Compound Discovery Report

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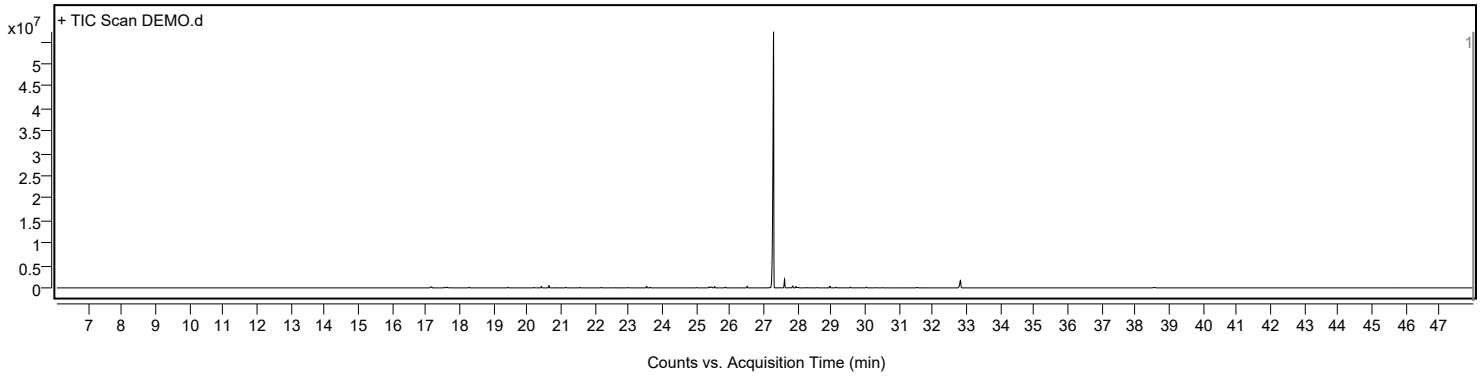
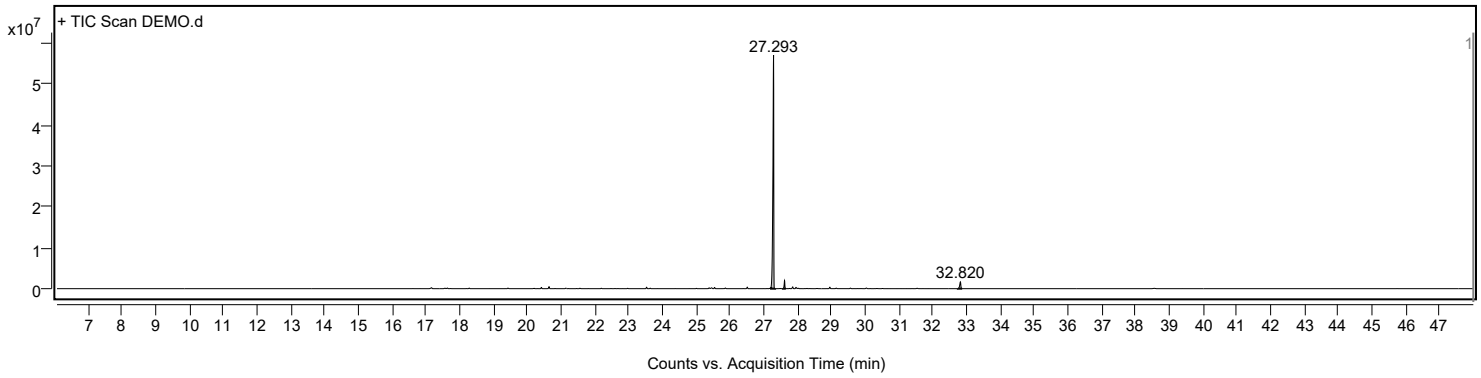
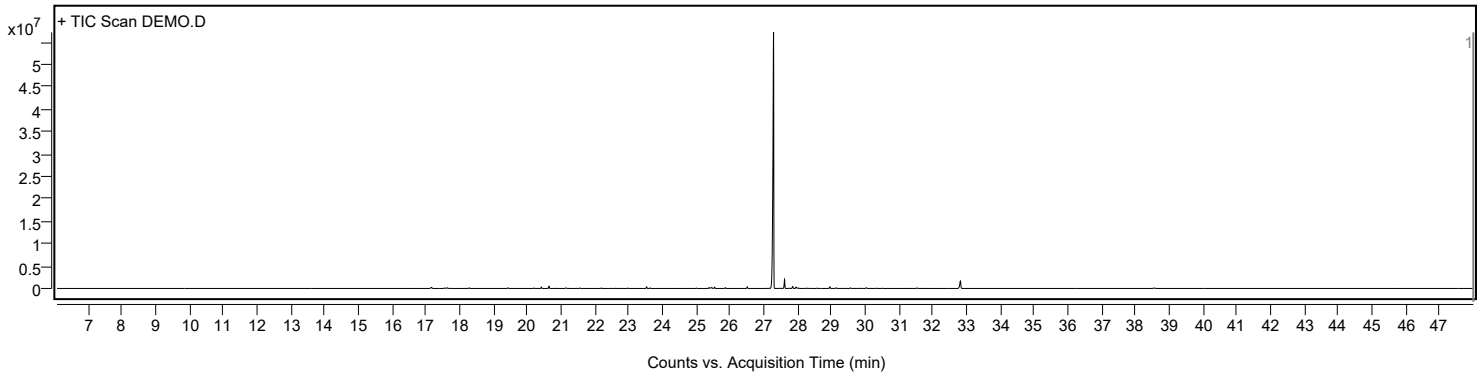
Sample Information

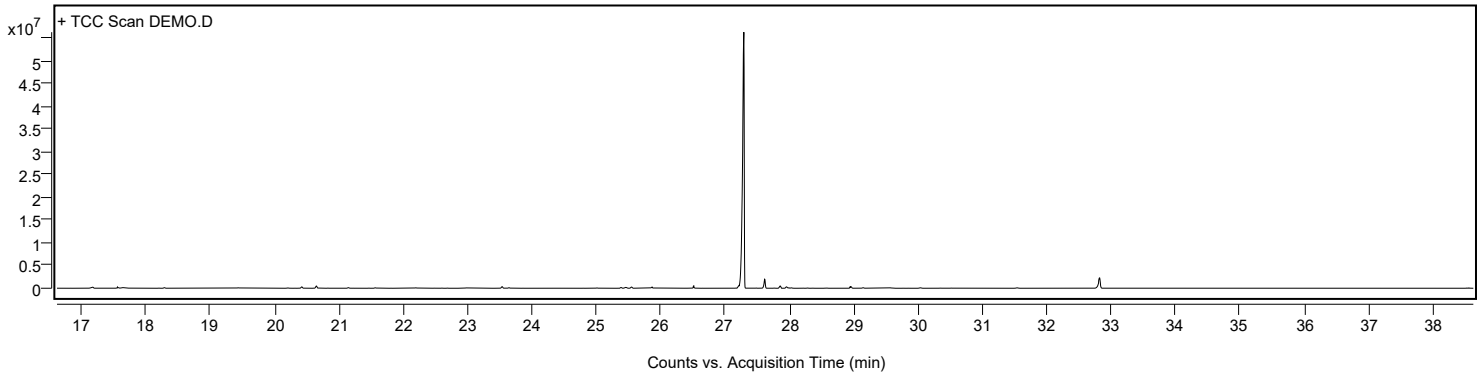
Name	DEMO	**Data File Path**	C:\Users\Lenovo\Desktop\DEMO.D
Sample ID	GCMS	**Acq. Time (Local)**	2569-02-19 15:29:07 (UTC+07:00)
Instrument	Q	**Method Path (Acq)**	D:\MassHunter\GCMS\1\methods\SD 60M-60meth gas1-4 80-280c Hold20 MST280 -S.M
MS Type	1	**Version (Acq SW)**	MassHunter GC/MS Acquisition 10.1.49 02-Nov-2025 Copyright © 1989-2025 Agilent Technologies, Inc.
Inj. Vol. (ul)	1	**IRM Status**	
Position		**Method Path (DA)**	C:\MassHunter\Methods\10.0\Default.m
Plate Pos.	eric	**Target Source Path**	C:\MassHunter\PCDL\default.csv
Operator		**Result Summary**	92 identified (93 found)

Sample Chromatograms









Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
1	Bicyclo[4.1.0]heptane,	C8 H12	16.626		54211-14-2	LibSearch	69.09	69.09			Chrom Decon

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
	7-methylene-										
2	Pentanoic acid, 4-oxo-	C5 H8 O3	16.834		123-76-2	LibSearch	50.77	50.77			Chrom Decon
3	2-Propanol, 1,1'-oxybis-	C6 H14 O3	17.170		110-98-5	LibSearch	89.77	89.77			Chrom Decon
4	Acetic acid, methoxy-, anhydride	C6 H10 O5	17.563		19500-95-9	LibSearch	69.08	69.08			Chrom Decon
5	1-Propanol, 2-(2-hydroxypropoxy)-	C6 H14 O3	17.575		106-62-7	LibSearch	85.15	85.15			Chrom Decon
6	1-Propanol, 2-(2-hydroxypropoxy)-	C6 H14 O3	17.640		106-62-7	LibSearch	83.56	83.56			Chrom Decon
7	1-Propanol, 2-(2-hydroxypropoxy)-	C6 H14 O3	17.737		106-62-7	LibSearch	79.03	79.03			Chrom Decon
8	1-Propanol, 2-(2-hydroxypropoxy)-	C6 H14 O3	18.203		106-62-7	LibSearch	76.66	76.66			Chrom Decon
9	2-Nonanone, 9-hydroxy-	C9 H18 O2	18.285		25368-56-3	LibSearch	83.73	83.73			Chrom Decon
10	Toluene	C7 H8	19.429		108-88-3	LibSearch	80.22	80.22			Chrom Decon
11	Benzyl acetate	C9 H10 O2	20.189		140-11-4	LibSearch	81.75	81.75			Chrom Decon
12	Allyl heptanoate	C10 H18 O2	20.216		142-19-8	LibSearch	83.37	83.37			Chrom Decon
13	Benzeneethanol, .alpha.,.alpha.-dimethyl-	C10 H14 O	20.312		100-86-7	LibSearch	62.88	62.88			Chrom Decon
14	Linalool <ethyl-, (Z)->	C11 H20 O	20.420		54592-32-4	LibSearch	96.86	96.86			Chrom Decon
15	2-Methylbenzyl benzoate	C15 H14 O2	20.601		80716-36-5	LibSearch	79.74	79.74			Chrom Decon
16	Linalool <ethyl-, (Z)->	C11 H20 O	20.648		54592-32-4	LibSearch	97.24	97.24			Chrom Decon
17	Rozanol, trans-	C10 H20 O2	20.829		65418-70-4	LibSearch	69.06	69.06			Chrom Decon
18	Rozanol, trans-	C10 H20 O2	21.147		65418-70-4	LibSearch	90.17	90.17			Chrom Decon
19	1,5-Heptadiene, 3,4-dimethyl-	C9 H16	21.215		1000061-77-9	LibSearch	64.93	64.93			Chrom Decon
20	Linalyl acetate	C12 H20 O2	21.466		115-95-7	LibSearch	55.44	55.44			Chrom Decon
21	2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-	C10 H18 O	21.563		106-25-2	LibSearch	83.84	83.84			Chrom Decon
22	Carbonic acid, monoamide, N-isobutyl-, benzyl ester	C12 H17 N O2	21.811		1000420-28-2	LibSearch	62.11	62.11			Chrom Decon
23	Citronellal <hydroxy->	C10 H20 O2	22.194		107-75-5	LibSearch	84.85	84.85			Chrom Decon
24	3-Hexen-1-ol, propanoate, (Z)-	C9 H16 O2	22.482		33467-74-2	LibSearch	72.60	72.60			Chrom Decon
25	Benzenepropanol, .alpha.,.alpha.-dimethyl-	C11 H16 O	22.605		103-05-9	LibSearch	78.22	78.22			Chrom Decon
26	5-methyl-2-(Z)-hepten-4-one	C8 H14 O	22.684		24608-84-2	LibSearch	62.94	62.94			Chrom Decon
27	Cyclopentane, (1,1-dimethylethyl)-	C9 H18	22.687		3875-52-3	LibSearch	61.77	61.77			Chrom Decon
28	2,3-Pentanedione	C5 H8 O2	22.823		600-14-6	LibSearch	66.28	66.28			Chrom Decon
29	6-Octen-1-ol, 3,7-dimethyl-, acetate	C12 H22 O2	22.974		150-84-5	LibSearch	81.73	81.73			Chrom Decon
30	2-Propanone, 1,1,1-trifluoro-	C3 H3 F3 O	23.397		421-50-1	LibSearch	57.33	57.33			Chrom Decon
31	Herbanate isomer I	C13 H20 O2	23.535		116126-82-0	LibSearch	95.14	95.14			Chrom Decon
32	Herbanate isomer II	C13 H20 O2	23.644		116126-82-0	LibSearch	90.41	90.41			Chrom Decon
33	Cyclopropyl 2-(5'-methyl-2'-furyl)cyclopropyl ketone	C12 H14 O2	23.859		1000139-92-9	LibSearch	44.09	44.09			Chrom Decon
34	(5Z)-3-Methyl-1,5-heptadiene	C8 H14	24.389		50763-51-4	LibSearch	44.90	44.90			Chrom Decon
35	3-Methylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester	C15 H10 Cl2 O3	24.796		1010331-26-9	LibSearch	62.68	62.68			Chrom Decon
36	2(3H)-Furanone, 5-hexyldihydro-	C10 H18 O2	25.009		706-14-9	LibSearch	81.73	81.73			Chrom Decon
37	2-Butanone, 3-methyl-1-phenyl-	C11 H14 O	25.295		2893-05-2	LibSearch	42.30	42.30			Chrom Decon
38	D-Alanine, N-(4-anisoyl)-, isohexyl ester	C17 H25 N O4	25.344		1000348-49-0	LibSearch	69.01	69.01			Chrom Decon
39	Hydroxycitronellal <diethyl-> acetal	C14 H30 O3	25.386		7779-94-4	LibSearch	89.78	89.78			Chrom Decon
40	benzamide, N-[4-[[2-[4-[(butylsulfonyl)amino]phenoxy]-1-oxotetradecyl]amino]-2-hydroxyphenyl]-	C37 H51 N3 O6 S	25.406		1000403-01-5	LibSearch	9.67	9.67			Chrom Decon
41	Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-, methylcarbamate	C17 H27 N O2	25.454		1918-11-2	LibSearch	84.98	84.98			Chrom Decon
42	Tricyclo[4.3.0.0(3,8)]nonan-7-one	C9 H12 O	25.466		103001-16-7	LibSearch	48.61	48.61			Chrom Decon
43	4-Amino-5-o-tolyl-4H-[1,2,4]triazole-3-thiol, 2TMS	C15 H26 N4 S Si2	25.476		1000509-47-9	LibSearch	1.70	1.70			Chrom Decon
44	Caryophyllene<Z->	C15 H24	25.547		118-65-0	LibSearch	79.00	79.00			Chrom Decon
45			25.563								Chrom Decon
46	Magnolan, (1RS,3RS,4aSR,9aRS)	C13 H16 O2	25.863		27606-09-3	LibSearch	65.73	65.73			Chrom Decon
47	Cyclaprop	C13 H18 O2	25.870		17511-60-3	LibSearch	63.13	63.13			Chrom Decon
48	Valeric anhydride	C10 H18 O3	26.391		2082-59-9	LibSearch	80.71	80.71			Chrom Decon
49	1,2-Ethanediol, monobenzoate	C9 H10 O3	26.510		94-33-7	LibSearch	64.24	64.24			Chrom Decon
50	Helional (Tropional)	C11 H12 O3	26.515		1205-17-0	LibSearch	97.01	97.01			Chrom Decon
51	4-tert-Octylphenol, TMS derivative	C17 H30 O Si	26.654		78721-87-6	LibSearch	42.24	42.24			Chrom Decon
52	Propanedinitrile, cyclohexyl(2-methylcyclohexyl)-	C16 H24 N2	27.171		74764-55-9	LibSearch	50.70	50.70			Chrom Decon
53	1,4-Pentadiene, 2-methyl-	C6 H10	27.182		763-30-4	LibSearch	39.87	39.87			Chrom Decon
54	[2-(3,3a,4,5,6,10c-Hexahydro-1H-pyrrolo[3,4-c]carbazol-2-yl)-ethyl]-dimethyl-amine	C18 H25 N3	27.259		1000297-41-9	LibSearch	27.87	27.87			Chrom Decon
55	Methyl dihydrojasmonate<cis->	C13 H22 O3	27.291		39647-11-5	LibSearch	97.09	97.09			Chrom Decon
56	Norbornen-2-ol acetate<endo-5->	C9 H12 O2	27.485		99295-40-6	LibSearch	53.23	53.23			Chrom Decon
57	Disulfide <allyl->	C6 H10 S2	27.492		2179-57-9	LibSearch	46.24	46.24			Chrom Decon

Compound Summary

Cpd	Name	Formula	RT	Mass	CAS	ID Source	Score	Score (Lib)	Score (DB)	Score (MFG)	Algorithm
58	Methyl dihydrojasmonate<trans->	C13 H22 O3	27.617		2630-39-9	LibSearch	98.23	98.23			Chrom Decon
59	Ethyl 1-(1-adamantylcarbonyl)piperidine-4-carboxylate	C19 H29 N O3	27.757		260553-08-0	LibSearch	44.17	44.17			Chrom Decon
60	Iso E Super <gamma->	C16 H26 O	27.768		68155-67-9	LibSearch	53.30	53.30			Chrom Decon
61	Fumaric acid, di(cis-hex-3-enyl) ester	C16 H24 O4	27.854		1000348-87-6	LibSearch	46.14	46.14			Chrom Decon
62	Amberonne (isomer 2)	C16 H26 O	27.855		1010470-69-8	LibSearch	91.02	91.02			Chrom Decon
63	[2,2'-Bifuran]-3-carboxylic acid, methyl ester	C10 H8 O4	27.867		5905-07-7	LibSearch	42.63	42.63			Chrom Decon
64	Helvetolide	C17 H32 O3	27.957		141773-73-1	LibSearch	93.34	93.34			Chrom Decon
65	Iso E Super <gamma->	C16 H26 O	27.987		68155-67-9	LibSearch	61.90	61.90			Chrom Decon
66	1-Octen-4-ol acetate	C10 H18 O2	28.032		150666-71-0	LibSearch	43.32	43.32			Chrom Decon
67	Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	C16 H24 O3	28.103		2511-22-0	LibSearch	47.18	47.18			Chrom Decon
68	Tiglate <(3Z)-hexenyl->	C11 H18 O2	28.217		67883-79-8	LibSearch	54.59	54.59			Chrom Decon
69	1-Oxaspiro[2.5]oct-5-ene, 8,8-dimethyl-4-methylene-	C10 H14 O	28.279		54345-60-7	LibSearch	69.34	69.34			Chrom Decon
70	Iron, acetyldicarbonyl[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadienyl]-	C14 H18 Fe O3	28.286		1000146-24-2	LibSearch	59.62	59.62			Chrom Decon
71	Diethylene glycol, O,O-di(pivaloyl)-	C14 H26 O5	28.347		1000308-76-7	LibSearch	57.16	57.16			Chrom Decon
72	Benzene, [1-methyl-1-(pentyloxy)ethyl]-	C14 H22 O	28.366		54932-79-5	LibSearch	50.47	50.47			Chrom Decon
73	4-(N-Methyl-N-methoxy)indancarboxamide	C12 H15 N O2	28.564		1000284-45-9	LibSearch	51.74	51.74			Chrom Decon
74	Helvetolide	C17 H32 O3	28.586		141773-73-1	LibSearch	73.00	73.00			Chrom Decon
75	Diethylene glycol, O,O-di(pivaloyl)-	C14 H26 O5	28.950		1000308-76-7	LibSearch	51.42	51.42			Chrom Decon
76	Tetradecanoate <isopropyl->	C17 H34 O2	28.960		110-27-0	LibSearch	85.97	85.97			Chrom Decon
77	2,2-Diethoxyacetophenone	C12 H16 O3	29.149		6175-45-7	LibSearch	59.63	59.63			Chrom Decon
78	Amberlyn	C16 H28 O	29.573		3738-00-9	LibSearch	74.08	74.08			Chrom Decon
79	N-Carboxyethylrhodanine	C6 H7 N O3 S2	29.684		7025-19-6	LibSearch	20.64	20.64			Chrom Decon
80	Hexanethioic acid, S-methyl ester	C7 H14 O S	29.768		2432-77-1	LibSearch	61.97	61.97			Chrom Decon
81	N-Carboxyethylrhodanine	C6 H7 N O3 S2	29.785		7025-19-6	LibSearch	20.68	20.68			Chrom Decon
82	Nortricyclyl bromide	C7 H9 Br	29.848		1000342-32-2	LibSearch	43.32	43.32			Chrom Decon
83	3,5-Hexadiyn-2-one	C6 H4 O	29.873		31097-80-0	LibSearch	49.41	49.41			Chrom Decon
84	Galaxolide	C18 H26 O	30.041		1222-05-5	LibSearch	77.71	77.71			Chrom Decon
85	Hexylacetylene	C8 H14	30.347		629-05-0	LibSearch	71.62	71.62			Chrom Decon
86	Cyclopentanemethanol	C6 H12 O	30.506		3637-61-4	LibSearch	61.41	61.41			Chrom Decon
87	Hexylacetylene	C8 H14	30.517		629-05-0	LibSearch	74.61	74.61			Chrom Decon
88	Undecyne<1->	C11 H20	31.540		2243-98-3	LibSearch	87.43	87.43			Chrom Decon
89	Ethylene brassylate	C15 H26 O4	32.820		105-95-3	LibSearch	95.19	95.19			Chrom Decon
90	2,6-Nonadienal, 3,7-dimethyl-	C11 H18 O	32.830		41448-29-7	LibSearch	45.84	45.84			Chrom Decon
91	2-Methyl-5-nitrobenzimidazole	C8 H7 N3 O2	38.536		1792-40-1	LibSearch	36.11	36.11			Chrom Decon
92	Benzene, 1-isocyano-3-methoxy-	C8 H7 N O	38.550		20600-55-9	LibSearch	51.42	51.42			Chrom Decon
93	Cinoxate	C14 H18 O4	38.564		104-28-9	LibSearch	71.97	71.97			Chrom Decon

Compound Details

Cpd. 1: Bicyclo[4.1.0]heptane, 7-methylene-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Bicyclo[4.1.0]heptane, 7-methylene-	C8 H12	16.626			54211-14-2	LibSearch	69.09	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		69.09			50		

Compound Discovery Report

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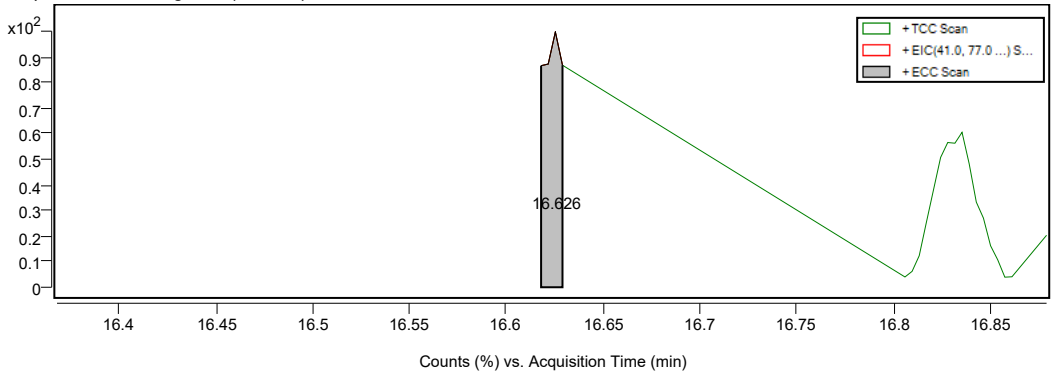
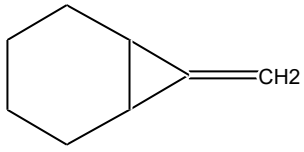
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Bicyclo[4.1.0]heptane, 7-methylene-	C8H12		LibSearch	16.626	3.159		54211-14-2	69.09		
Spiro[bicyclo[3.1.0]hexane-2,1'-cyclopropane]	C8H12		LibSearch	16.626	3.693		1000460-73-6	67.03		
Bicyclo[3.1.0]hexane, 6-methylene-	C7H10		LibSearch	16.626	5.159		54211-16-4	63.63		
(2Z,4Z,6E)-2,4,6-Undecatriene	C11H18		LibSearch	16.626	-2.357		85615-64-1	61.81		
1,4-Methano-1H-Cyclopropa[d]pyridazine, 4,4a,5,5a-tetrahydro-6,6-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,5a.alpha.)-	C8H12N2		LibSearch	16.626			109746-10-3	60.93		
Bicyclo[3.2.0]hept-6-ene	C7H10		LibSearch	16.626	4.559		4927-03-1	60.90		
1-Methylene-2-vinylcyclopentane	C8H12		LibSearch	16.626	3.009		6196-78-7	60.44		
Sabinene	C10H16		LibSearch	16.626			3387-41-5	60.34		
3-Methylenecycloheptene	C8H12		LibSearch	16.626	1.826		34564-56-2	58.62		
Phellandrene <alpha->	C10H16		LibSearch	16.626			99-83-2	58.32		
Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)-	C10H16		LibSearch	16.626	1.676		3387-41-5	58.23		
Bicyclo[3.1.0]hex-2-ene, 4-methyl-1-(1-methylethyl)-	C10H16		LibSearch	16.626	2.076		28634-89-1	58.19		
.beta.-Phellandrene	C10H16		LibSearch	16.626	0.559		555-10-2	57.97		
Thujene <alpha->	C10H16		LibSearch	16.626			2867-05-2	57.76		
Sabinene	C10H16		LibSearch	16.626			3387-41-5	57.20		
Bicyclo[3.1.0]hex-2-ene, 4-methyl-1-(1-methylethyl)-	C10H16		LibSearch	16.626	2.076		28634-89-1	56.80		
.alpha.-Phellandrene	C10H16		LibSearch	16.626	0.476		99-83-2	56.38		
Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)-	C10H16		LibSearch	16.626	1.593		2867-05-2	56.35		
Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)-	C10H16		LibSearch	16.626	1.676		3387-41-5	56.28		
Nortricyclyl bromide	C7H9Br		LibSearch	16.626	3.643		1000342-32-2	55.99		
.alpha.-Phellandrene	C10H16		LibSearch	16.626	0.476		99-83-2	55.84		
1,3,6-Heptatriene, 5-methyl-, (E)-	C8H12		LibSearch	16.626	4.276		818-48-4	55.48		
3-Methylene-1,6-heptadiene	C8H12		LibSearch	16.626	3.893		16626-48-5	55.39		
Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)-	C10H16		LibSearch	16.626	1.593		2867-05-2	55.30		
Bicyclo[3.1.0]hex-2-ene, 2-methyl-5-(1-methylethyl)-	C10H16		LibSearch	16.626	1.593		2867-05-2	55.11		
1,3-Cyclohexadiene, 5,6-dimethyl-	C8H12		LibSearch	16.626	3.193		5715-27-5	55.01		
Cyclopentane, 1-ethenyl-3-methylene-	C8H12		LibSearch	16.626	3.009		29668-63-1	54.79		
Cyclohexene, 4-methylene-1-(1-methylethyl)-	C10H16		LibSearch	16.626	0.076		99-84-3	54.68		
Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)-	C10H16		LibSearch	16.626	1.676		3387-41-5	54.66		
Phellandrene<alpha->	C10H16		LibSearch	16.626	8.776		99-83-2	54.48		
.beta.-Phellandrene	C10H16		LibSearch	16.626	0.559		555-10-2	54.17		
Thujene<alpha->	C10H16		LibSearch	16.626	11.006		2867-05-2	54.08		
Bicyclo[3.1.0]hexane, 4-methylene-1-(1-methylethyl)-	C10H16		LibSearch	16.626	1.676		3387-41-5	53.91		
Cyclopropane, 1-ethenyl-2-hexenyl-, [1.alpha.,2.beta.(E)]-(.+/-.)-	C11H18		LibSearch	16.626	-1.307		22822-99-7	53.82		
Cyclopentadiene, 2,5,5-trimethyl-	C8H12		LibSearch	16.626	3.493		7086-15-9	53.59		
Cyclobutane, 2-ethylidene-1-vinyl-	C8H12		LibSearch	16.626	3.059		1000150-32-4	53.57		
Bicyclo[4.1.0]heptane, 7-methylene-	C8H12		LibSearch	16.626	3.159		54211-14-2	53.56		
Octatriene, 1,3-trans-5-trans-	C8H12		LibSearch	16.626	2.909		33580-04-0	53.51		
Pinene <beta->	C10H16		LibSearch	16.626			127-91-3	53.50		
1,3,6-Octatriene, (Z,E)-	C8H12		LibSearch	16.626	2.909		22038-68-2	53.31		
Cyclopentadiene, 1,5,5-trimethyl-	C8H12		LibSearch	16.626	3.493		4249-09-6	53.23		
Bis[bicyclo[3.2.0]hept-2-en-4-yl]ether	C14H18O		LibSearch	16.626	-7.141		1000153-89-5	53.21		
Cyclopentene, 3-ethylidene-1-methyl-	C8H12		LibSearch	16.626	2.376		62338-00-5	53.14		
Tricyclo[4.1.0.0(2,4)]heptane, 5-(phenylthio)-, (1.alpha.,2.beta.,4.beta.,5.alpha.,6.alpha.)-	C13H14S		LibSearch	16.626	-8.857		71055-11-3	53.00		
1,3,6-Heptatriene, 5-methyl-	C8H12		LibSearch	16.626	4.276		925-52-0	52.89		
Spiro[2.4]heptane, 4-methylene-	C8H12		LibSearch	16.626	2.943		24308-54-1	52.62		
(E,E,E)-2,4,6-Octatriene	C8H12		LibSearch	16.626	2.626		15192-80-0	52.61		
E,Z-3-Ethylidenecyclohexene	C8H12		LibSearch	16.626	1.859		16631-62-2	52.58		
Pinene <alpha->	C10H16		LibSearch	16.626			80-56-8	52.56		
2,4,6-Octatrienal	C8H10O		LibSearch	16.626	-0.524		17609-31-3	52.53		

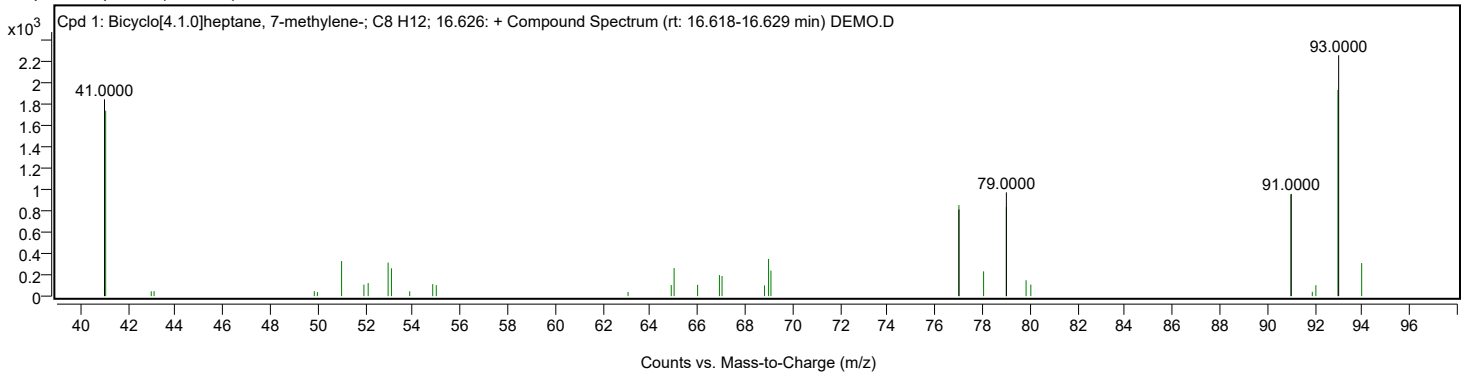
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



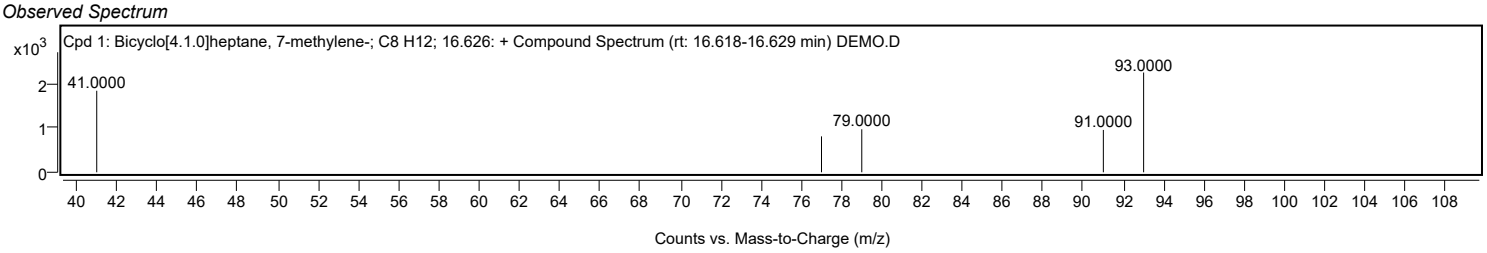
Bicyclo[4.1.0]heptane, 7-methylene-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			69.09			NIST.L

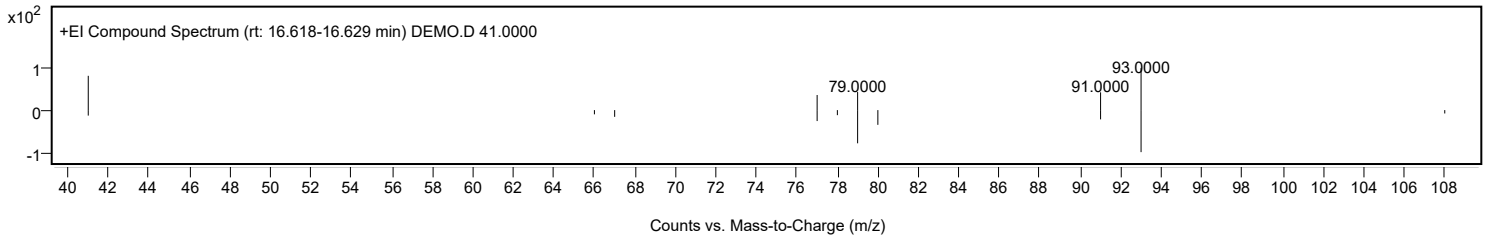
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			69.09			NIST.L

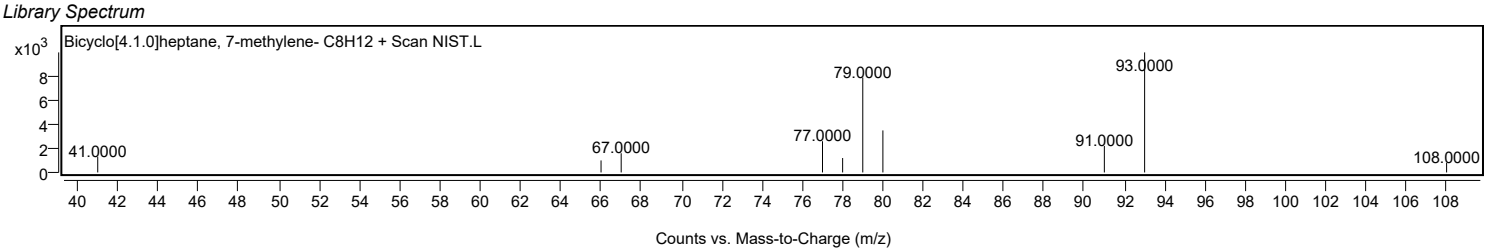
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 2: Pentanoic acid, 4-oxo-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Pentanoic acid, 4-oxo-	C5 H8 O3	16.834			123-76-2	LibSearch	50.77	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		50.77			50		

Compound Discovery Report

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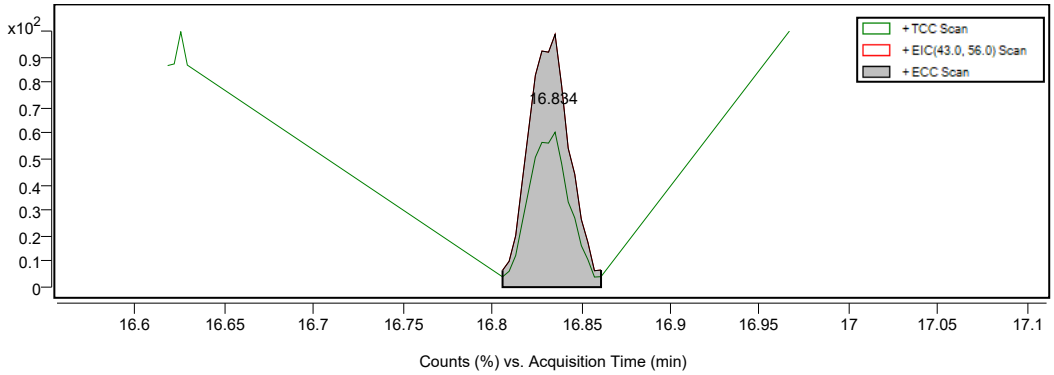
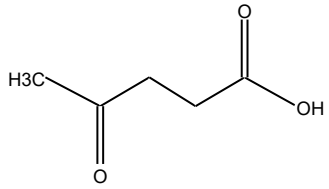
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Pentanoic acid, 4-oxo-	C5H8O3		LibSearch	16.834	-0.016		123-76-2	50.77		
Isobutyl acetate	C6H12O2		LibSearch	16.834	4.818		110-19-0	49.73		
Isobutyl acetate	C6H12O2		LibSearch	16.834	4.818		110-19-0	49.25		
Pentanoic acid, 4-oxo-	C5H8O3		LibSearch	16.834	-0.016		123-76-2	48.67		
Pentanoic acid, 4-oxo-	C5H8O3		LibSearch	16.834	-0.016		123-76-2	48.56		
Acetic acid, butyl ester	C6H12O2		LibSearch	16.834	3.751		123-86-4	47.77		
Butyl acetate	C6H12O2		LibSearch	16.834	13.524		123-86-4	46.68		
Acetate <isobutyl->	C6H12O2		LibSearch	16.834			110-19-0	46.02		
Isobutyl acetate	C6H12O2		LibSearch	16.834	4.818		110-19-0	45.75		
Isobutyl acetate	C6H12O2		LibSearch	16.834	4.818		110-19-0	44.98		
sec-Butyl acetate	C6H12O2		LibSearch	16.834	4.818		105-46-4	44.62		
Isobutyl acetate	C6H12O2		LibSearch	16.834	14.024		110-19-0	44.33		
Pentanoic acid, 4-oxo-	C5H8O3		LibSearch	16.834	-0.016		123-76-2	44.00		
Acetate <butyl->	C6H12O2		LibSearch	16.834			123-86-4	43.77		
Pentanoic acid, 4-oxo-	C5H8O3		LibSearch	16.834	-0.016		123-76-2	43.32		
sec-Butyl acetate	C6H12O2		LibSearch	16.834	4.818		105-46-4	42.40		
Acetic acid, butyl ester	C6H12O2		LibSearch	16.834	3.751		123-86-4	42.39		
sec-Butyl acetate	C6H12O2		LibSearch	16.834	4.818		105-46-4	41.99		
Acetic acid, butyl ester	C6H12O2		LibSearch	16.834	3.751		123-86-4	41.42		
sec-Butyl acetate	C6H12O2		LibSearch	16.834	4.818		105-46-4	40.31		
sec-Butyl acetate	C6H12O2		LibSearch	16.834	4.818		105-46-4	40.07		
Isobutyl acetate	C6H12O2		LibSearch	16.834	4.818		110-19-0	38.99		
Acetic acid, butyl ester	C6H12O2		LibSearch	16.834	3.751		123-86-4	38.79		
Acetic acid, hexyl ester	C8H16O2		LibSearch	16.834	0.434		142-92-7	37.12		
2-Acetylamino-2-cyano-acetamide	C5H7N3O2		LibSearch	16.834	-8.316		14056-39-4	36.85		
3,5-Dimethyl-1,6-heptadien-4-ol	C9H16O		LibSearch	16.834	1.334		19549-66-7	33.77		
Acetic acid, hexyl ester	C8H16O2		LibSearch	16.834	0.434		142-92-7	33.51		
1-Pentanol, 2-methyl-, acetate	C8H16O2		LibSearch	16.834	1.501		7789-99-3	33.21		
1,3-Propanediol, 2,2-dimethyl-, diacetate	C9H16O4		LibSearch	16.834	-2.599		13431-57-7	32.93		
O-Hexylhydroxylamine	C6H15NO		LibSearch	16.834	1.218		1000426-05-8	32.84		
Hexyl acetate	C8H16O2		LibSearch	16.834	8.784		142-92-7	32.53		
Hexyl acetate	C8H16O2		LibSearch	16.834			142-92-7	32.13		
Isobutyl chloroformate	C5H9ClO2		LibSearch	16.834	3.534		543-27-1	31.63		
Acetic acid, hexyl ester	C8H16O2		LibSearch	16.834	0.434		142-92-7	31.09		
Acetic acid, hexyl ester	C8H16O2		LibSearch	16.834	0.434		142-92-7	30.36		
Ethanethioic acid, S-butyl ester	C6H12OS		LibSearch	16.834	0.101		928-47-2	30.34		
Dichloroacetic acid, hexyl ester	C8H14Cl2O2		LibSearch	16.834	-5.316		37079-04-2	29.95		
1-Pentanol, 2-methyl-, acetate	C8H16O2		LibSearch	16.834	1.501		7789-99-3	28.49		
2-Aminopentanenitrile, N-acetyl-	C7H12N2O		LibSearch	16.834	-4.799		40652-09-3	27.86		
N'-Hydroxypropimidamide	C3H8N2O		LibSearch	16.834	1.918		29335-36-2	27.62		
2-Methylpentyl formate	C7H14O2		LibSearch	16.834	1.551		381670-34-4	27.59		
2-Methyl-1-hexanol	C7H16O		LibSearch	16.834	1.901		1000427-67-0	27.34		
Acetic acid, hexyl ester	C8H16O2		LibSearch	16.834	0.434		142-92-7	27.20		
Heptyl acetate	C9H18O2		LibSearch	16.834	4.814		112-06-1	27.01		
Azetidine, 1-acetyl-2-methyl-	C6H11NO		LibSearch	16.834	2.018		50837-77-9	26.86		
1-Pentanol, 2-methyl-, acetate	C8H16O2		LibSearch	16.834	1.501		7789-99-3	26.80		
1-Pentanol, 2-methyl-, acetate	C8H16O2		LibSearch	16.834	1.501		7789-99-3	26.40		
Buten-2-ol acetate <2-methyl-3->	C7H12O2		LibSearch	16.834			24509-88-4	25.83		
Buten-2-ol acetate<2-methyl-3->	C7H12O2		LibSearch	16.834	13.954		24509-88-4	25.64		
Acetic acid, heptyl ester	C9H18O2		LibSearch	16.834	-1.216		112-06-1	25.46		

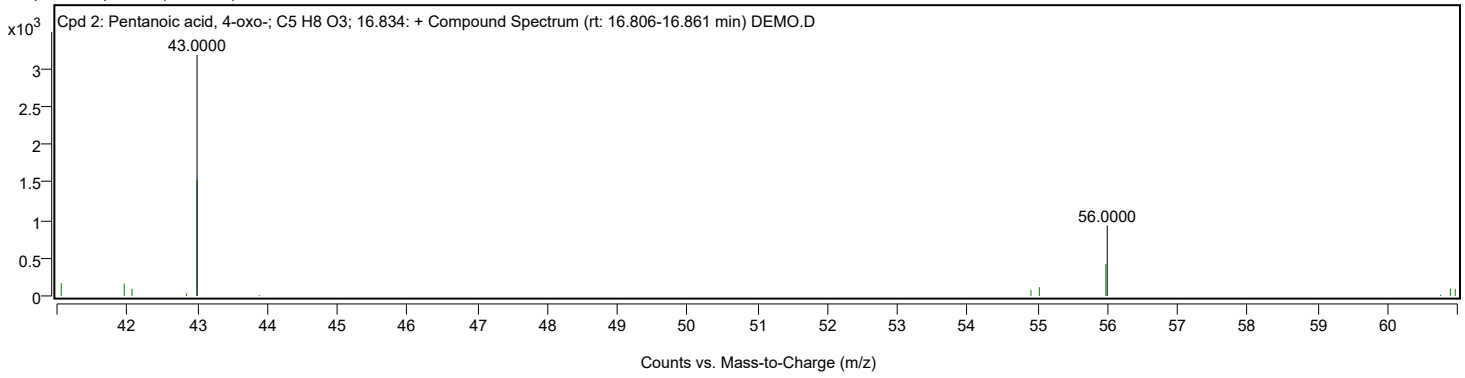
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



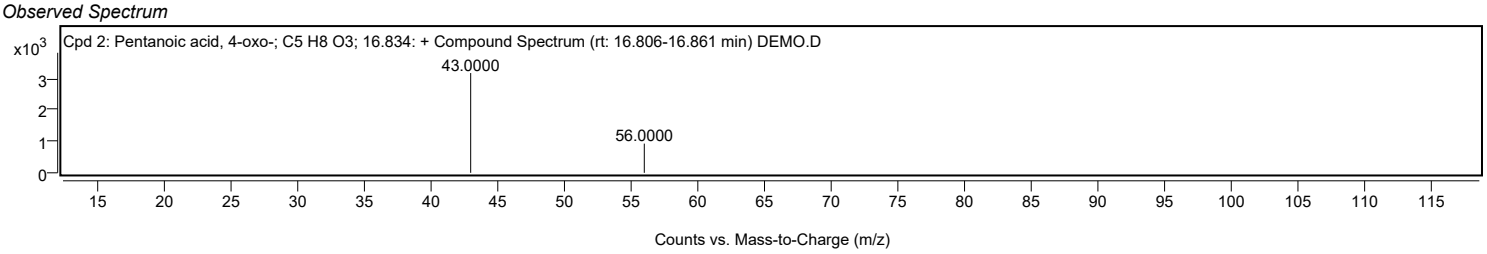
Pentanoic acid, 4-oxo-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			50.77			NIST.L

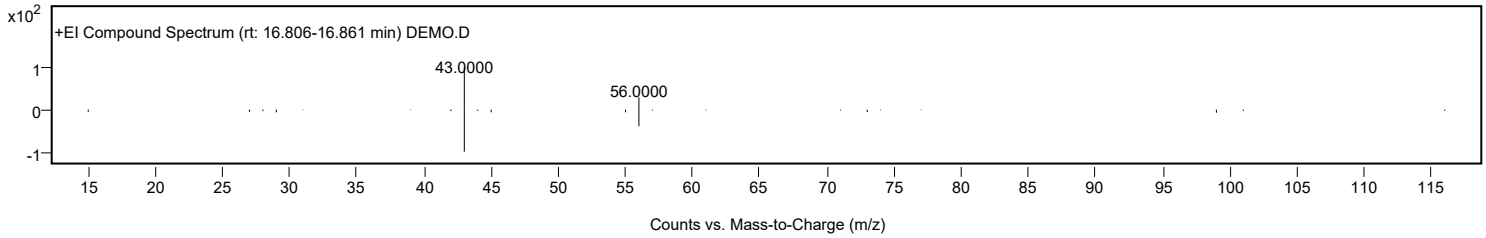
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			50.77			NIST.L

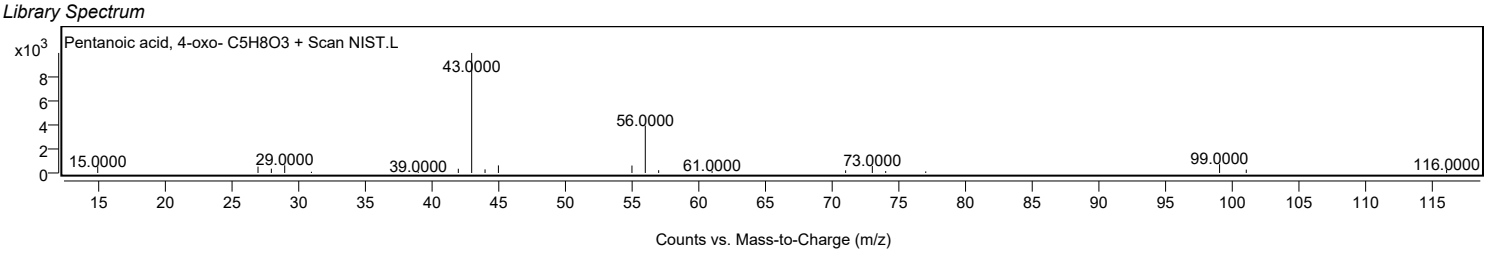
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 3: 2-Propanol, 1,1'-oxybis-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
2-Propanol, 1,1'-oxybis-	C6 H14 O3	17.170			110-98-5	LibSearch	89.77	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		89.77			50		

Compound Discovery Report

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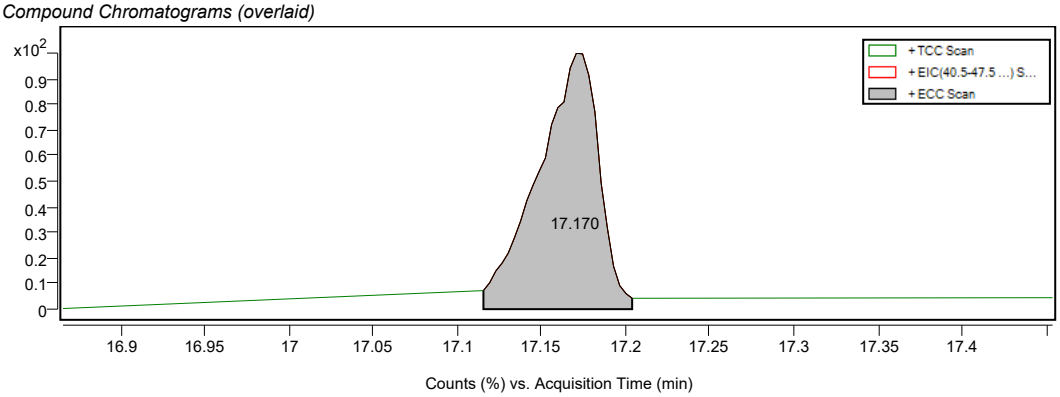
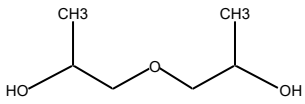
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
2-Propanol, 1,1'-oxybis-	C6H14O3		LibSearch	17.170	0.203		110-98-5	89.77		
2-Propanol, 1,1'-oxybis-	C6H14O3		LibSearch	17.170	0.203		110-98-5	88.22		
Dipropylene glycol (isomer 1)	C6H14O3		LibSearch	17.170			1000506-25-3	88.17		
Dipropylene glycol (isomer 1)	C6H14O3		LibSearch	17.170	0.203		1000506-25-3	88.17		
2-Propanol, 1,1'-oxybis-	C6H14O3		LibSearch	17.170	0.203		110-98-5	87.30		
2-Propanol, 1,1'-oxybis-	C6H14O3		LibSearch	17.170	0.203		110-98-5	86.13		
(S)-Isopropyl lactate	C6H12O3		LibSearch	17.170	2.453		63697-00-7	78.08		
Propyl nitrite	C3H7NO2		LibSearch	17.170	8.686		543-67-9	76.26		
Ethanol, 2-(1-methylethoxy)-	C5H12O2		LibSearch	17.170	4.286		109-59-1	75.80		
Butan-2-ol	C4H10O		LibSearch	17.170			78-92-2	74.67		
Ethoxy ethanol<2->	C4H10O2		LibSearch	17.170	14.840		110-80-5	74.01		
Ethoxy ethanol <2->	C4H10O2		LibSearch	17.170			110-80-5	73.74		
Ethanol, 2-(1-methylethoxy)-	C5H12O2		LibSearch	17.170	4.286		109-59-1	73.55		
Ethanol, 2-(1-methylethoxy)-	C5H12O2		LibSearch	17.170	4.286		109-59-1	73.47		
(2R,4R)-(-)-Pentanediol	C5H12O2		LibSearch	17.170	3.120		42075-32-1	73.38		
2,4-Pentanediol	C5H12O2		LibSearch	17.170	3.120		625-69-4	73.14		
Ethanol, 2-(1-methylethoxy)-	C5H12O2		LibSearch	17.170	4.286		109-59-1	72.39		
(2S,4S)-(+)-Pentanediol	C5H12O2		LibSearch	17.170	3.120		72345-23-4	72.22		
(2R,4R)-(-)-Pentanediol	C5H12O2		LibSearch	17.170	3.120		42075-32-1	72.02		
2,4-Pentanediol	C5H12O2		LibSearch	17.170	3.120		625-69-4	71.74		
2-Propanol, 1-methoxy-2-methyl-	C5H12O2		LibSearch	17.170	5.736		3587-64-2	71.04		
Ethanol, 2-[2-(ethenyloxy)ethoxy]-	C6H12O3		LibSearch	17.170	0.470		929-37-3	69.91		
N-Hydroxymethylacetamide	C3H7NO2		LibSearch	17.170	1.136		625-51-4	69.88		
2,4-Pentanediol	C5H12O2		LibSearch	17.170	3.120		625-69-4	69.80		
Butanediol<2,3->	C4H10O2		LibSearch	17.170	14.140		513-85-9	69.65		
Ethanol, 2-[2-(ethenyloxy)ethoxy]-	C6H12O3		LibSearch	17.170	0.470		929-37-3	69.60		
Acetaldehyde, tetramer	C8H16O4		LibSearch	17.170	-2.164		108-62-3	69.54		
2-Butanamine, N-nitro-	C4H10N2O2		LibSearch	17.170	1.586		3335-65-7	69.31		
Formic acid, 1-methylethyl ester	C4H8O2		LibSearch	17.170	6.853		625-55-8	68.97		
3-Methoxycarbonyl-3-methyl-1,2,4-trioxolane	C5H8O5		LibSearch	17.170	1.036		105949-86-8	68.16		
Metaldehyde isomer I	C8H16O4		LibSearch	17.170			108-62-3	68.07		
2-Butanol	C4H10O		LibSearch	17.170	7.486		78-92-2	68.00		
Propanoic acid, 2-hydroxy-, methyl ester, (.+/-.)-	C4H8O3		LibSearch	17.170	4.703		547-64-8	67.55		
Acetaldehyde, tetramer	C8H16O4		LibSearch	17.170	-2.164		108-62-3	67.52		
2,3-Butanediol	C4H10O2		LibSearch	17.170	4.786		513-85-9	67.50		
Propane, 2,2',2''-[methylidynetris(oxy)]tris-	C10H22O3		LibSearch	17.170	0.720		4447-60-3	67.35		
Metaldehyde isomer II	C8H16O4		LibSearch	17.170			108-62-3	67.32		
Formate <propyl->	C4H8O2		LibSearch	17.170			110-74-7	67.28		
[1,4,7]Trioxonane	C6H12O3		LibSearch	17.170	-0.264		27725-91-3	67.22		
2-Butanol	C4H10O		LibSearch	17.170	7.486		78-92-2	67.00		
2-Methyl-2,3-pentanediol	C6H14O2		LibSearch	17.170	2.636		7795-80-4	66.85		
Lactic acid	C3H6O3		LibSearch	17.170			50-21-5	66.79		
Propanoic acid, 2-methyl-, 1-methylethyl ester	C7H14O2		LibSearch	17.170	4.570		617-50-5	66.70		
N-Methoxydiacetamide	C5H9NO3		LibSearch	17.170	1.653		128459-09-6	66.66		
Isopropyl Alcohol	C3H8O		LibSearch	17.170	9.136		67-63-0	66.45		
Isopropyl isobutyrate	C7H14O2		LibSearch	17.170	14.090		617-50-5	66.12		
Butadienol <2,3->	C4H10O2		LibSearch	17.170			513-85-9	66.06		
2,3-Butanediol, [R-(R*,R*)]-	C4H10O2		LibSearch	17.170	4.786		24347-58-8	66.03		
Ethanol, 2-(2-methoxyethoxy)-	C5H12O3		LibSearch	17.170	1.953		111-77-3	65.85		
Propanoic acid, 2-hydroxy-, methyl ester, (.+/-.)-	C4H8O3		LibSearch	17.170	4.703		547-64-8	65.73		

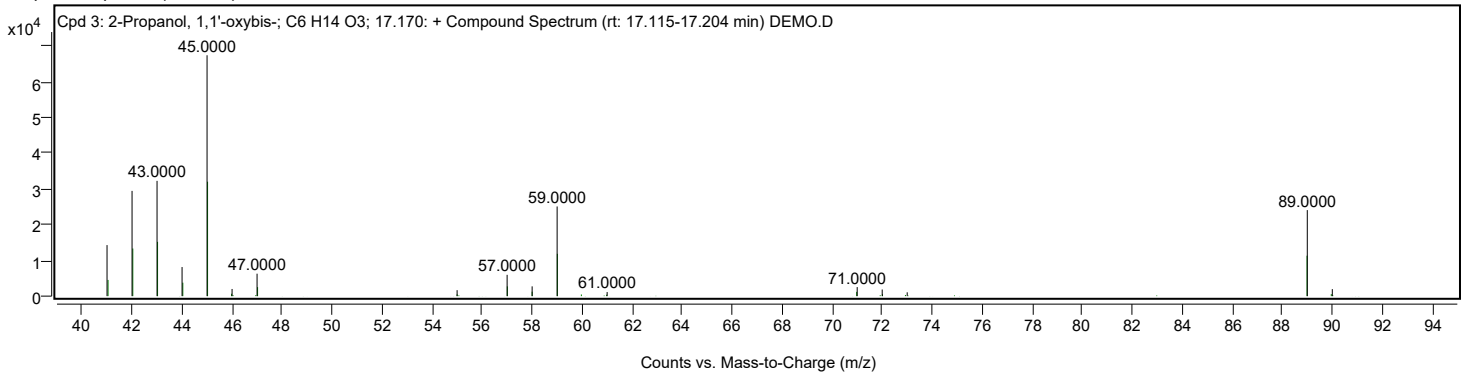
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



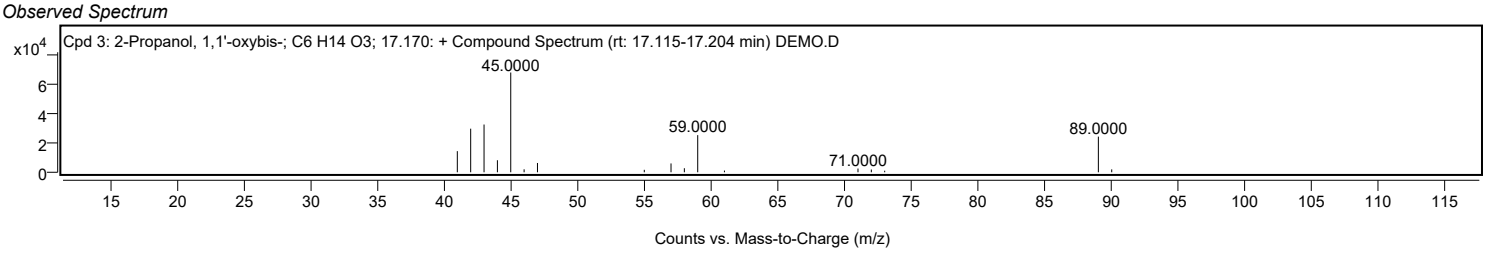
2-Propanol, 1,1'-oxybis-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			89.77			NIST.L

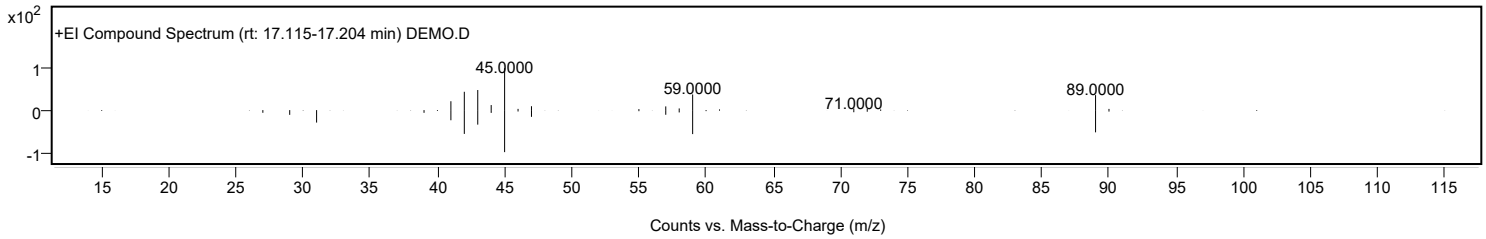
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			89.77			NIST.L

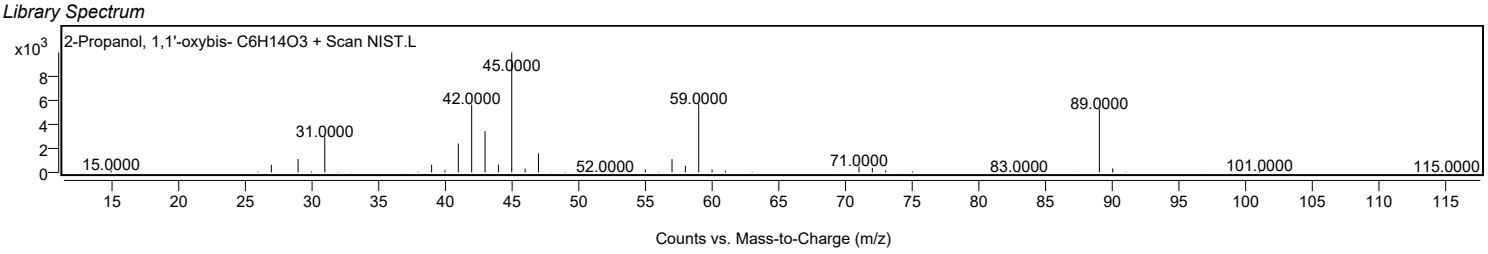
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 4: Acetic acid, methoxy-, anhydride

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Acetic acid, methoxy-, anhydride	C6 H10 O5	17.563			19500-95-9	LibSearch	69.08	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		69.08			12		

Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Acetic acid, methoxy-, anhydride	C6H10O5		LibSearch	17.563	-0.321		19500-95-9	69.08		
Acetic acid, methoxy-	C3H6O3		LibSearch	17.563	5.029		625-45-6	68.62		
Ethane, 1,2-dimethoxy-	C4H10O2		LibSearch	17.563	8.046		110-71-4	61.90		
Ethane, 1,2-dimethoxy-	C4H10O2		LibSearch	17.563	8.046		110-71-4	58.83		
Ethane, 1,2-dimethoxy-	C4H10O2		LibSearch	17.563	8.046		110-71-4	56.63		
Ethane, 1,2-dimethoxy-	C4H10O2		LibSearch	17.563	8.046		110-71-4	56.37		
Hydrazine, ethyl-	C2H8N2		LibSearch	17.563	6.529		624-80-6	51.10		
Hydrazine, ethyl-	C2H8N2		LibSearch	17.563	6.529		624-80-6	50.25		
Propanedioic acid	C3H4O4		LibSearch	17.563	0.363		141-82-2	29.80		
Nitrous acid, ethyl ester	C2H5NO2		LibSearch	17.563	10.729		109-95-5	28.74		
2-Hydroxyethyl vinyl sulfide	C4H8OS		LibSearch	17.563	2.529		3090-56-0	23.58		
1,3,4-Thiadiazol-2-amine, 5-[2-(2-methoxy)ethyl]-	C5H9N3OS		LibSearch	17.563	-5.404		15884-90-9	22.13		

Compound Discovery Report

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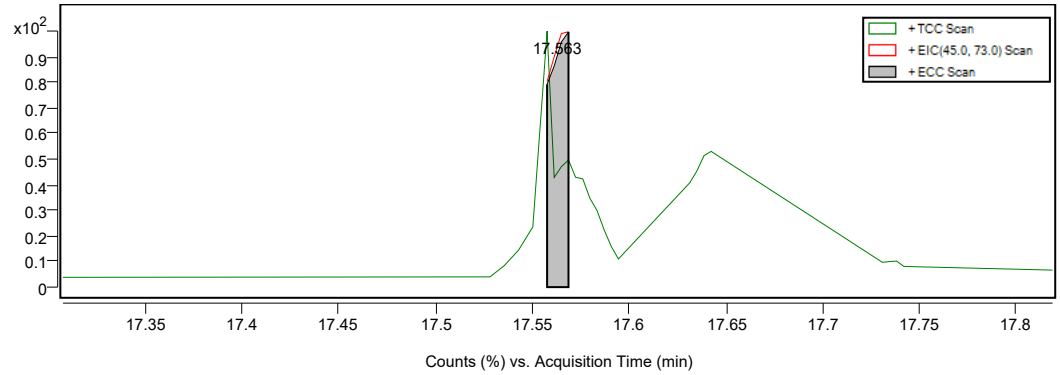
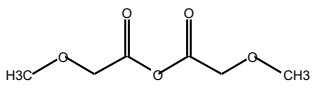
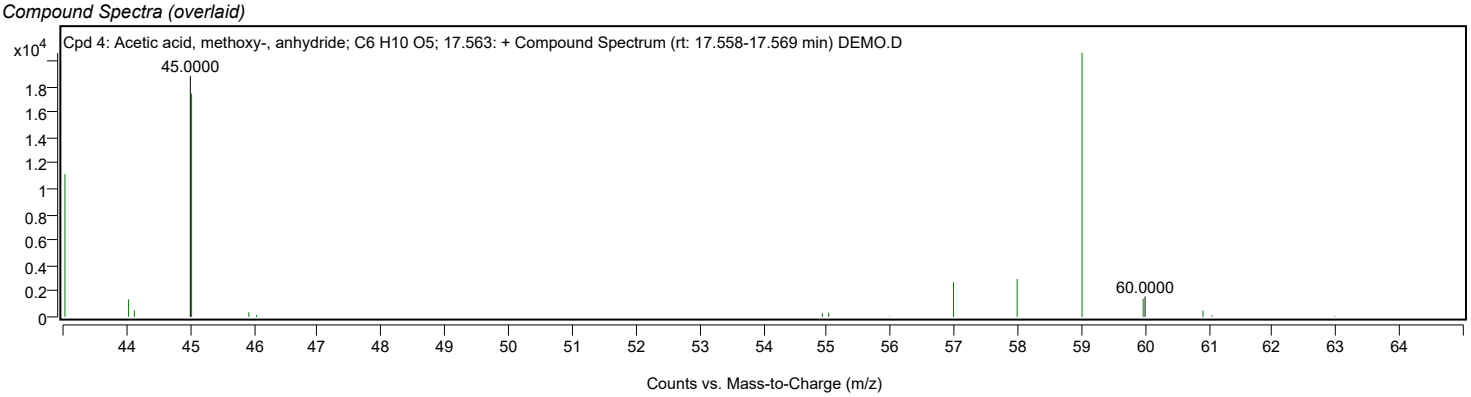
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



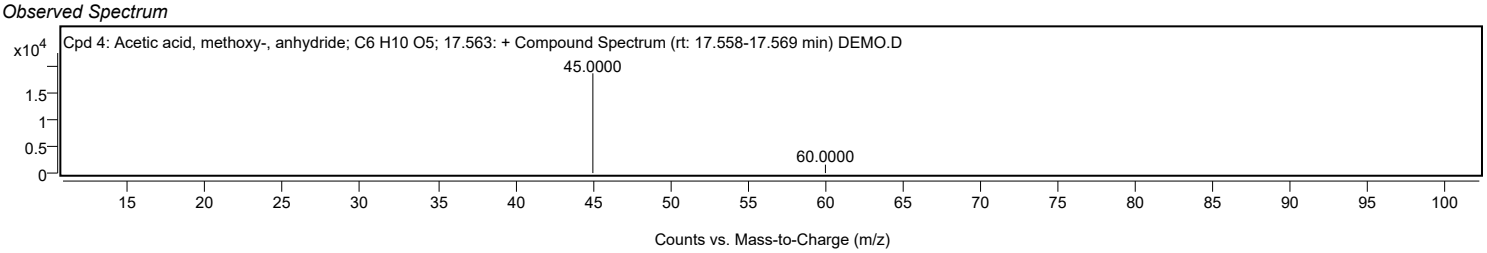
Acetic acid, methoxy-, anhydride

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			69.08			NIST.L

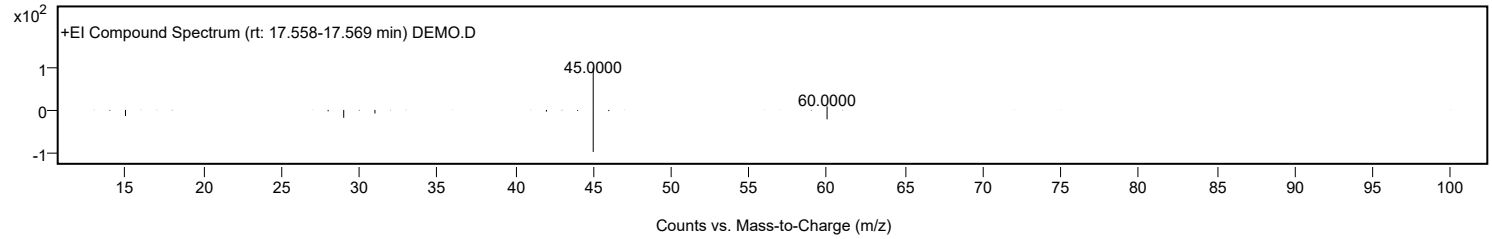
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			69.08			NIST.L

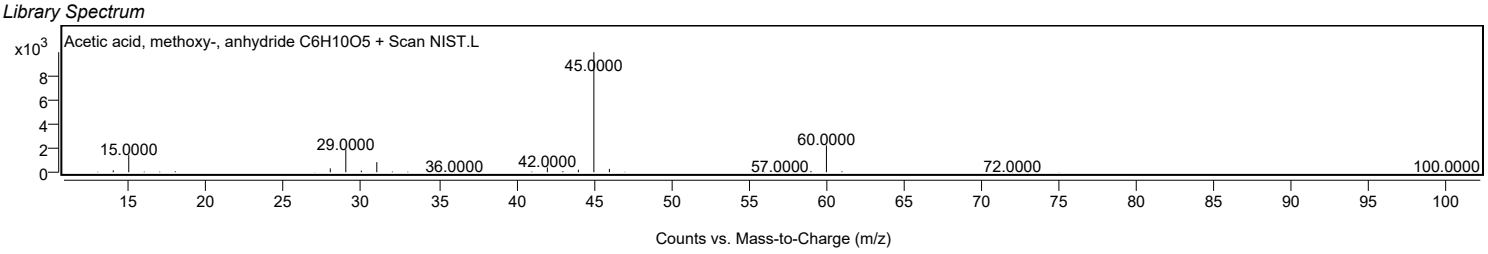
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 5: 1-Propanol, 2-(2-hydroxypropoxy)-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
1-Propanol, 2-(2-hydroxypropoxy)-	C6 H14 O3	17.575			106-62-7	LibSearch	85.15	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		85.15			50		

Compound Discovery Report

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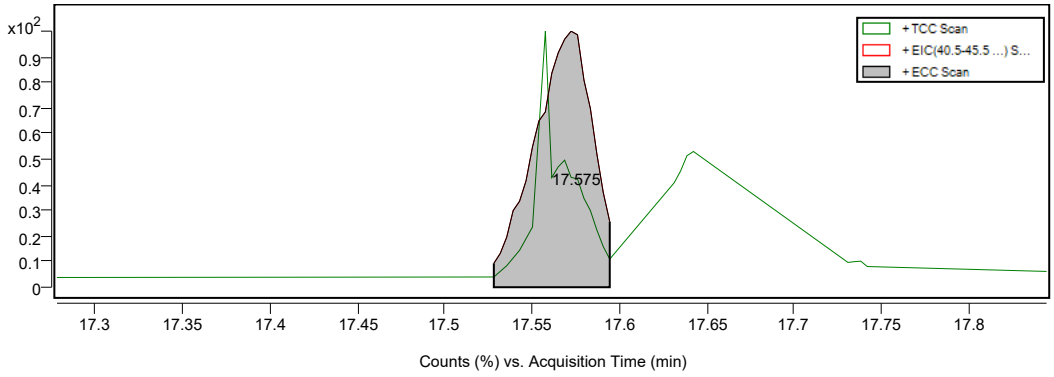
Compound ID Table

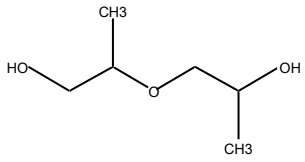
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.575	0.342		106-62-7	85.15		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.575			106-62-7	85.15		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.575			106-62-7	84.73		
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.575	0.342		106-62-7	84.73		
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.575	0.342		106-62-7	84.69		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.575			106-62-7	84.69		
1-Propanol, 2,2'-oxybis-	C6H14O3		LibSearch	17.575	0.059		108-61-2	84.48		
DPG 1-Propanol, 2,2'-oxybis-	C6H14O3		LibSearch	17.575			108-61-2	84.48		
Dipropylene glycol (isomer 2)	C6H14O3		LibSearch	17.575	0.609		1000506-25-4	83.47		
Dipropylene glycol (isomer 2)	C6H14O3		LibSearch	17.575			1000506-25-4	83.47		
Dipropylene glycol (isomer 3)	C6H14O3		LibSearch	17.575			1000506-25-5	83.27		
Dipropylene glycol (isomer 3)	C6H14O3		LibSearch	17.575	0.609		1000506-25-5	83.27		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.575			106-62-7	80.48		
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.575	0.342		106-62-7	80.48		
2-(2-methoxyethoxy)propanoic acid, O-acetyl-	C8H14O5		LibSearch	17.575	-2.541		1000506-61-7	80.30		
1,4,7-Trimethyl-3,6-dioxaoctane-1,8-diol	C9H20O4		LibSearch	17.575	-4.825		1000423-63-2	80.07		
1-Propanol, 3,3'-oxybis-	C6H14O3		LibSearch	17.575	-2.075		2396-61-4	77.15		
2-Propanol, 1-[1-methyl-2-(2-propenyloxy)ethoxy]-	C9H18O3		LibSearch	17.575	-1.691		55956-25-7	74.29		
Ethanol, 1-methoxy-, acetate	C5H10O3		LibSearch	17.575	5.959		4382-77-8	72.86		
2-Propanol, 1-(2-butoxy-1-methylethoxy)-	C10H22O3		LibSearch	17.575	-3.508		29911-28-2	72.68		
Guanidine	CH5N3		LibSearch	17.575			113-00-8	71.54		
Pentanol <3->	C5H12O		LibSearch	17.575			584-02-1	70.96		
2-Propanol, 1-(2-methoxy-1-methylethoxy)-	C7H16O3		LibSearch	17.575	1.459		20324-32-7	70.23		
Hexylene glycol	C6H14O2		LibSearch	17.575	3.042		107-41-5	69.95		
Propanoic acid, 2-hydroxy-2-methyl-, methyl ester	C5H10O3		LibSearch	17.575	4.625		2110-78-3	69.91		
2-Propanol, 1-(2-methoxy-1-methylethoxy)-	C7H16O3		LibSearch	17.575	1.459		20324-32-7	69.43		
2,4-Diethyl-6-methyl-1,3,5-trioxane	C8H16O3		LibSearch	17.575	-0.241		117888-04-7	69.03		
2-Propanol, 1-(2-butoxy-1-methylethoxy)-	C10H22O3		LibSearch	17.575	-3.508		29911-28-2	68.88		
Methane, diethoxy-	C5H12O2		LibSearch	17.575	6.409		462-95-3	68.71		
Propane, 1,2-dimethoxy-	C5H12O2		LibSearch	17.575	7.475		7778-85-0	68.61		
Propanoic acid, 2-hydroxy-2-methyl-, methyl ester	C5H10O3		LibSearch	17.575	4.625		2110-78-3	68.25		
Ethanol, 2-(1,1-dimethylethoxy)-	C6H14O2		LibSearch	17.575	3.375		7580-85-0	67.73		
Ethanol, 2-(1,1-dimethylethoxy)-	C6H14O2		LibSearch	17.575	3.375		7580-85-0	67.64		
Guanidine, monothiocyanate	C2H4N4S		LibSearch	17.575	-1.041		56960-89-5	67.59		
2-Propanol, 1,1'-[(1-methyl-1,2-ethanediyl)bis(oxy)]bis-	C9H20O4		LibSearch	17.575	-4.558		1638-16-0	67.44		
Butan-2-ol	C4H10O		LibSearch	17.575			78-92-2	67.36		
Pinacol	C6H14O2		LibSearch	17.575			76-09-5	66.98		
Propanoic acid, 2-hydroxy-2-methyl-, methyl ester	C5H10O3		LibSearch	17.575	4.625		2110-78-3	66.72		
Silane, dimethyl-	C2H8Si		LibSearch	17.575			1111-74-6	66.54		
Propionic acid, 2-isopropoxy-, methyl ester	C7H14O3		LibSearch	17.575	3.709		1000151-15-1	66.46		
Ethoxy ethanol<2->	C4H10O2		LibSearch	17.575	15.245		110-80-5	66.37		
Isopropyl methyl carbonate	C5H10O3		LibSearch	17.575	5.959		51729-83-0	66.29		
Propyl alcohol	C3H8O		LibSearch	17.575			71-23-8	66.10		
Silane, dimethyl-	C2H8Si		LibSearch	17.575			1111-74-6	66.09		
2-Propanol, 1-(2-methoxy-1-methylethoxy)-	C7H16O3		LibSearch	17.575	1.459		20324-32-7	66.08		
Tetraglyme	C10H22O5		LibSearch	17.575	-5.675		143-24-8	66.01		
Tetraglyme	C10H22O5		LibSearch	17.575	-5.675		143-24-8	65.96		
Ethoxy ethanol <2->	C4H10O2		LibSearch	17.575			110-80-5	65.81		
Butanoic acid, 4-methoxy-	C5H10O3		LibSearch	17.575	1.725		29006-02-8	65.47		
Methane, diethoxy-	C5H12O2		LibSearch	17.575	6.409		462-95-3	65.41		

Compound Chromatograms (overlaid)

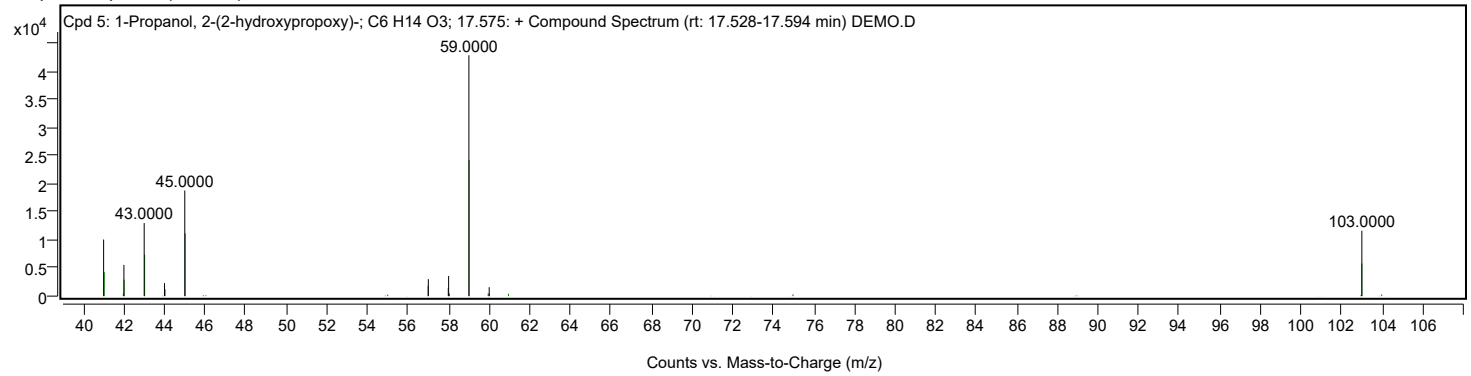


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



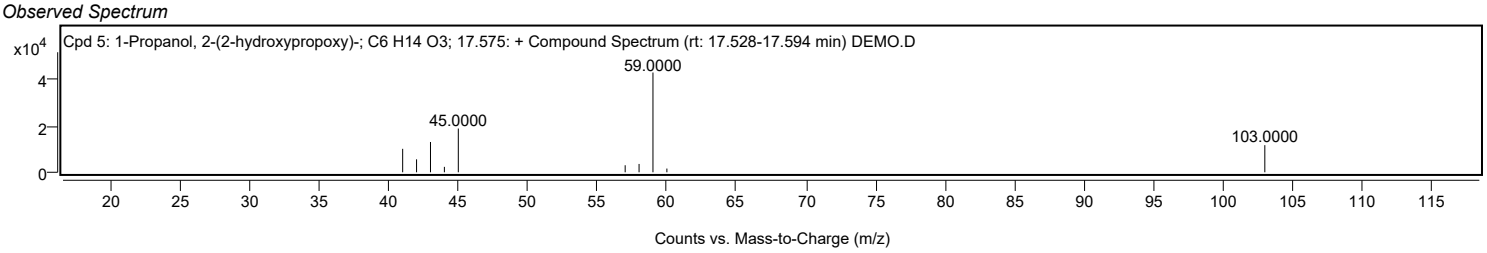
1-Propanol, 2-(2-hydroxypropoxy)-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			85.15			NIST.L

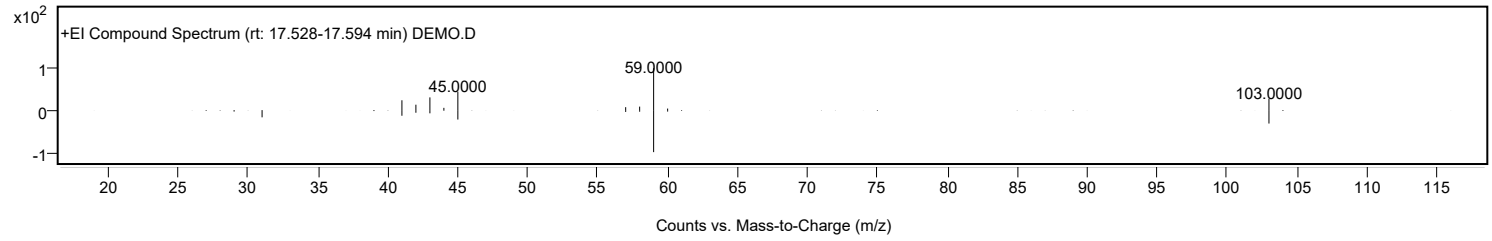
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			85.15			NIST.L

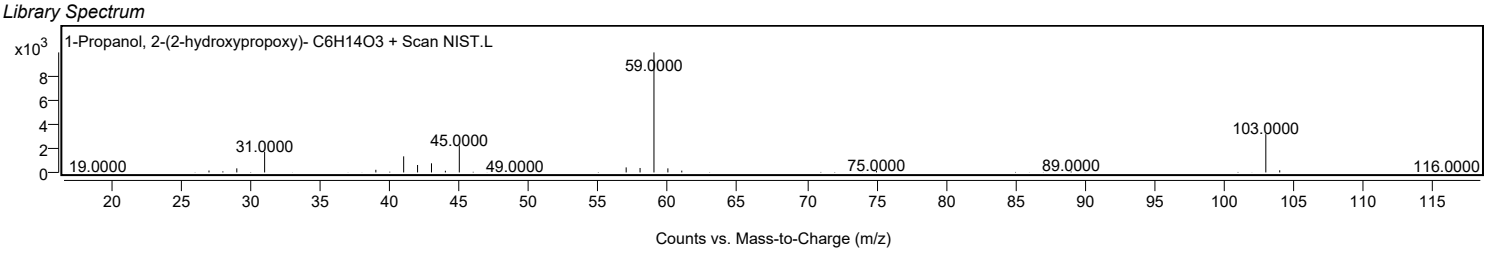
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 6: 1-Propanol, 2-(2-hydroxypropoxy)-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
1-Propanol, 2-(2-hydroxypropoxy)-	C6 H14 O3	17.640			106-62-7	LibSearch	83.56	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		83.56			50		

Compound Discovery Report

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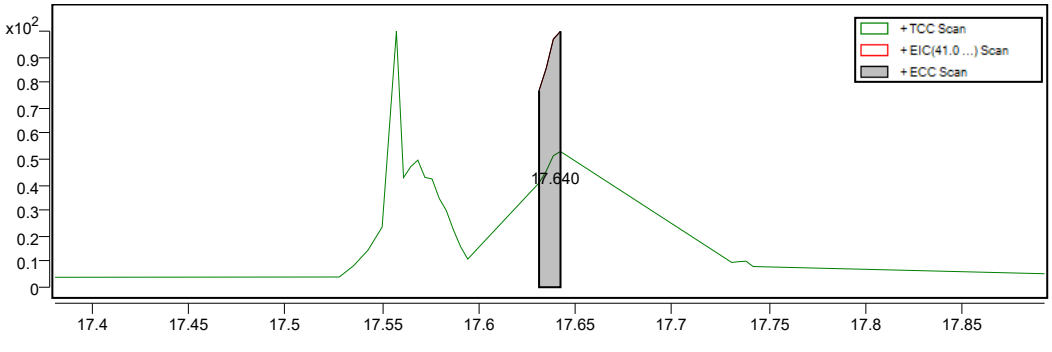
Compound ID Table

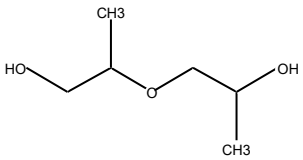
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.640	0.406		106-62-7	83.56		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.640			106-62-7	83.56		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.640			106-62-7	82.84		
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.640	0.406		106-62-7	82.84		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.640			106-62-7	82.70		
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.640	0.406		106-62-7	82.70		
1-Propanol, 2,2'-oxybis-	C6H14O3		LibSearch	17.640	0.123		108-61-2	82.17		
DPG 1-Propanol, 2,2'-oxybis-	C6H14O3		LibSearch	17.640			108-61-2	82.17		
Dipropylene glycol (isomer 2)	C6H14O3		LibSearch	17.640	0.673		1000506-25-4	81.58		
Dipropylene glycol (isomer 2)	C6H14O3		LibSearch	17.640			1000506-25-4	81.58		
Dipropylene glycol (isomer 3)	C6H14O3		LibSearch	17.640			1000506-25-5	81.22		
Dipropylene glycol (isomer 3)	C6H14O3		LibSearch	17.640	0.673		1000506-25-5	81.22		
2-(2-methoxyethoxy)propanoic acid, O-acetyl-	C8H14O5		LibSearch	17.640	-2.477		1000506-61-7	79.21		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.640			106-62-7	78.51		
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.640	0.406		106-62-7	78.51		
1,4,7-Trimethyl-3,6-dioxaoctane-1,8-diol	C9H20O4		LibSearch	17.640	-4.760		1000423-63-2	76.17		
Ethanol, 1-methoxy-, acetate	C5H10O3		LibSearch	17.640	6.023		4382-77-8	74.45		
1-Propanol, 3,3'-oxybis-	C6H14O3		LibSearch	17.640	-2.010		2396-61-4	73.89		
2-Propanol, 1-[1-methyl-2-(2-propenyloxy)ethoxy]-	C9H18O3		LibSearch	17.640	-1.627		55956-25-7	72.53		
2-Propanol, 1-(2-butoxy-1-methylethoxy)-	C10H22O3		LibSearch	17.640	-3.444		29911-28-2	71.53		
Methane, diethoxy-	C5H12O2		LibSearch	17.640	6.473		462-95-3	71.37		
Propanoic acid, 2-hydroxy-2-methyl-, methyl ester	C5H10O3		LibSearch	17.640	4.690		2110-78-3	70.41		
2,4-Diethyl-6-methyl-1,3,5-trioxane	C8H16O3		LibSearch	17.640	-0.177		117888-04-7	69.59		
Pentanol <3->	C5H12O		LibSearch	17.640			584-02-1	69.33		
2-Propanol, 1-(2-methoxy-1-methylethoxy)-	C7H16O3		LibSearch	17.640	1.523		20324-32-7	68.97		
Butan-2-ol	C4H10O		LibSearch	17.640			78-92-2	68.87		
Propanoic acid, 2-hydroxy-2-methyl-, methyl ester	C5H10O3		LibSearch	17.640	4.690		2110-78-3	68.66		
2-Propanol, 1-(2-methoxy-1-methylethoxy)-	C7H16O3		LibSearch	17.640	1.523		20324-32-7	68.26		
Ethanol, 2-(1,1-dimethylethoxy)-	C6H14O2		LibSearch	17.640	3.440		7580-85-0	67.83		
2-Propanol, 1-(2-butoxy-1-methylethoxy)-	C10H22O3		LibSearch	17.640	-3.444		29911-28-2	67.57		
Methane, diethoxy-	C5H12O2		LibSearch	17.640	6.473		462-95-3	67.21		
Propanoic acid, 2-hydroxy-2-methyl-, methyl ester	C5H10O3		LibSearch	17.640	4.690		2110-78-3	67.02		
Propane, 1,2-dimethoxy-	C5H12O2		LibSearch	17.640	7.540		7778-85-0	66.85		
Ethanol, 2-(1,1-dimethylethoxy)-	C6H14O2		LibSearch	17.640	3.440		7580-85-0	66.83		
Tetraglyme	C10H22O5		LibSearch	17.640	-5.610		143-24-8	66.15		
Propionic acid, 2-isopropoxy-, methyl ester	C7H14O3		LibSearch	17.640	3.773		1000151-15-1	66.11		
Tetraglyme	C10H22O5		LibSearch	17.640	-5.610		143-24-8	66.11		
Hexylene glycol	C6H14O2		LibSearch	17.640	3.106		107-41-5	65.98		
Butanoic acid, 2-hydroxy-, ethyl ester	C6H12O3		LibSearch	17.640	1.856		52089-54-0	65.96		
2-Propanol, 1,1'-[(1-methyl-1,2-ethanediyl)bis(oxy)]bis-	C9H20O4		LibSearch	17.640	-4.494		1638-16-0	65.51		
2-Butanol, 3-methoxy-	C5H12O2		LibSearch	17.640	6.106		53778-72-6	65.42		
Ethanol, 2-(1,1-dimethylethoxy)-	C6H14O2		LibSearch	17.640	3.440		7580-85-0	64.97		
Pinacol	C6H14O2		LibSearch	17.640			76-09-5	64.70		
1-(1-tert-Butoxypropan-2-yloxy)propan-2-ol	C10H22O3		LibSearch	17.640	-2.044		132739-31-2	64.45		
Methane, diethoxy-	C5H12O2		LibSearch	17.640	6.473		462-95-3	64.44		
1-Propanol, 2-methoxy-	C4H10O2		LibSearch	17.640	6.423		1589-47-5	64.38		
Acetic acid, [2-(2-methoxyethoxy)ethoxy]-	C7H14O5		LibSearch	17.640	-4.044		16024-58-1	64.34		
Tetraglyme	C10H22O5		LibSearch	17.640	-5.610		143-24-8	64.31		
Tetraglyme	C10H22O5		LibSearch	17.640	-5.610		143-24-8	64.11		
2,5,8,11-Tetraoxadodecane	C8H18O4		LibSearch	17.640	-1.027		112-49-2	64.06		

Compound Chromatograms (overlaid)

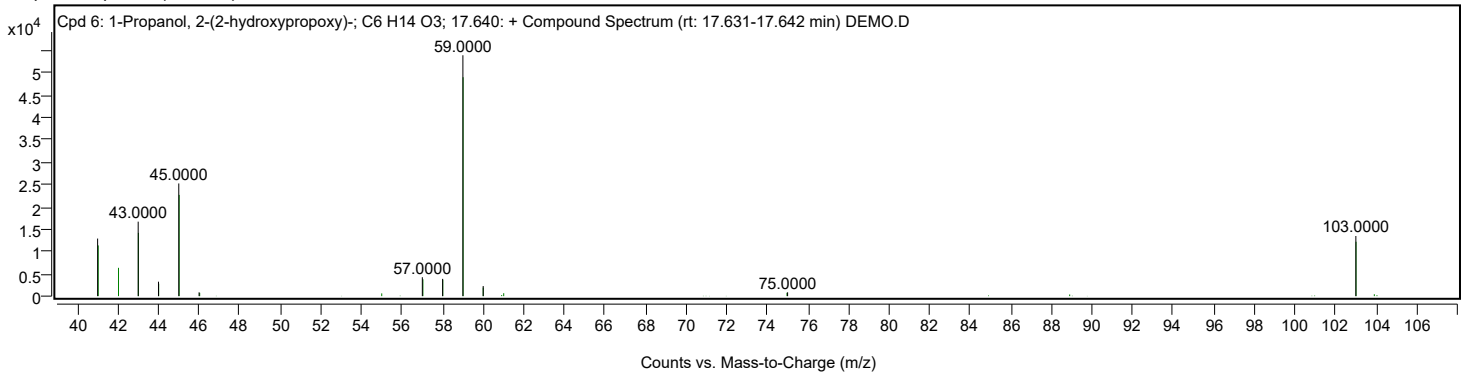


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



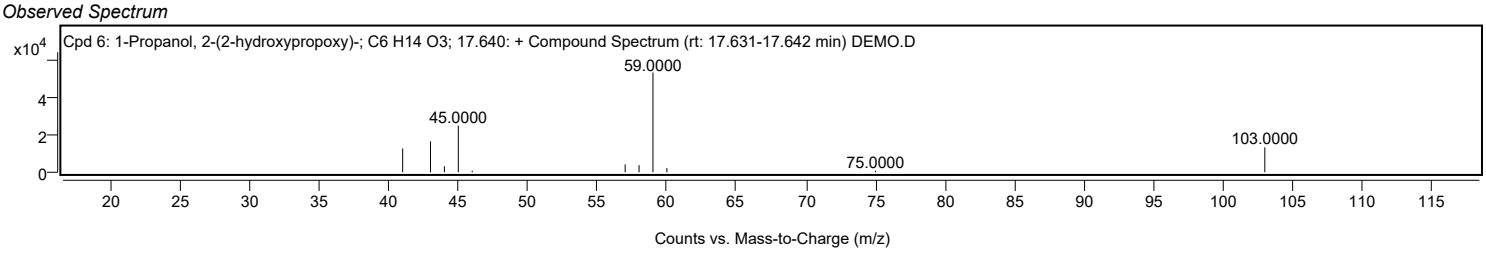
1-Propanol, 2-(2-hydroxypropoxy)-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			83.56			NIST.L

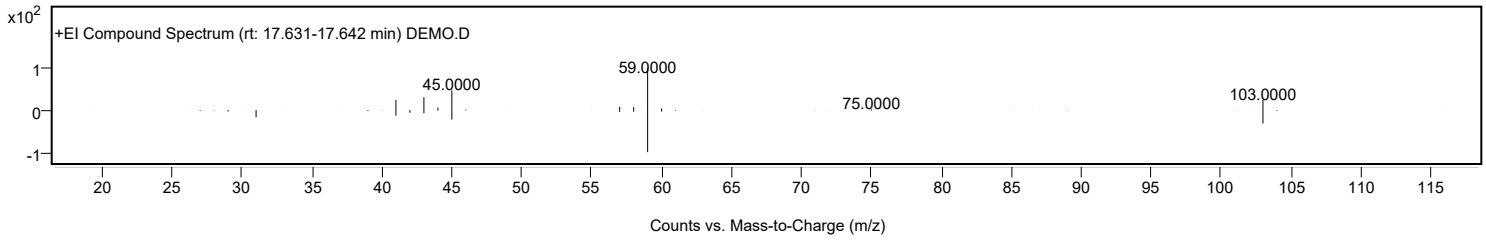
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			83.56			NIST.L

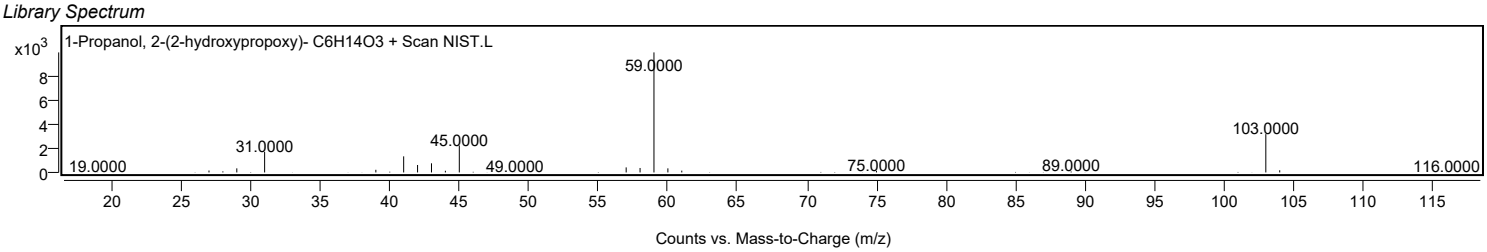
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 7: 1-Propanol, 2-(2-hydroxypropoxy)-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
1-Propanol, 2-(2-hydroxypropoxy)-	C6 H14 O3	17.737			106-62-7	LibSearch	79.03	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		79.03			50		

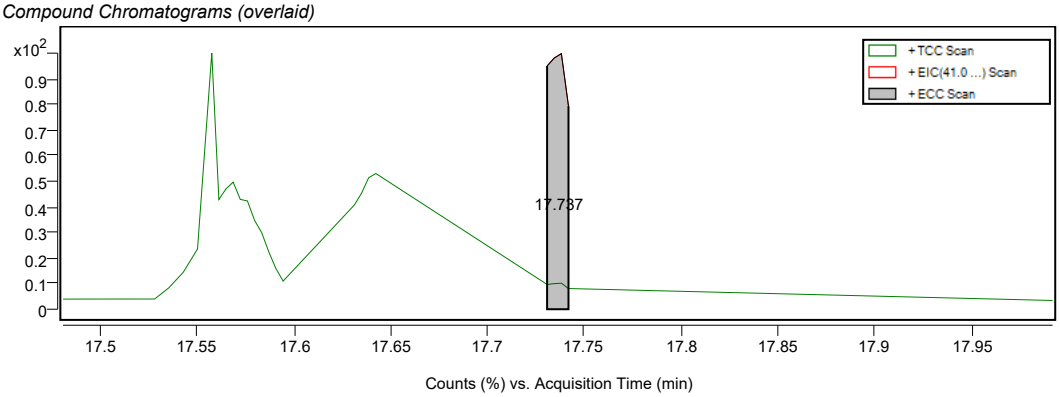
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

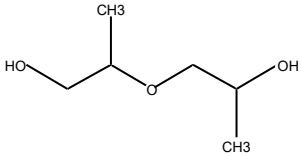
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.737	0.504		106-62-7	79.03		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.737			106-62-7	79.03		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.737			106-62-7	78.95		
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.737	0.504		106-62-7	78.95		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.737			106-62-7	77.92		
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.737	0.504		106-62-7	77.92		
1-Propanol, 2,2'-oxybis-	C6H14O3		LibSearch	17.737	0.220		108-61-2	77.01		
DPG 1-Propanol, 2,2'-oxybis-	C6H14O3		LibSearch	17.737			108-61-2	77.01		
Dipropylene glycol (isomer 2)	C6H14O3		LibSearch	17.737			1000506-25-4	76.74		
Dipropylene glycol (isomer 2)	C6H14O3		LibSearch	17.737	0.770		1000506-25-4	76.74		
Dipropylene glycol (isomer 3)	C6H14O3		LibSearch	17.737			1000506-25-5	76.19		
Dipropylene glycol (isomer 3)	C6H14O3		LibSearch	17.737	0.770		1000506-25-5	76.19		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.737			106-62-7	74.02		
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	17.737	0.504		106-62-7	74.02		
2-(2-methoxyethoxy)propanoic acid, O-acetyl-	C8H14O5		LibSearch	17.737	-2.380		1000506-61-7	72.53		
1,4,7-Trimethyl-3,6-dioxaoctane-1,8-diol	C9H20O4		LibSearch	17.737	-4.663		1000423-63-2	70.94		
2-Propanol, 1-[1-methyl-2-(2-propenyloxy)ethoxy]-	C9H18O3		LibSearch	17.737	-1.530		55956-25-7	70.24		
2-Propanol, 1-(2-butoxy-1-methylethoxy)-	C10H22O3		LibSearch	17.737	-3.346		29911-28-2	66.78		
1-Propanol, 3,3'-oxybis-	C6H14O3		LibSearch	17.737	-1.913		2396-61-4	66.07		
Ethanol, 2-(1,1-dimethylethoxy)-	C6H14O2		LibSearch	17.737	3.537		7580-85-0	65.48		
Ethanol, 2-(1,1-dimethylethoxy)-	C6H14O2		LibSearch	17.737	3.537		7580-85-0	65.25		
2,4-Diethyl-6-methyl-1,3,5-trioxane	C8H16O3		LibSearch	17.737	-0.080		117888-04-7	65.00		
2-Propanol, 1-(2-methoxy-1-methylethoxy)-	C7H16O3		LibSearch	17.737	1.620		20324-32-7	64.87		
2-Propanol, 1-(2-methoxy-1-methylethoxy)-	C7H16O3		LibSearch	17.737	1.620		20324-32-7	64.71		
2-Butanol	C4H10O		LibSearch	17.737	8.054		78-92-2	63.88		
2-Propanol, 1-(2-butoxy-1-methylethoxy)-	C10H22O3		LibSearch	17.737	-3.346		29911-28-2	63.60		
Methane, diethoxy-	C5H12O2		LibSearch	17.737	6.570		462-95-3	63.12		
Propanoic acid, 2-hydroxy-2-methyl-, methyl ester	C5H10O3		LibSearch	17.737	4.787		2110-78-3	62.97		
Ethanol, 2-(1,1-dimethylethoxy)-	C6H14O2		LibSearch	17.737	3.537		7580-85-0	62.80		
Isopropyl methyl carbonate	C5H10O3		LibSearch	17.737	6.120		51729-83-0	62.49		
Hexylene glycol	C6H14O2		LibSearch	17.737	3.204		107-41-5	62.34		
2-Propanol, 1,1'-[(1-methyl-1,2-ethanediyl)bis(oxy)]bis-	C9H20O4		LibSearch	17.737	-4.396		1638-16-0	61.52		
2-Butanol	C4H10O		LibSearch	17.737	8.054		78-92-2	61.11		
Propanoic acid, 2-hydroxy-2-methyl-, methyl ester	C5H10O3		LibSearch	17.737	4.787		2110-78-3	60.99		
1-Ethoxypentan-3-ol	C7H16O2		LibSearch	17.737	1.820		100910-92-7	60.81		
Propionic acid, 2-isopropoxy-, methyl ester	C7H14O3		LibSearch	17.737	3.870		1000151-15-1	60.55		
Methane, diethoxy-	C5H12O2		LibSearch	17.737	6.570		462-95-3	60.45		
1-(1-tert-Butoxypropan-2-yloxy)propan-2-ol	C10H22O3		LibSearch	17.737	-1.946		132739-31-2	59.80		
Pinacol	C6H14O2		LibSearch	17.737			76-09-5	59.62		
Ethanol, 2-(1,1-dimethylethoxy)-	C6H14O2		LibSearch	17.737	3.537		7580-85-0	59.37		
2-Butanol	C4H10O		LibSearch	17.737	8.054		78-92-2	58.50		
Propanoic acid, 2-hydroxy-2-methyl-, methyl ester	C5H10O3		LibSearch	17.737	4.787		2110-78-3	58.33		
Pentanol <3->	C5H12O		LibSearch	17.737			584-02-1	58.16		
Hydrazine, 1-methyl-1-(2-methylpropyl)-	C5H14N2		LibSearch	17.737	5.304		20240-63-5	58.10		
Hexylene glycol	C6H14O2		LibSearch	17.737	3.204		107-41-5	57.99		
Methane, diethoxy-	C5H12O2		LibSearch	17.737	6.570		462-95-3	57.91		
Hexylene glycol	C6H14O2		LibSearch	17.737	3.204		107-41-5	57.89		
2-Propanol, 1-(1-methylethoxy)-	C6H14O2		LibSearch	17.737	4.537		3944-36-3	57.66		
2-Methyl-2,3-pentanediol	C6H14O2		LibSearch	17.737	3.204		7795-80-4	57.42		
Isopropyl Alcohol	C3H8O		LibSearch	17.737	9.704		67-63-0	56.93		

Compound Chromatograms (overlaid)

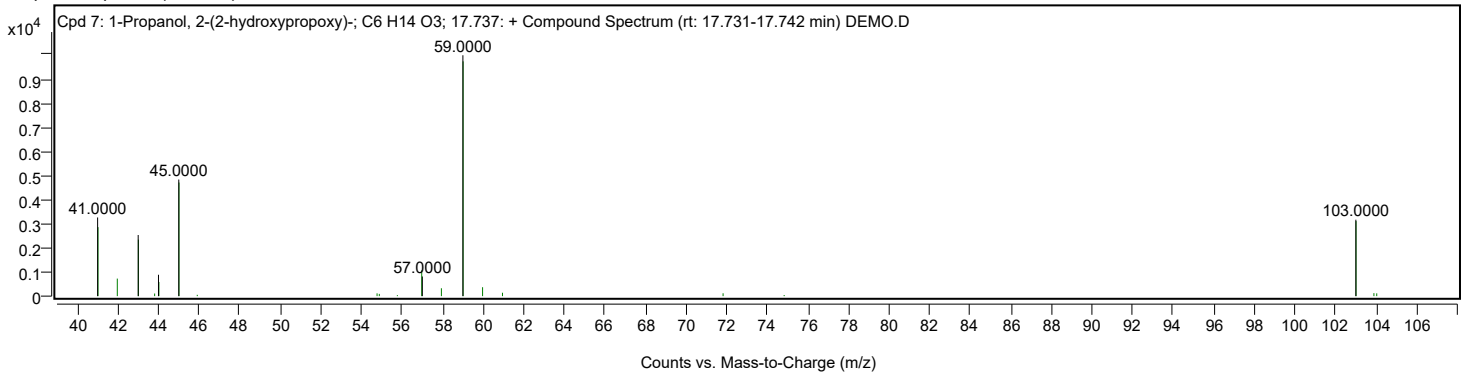


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



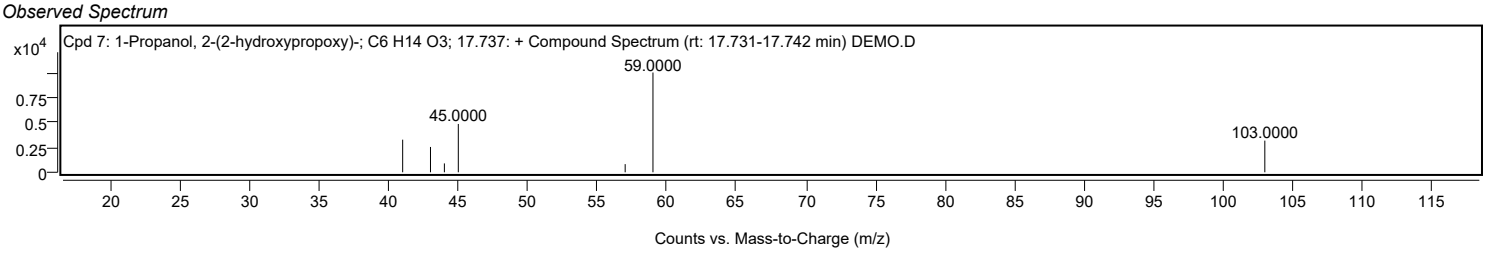
1-Propanol, 2-(2-hydroxypropoxy)-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			79.03			NIST.L

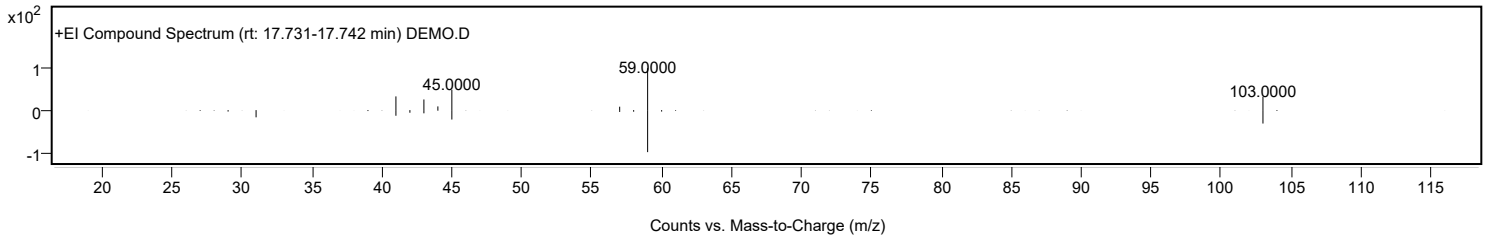
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			79.03			NIST.L

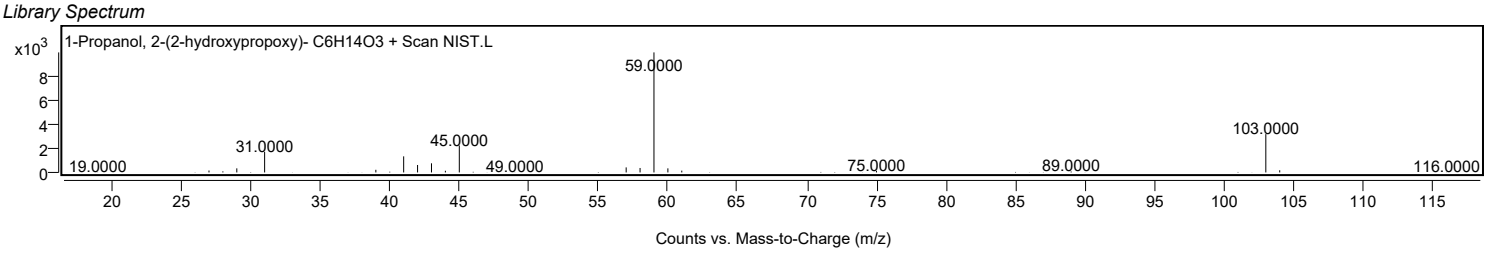
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 8: 1-Propanol, 2-(2-hydroxypropoxy)-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
1-Propanol, 2-(2-hydroxypropoxy)-	C6 H14 O3	18.203			106-62-7	LibSearch	76.66	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		76.66			50		

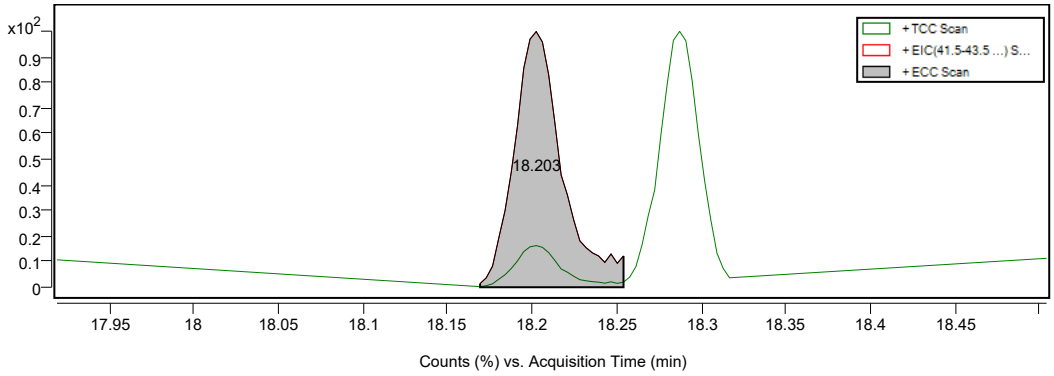
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

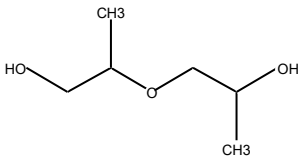
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	18.203	0.969		106-62-7	76.66		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	18.203			106-62-7	76.66		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	18.203			106-62-7	75.89		
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	18.203	0.969		106-62-7	75.89		
2-(2-methoxyethoxy)propanoic acid, O-acetyl-	C8H14O5		LibSearch	18.203	-1.914		1000506-61-7	74.79		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	18.203			106-62-7	74.20		
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	18.203	0.969		106-62-7	74.20		
DPG 1-Propanol, 2,2'-oxybis-	C6H14O3		LibSearch	18.203			108-61-2	73.99		
1-Propanol, 2,2'-oxybis-	C6H14O3		LibSearch	18.203	0.686		108-61-2	73.99		
Dipropylene glycol (isomer 2)	C6H14O3		LibSearch	18.203			1000506-25-4	73.88		
Dipropylene glycol (isomer 2)	C6H14O3		LibSearch	18.203	1.236		1000506-25-4	73.88		
Dipropylene glycol (isomer 3)	C6H14O3		LibSearch	18.203			1000506-25-5	73.57		
Dipropylene glycol (isomer 3)	C6H14O3		LibSearch	18.203	1.236		1000506-25-5	73.57		
1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	18.203	0.969		106-62-7	71.96		
DPG 1-Propanol, 2-(2-hydroxypropoxy)-	C6H14O3		LibSearch	18.203			106-62-7	71.96		
1,4,7-Trimethyl-3,6-dioxaoctane-1,8-diol	C9H20O4		LibSearch	18.203	-4.197		1000423-63-2	69.46		
2-Propanol, 1-(2-butoxy-1-methylethoxy)-	C10H22O3		LibSearch	18.203	-2.881		29911-28-2	64.46		
2,4-Diethyl-6-methyl-1,3,5-trioxane	C8H16O3		LibSearch	18.203	0.386		117888-04-7	64.34		
Ethanol, 2-(1,1-dimethylethoxy)-	C6H14O2		LibSearch	18.203	4.003		7580-85-0	62.13		
2-Propanol, 1-(2-methoxy-1-methylethoxy)-	C7H16O3		LibSearch	18.203	2.086		20324-32-7	62.10		
2-Propanol, 1-[1-methyl-2-(2-propenyloxy)ethoxy]-	C9H18O3		LibSearch	18.203	-1.064		55956-25-7	61.94		
2-Propanol, 1-(2-methoxy-1-methylethoxy)-	C7H16O3		LibSearch	18.203	2.086		20324-32-7	61.38		
1-Propanol, 3,3'-oxybis-	C6H14O3		LibSearch	18.203	-1.447		2396-61-4	61.28		
2-Propanol, 1-(2-butoxy-1-methylethoxy)-	C10H22O3		LibSearch	18.203	-2.881		29911-28-2	61.09		
Ethanol, 2-(1,1-dimethylethoxy)-	C6H14O2		LibSearch	18.203	4.003		7580-85-0	60.68		
Methane, diethoxy-	C5H12O2		LibSearch	18.203	7.036		462-95-3	60.66		
2-Propanol, 1,1'-[(1-methyl-1,2-ethanediyl)bis(oxy)]bis-	C9H20O4		LibSearch	18.203	-3.931		1638-16-0	60.30		
Ethanol, 2-(1,1-dimethylethoxy)-	C6H14O2		LibSearch	18.203	4.003		7580-85-0	60.05		
1-Ethoxypentan-3-ol	C7H16O2		LibSearch	18.203	2.286		100910-92-7	59.01		
Hexylene glycol	C6H14O2		LibSearch	18.203	3.669		107-41-5	58.91		
1-(1-tert-Butoxypropan-2-yloxy)propan-2-ol	C10H22O3		LibSearch	18.203	-1.481		132739-31-2	58.89		
Isopropyl methyl carbonate	C5H10O3		LibSearch	18.203	6.586		51729-83-0	58.32		
Methane, diethoxy-	C5H12O2		LibSearch	18.203	7.036		462-95-3	57.33		
Methane, diethoxy-	C5H12O2		LibSearch	18.203	7.036		462-95-3	56.88		
Propanoic acid, 2-hydroxy-2-methyl-, methyl ester	C5H10O3		LibSearch	18.203	5.253		2110-78-3	56.47		
Propionic acid, 2-isopropoxy-, methyl ester	C7H14O3		LibSearch	18.203	4.336		1000151-15-1	56.17		
Propanoic acid, 2-hydroxy-2-methyl-, methyl ester	C5H10O3		LibSearch	18.203	5.253		2110-78-3	55.94		
Acetic acid, [2-(2-methoxyethoxy)ethoxy]-	C7H14O5		LibSearch	18.203	-3.481		16024-58-1	55.57		
Hexylene glycol	C6H14O2		LibSearch	18.203	3.669		107-41-5	55.53		
2-Butanol, 3-methoxy-	C5H12O2		LibSearch	18.203	6.669		53778-72-6	55.29		
Guanidine, monothiocyanate	C2H4N4S		LibSearch	18.203	-0.414		56960-89-5	55.29		
Pinacol	C6H14O2		LibSearch	18.203			76-09-5	54.74		
3-Methyl-oxirane-2-carboxylic acid, methyl ester	C5H8O3		LibSearch	18.203	5.903		1000194-20-4	54.46		
Hexylene glycol	C6H14O2		LibSearch	18.203	3.669		107-41-5	54.14		
2-Propanol, 1-(2-methoxy-1-methylethoxy)-	C7H16O3		LibSearch	18.203	2.086		20324-32-7	54.00		
2,3-Butanediol, 2,3-dimethyl-	C6H14O2		LibSearch	18.203	4.853		76-09-5	53.69		
2-Butanol, 3-methoxy-	C5H12O2		LibSearch	18.203	6.669		53778-72-6	53.44		
2-Propanol, 1-(2-methoxypropoxy)-	C7H16O3		LibSearch	18.203	2.086		13429-07-7	53.26		
2-Propanol, 1-(2-ethoxypropoxy)-	C8H18O3		LibSearch	18.203	0.436		10143-32-5	53.15		
2-(2-(2-(2-Methoxyethoxy)ethoxy)ethoxy)acetic acid	C9H18O6		LibSearch	18.203	-8.064		16024-60-5	52.65		

Compound Chromatograms (overlaid)

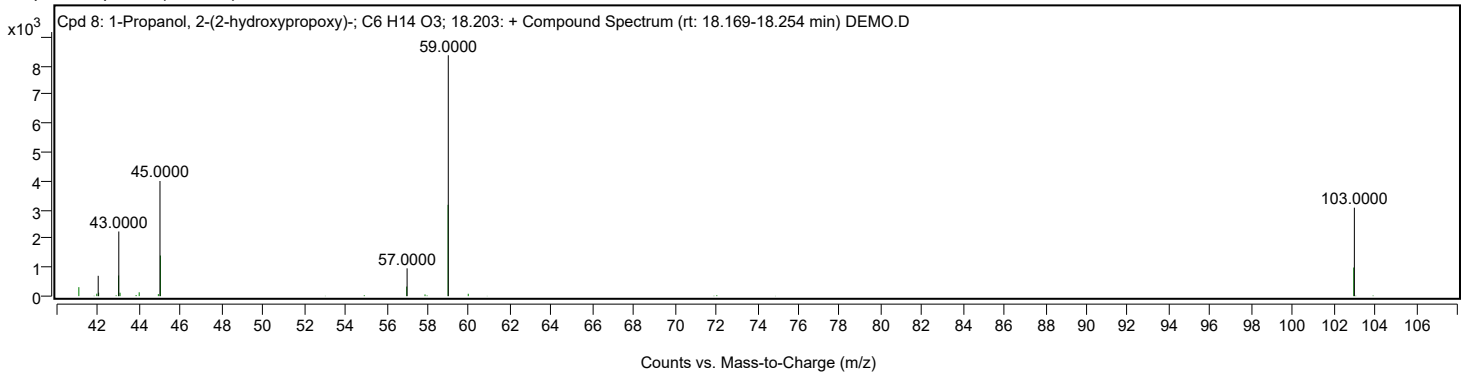


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



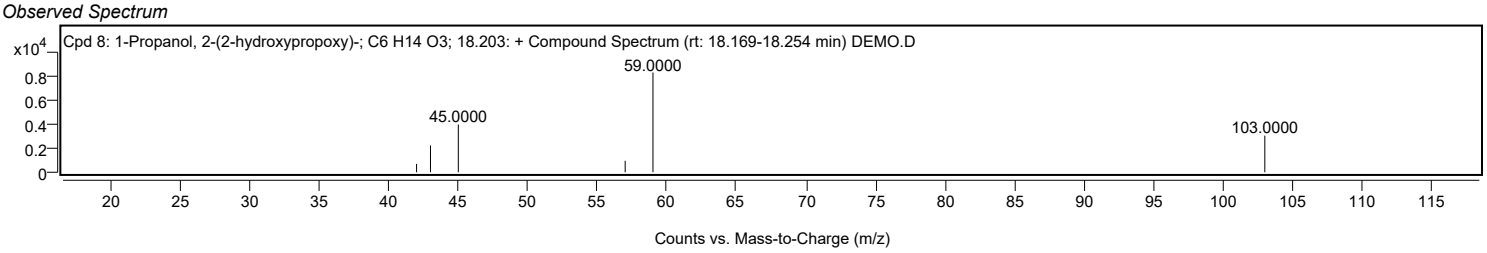
1-Propanol, 2-(2-hydroxypropoxy)-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			76.66			NIST.L

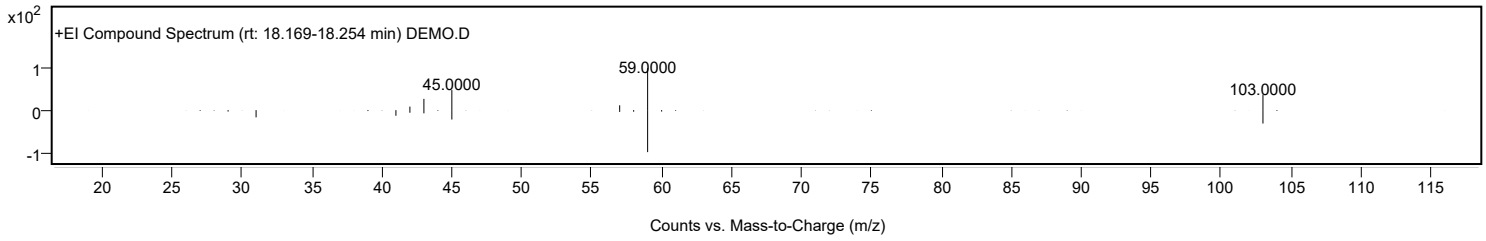
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			76.66			NIST.L

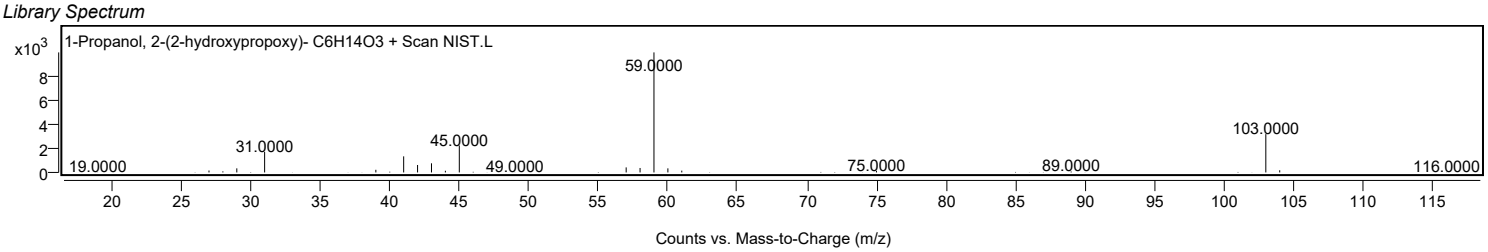
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 9: 2-Nonanone, 9-hydroxy-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
2-Nonanone, 9-hydroxy-	C9 H18 O2	18.285			25368-56-3	LibSearch	83.73	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		83.73			50		

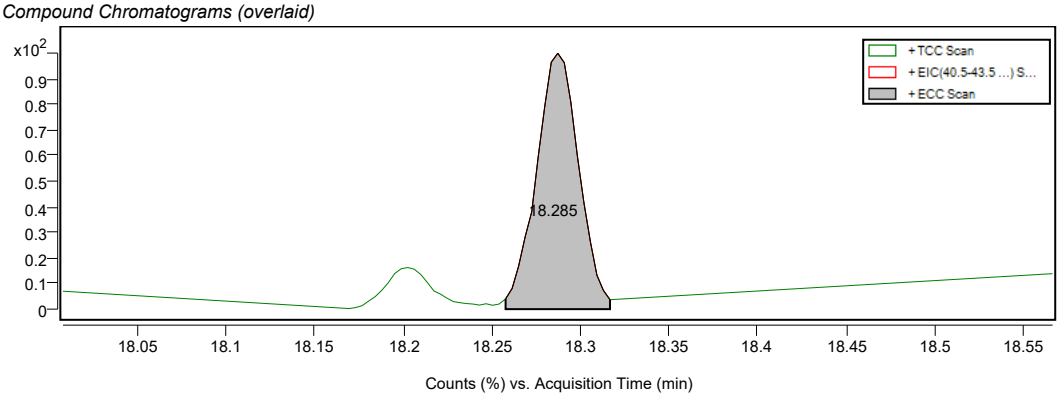
Compound Discovery Report

Agilent | Trusted Answers

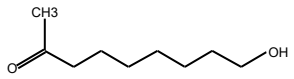
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
2-Nonanone, 9-hydroxy-	C9H18O2		LibSearch	18.285	-3.299		25368-56-3	83.73		
1,8-Nonanediol, 8-methyl-	C10H22O2		LibSearch	18.285	-4.215		54725-73-4	82.43		
Dihydromyrcenol	C10H20O		LibSearch	18.285	7.935		18479-58-8	78.30		
2-Octanol, 2,6-dimethyl-	C10H22O		LibSearch	18.285	0.901		18479-57-7	77.98		
Tetrahydromyrcenol	C10H22O		LibSearch	18.285			18479-57-7	77.76		
Pentanol <3->	C5H12O		LibSearch	18.285			584-02-1	76.12		
Dihydromyrcenol	C10H20O		LibSearch	18.285			18479-58-8	75.10		
Heptanol<2,6-dimethyl-2->	C9H20O		LibSearch	18.285	10.805		13254-34-7	74.44		
2-Decanol, methyl ether	C11H24O		LibSearch	18.285	-0.482		1000333-83-9	74.04		
6-Methylheptane-1,6-diol	C8H18O2		LibSearch	18.285	-0.899		5392-57-4	73.98		
Oxetane, 2,2,3-trimethyl-	C6H12O		LibSearch	18.285	7.218		23120-43-6	73.51		
2-Hexanol, 2,3-dimethyl-	C8H18O		LibSearch	18.285	4.218		19550-03-9	73.39		
7-Octen-2-ol, 2,6-dimethyl-	C10H20O		LibSearch	18.285	1.068		18479-58-8	73.33		
3-Heptanol, 4-methyl-	C8H18O		LibSearch	18.285	3.035		14979-39-6	73.15		
meso-3,4-Hexanediol	C6H14O2		LibSearch	18.285	2.585		22520-39-4	73.11		
2-Octanol, 2,6-dimethyl-	C10H22O		LibSearch	18.285	0.901		18479-57-7	73.05		
3-Hexene, 1-(1-methoxyethoxy)-, (E)-	C9H18O2		LibSearch	18.285	1.418		54340-97-5	72.60		
3-Hexene, 1-(1-methoxyethoxy)-, (Z)-	C9H18O2		LibSearch	18.285	1.418		54340-96-4	72.56		
o-Menthan-8-ol	C10H20O		LibSearch	18.285	-0.582		343855-44-7	72.42		
2-Hexanol, 2,5-dimethyl-, (S)-	C8H18O		LibSearch	18.285	4.218		3730-60-7	72.36		
2-Methyl-2-nonanol	C10H22O		LibSearch	18.285	-0.165		10297-57-1	72.33		
Hydroxy citronellol	C10H22O2		LibSearch	18.285	-4.545		107-74-4	72.18		
2-Hexanol, 2,3-dimethyl-	C8H18O		LibSearch	18.285	4.218		19550-03-9	71.94		
Dimetol	C9H20O		LibSearch	18.285			13254-34-7	71.93		
Hydroxycitronellol	C10H22O2		LibSearch	18.285			107-74-4	71.83		
2-Propanone, 1-cyclopentyl-	C8H14O		LibSearch	18.285	1.701		1122-98-1	71.46		
2-Heptanol, 2-methyl-	C8H18O		LibSearch	18.285	3.151		625-25-2	71.26		
2-Heptanol, 2-methyl-	C8H18O		LibSearch	18.285	3.151		625-25-2	71.24		
3-Hexanol, 4-ethyl-	C8H18O		LibSearch	18.285	3.035		19780-44-0	71.24		
4-Pentene-2-ol, 2-methyl	C6H12O		LibSearch	18.285	6.635		624-97-5	70.90		
2-Propanone, 1-cyclohexyl-	C9H16O		LibSearch	18.285	-0.299		103-78-6	70.89		
Cyclohexane, (ethoxymethoxy)-	C9H18O2		LibSearch	18.285	-0.565		54699-29-5	70.84		
7-Octen-2-ol, 2,6-dimethyl-	C10H20O		LibSearch	18.285	1.068		18479-58-8	70.57		
2-Pentanol, 2,3-dimethyl-	C7H16O		LibSearch	18.285	5.868		4911-70-0	70.30		
2,3-Dimethyloxirane-2-carboxylic acid, methyl ester	C6H10O3		LibSearch	18.285	4.768		1000306-64-4	70.27		
Terpineol <trans-dihydro-alpha->	C10H20O		LibSearch	18.285			5114-00-1	70.21		
2-Pentanol, 2,4-dimethyl-	C7H16O		LibSearch	18.285	5.868		625-06-9	70.20		
Terpineol<cis-dihydro-alpha->	C10H20O		LibSearch	18.285	4.195		7322-63-6	70.04		
2-Octanol, 2-methyl-6-methylene-	C10H20O		LibSearch	18.285	0.385		18479-59-9	70.00		
2,3,3-Trimethyl-2-pentanol	C8H18O		LibSearch	18.285	4.551		23171-85-9	69.92		
2-Dodecanol, 2-methyl-	C13H28O		LibSearch	18.285	-5.132		1653-37-8	69.71		
Octanol<3->	C8H18O		LibSearch	18.285	10.845		589-98-0	69.53		
2-Heptanol, 2,6-dimethyl-	C9H20O		LibSearch	18.285	2.568		13254-34-7	69.52		
3-Heptanol, 4-methyl-	C8H18O		LibSearch	18.285	3.035		14979-39-6	69.52		
3-Ethyl-2-methyl-2-heptanol	C10H22O		LibSearch	18.285	0.901		19780-59-7	69.48		
2-Methyl-2-decanol	C11H24O		LibSearch	18.285	-1.815		3396-02-9	69.19		
3-Pentadecanol	C15H32O		LibSearch	18.285	-9.632		53346-71-7	69.17		
2-Hexanol, 2-methyl-	C7H16O		LibSearch	18.285	4.801		625-23-0	69.13		
Butane, 2-methoxy-3-methyl-	C6H14O		LibSearch	18.285	8.868		62016-49-3	69.06		
2-Propanone, 1-cyclopentyl-	C8H14O		LibSearch	18.285	1.701		1122-98-1	68.91		

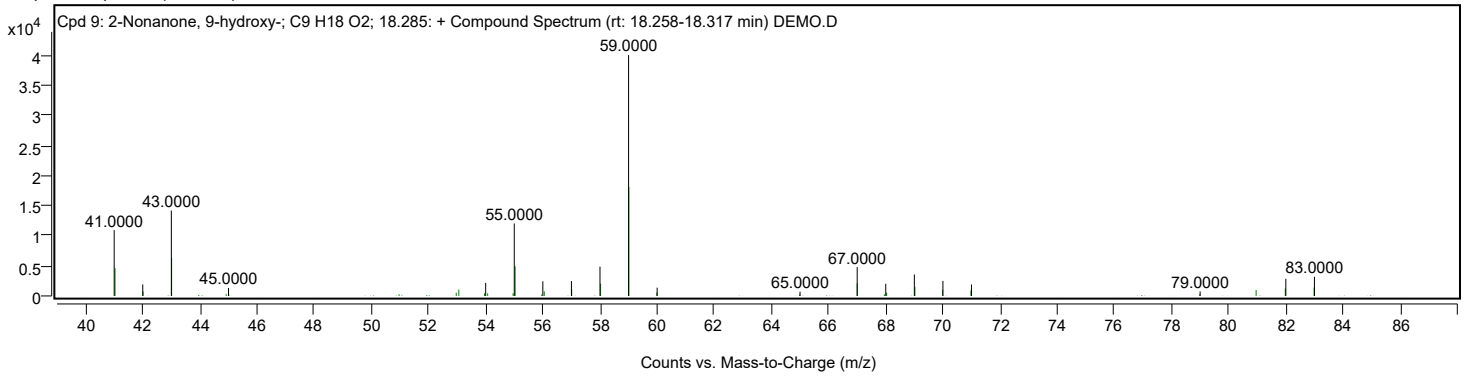
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



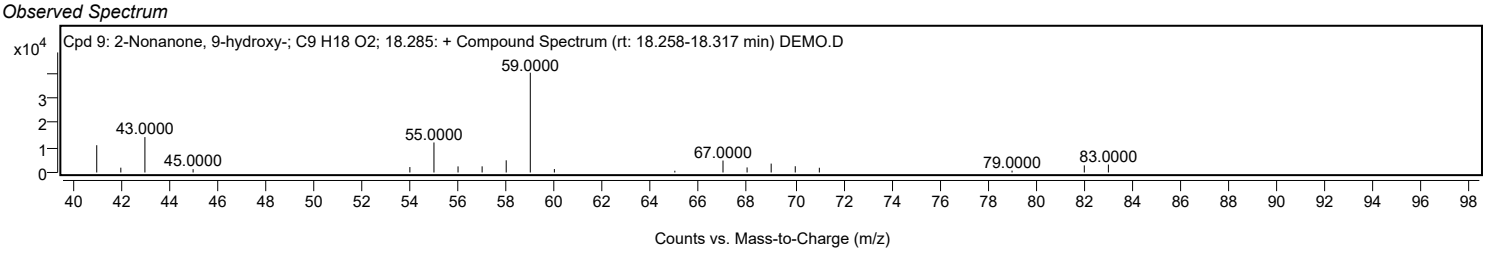
2-Nonanone, 9-hydroxy-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			83.73			NIST.L

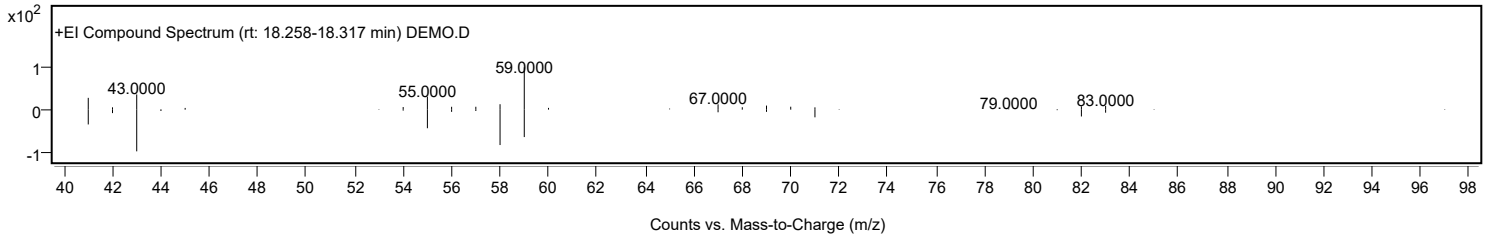
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			83.73			NIST.L

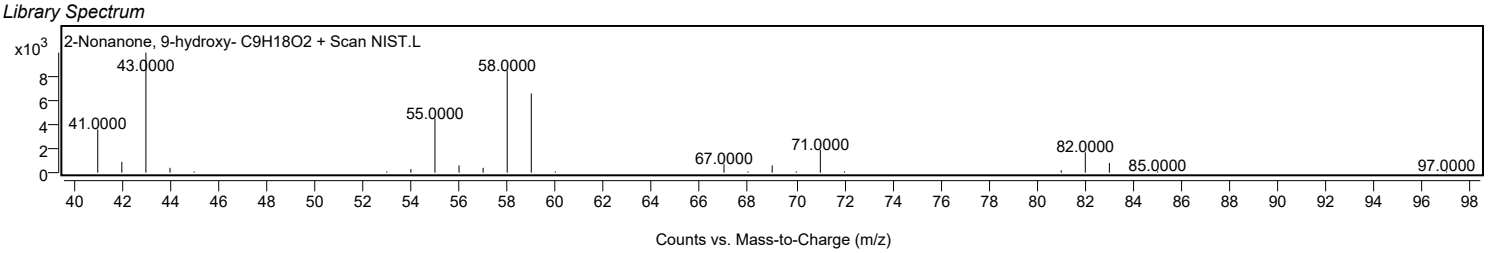
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 10: Toluene

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Toluene	C7 H8	19.429			108-88-3	LibSearch	80.22	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		80.22			50		

Compound Discovery Report

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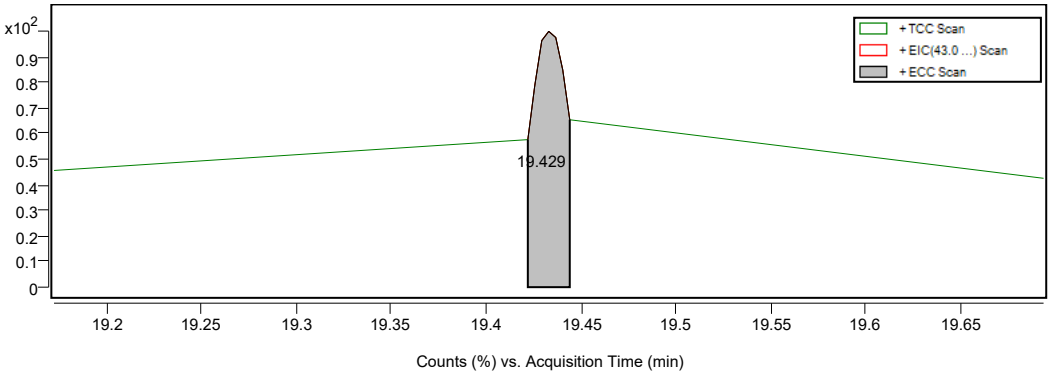
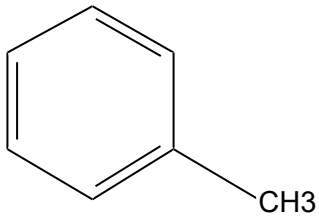
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Toluene	C7H8		LibSearch	19.429			108-88-3	80.22		
Toluene	C7H8		LibSearch	19.429	6.196		108-88-3	80.13		
Toluene	C7H8		LibSearch	19.429	6.196		108-88-3	79.57		
Toluene	C7H8		LibSearch	19.429	6.196		108-88-3	78.94		
Toluene	C7H8		LibSearch	19.429	6.196		108-88-3	78.76		
Toluene	C7H8		LibSearch	19.429	6.196		108-88-3	77.70		
Spiro[2,4]hepta-4,6-diene	C7H8		LibSearch	19.429	7.463		765-46-8	76.34		
Cycloheptatriene	C7H8		LibSearch	19.429			544-25-2	76.02		
Toluene	C7H8		LibSearch	19.429	6.196		108-88-3	74.17		
Cyclobutene, 2-propenylidene-	C7H8		LibSearch	19.429	7.179		52097-85-5	73.76		
1,5-Heptadien-3-yne	C7H8		LibSearch	19.429	7.213		3511-27-1	73.73		
Toluene	C7H8		LibSearch	19.429	6.196		108-88-3	72.96		
1,3,5-Cycloheptatriene	C7H8		LibSearch	19.429	6.329		544-25-2	72.71		
1,3,5-Cycloheptatriene	C7H8		LibSearch	19.429	6.329		544-25-2	71.67		
1,5-Hexadien-3-yne, 2-methyl-	C7H8		LibSearch	19.429	7.896		820-54-2	71.25		
1,6-Heptadien-3-yne	C7H8		LibSearch	19.429	7.513		5150-80-1	71.02		
Bicyclo[2.2.2]oct-7-en-2-one, 5-methylene-	C9H10O		LibSearch	19.429	1.396		1000217-18-1	70.96		
Benzeneethanol, .alpha.-methyl-	C9H12O		LibSearch	19.429	0.179		698-87-3	70.25		
Benzeneethanol, .alpha.-methyl-	C9H12O		LibSearch	19.429	0.179		698-87-3	69.69		
1,3,5-Cycloheptatriene	C7H8		LibSearch	19.429	6.329		544-25-2	69.64		
1,6-Heptadien-3-yne	C7H8		LibSearch	19.429	7.513		5150-80-1	69.27		
Spiro[2,4]hepta-4,6-diene	C7H8		LibSearch	19.429	7.463		765-46-8	68.93		
4-Benzyloxy-3-hydroxy-2-methyl-1-butene	C12H16O2		LibSearch	19.429	-5.504		1000432-17-9	68.22		
Hydroxylamine, O-(phenylmethyl)-	C7H9NO		LibSearch	19.429	0.879		622-33-3	68.20		
Spiro[3.3]hepta-1,5-diene	C7H8		LibSearch	19.429	7.463		22635-78-5	68.09		
Benzyl 2-chloroethyl sulfone	C9H11ClO2S		LibSearch	19.429	-9.304		66998-67-2	67.99		
Hydroxylamine, O-(phenylmethyl)-	C7H9NO		LibSearch	19.429	0.879		622-33-3	67.84		
N-Hydroxymethyl-2-phenylacetamide	C9H11NO2		LibSearch	19.429	-7.821		6291-06-1	67.71		
Benzene, (propoxymethyl)-	C10H14O		LibSearch	19.429	-0.037		937-61-1	67.51		
Gardenia ether	C12H18O		LibSearch	19.429			122-73-6	67.25		
Phenylethyl Alcohol	C8H10O		LibSearch	19.429	0.496		60-12-8	67.24		
Bicyclo[3.2.0]hepta-2,6-diene	C7H8		LibSearch	19.429	7.663		2422-86-8	67.16		
Benzene, (butoxymethyl)-	C11H16O		LibSearch	19.429	-1.687		588-67-0	66.94		
Benzene, (butoxymethyl)-	C11H16O		LibSearch	19.429	-1.687		588-67-0	66.85		
Tetracyclo[3.2.0.0(2,7).0(4,6)]heptane	C7H8		LibSearch	19.429	12.379		278-06-8	66.82		
Phenyl ethyl alcohol	C8H10O		LibSearch	19.429	7.679		60-12-8	66.78		
1-(Benzyloxy)-3,5-dinitrobenzene	C13H10N2O5		LibSearch	19.429	-19.471		128923-97-7	66.66		
Benzaldehyde, 4-benzyloxy-3-methoxy-2-nitro-	C15H13NO5		LibSearch	19.429	-21.054		2450-27-3	66.58		
4-Benzyloxy-3-methoxy-2-nitrobenzoic acid	C15H13NO6		LibSearch	19.429	-23.854		3584-32-5	66.24		
Phenethyl alcohol	C8H10O		LibSearch	19.429			60-12-8	66.20		
Benzene, (butoxymethyl)-	C11H16O		LibSearch	19.429	-1.687		588-67-0	66.19		
Benzyl 4-nitrophenyl carbonate	C14H11NO5		LibSearch	19.429	-17.321		13795-24-9	66.12		
Benzyl isopentyl ether	C12H18O		LibSearch	19.429	-2.271		122-73-6	65.99		
Phenylethyl Alcohol	C8H10O		LibSearch	19.429	0.496		60-12-8	65.97		
1,5-Hexadien-3-yne, 2-methyl-	C7H8		LibSearch	19.429	7.896		820-54-2	65.65		
N-(Benzyloxy)-2,2,2-trifluoroacetamide	C9H8F3NO2		LibSearch	19.429	-2.287		174075-91-3	65.53		
Thiocyanic acid, phenylmethyl ester	C8H7NS		LibSearch	19.429	-3.721		3012-37-1	65.46		
Benzene, 1,1'-[oxybis(methylene)]bis-	C14H14O		LibSearch	19.429	-7.937		103-50-4	65.45		
Phenylethyl Alcohol	C8H10O		LibSearch	19.429	0.496		60-12-8	65.26		
Benzyl ether	C14H14O		LibSearch	19.429			103-50-4	64.99		

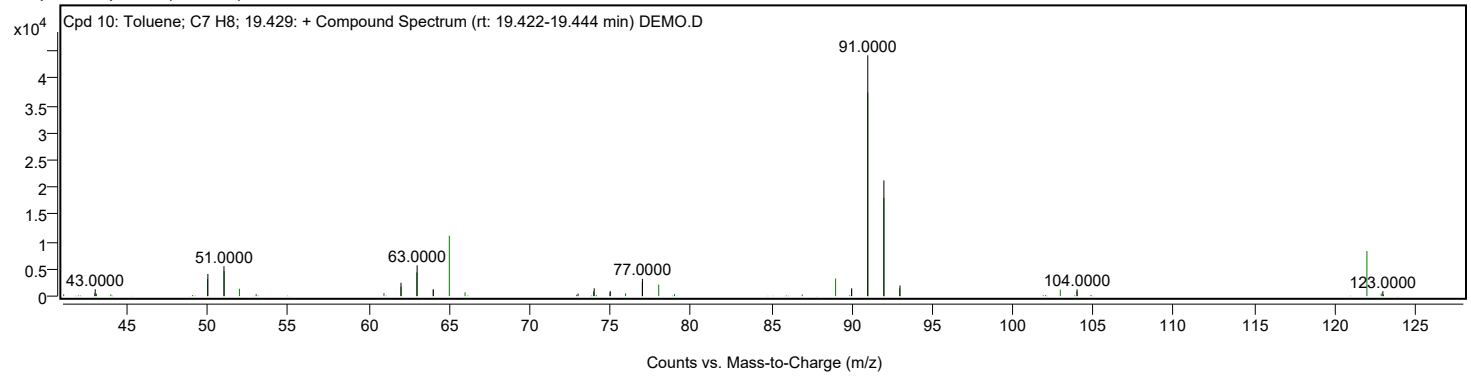
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



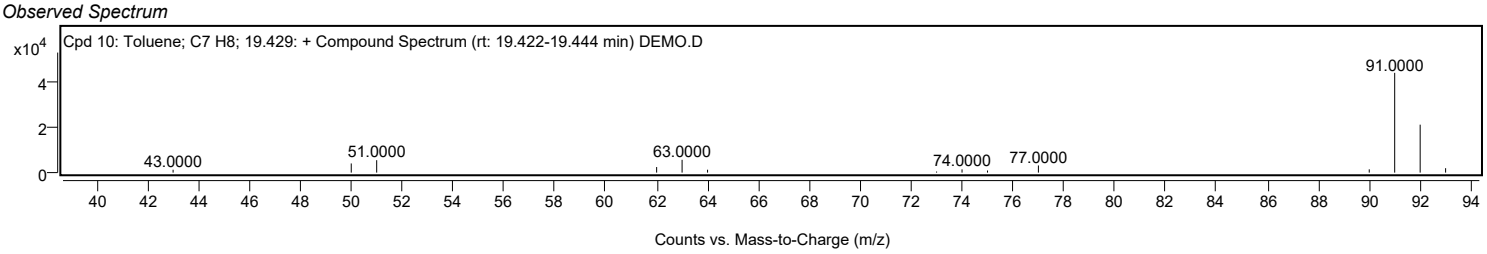
Toluene

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			80.22			PWNose.xml

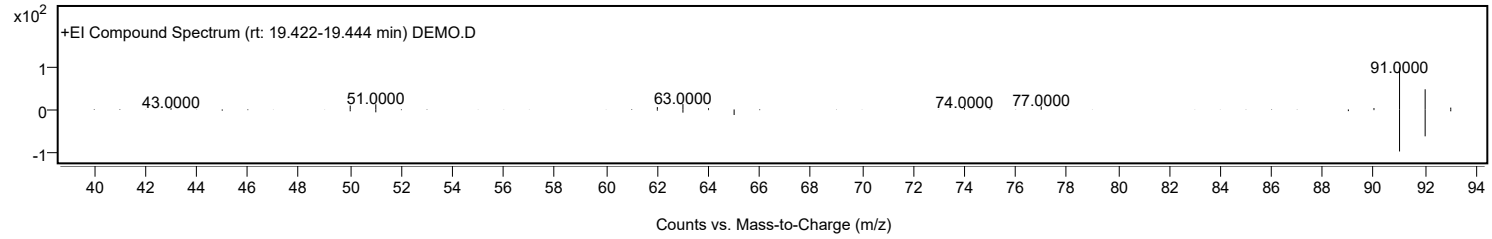
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			80.22			PWNose.xml

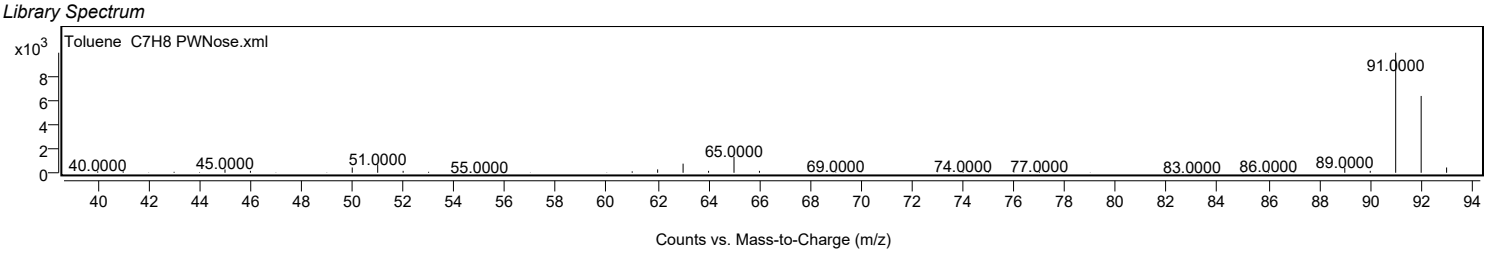
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 11: Benzyl acetate

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Benzyl acetate	C9 H10 O2	20.189			140-11-4	LibSearch	81.75	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		81.75			50		

Compound Discovery Report

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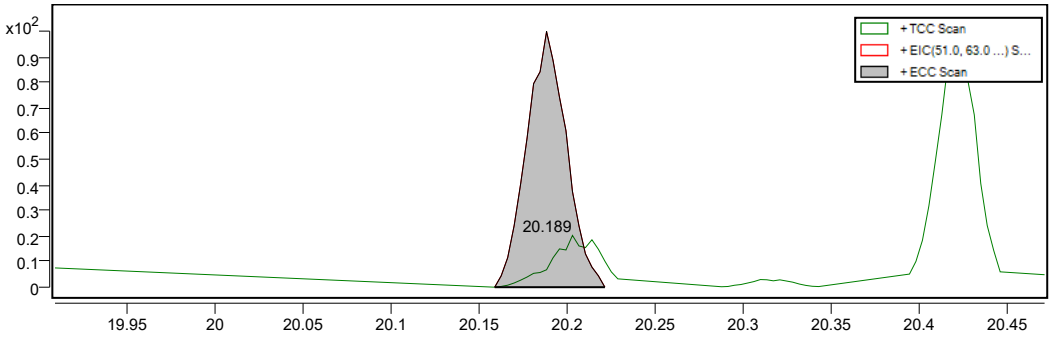
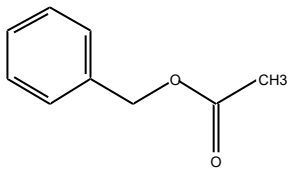
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Benzyl acetate	C9H10O2		LibSearch	20.189			140-11-4	81.75		
Acetic acid, phenylmethyl ester	C9H10O2		LibSearch	20.189	0.855		140-11-4	81.31		
Acetic acid, phenylmethyl ester	C9H10O2		LibSearch	20.189	0.855		140-11-4	80.68		
Acetic acid, phenylmethyl ester	C9H10O2		LibSearch	20.189	0.855		140-11-4	79.66		
Acetic acid, phenylmethyl ester	C9H10O2		LibSearch	20.189	0.855		140-11-4	79.24		
Benzyl acetate	C9H10O2		LibSearch	20.189	6.229		140-11-4	77.88		
Acetic acid, phenylmethyl ester	C9H10O2		LibSearch	20.189	0.855		140-11-4	73.95		
Carbonic acid, monoamide, N-propyl-, benzyl ester	C11H15NO2		LibSearch	20.189	-5.761		1000420-28-1	70.32		
4-Methylphenol, n-propyl ether	C10H14O		LibSearch	20.189	0.489		1000395-16-2	70.07		
Benzyl 3-hydroxypropanoate	C10H12O3		LibSearch	20.189	-4.845		1000090-68-8	69.25		
Acetic acid, 2-methylphenyl ester	C9H10O2		LibSearch	20.189	0.622		533-18-6	69.14		
Acetic acid, 2-methylphenyl ester	C9H10O2		LibSearch	20.189	0.622		533-18-6	68.57		
Carbonic acid, monoamide, N-butyl-, benzyl ester	C12H17NO2		LibSearch	20.189	-7.411		1000420-28-3	68.50		
4-Methylphenol, isopropyl ether	C10H14O		LibSearch	20.189	1.572		1000395-16-4	67.80		
m-Cresyl acetate	C9H10O2		LibSearch	20.189	0.622		122-46-3	67.47		
Benzylcarbamate	C8H9NO2		LibSearch	20.189	-1.528		621-84-1	67.17		
Benzylcarbamate	C8H9NO2		LibSearch	20.189	-1.528		621-84-1	66.93		
*EU Benzyl alcohol	C7H8O		LibSearch	20.189			100-51-6	66.92		
Acetic acid, 2-methylphenyl ester	C9H10O2		LibSearch	20.189	0.622		533-18-6	66.80		
Carbonic acid, monoamide, N-pentyl-, benzyl ester	C13H19NO2		LibSearch	20.189	-9.078		1000420-28-5	66.72		
Carbamic acid, methyl-, phenylmethyl ester	C9H11NO2		LibSearch	20.189	-2.445		30379-59-0	66.69		
Cresol <para-> acetate	C9H10O2		LibSearch	20.189			140-39-6	66.65		
Acetic acid, 4-methylphenyl ester	C9H10O2		LibSearch	20.189	0.622		140-39-6	66.63		
Carbonic acid, monoamide, N-isobutyl-, benzyl ester	C12H17NO2		LibSearch	20.189	-6.345		1000420-28-2	66.51		
Benzyl alcohol	C7H8O		LibSearch	20.189			100-51-6	66.37		
m-Cresyl acetate	C9H10O2		LibSearch	20.189	0.622		122-46-3	66.34		
m-Cresyl acetate	C9H10O2		LibSearch	20.189	0.622		122-46-3	65.95		
m-Cresyl acetate	C9H10O2		LibSearch	20.189	0.622		122-46-3	65.83		
Acetic acid, 2-methylphenyl ester	C9H10O2		LibSearch	20.189	0.622		533-18-6	65.56		
Acetic acid, 4-methylphenyl ester	C9H10O2		LibSearch	20.189	0.622		140-39-6	65.38		
Benzylcarbamate	C8H9NO2		LibSearch	20.189	-1.528		621-84-1	65.22		
Benzyl alcohol	C7H8O		LibSearch	20.189	2.922		100-51-6	65.00		
Cresol acetate<ortho->	C9H10O2		LibSearch	20.189	7.209		533-18-6	64.86		
Carbonic acid, monoamide, N-hexyl-, benzyl ester	C14H21NO2		LibSearch	20.189	-10.728		1000420-28-7	64.71		
Benzyl glycolate	C9H10O3		LibSearch	20.189	-3.178		30379-58-9	64.71		
Cresol acetate<para-	C9H10O2		LibSearch	20.189	5.839		140-39-6	64.70		
Benzyl formate	C8H8O2		LibSearch	20.189			104-57-4	64.51		
Benzyl alcohol	C7H8O		LibSearch	20.189	2.922		100-51-6	64.42		
Benzyl alcohol	C7H8O		LibSearch	20.189	2.922		100-51-6	64.41		
Acetic acid, 4-methylphenyl ester	C9H10O2		LibSearch	20.189	0.622		140-39-6	64.18		
L-Alanine, N-[(phenylmethoxy)carbonyl]-	C11H13NO4		LibSearch	20.189	-10.628		1142-20-7	64.12		
Benzyl propanoate	C10H12O2		LibSearch	20.189			122-63-4	64.07		
Carbonic acid, monoamide, N-3-methylbutyl-, benzyl ester	C13H19NO2		LibSearch	20.189	-8.011		1000420-28-4	64.02		
Cresol acetate <o->	C9H10O2		LibSearch	20.189			533-18-6	64.02		
L-Alanine, N-[(phenylmethoxy)carbonyl]-	C11H13NO4		LibSearch	20.189	-10.628		1142-20-7	63.92		
N-(Benzyloxycarbonyl)-3,3,3-trifluoroalanine ethyl ester	C13H14F3NO4		LibSearch	20.189	-8.028		134356-87-9	63.86		
DL-Alanine, N-[(phenylmethoxy)carbonyl]-	C11H13NO4		LibSearch	20.189	-10.628		4132-86-9	63.79		
L-Asparagine, N2-[(phenylmethoxy)carbonyl]-	C12H14N2O5		LibSearch	20.189	-19.111		2304-96-3	63.60		
Benzyl alcohol	C7H8O		LibSearch	20.189	11.419		100-51-6	63.44		
N-Cbz-glycylglycine p-nitrophenyl ester	C18H17N3O7		LibSearch	20.189	-34.678		13574-81-7	63.41		

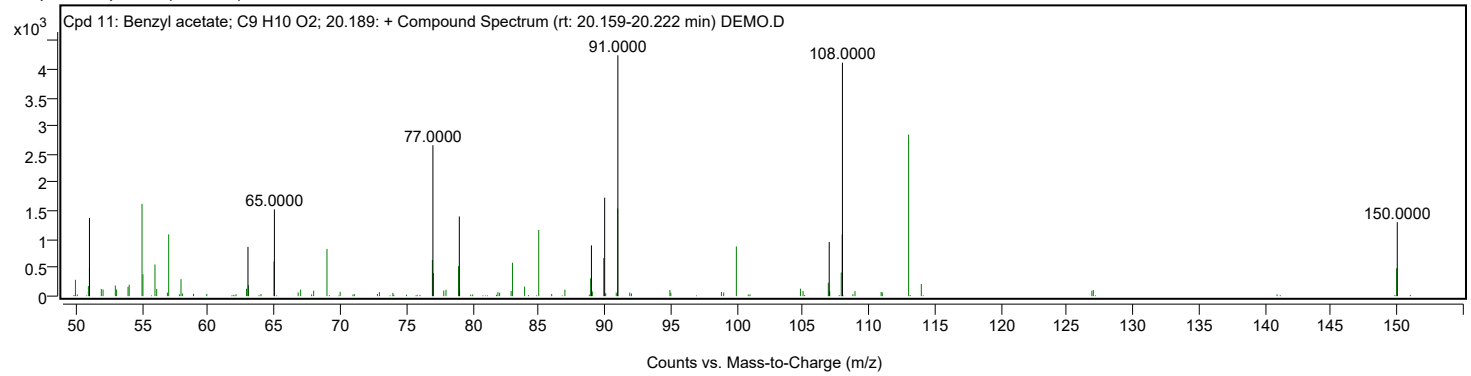
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



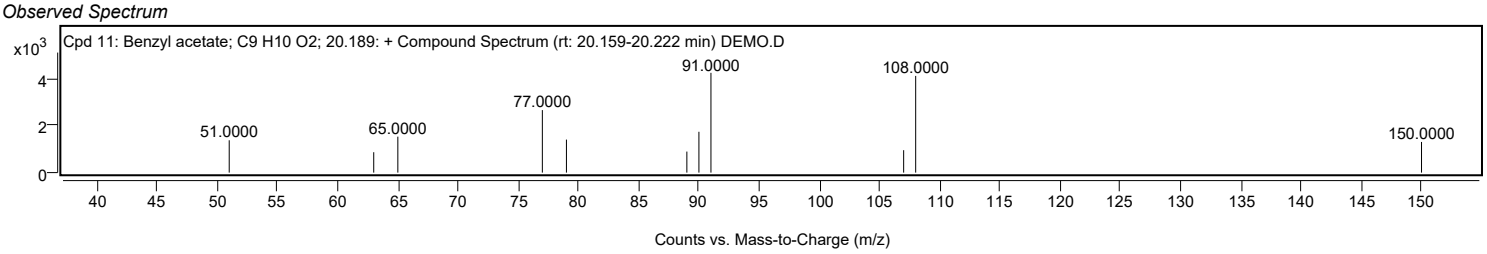
Benzyl acetate

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			81.75			PWNose.xml

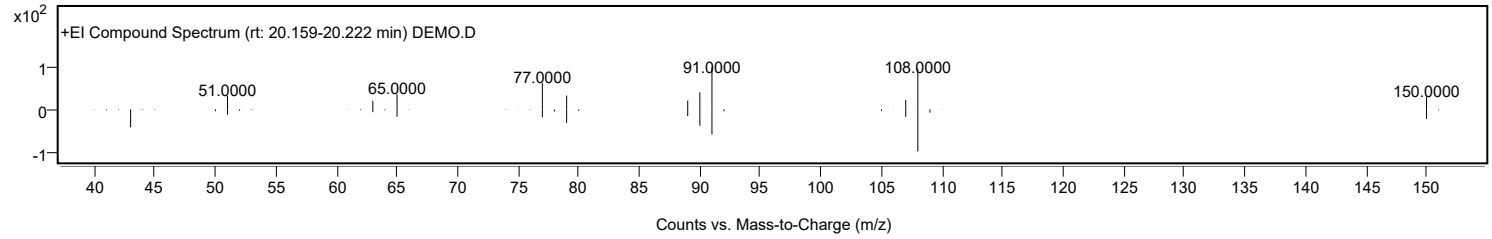
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			81.75			PWNose.xml

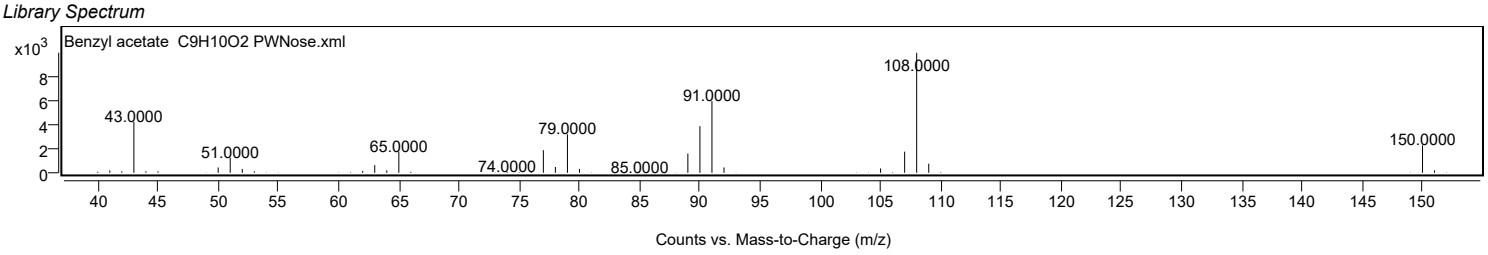
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 12: Allyl heptanoate

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Allyl heptanoate	C10 H18 O2	20.216			142-19-8	LibSearch	83.37	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		83.37			50		

Compound Discovery Report

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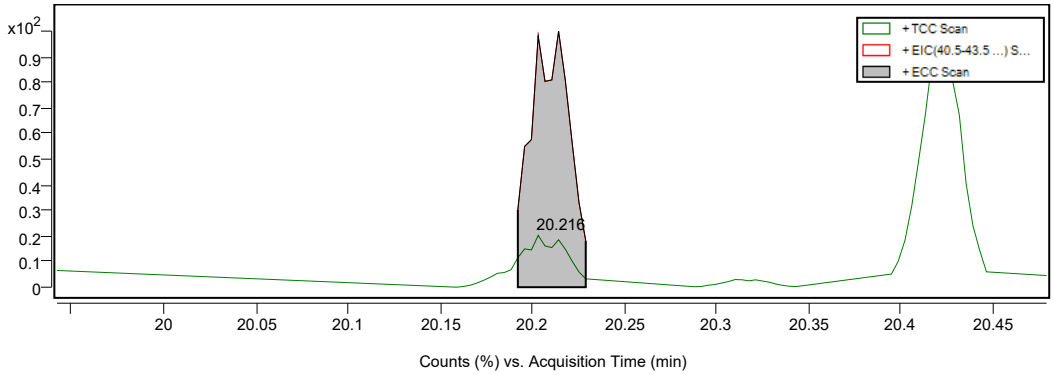
Compound ID Table

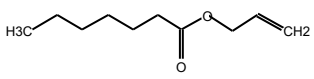
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Allyl heptanoate	C10H18O2		LibSearch	20.216	0.666		142-19-8	83.37		
Allyl heptanoate	C10H18O2		LibSearch	20.216	0.666		142-19-8	82.05		
Heptanoate <allyl->	C10H18O2		LibSearch	20.216			142-19-8	80.61		
Allyl heptanoate	C10H18O2		LibSearch	20.216	5.356		142-19-8	80.40		
Allyl heptanoate	C10H18O2		LibSearch	20.216	0.666		142-19-8	77.65		
Allyl heptanoate	C10H18O2		LibSearch	20.216	0.666		142-19-8	76.71		
2,3-Nonanedione	C9H16O2		LibSearch	20.216	0.416		1000430-93-9	76.28		
2-Oxooctanoic acid	C8H14O3		LibSearch	20.216	-1.601		328-51-8	71.22		
2-Methyl-4-decanone	C11H22O		LibSearch	20.216	0.432		6628-25-7	67.39		
Heptanoic acid, anhydride	C14H26O3		LibSearch	20.216	-8.384		626-27-7	66.15		
Heptanoic acid, 3-buten-1-yl ester	C11H20O2		LibSearch	20.216	-0.984		1000160-10-9	65.68		
.+/-.-beta.,.beta.-Dimethyl-.gamma.-(hydroxy-methyl)-.gamma.-butyrolactone	C7H12O3		LibSearch	20.216	-0.834		52398-48-8	65.51		
Hexane, 1-(ethenyloxy)-	C8H16O		LibSearch	20.216	5.516		5363-64-4	65.49		
Methyl-2-pentanone<4->	C6H12O		LibSearch	20.216	17.716		108-10-1	65.34		
5-Undecanone	C11H22O		LibSearch	20.216	-0.634		33083-83-9	65.30		
Oxalic acid, cyclobutyl isohexyl ester	C12H20O4		LibSearch	20.216	-4.901		1000309-69-6	64.85		
5-Undecanone	C11H22O		LibSearch	20.216	-0.634		33083-83-9	64.44		
5-Nonanone, 2,2,8,8-tetramethyl-	C13H26O		LibSearch	20.216	-1.118		5709-95-5	64.23		
Oxalic acid, allyl isohexyl ester	C11H18O4		LibSearch	20.216	-2.701		1000309-23-3	64.21		
2,5-Pyrrolidinedione, 1-methyl-	C5H7NO2		LibSearch	20.216	2.016		1121-07-9	64.19		
.+/-.-beta.,.beta.-Dimethyl-.gamma.-(hydroxy-methyl)-.gamma.-butyrolactone	C7H12O3		LibSearch	20.216	-0.834		52398-48-8	64.12		
Pentanoic acid, 2,2-dimethyl-, ethenyl ester	C9H16O2		LibSearch	20.216	3.732		44970-05-0	63.98		
Pentane, 2,4-dimethyl-	C7H16		LibSearch	20.216	10.399		108-08-7	63.82		
Hexane <2-methyl->	C7H16		LibSearch	20.216			591-76-4	63.79		
Pentanoic acid, 2-propenyl ester	C8H14O2		LibSearch	20.216	3.982		6321-45-5	63.74		
Dichloroacetic acid, hexyl ester	C8H14Cl2O2		LibSearch	20.216	-1.934		37079-04-2	63.63		
Heptanethioic acid, S-methyl ester	C8H16OS		LibSearch	20.216	0.166		2432-82-8	63.58		
Pentanoic acid, 2-propenyl ester	C8H14O2		LibSearch	20.216	3.982		6321-45-5	63.34		
1-Propoxypropan-2-yl heptanoate	C13H26O3		LibSearch	20.216	-4.668		1000367-12-5	63.14		
2,5-Pyrrolidinedione, 1-methyl-	C5H7NO2		LibSearch	20.216	2.016		1121-07-9	63.10		
Allyl isovalerate	C8H14O2		LibSearch	20.216	14.396		2835-39-4	63.07		
trans-2-Hexenyl heptanoate	C13H24O2		LibSearch	20.216	-4.601		1000433-23-3	63.03		
Hexane, 2-methyl-	C7H16		LibSearch	20.216	9.332		591-76-4	62.99		
2,5-Pyrrolidinedione, 1-methyl-	C5H7NO2		LibSearch	20.216	2.016		1121-07-9	62.99		
Furan, tetrahydro-2,2,4,4-tetramethyl-	C8H16O		LibSearch	20.216	5.916		3358-28-9	62.98		
Pentane, 2,4-dimethyl-	C7H16		LibSearch	20.216	10.399		108-08-7	62.81		
2-Butanone, 3,3-dimethyl-	C6H12O		LibSearch	20.216	9.066		75-97-8	62.78		
Ambersage	C11H20O2		LibSearch	20.216	1.636		53338-05-9	62.77		
Oxalic acid, allyl hexyl ester	C11H18O4		LibSearch	20.216	-3.768		1000309-23-4	62.75		
Heptanoic acid, anhydride	C14H26O3		LibSearch	20.216	-8.384		626-27-7	62.65		
Hexane, 2-methyl-	C7H16		LibSearch	20.216	9.332		591-76-4	62.64		
4,4-Dimethylpentanoic acid, O-acetyl-	C9H16O3		LibSearch	20.216	1.299		1000506-53-9	62.60		
Nonan-3-one	C9H18O		LibSearch	20.216			925-78-0	62.49		
Heptanoic acid, anhydride	C14H26O3		LibSearch	20.216	-8.384		626-27-7	62.48		
Furan, tetrahydro-2,2,4,4-tetramethyl-	C8H16O		LibSearch	20.216	5.916		3358-28-9	62.41		
tert-Butyl acrylate	C7H12O2		LibSearch	20.216	7.049		1663-39-4	62.36		
Hexane, 2-methyl-	C7H16		LibSearch	20.216	9.332		591-76-4	62.36		
Pentane, 2,4-dimethyl-	C7H16		LibSearch	20.216	10.399		108-08-7	62.28		
6-Caprolactam	C6H11NO		LibSearch	20.216			105-60-2	62.26		
Pentanoic acid, 2-propenyl ester	C8H14O2		LibSearch	20.216	3.982		6321-45-5	62.03		

Compound Chromatograms (overlaid)

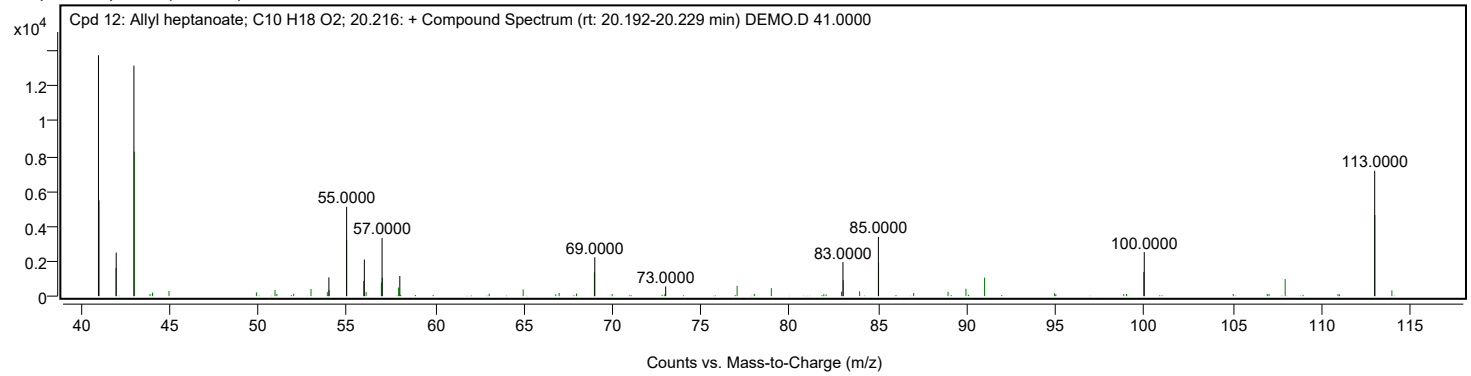


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



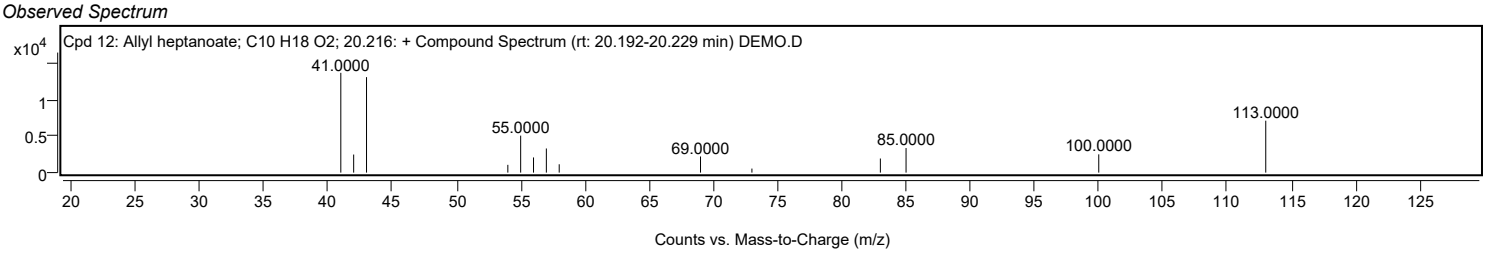
Allyl heptanoate

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			83.37			NIST.L

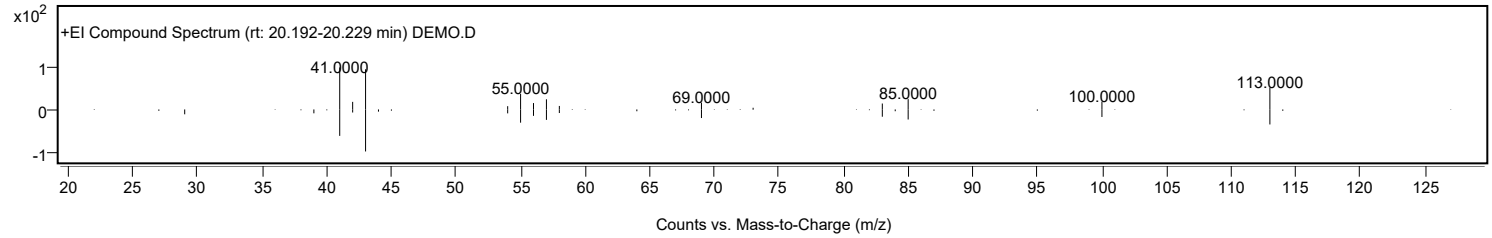
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			83.37			NIST.L

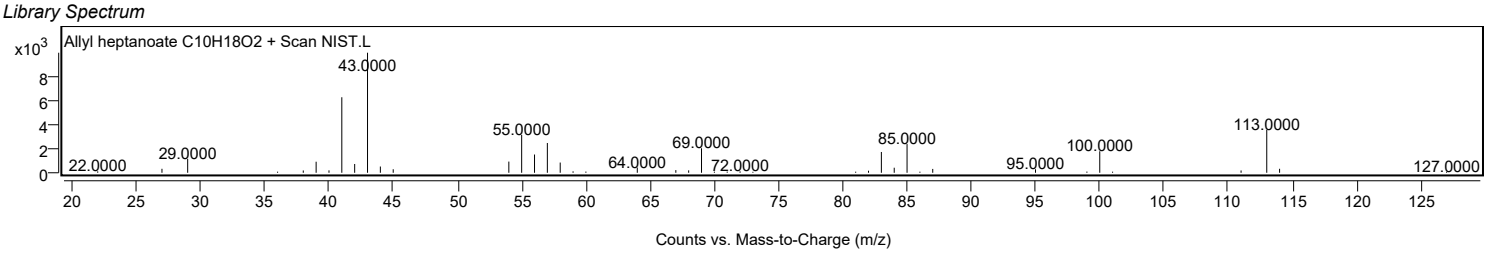
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 13: Benzeneethanol, .alpha.,.alpha.-dimethyl-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Benzeneethanol, .alpha.,.alpha.-dimethyl-	C10 H14 O	20.312			100-86-7	LibSearch	62.88	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		62.88			50		

Compound Discovery Report

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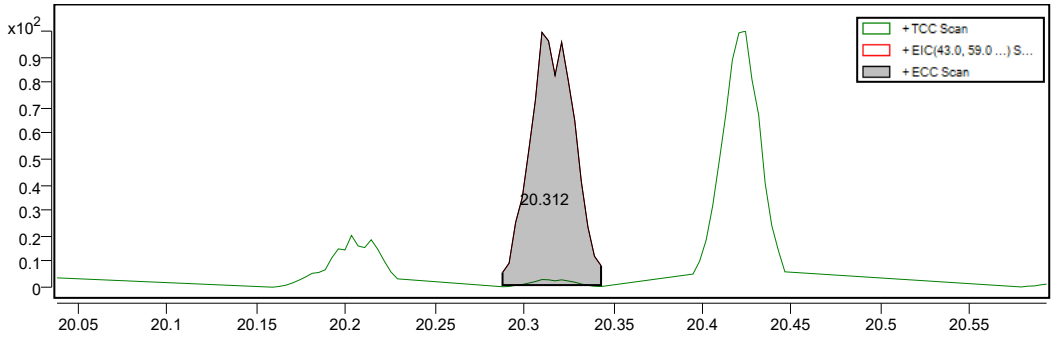
Compound ID Table

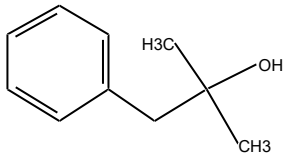
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Benzeneethanol, .alpha.,.alpha.-dimethyl-	C10H14O		LibSearch	20.312	0.578		100-86-7	62.88		
Benzeneethanol, .alpha.-ethyl-	C10H14O		LibSearch	20.312	-0.588		701-70-2	61.22		
Phenyl-tert-butanol	C10H14O		LibSearch	20.312			100-86-7	61.15		
Benzeneethanol, .alpha.,.alpha.-dimethyl-	C10H14O		LibSearch	20.312	0.578		100-86-7	60.36		
Toluene	C7H8		LibSearch	20.312	7.078		108-88-3	60.26		
Propanal benzyl isopropyl acetal	C13H20O2		LibSearch	20.312	-3.255		1010431-62-8	60.09		
Benzeneethanol, .alpha.-ethyl-	C10H14O		LibSearch	20.312	-0.588		701-70-2	58.76		
Phenyl-tert-butanol	C10H14O		LibSearch	20.312	6.522		100-86-7	57.72		
Benzyl isopentyl ether	C12H18O		LibSearch	20.312	-1.388		122-73-6	57.48		
Toluene	C7H8		LibSearch	20.312			108-88-3	57.36		
Toluene	C7H8		LibSearch	20.312	7.078		108-88-3	57.24		
Toluene	C7H8		LibSearch	20.312	7.078		108-88-3	57.24		
Benzeneethanol, .alpha.,.alpha.-dimethyl-	C10H14O		LibSearch	20.312	0.578		100-86-7	57.08		
Toluene	C7H8		LibSearch	20.312	7.078		108-88-3	56.96		
Benzeneethanol, .alpha.-methyl-	C9H12O		LibSearch	20.312	1.062		698-87-3	56.88		
Gardenia ether	C12H18O		LibSearch	20.312			122-73-6	55.45		
2-Benzyloxy-3-methyl-1,4-butanediol	C12H18O3		LibSearch	20.312	-8.422		88481-61-2	54.21		
Benzeneethanol, .alpha.,.alpha.-dimethyl-	C10H14O		LibSearch	20.312	0.578		100-86-7	53.65		
Benzeneethanol, .alpha.-methyl-	C9H12O		LibSearch	20.312	1.062		698-87-3	53.62		
Benzeneethanol, .alpha.-ethyl-	C10H14O		LibSearch	20.312	-0.588		701-70-2	53.43		
Toluene	C7H8		LibSearch	20.312	7.078		108-88-3	53.12		
Phenylacetamide, N-propyl-	C11H15NO		LibSearch	20.312	-6.205		1000407-22-1	52.89		
Toluene	C7H8		LibSearch	20.312	7.078		108-88-3	52.01		
Benzene, (butoxymethyl)-	C11H16O		LibSearch	20.312	-0.805		588-67-0	51.57		
N-Hydroxymethyl-2-phenylacetamide	C9H11NO2		LibSearch	20.312	-6.938		6291-06-1	51.39		
Bicyclo[2.2.2]oct-7-en-2-one, 5-methylene-	C9H10O		LibSearch	20.312	2.278		1000217-18-1	51.06		
Toluene	C7H8		LibSearch	20.312	7.078		108-88-3	51.05		
Benzeneethanol, .alpha.-methyl-	C9H12O		LibSearch	20.312	1.062		698-87-3	50.49		
Benzyl isopentyl ether	C12H18O		LibSearch	20.312	-1.388		122-73-6	50.05		
Benzeneethanol, .alpha.,.alpha.-dimethyl-	C10H14O		LibSearch	20.312	0.578		100-86-7	49.85		
Isoamyl benzyl ether	C12H18O		LibSearch	20.312	-0.328		122-73-6	49.83		
Benzyl isopentyl ether	C12H18O		LibSearch	20.312	-1.388		122-73-6	49.34		
Benzeneacetamide, N-methyl-	C9H11NO		LibSearch	20.312	-2.905		6830-82-6	49.31		
Phenylethyl Alcohol	C8H10O		LibSearch	20.312	1.378		60-12-8	49.06		
Benzene, (2-methylpropyl)-	C10H14		LibSearch	20.312	3.178		538-93-2	49.00		
Benzenemethanol, .alpha.-methyl-	C8H10O		LibSearch	20.312	2.728		98-85-1	48.67		
Benzene, (3-methylpentyl)-	C12H18		LibSearch	20.312	-0.138		54410-69-4	48.60		
Benzene, (2-methylpropyl)-	C10H14		LibSearch	20.312	3.178		538-93-2	47.96		
Benzeneethanol, .alpha.-methyl-	C9H12O		LibSearch	20.312	1.062		698-87-3	47.69		
2-Butanol, 1-(phenylmethoxy)-	C11H16O2		LibSearch	20.312	-3.505		14869-00-2	47.46		
Benzene, 1,1'-[oxybis(methylene)]bis-	C14H14O		LibSearch	20.312	-7.055		103-50-4	47.42		
Benzeneacetamide, N-methyl-	C9H11NO		LibSearch	20.312	-2.905		6830-82-6	46.99		
Benzyl ether	C14H14O		LibSearch	20.312			103-50-4	46.68		
Benzeneacetamide	C8H9NO		LibSearch	20.312	-1.388		103-81-1	46.63		
Benzene, (2-ethylbutyl)-	C12H18		LibSearch	20.312	-0.138		19219-85-3	46.60		
Benzene, 1,1'-[methylenebis(oxymethylene)]bis-	C15H16O2		LibSearch	20.312	-9.972		2749-70-4	46.37		
Benzene, 1,1'-[oxybis(methylene)]bis-	C14H14O		LibSearch	20.312	-7.055		103-50-4	46.23		
2-Hydroxypropyl phenylacetate	C11H14O3		LibSearch	20.312	-5.038		1000433-20-9	46.19		
Benzene, undecyl-	C17H28		LibSearch	20.312	-9.488		6742-54-7	46.18		
Butanamide, 3-hydroxy-3-methyl-N-benzyloxy-	C12H17NO3		LibSearch	20.312	-10.655		1010185-71-6	45.86		

Compound Chromatograms (overlaid)

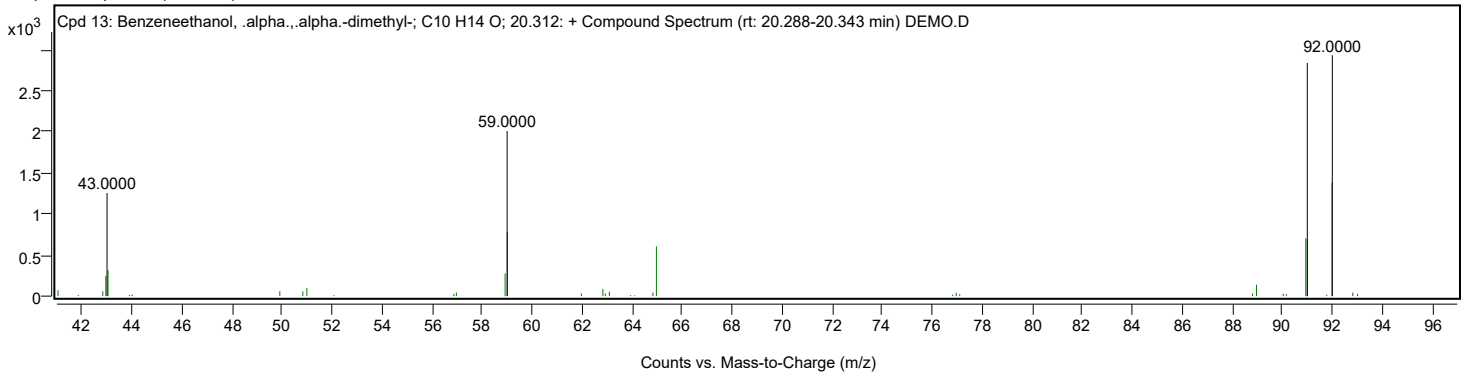


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



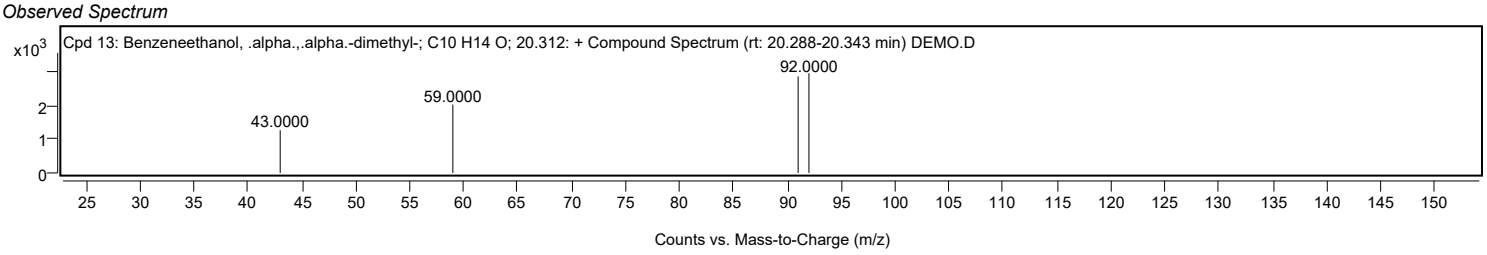
Benzeneethanol, .alpha.,.alpha.-dimethyl-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			62.88			NIST.L

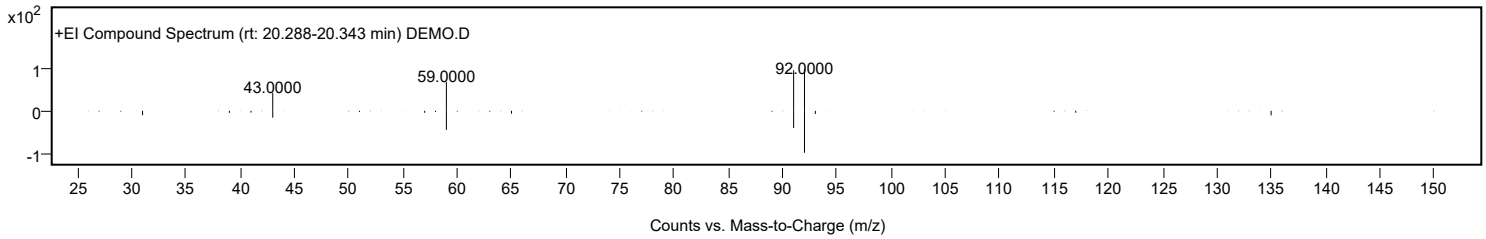
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			62.88			NIST.L

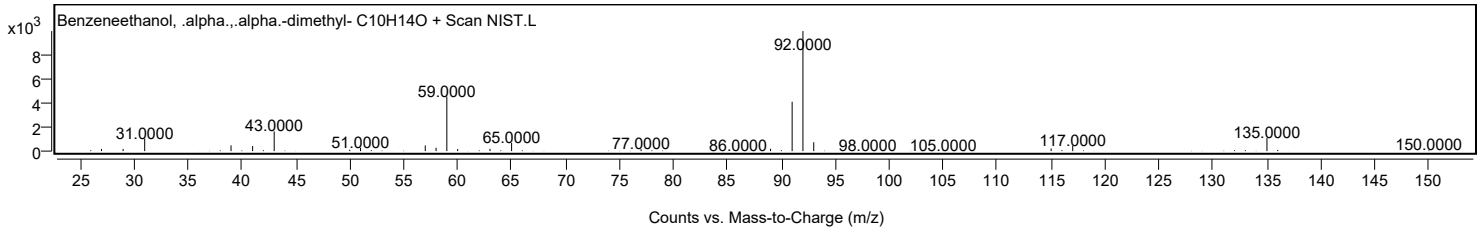
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 14: Linalool <ethyl-, (Z)->

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Linalool <ethyl-, (Z)->	C11 H20 O	20.420			54592-32-4	LibSearch	96.86	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		96.86			50		

Compound Discovery Report

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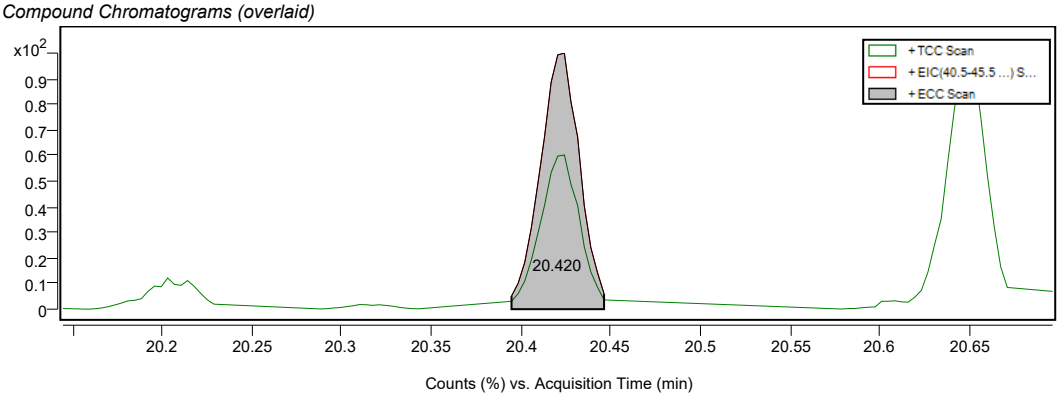
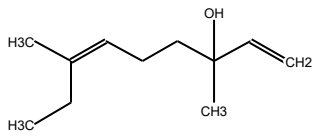
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Linalool <ethyl-, (Z)->	C11H20O		LibSearch	20.420			54592-32-4	96.86		
Linalool <ethyl-, (E)->	C11H20O		LibSearch	20.420			92590-71-1	96.37		
Ethyllinalool	C11H20O		LibSearch	20.420	0.720		1000430-72-3	94.03		
Nona-1,6-dien-3-ol <3,7-dimethyl-> acetate	C13H22O2		LibSearch	20.420			61931-80-4	89.20		
Linalool	C10H18O		LibSearch	20.420			78-70-6	88.69		
Linalool	C10H18O		LibSearch	20.420	9.100		78-70-6	87.79		
Linalool	C10H18O		LibSearch	20.420			78-70-6	87.52		
cis-Ethyl-linalyl acetate	C13H22O2		LibSearch	20.420	-2.430		1000430-70-6	86.36		
trans-Ethyl-linalyl acetate	C13H22O2		LibSearch	20.420	-2.430		1000430-70-7	85.97		
Linalool	C10H18O		LibSearch	20.420	2.387		78-70-6	85.94		
1,6-Nonadien-3-ol, 3,7-dimethyl-	C11H20O		LibSearch	20.420	0.703		10339-55-6	85.93		
Linalool	C10H18O		LibSearch	20.420	2.387		78-70-6	85.20		
Linalool	C10H18O		LibSearch	20.420	2.387		78-70-6	84.88		
1,2-Dihydropyridine, 1-(1-oxobutyl)-	C9H13NO		LibSearch	20.420	-0.097		1000132-46-2	84.53		
*EU Linalol	C10H18O		LibSearch	20.420			78-70-6	84.42		
Linalool butanoate	C14H24O2		LibSearch	20.420	-5.110		78-36-4	83.48		
Dihydro carveol <neoiso->	C10H18O		LibSearch	20.420			18675-34-8	82.83		
Linalool	C10H18O		LibSearch	20.420	2.387		78-70-6	82.48		
Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, (1.alpha.,2.alpha.,5.beta.)-	C10H18O		LibSearch	20.420	0.487		18675-33-7	82.22		
Dihydro carveol<neoiso->	C10H18O		LibSearch	20.420	3.490		18675-34-8	82.08		
Undec-9Z-en-1-al	C11H20O		LibSearch	20.420			390745-03-6	81.43		
Linalool isobutanoate	C14H24O2		LibSearch	20.420	-3.010		78-35-3	81.35		
Linalyl acetate	C12H20O2		LibSearch	20.420			115-95-7	81.31		
Linalool formate	C11H18O2		LibSearch	20.420	4.000		115-99-1	81.26		
Undec-9Z-en-1-al	C11H20O		LibSearch	20.420	-0.750		390745-03-6	81.11		
Thujanol<iso-3->	C10H18O		LibSearch	20.420	7.480		7712-79-0	81.09		
Linalool acetate	C12H20O2		LibSearch	20.420	2.260		115-95-7	81.04		
(-)-Isopinocampheol, 2-methylpropionate	C14H24O2		LibSearch	20.420	-2.913		1000462-98-0	80.81		
Thujanol<neo-3->	C10H18O		LibSearch	20.420	6.820		21653-18-9	80.72		
Undec-9E-en-1-al	C11H20O		LibSearch	20.420	-0.280		143-14-6	80.70		
Linalool butyrate	C14H24O2		LibSearch	20.420			78-36-4	80.31		
13-Tetradece-11-yn-1-ol	C14H24O		LibSearch	20.420	-7.297		1000131-00-4	80.28		
Fenchol <endo->	C10H18O		LibSearch	20.420			14575-74-7	80.27		
Dihydro carveol	C10H18O		LibSearch	20.420	4.970		38049-26-2	80.24		
Undec-10-en-1-al	C11H20O		LibSearch	20.420	0.240		112-45-8	80.24		
Linalyl formate	C11H18O2		LibSearch	20.420			115-99-1	80.23		
Linalyl acetate	C12H20O2		LibSearch	20.420	-0.780		115-95-7	80.13		
Lilac aldehyde C	C10H16O2		LibSearch	20.420	0.470		53447-48-6	80.05		
Undecenal<8Z->	C11H20O		LibSearch	20.420	0.220		147159-49-7	80.02		
Fenchol <exo->	C10H18O		LibSearch	20.420			22627-95-8	80.01		
Dihydro carveol <iso->	C10H18O		LibSearch	20.420			18675-35-9	79.97		
Fenchol, exo-	C10H18O		LibSearch	20.420	1.453		22627-95-8	79.94		
Dihydro carveol<iso->	C10H18O		LibSearch	20.420	4.080		18675-35-9	79.89		
Myrtanol acetate<trans->	C12H20O2		LibSearch	20.420	-3.550		90934-53-5	79.88		
Linalool isobutyrate	C14H24O2		LibSearch	20.420			78-35-3	79.83		
Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, (1.alpha.,2.beta.,5.alpha.)-	C10H18O		LibSearch	20.420	0.487		38049-26-2	79.70		
Linalyl acetate	C12H20O2		LibSearch	20.420	-0.780		115-95-7	79.64		
Thujanol<neoiso-3->	C10H18O		LibSearch	20.420	6.920		21653-19-0	79.60		
1,5-Dimethyl-1-vinyl-4-hexenyl butyrate	C14H24O2		LibSearch	20.420	-4.097		78-36-4	79.51		
Nerolidol	C15H26O		LibSearch	20.420	-5.647		142-50-7	79.40		

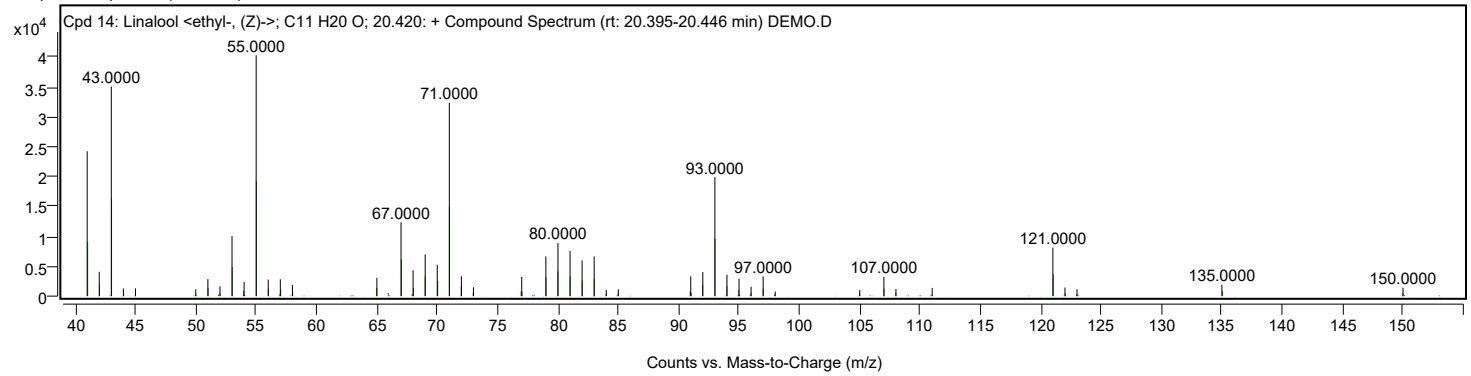
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



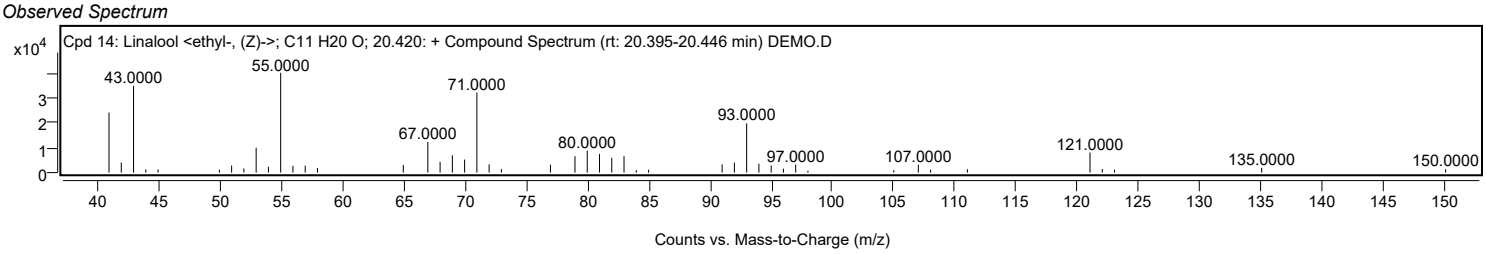
Linalool <ethyl-, (Z)->

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			96.86			PWNose.xml

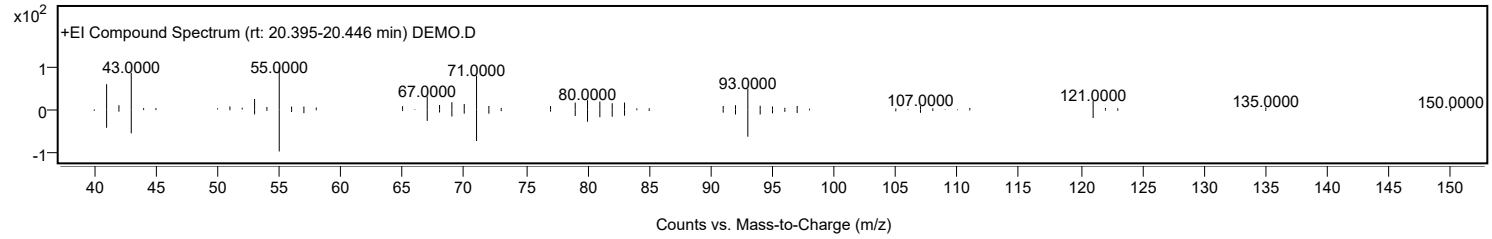
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			96.86			PWNose.xml

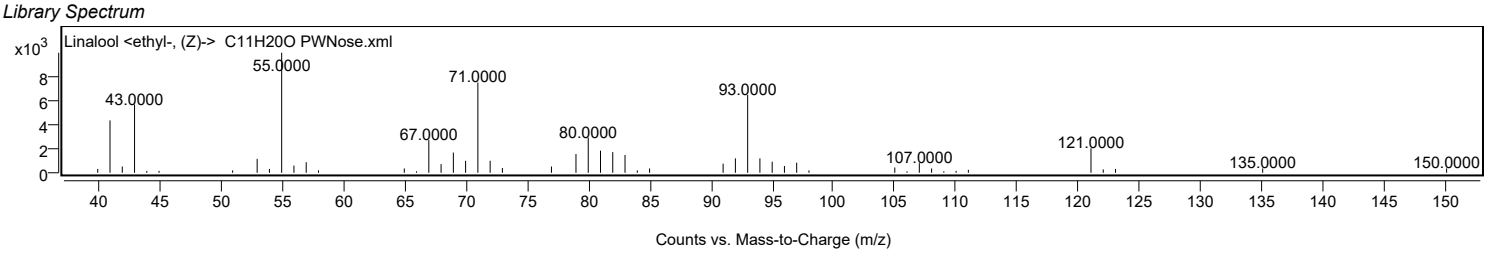
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 15: 2-Methylbenzyl benzoate

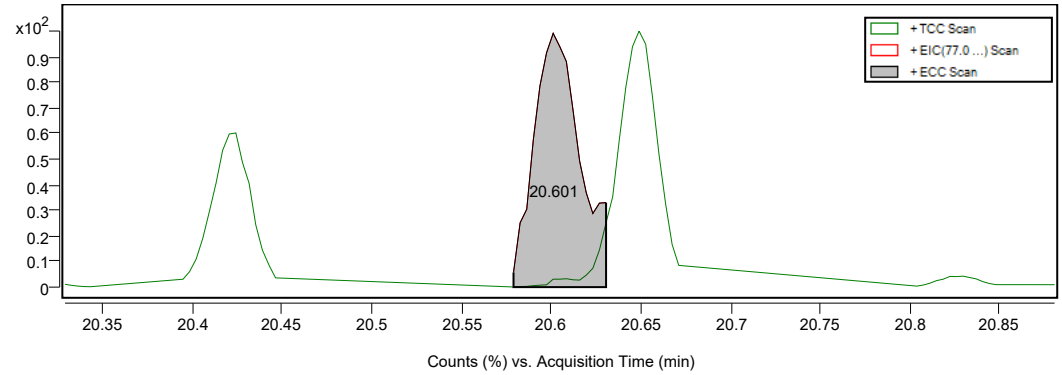
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
2-Methylbenzyl benzoate	C15 H14 O2	20.601			80716-36-5	LibSearch	79.74	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		79.74			50		

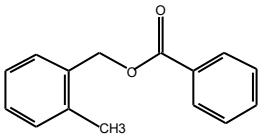
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
2-Methylbenzyl benzoate	C15H14O2		LibSearch	20.601	-10.182		80716-36-5	79.74		
Benzoic acid, 2-phenylethyl ester	C15H14O2		LibSearch	20.601	-9.949		94-47-3	74.59		
Benzoate <phenethyl->	C15H14O2		LibSearch	20.601			94-47-3	73.32		
Benzoic acid, 2-phenylethyl ester	C15H14O2		LibSearch	20.601	-9.949		94-47-3	71.41		
Diglycolic acid, di(phenethyl) ester	C20H22O5		LibSearch	20.601	-22.282		1000382-16-8	69.96		
Diethylmalonic acid, diphenethyl ester	C23H28O4		LibSearch	20.601	-24.582		1010369-56-1	68.45		
Adipic acid, di(2-phenylethyl) ester	C22H26O4		LibSearch	20.601	-24.332		1000324-58-0	68.18		
Succinic acid, di(2-phenylethyl) ester	C20H22O4		LibSearch	20.601	-21.015		1000325-04-3	67.46		
Phenylethyl 2-ethylhexanoate	C16H24O2		LibSearch	20.601	-9.249		1000431-57-7	66.67		
Benzoic acid, 2-phenylethyl ester	C15H14O2		LibSearch	20.601	-9.949		94-47-3	65.95		
Succinic acid, di(2-phenylethyl) ester	C20H22O4		LibSearch	20.601	-21.015		1000325-04-3	65.86		
Fumaric acid, di(2-phenylethyl) ester	C20H20O4		LibSearch	20.601	-21.149		1000339-35-3	65.43		
Oxalic acid, di(2-phenylethyl) ester	C18H18O4		LibSearch	20.601	-17.699		1000309-66-5	65.34		
Glutaric acid, di(phenethyl) ester	C21H24O4		LibSearch	20.601	-22.665		1000358-69-4	65.24		
Diethylmalonic acid, monochloride, phenethyl ester	C15H19ClO3		LibSearch	20.601	-12.465		1000369-56-2	65.23		
Oxalic acid, pentyl 2-phenylethyl ester	C15H20O4		LibSearch	20.601	-11.449		1010309-65-8	65.15		
Butylphosphonic acid, di(2-phenylethyl) ester	C20H27O3P		LibSearch	20.601			1000315-10-4	64.74		
Oxalic acid, heptyl 2-phenylethyl ester	C17H24O4		LibSearch	20.601	-14.765		1000309-66-1	64.64		
Oxalic acid, isobutyl 2-phenylethyl ester	C14H18O4		LibSearch	20.601	-8.732		1000309-65-6	64.63		
2-Methylbenzyl benzoate	C15H14O2		LibSearch	20.601	-10.182		80716-36-5	64.49		
Oxalic acid, butyl 2-phenylethyl ester	C14H18O4		LibSearch	20.601	-9.799		1000309-65-7	64.47		
Oxalic acid, hexyl 2-phenylethyl ester	C16H22O4		LibSearch	20.601	-13.115		1000309-66-0	64.35		
Diglycolic acid, hexyl phenethyl ester	C18H26O5		LibSearch	20.601	-17.699		1000382-16-1	64.12		
Dimethylmalonic acid, pentyl 2-phenethyl ester	C18H26O4		LibSearch	20.601	-15.015		1000361-61-7	64.07		
Phthalic acid, di(2-phenylethyl) ester	C24H22O4		LibSearch	20.601	-29.149		1000309-78-0	63.69		
Oxalic acid, octyl 2-phenylethyl ester	C18H26O4		LibSearch	20.601	-16.432		1000309-66-2	63.24		
Diglycolic acid, pentyl phenethyl ester	C17H24O5		LibSearch	20.601	-16.032		1010382-15-9	63.22		
Succinic acid, 3-methylbut-2-yl phenethyl ester	C17H24O4		LibSearch	20.601	-12.632		1000389-74-3	63.16		
Butylphosphonic acid, isobutyl 2-phenylethyl ester	C16H27O3P		LibSearch	20.601			1000315-10-3	62.87		
trans-2,3-Di-(.alpha.-phenylethyl)-1-phthalimido-azimine	C24H22N4O2		LibSearch	20.601	-36.632		1000055-44-8	62.55		
Oxalic acid, nonyl 2-phenylethyl ester	C19H28O4		LibSearch	20.601	-18.082		1000309-66-3	62.32		
Oxalic acid, 2-phenylethyl propyl ester	C13H16O4		LibSearch	20.601	-8.149		1000309-65-5	62.30		
Glutaric acid, 8-chlorooctyl phenethyl ester	C21H31ClO4		LibSearch	20.601	-25.149		1000391-79-7	62.27		
Octanoic acid, 2-phenylethyl ester	C16H24O2		LibSearch	20.601	-10.332		5457-70-5	62.10		
Butylphosphonic acid, butyl 2-phenylethyl ester	C16H27O3P		LibSearch	20.601			1000315-09-3	61.55		
Dimethylmalonic acid, isobutyl 2-phenethyl ester	C17H24O4		LibSearch	20.601	-12.299		1000361-61-5	61.44		
Acetic acid, methoxy-, 2-phenylethyl ester	C11H14O3		LibSearch	20.601	-3.299		84682-19-9	61.36		
Oxalic acid, decyl 2-phenylethyl ester	C20H30O4		LibSearch	20.601	-19.732		1000309-66-4	61.22		
Benzene, 1,1'-(1,2-dimethyl-1,2-ethanediyl)bis-, (R*,S*)-	C16H18		LibSearch	20.601	-6.682		4613-11-0	61.08		
Diglycolic acid, ethyl phenethyl ester	C14H18O5		LibSearch	20.601	-11.065		1000382-15-5	60.88		
Dimethylmalonic acid, butyl 2-phenethyl ester	C17H24O4		LibSearch	20.601	-13.365		1000361-61-6	60.73		
Dimethylmalonic acid, ethyl 2-phenethyl ester	C15H20O4		LibSearch	20.601	-10.049		1000361-61-3	60.67		
Butylphosphonic acid, pentyl 2-phenylethyl ester	C17H29O3P		LibSearch	20.601			1000315-09-4	60.57		
1,3,5-Triazine, hexahydro-1,3,5-triphenyl-	C21H21N3		LibSearch	20.601	-25.732		91-78-1	60.56		
Benzene, 1,1'-(1,2-dimethyl-1,2-ethanediyl)bis-, (R*,R*)-(.+/-.)-	C16H18		LibSearch	20.601	-6.682		2726-21-8	60.29		
Oxalic acid, ethyl 2-phenylethyl ester	C12H14O4		LibSearch	20.601	-6.482		1000309-65-4	60.21		
Dimethylmalonic acid, isohexyl 2-phenethyl ester	C19H28O4		LibSearch	20.601	-15.599		1000361-61-8	59.93		
Nonanoic acid, 2-phenylethyl ester	C17H26O2		LibSearch	20.601	-11.982		57943-67-6	59.92		
Diethylmalonic acid, ethyl phenethyl ester	C17H24O4		LibSearch	20.601	-13.365		1000369-54-5	59.79		
Succinic acid, 2-phenylethyl propyl ester	C15H20O4		LibSearch	20.601	-11.449		1000325-03-3	59.76		

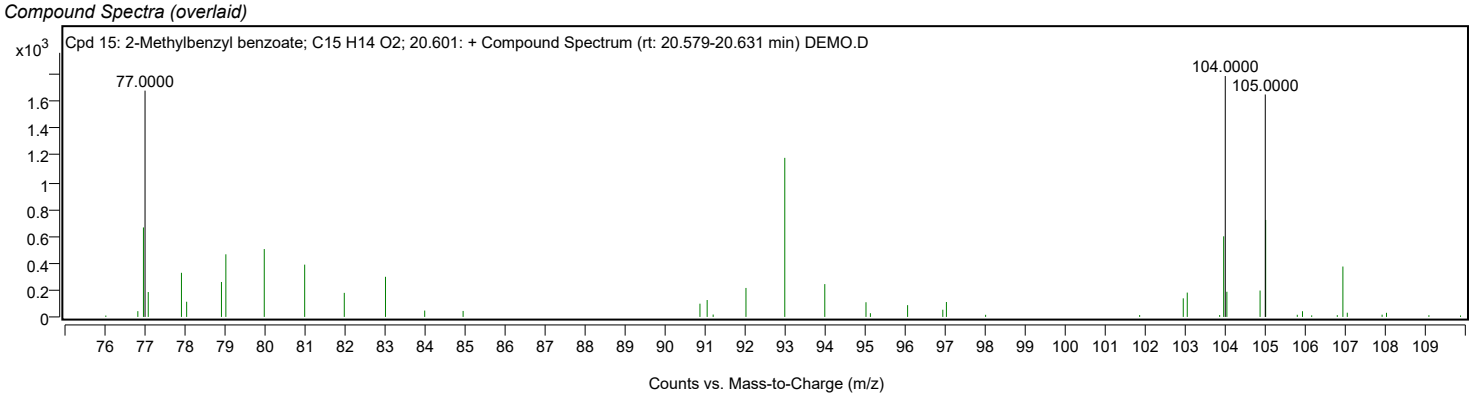
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



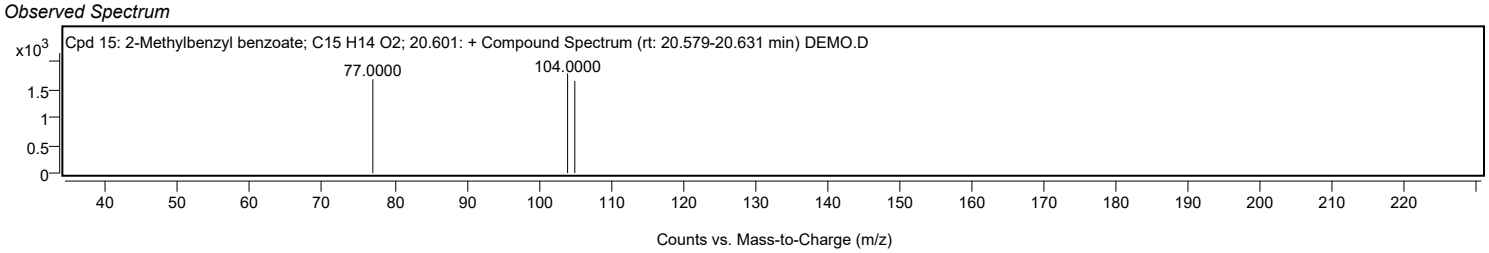
2-Methylbenzyl benzoate

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			79.74			NIST.L

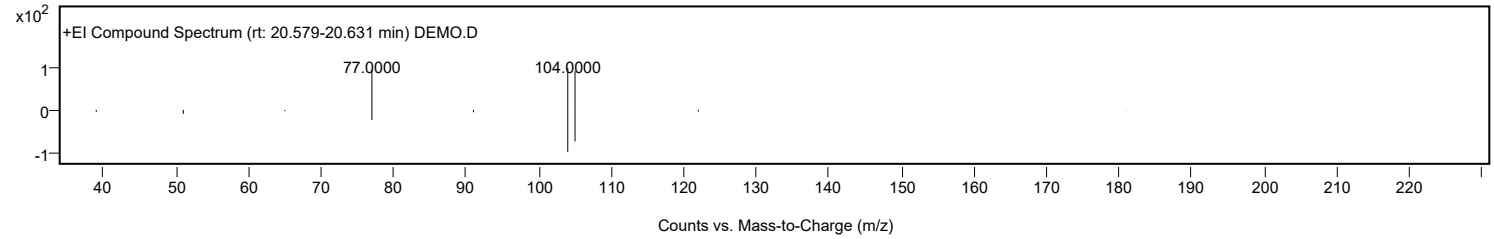
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			79.74			NIST.L

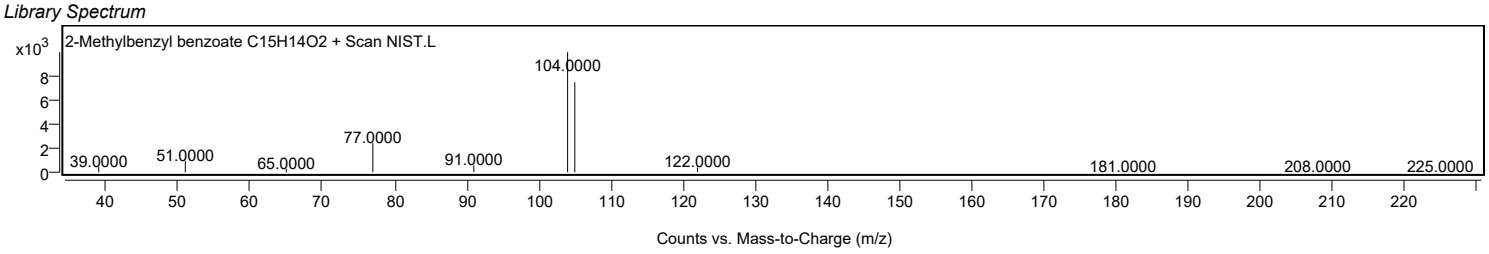
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 16: Linalool <ethyl-, (Z)->

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Linalool <ethyl-, (Z)->	C11 H20 O	20.648			54592-32-4	LibSearch	97.24	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		97.24			50		

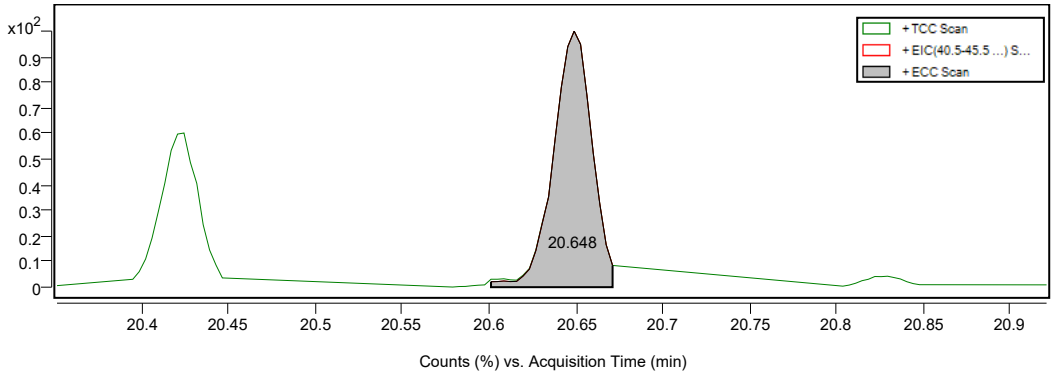
Compound Discovery Report

Agilent | Trusted Answers

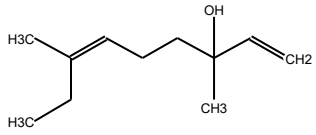
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Linalool <ethyl-, (Z)->	C11H20O		LibSearch	20.648			54592-32-4	97.24		
Linalool <ethyl-, (E)->	C11H20O		LibSearch	20.648			92590-71-1	97.19		
Ethyllinalool	C11H20O		LibSearch	20.648	0.948		1000430-72-3	94.27		
Nona-1,6-dien-3-ol <3,7-dimethyl-> acetate	C13H22O2		LibSearch	20.648			61931-80-4	89.96		
Linalool	C10H18O		LibSearch	20.648			78-70-6	88.74		
Linalool	C10H18O		LibSearch	20.648	9.328		78-70-6	88.35		
Linalool	C10H18O		LibSearch	20.648			78-70-6	87.71		
cis-Ethyl-linalyl acetate	C13H22O2		LibSearch	20.648	-2.202		1000430-70-6	86.92		
trans-Ethyl-linalyl acetate	C13H22O2		LibSearch	20.648	-2.202		1000430-70-7	86.82		
Linalool	C10H18O		LibSearch	20.648	2.615		78-70-6	86.61		
1,6-Nonadien-3-ol, 3,7-dimethyl-	C11H20O		LibSearch	20.648	0.931		10339-55-6	86.24		
Linalool	C10H18O		LibSearch	20.648	2.615		78-70-6	85.75		
1,2-Dihydropyridine, 1-(1-oxobutyl)-	C9H13NO		LibSearch	20.648	0.131		1000132-46-2	85.55		
*EU Linalol	C10H18O		LibSearch	20.648			78-70-6	85.36		
Linalool	C10H18O		LibSearch	20.648	2.615		78-70-6	85.32		
Linalool butanoate	C14H24O2		LibSearch	20.648	-4.882		78-36-4	84.53		
Linalool	C10H18O		LibSearch	20.648	2.615		78-70-6	83.24		
Thujanol<iso-3->	C10H18O		LibSearch	20.648	7.708		7712-79-0	82.99		
Linalool formate	C11H18O2		LibSearch	20.648	4.228		115-99-1	82.67		
Linalool acetate	C12H20O2		LibSearch	20.648	2.488		115-95-7	82.44		
Thujanol<neo-3->	C10H18O		LibSearch	20.648	7.048		21653-18-9	82.42		
Linalool isobutanoate	C14H24O2		LibSearch	20.648	-2.782		78-35-3	82.42		
Dihydro carveol <neoiso->	C10H18O		LibSearch	20.648			18675-34-8	82.41		
Dihydro carveol<neoiso->	C10H18O		LibSearch	20.648	3.718		18675-34-8	82.27		
Linalyl acetate	C12H20O2		LibSearch	20.648			115-95-7	82.04		
Cyclohexanol, 2-methyl-5-(1-methylethenyl)-, (1.alpha.,2.alpha.,5.beta.)-	C10H18O		LibSearch	20.648	0.715		18675-33-7	81.88		
(-)-Isopinocampheol, 2-methylpropionate	C14H24O2		LibSearch	20.648	-2.685		1000462-98-0	81.54		
Linalyl formate	C11H18O2		LibSearch	20.648			115-99-1	81.26		
Linalool butyrate	C14H24O2		LibSearch	20.648			78-36-4	80.92		
Thujanol<3->	C10H18O		LibSearch	20.648	6.388		21653-20-3	80.86		
Linalyl acetate	C12H20O2		LibSearch	20.648	-0.552		115-95-7	80.85		
Linalool isobutyrate	C14H24O2		LibSearch	20.648			78-35-3	80.78		
Linalyl acetate	C12H20O2		LibSearch	20.648	-0.552		115-95-7	80.75		
Thujanol<neoiso-3->	C10H18O		LibSearch	20.648	7.148		21653-19-0	80.63		
Undec-9Z-en-1-al	C11H20O		LibSearch	20.648	-0.522		390745-03-6	80.52		
1,5-Dimethyl-1-vinyl-4-hexenyl butyrate	C14H24O2		LibSearch	20.648	-3.869		78-36-4	80.48		
Dihydro carveol	C10H18O		LibSearch	20.648	5.198		38049-26-2	80.43		
Undec-9Z-en-1-al	C11H20O		LibSearch	20.648			390745-03-6	80.39		
Lilac aldehyde C	C10H16O2		LibSearch	20.648	0.698		53447-48-6	80.37		
1,6-Octadien-3-ol, 3,7-dimethyl-, formate	C11H18O2		LibSearch	20.648	-0.519		115-99-1	80.08		
Undec-9E-en-1-al	C11H20O		LibSearch	20.648	-0.052		143-14-6	80.05		
1-Octyn-3-ol	C8H14O		LibSearch	20.648	4.365		818-72-4	79.92		
Fenchol <endo->	C10H18O		LibSearch	20.648			14575-74-7	79.75		
Undecenal<8Z->	C11H20O		LibSearch	20.648	0.448		147159-49-7	79.59		
Myrtanol acetate<trans->	C12H20O2		LibSearch	20.648	-3.322		90934-53-5	79.56		
Nerolidol	C15H26O		LibSearch	20.648	-5.419		142-50-7	79.50		
Fenchol, exo-	C10H18O		LibSearch	20.648	1.681		22627-95-8	79.48		
Lilac aldehyde D	C10H16O2		LibSearch	20.648	0.698		53447-47-5	79.46		
Neryl isobutanoate	C14H24O2		LibSearch	20.648	-7.782		2345-24-6	79.35		
Cyclohexanol, 1-methyl-4-(1-methylethenyl)-, cis-	C10H18O		LibSearch	20.648	1.348		7299-41-4	79.20		

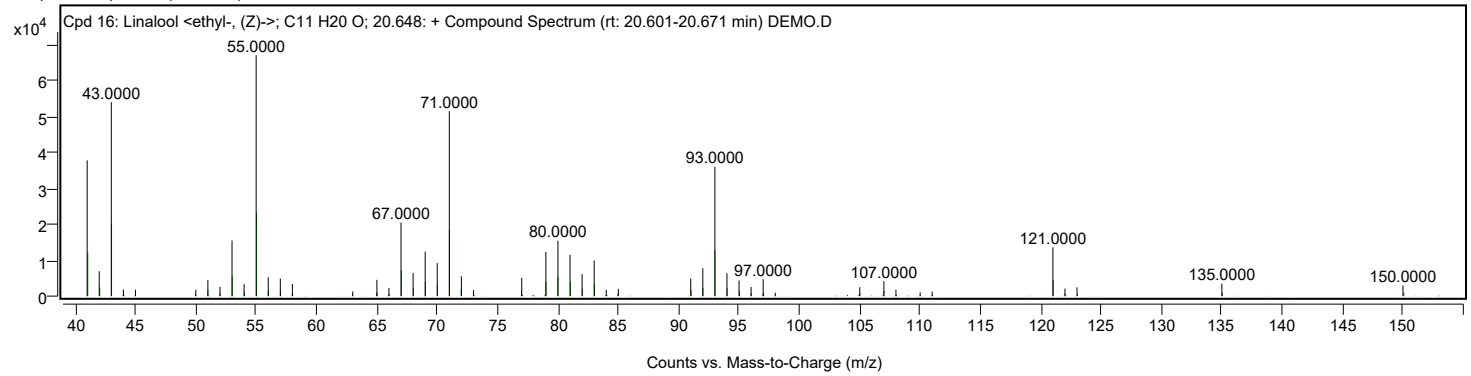
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



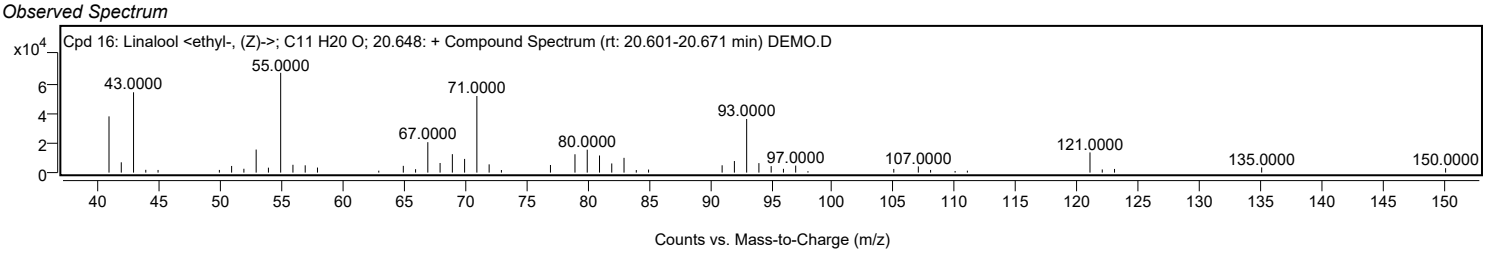
Linalool <ethyl-, (Z)->

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			97.24			PWNose.xml

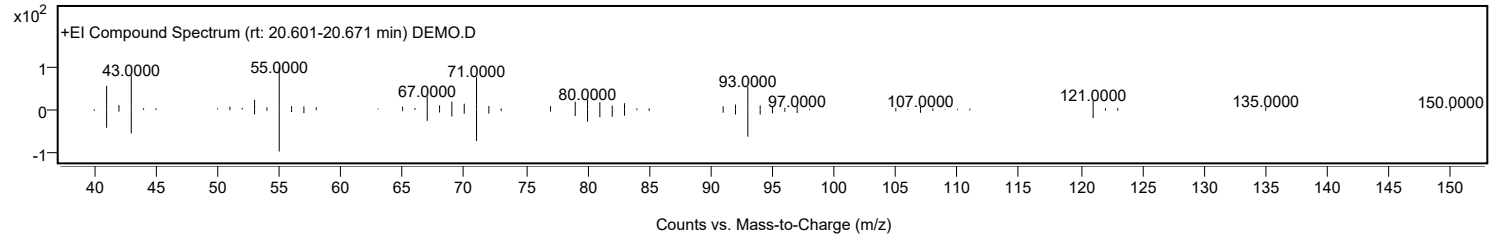
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			97.24			PWNose.xml

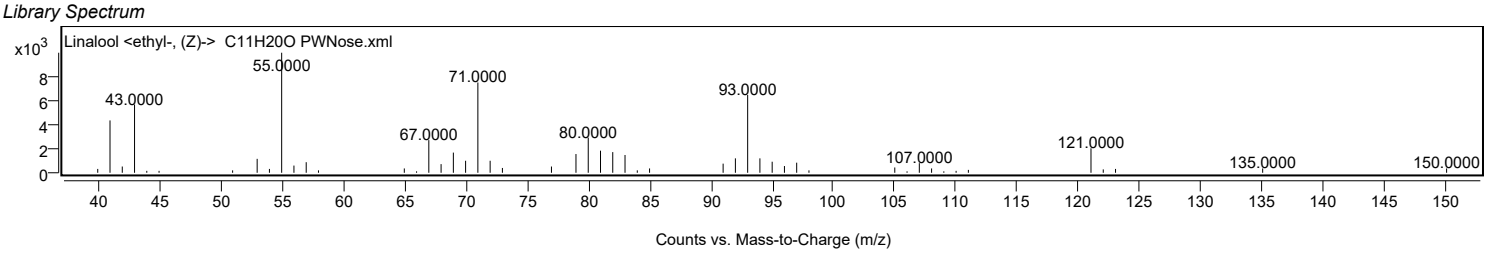
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 17: Rozanol, trans-

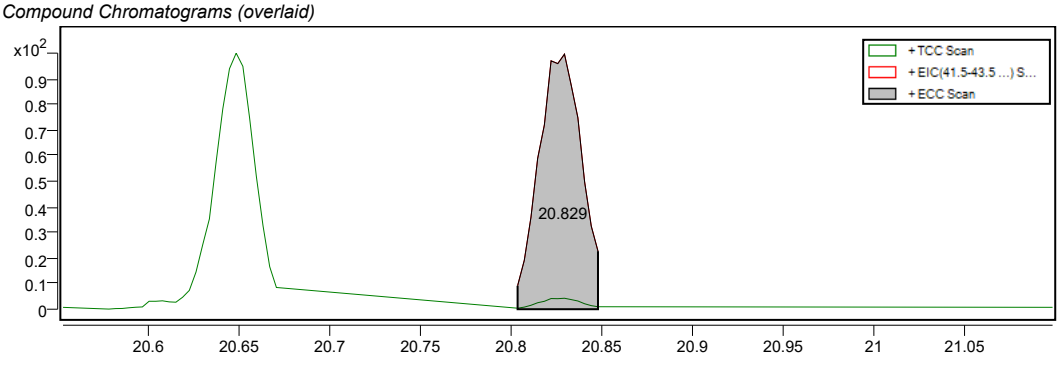
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Rozanol, trans-	C10 H20 O2	20.829			65418-70-4	LibSearch	69.06	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		69.06			50		

Compound ID Table

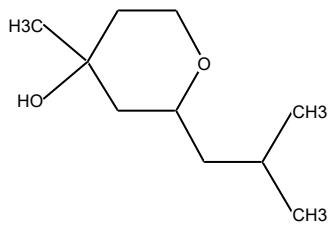
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Rozanol, trans-	C10H20O2		LibSearch	20.829			65418-70-4	69.06		
Rozanol, cis-	C10H20O2		LibSearch	20.829			65418-69-1	68.48		
Florosa	C10H20O2		LibSearch	20.829			63500-71-0	63.45		
Acetaldehyde isopentyl propyl acetal	C10H22O2		LibSearch	20.829	3.512		1000431-62-2	61.87		
Undecanol-5	C11H24O		LibSearch	20.829	-0.455		37493-70-2	59.69		
3-Octanol, 2,3-dimethyl-	C10H22O		LibSearch	20.829	3.445		19781-10-3	59.51		
Ethane <1,1-Di-2-methylbutoxy-> (isomer I)	C12H26O2		LibSearch	20.829			13535-43-8	58.63		
Ethane <1,1-Di-2-methylbutoxy-> (isomer II)	C12H26O2		LibSearch	20.829			13535-43-8	58.31		
Pentane, 2,2'-oxybis-	C10H22O		LibSearch	20.829	4.779		56762-00-6	57.25		
Undecanol-5	C11H24O		LibSearch	20.829	-0.455		37493-70-2	56.90		
Butane, 1,1'-[ethylidenebis(oxy)]bis[2-methyl-	C12H26O2		LibSearch	20.829	1.262		13535-43-8	56.86		
Undecanol <5->	C11H24O		LibSearch	20.829			37493-70-2	56.68		
3-Hydroxy-3-methylheptane-2,6-dione	C8H14O3		LibSearch	20.829	1.162		1000444-74-8	56.67		
Undecanol<5->	C11H24O		LibSearch	20.829	1.309		37493-70-2	56.55		
1,3-Dioxan-4-one, 2-(1,1-dimethylethyl)-5-methyl-, (2s-cis)-	C9H16O3		LibSearch	20.829	-0.338		107289-32-7	56.08		
Pentane, 2,2'-[ethylidenebis(oxy)]bis-	C12H26O2		LibSearch	20.829	1.262		54889-47-3	55.86		
Butanoic acid <1-methyl-, 2-oxopropyl-> ester	C8H14O3		LibSearch	20.829			84642-61-5	55.49		
Pyruvate <isoamyl->	C8H14O3		LibSearch	20.829			7779-72-8	55.41		
Acetic acid, 2-methylhex-3-yl ester	C9H18O2		LibSearch	20.829	4.912		1000368-35-1	55.20		
4-Nonanol, 4-methyl-	C10H22O		LibSearch	20.829	2.379		23418-38-4	55.02		
Pentanal, 2-methyl-	C6H12O		LibSearch	20.829	8.462		123-15-9	54.85		
4-Isopropoxy-2-butanone	C7H14O2		LibSearch	20.829	6.412		32541-58-5	54.50		
Pentane, 1-butoxy-	C9H20O		LibSearch	20.829	4.295		18636-66-3	54.12		
Hexanoic acid, 3-oxo-, ethyl ester	C8H14O3		LibSearch	20.829	2.162		3249-68-1	54.04		
2-Ethoxytetrahydrofuran	C6H12O2		LibSearch	20.829	7.079		13436-46-9	53.67		
Hexanoate <3-oxo-, ethyl->	C8H14O3		LibSearch	20.829			3249-68-1	53.64		
1,3-Dioxepane, 2-methyl-2-propyl-	C9H18O2		LibSearch	20.829	1.645		1000115-98-1	53.34		
4-sec-Butoxy-2-butanone	C8H16O2		LibSearch	20.829	4.762		57545-63-8	53.29		
3-Methyl-4-decanol	C11H24O		LibSearch	20.829	0.612		55816-17-6	53.21		
3-Pentanol, 2,3,4-trimethyl-	C8H18O		LibSearch	20.829	7.829		3054-92-0	53.20		
4-Nonanol, 4-methyl-	C10H22O		LibSearch	20.829	2.379		23418-38-4	53.05		
2,5-Dimethyl-3-hexanol acetate	C10H20O2		LibSearch	20.829	4.329		91008-85-4	53.04		
Butanoic acid, anhydride	C8H14O3		LibSearch	20.829	2.162		106-31-0	52.84		
Acetaldehyde dipentyl acetal	C12H26O2		LibSearch	20.829	-0.871		1000431-43-0	52.71		
Acetaldehyde diisoamyl acetal	C12H26O2		LibSearch	20.829	1.262		1000430-80-1	52.63		
Sulfurous acid, bis(2-pentyl) ester	C10H22O3S		LibSearch	20.829	-4.338		1000309-15-3	52.54		
1-Allyl-cyclohexane-1,2-diol	C9H16O2		LibSearch	20.829	-0.971		1000143-28-3	52.50		
Amyl ether	C10H22O		LibSearch	20.829			693-65-2	52.41		
1,3-Dioxan-4-one, 2-(1,1-dimethylethyl)-6-methyl-	C9H16O3		LibSearch	20.829	-0.338		113505-75-2	52.23		
4-Heptanol, acetate	C9H18O2		LibSearch	20.829	3.845		5921-84-6	52.19		
1,6:3,4-Dianhydro-2-O-acetyl-.beta.-d-talopyranose	C8H10O5		LibSearch	20.829	1.195		1000139-89-4	52.15		
dl-Mevalonic acid lactone	C6H10O3		LibSearch	20.829	1.562		674-26-0	52.08		
Ethane-1,1-diol dibutanoate	C10H18O4		LibSearch	20.829	-0.605		25572-25-2	52.03		
6-Methyl-2-heptanol, 2-methylpropionate	C12H24O2		LibSearch	20.829	1.012		1000447-36-7	51.94		
2,4-Dimethyl-3-pentanol acetate	C9H18O2		LibSearch	20.829	5.979		84612-74-8	51.86		
1,2-propanediol butyrate	C7H14O3		LibSearch	20.829	3.112		1000458-47-5	51.78		
dl-Mevalonic acid lactone	C6H10O3		LibSearch	20.829	1.562		674-26-0	51.44		
2-(Oxolan-2-yl)-1,2-oxazinane	C8H15NO2		LibSearch	20.829	-0.021		1000445-08-1	51.43		
Hexanoic acid, 3-oxo-, ethyl ester	C8H14O3		LibSearch	20.829	2.162		3249-68-1	51.27		
n-Amyl ether	C10H22O		LibSearch	20.829	2.645		693-65-2	51.19		

Compound Chromatograms (overlaid)

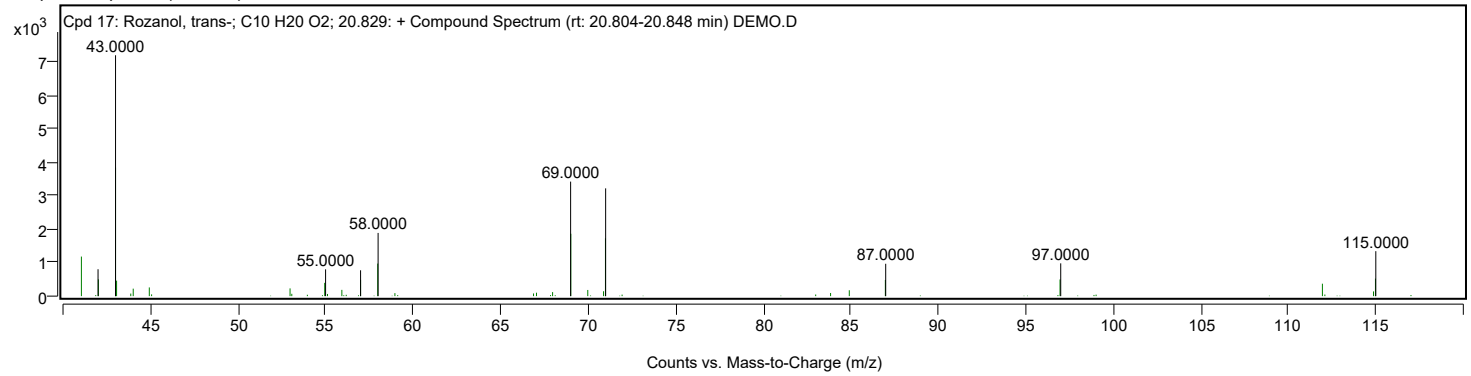


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



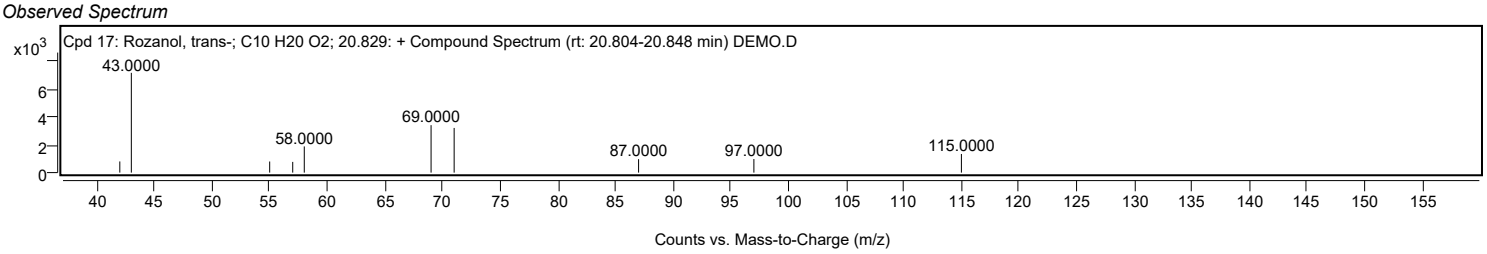
Rozanol, trans-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			69.06			PWNose.xml

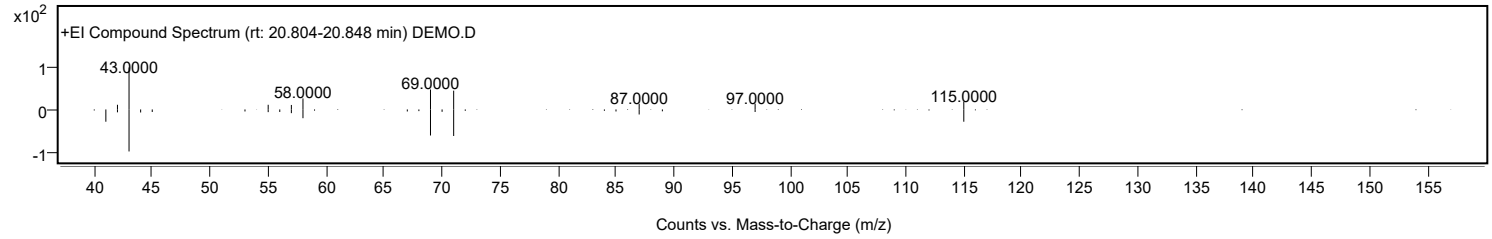
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			69.06			PWNose.xml

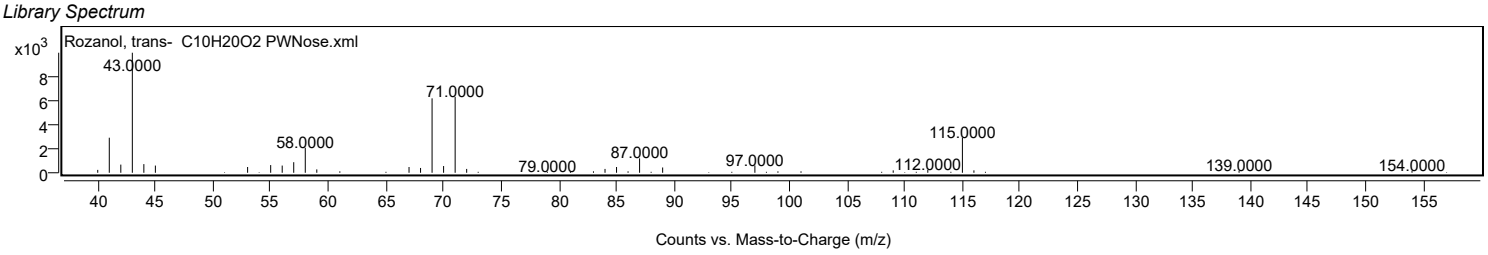
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 18: Rozanol, trans-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Rozanol, trans-	C10 H20 O2	21.147			65418-70-4	LibSearch	90.17	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		90.17			50		

Compound Discovery Report

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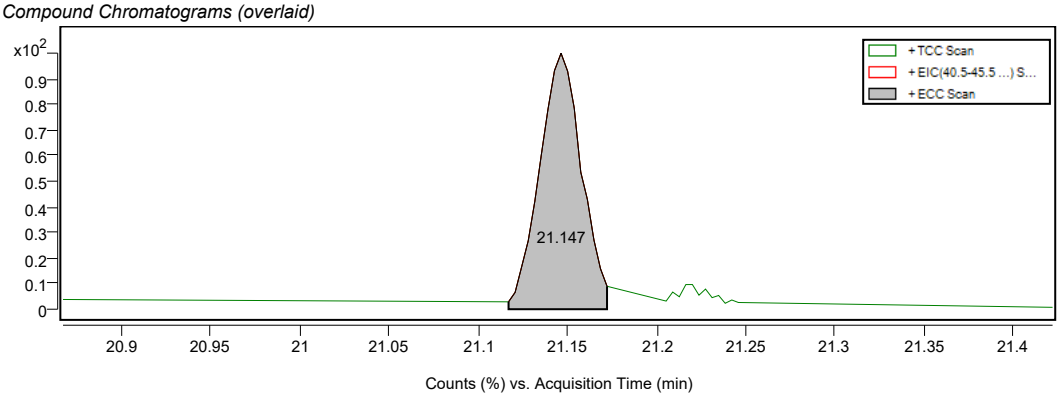
Compound ID Table

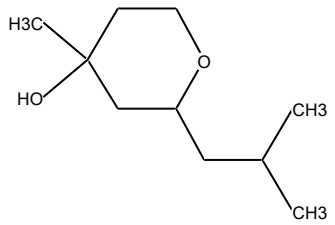
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Rozanol, trans-	C10H20O2		LibSearch	21.147			65418-70-4	90.17		
Rozanol, cis-	C10H20O2		LibSearch	21.147			65418-69-1	89.87		
Florosa	C10H20O2		LibSearch	21.147			63500-71-0	78.64		
Pyruvate <isoamyl->	C8H14O3		LibSearch	21.147			7779-72-8	74.65		
Ethane <1,1-Di-2-methylbutoxy-> (isomer I)	C12H26O2		LibSearch	21.147			13535-43-8	73.65		
Ethane <1,1-Di-2-methylbutoxy-> (isomer II)	C12H26O2		LibSearch	21.147			13535-43-8	73.48		
Butane, 1,1'-[ethylidenebis(oxy)]bis[2-methyl-	C12H26O2		LibSearch	21.147	1.580		13535-43-8	72.98		
1,3-Dimethylbutyl isobutyrate	C10H20O2		LibSearch	21.147	4.647		1000429-31-6	72.12		
6-Methyl-2-heptanol, 2-methylpropionate	C12H24O2		LibSearch	21.147	1.330		1000447-36-7	72.05		
4-sec-Butoxy-2-butanone	C8H16O2		LibSearch	21.147	5.080		57545-63-8	72.02		
1,3-Dimethylbutyl butyrate	C10H20O2		LibSearch	21.147	3.580		5332-88-7	71.88		
Oxirane, (3-methylbutyl)-	C7H14O		LibSearch	21.147	8.763		53229-41-7	71.01		
1-Butanol, 2,3-dimethyl-	C6H14O		LibSearch	21.147	8.947		19550-30-2	70.63		
Pentan-1-ol <2-methyl->	C6H14O		LibSearch	21.147			105-30-6	70.40		
1-Methylpentyl isobutyrate	C10H20O2		LibSearch	21.147	3.580		1000429-31-7	70.40		
Pentane, 2,2'-[ethylidenebis(oxy)]bis-	C12H26O2		LibSearch	21.147	1.580		54889-47-3	70.16		
Pentane, 2,2'-oxybis-	C10H22O		LibSearch	21.147	5.097		56762-00-6	70.08		
Pentane, 1-(2-propenyloxy)-	C8H16O		LibSearch	21.147	6.447		23186-70-1	69.99		
Amyl ether	C10H22O		LibSearch	21.147			693-65-2	69.70		
1-Trifluoroacetoxy-2-methylpentane	C8H13F3O2		LibSearch	21.147	8.580		155089-96-6	69.65		
Isobutyrate <3-Methyl pentyl->	C10H20O2		LibSearch	21.147			84254-84-2	69.58		
1-Butanol, 2,3-dimethyl-	C6H14O		LibSearch	21.147	8.947		19550-30-2	69.52		
1,3-Dioxan-4-one, 2-(1,1-dimethylethyl)-5-methyl-, (2s-cis)-	C9H16O3		LibSearch	21.147	-0.020		107289-32-7	69.51		
Allyl butanoate	C7H12O2		LibSearch	21.147	16.547		2051-78-7	69.41		
2-Ethyl-1-butanol, trifluoroacetate	C8H13F3O2		LibSearch	21.147	8.580		116464-98-3	69.07		
2,4-Dimethyl-3-pentanol acetate	C9H18O2		LibSearch	21.147	6.297		84612-74-8	69.06		
8-Hydroxy-2-octanone	C8H16O2		LibSearch	21.147	1.230		25368-54-1	68.91		
Acetic acid, 2-methylhex-3-yl ester	C9H18O2		LibSearch	21.147	5.230		1000368-35-1	68.90		
3-Octanol, 2,3-dimethyl-	C10H22O		LibSearch	21.147	3.763		19781-10-3	68.89		
2,5-Dimethyl-3-hexanol acetate	C10H20O2		LibSearch	21.147	4.647		91008-85-4	68.84		
Ethanedioic acid, bis(3-methylbutyl) ester	C12H22O4		LibSearch	21.147	-2.520		2051-00-5	68.64		
Propanoic acid, 2-methyl-, 2-methylpentyl ester	C10H20O2		LibSearch	21.147	3.580		84254-82-0	68.61		
Butanoic acid <1-methyl-, 2-oxopropyl-> ester	C8H14O3		LibSearch	21.147			84642-61-5	68.59		
1-Butanol, 2,3-dimethyl-	C6H14O		LibSearch	21.147	8.947		19550-30-2	68.53		
Propanoic acid, 2-methyl-, 1-methylbutyl ester	C9H18O2		LibSearch	21.147	5.230		54340-93-1	68.49		
Butanoic acid, 1-methyloctyl ester	C13H26O2		LibSearch	21.147	-2.470		69727-42-0	68.43		
5-Methyl-2-hexanol, 2-methylpropionate	C11H22O2		LibSearch	21.147	2.980		1000447-34-4	68.35		
Vinyldimethylcarbinol	C5H10O		LibSearch	21.147			115-18-4	68.26		
Butanoic acid, 1-methylhexyl ester	C11H22O2		LibSearch	21.147	0.847		39026-94-3	68.19		
Acetaldehyde dipentyl acetal	C12H26O2		LibSearch	21.147	-0.553		1000431-43-0	68.08		
Pentyl isobutanoate	C9H18O2		LibSearch	21.147	11.527		2445-72-9	68.07		
Oxalic acid, isohexyl pentyl ester	C13H24O4		LibSearch	21.147	-5.253		1000309-32-8	68.06		
Butanoate <allyl->	C7H12O2		LibSearch	21.147			2051-78-7	67.98		
Oxirane, pentyl-	C7H14O		LibSearch	21.147	7.697		5063-65-0	67.91		
2-Nonanol, 2-methylpropionate	C13H26O2		LibSearch	21.147	-1.403		69121-76-2	67.80		
n-Amyl ether	C10H22O		LibSearch	21.147	2.963		693-65-2	67.76		
Propanoic acid, 2-methyl-, 3-methylbutyl ester	C9H18O2		LibSearch	21.147	5.230		2050-01-3	67.74		
Pentyl isobutanoate	C9H18O2		LibSearch	21.147			2445-72-9	67.51		
Isopropyl isobutyrate	C7H14O2		LibSearch	21.147	18.067		617-50-5	67.48		
Oxalic acid, pentyl propyl ester	C10H18O4		LibSearch	21.147	-1.353		1000309-25-7	67.41		

Compound Chromatograms (overlaid)

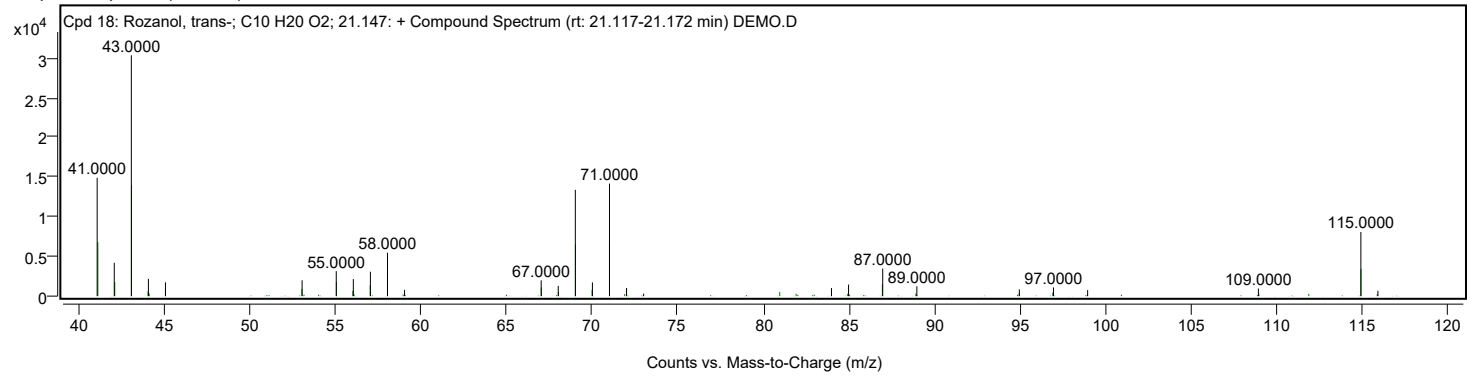


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



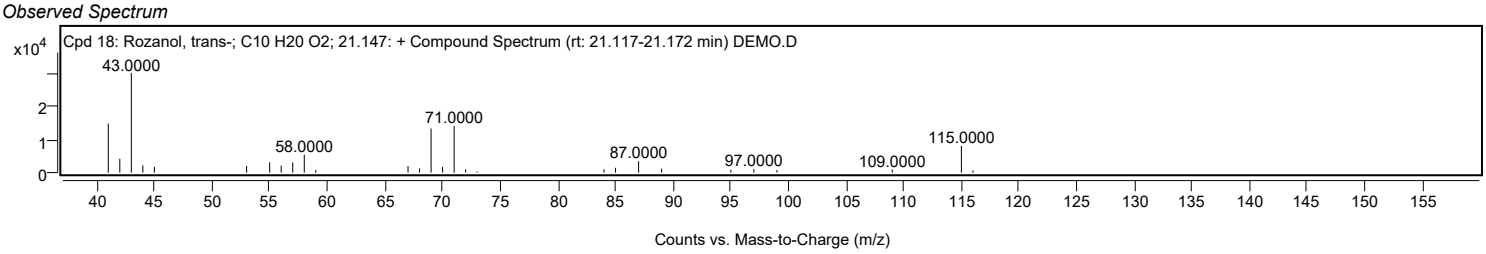
Rozanol, trans-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			90.17			PWNose.xml

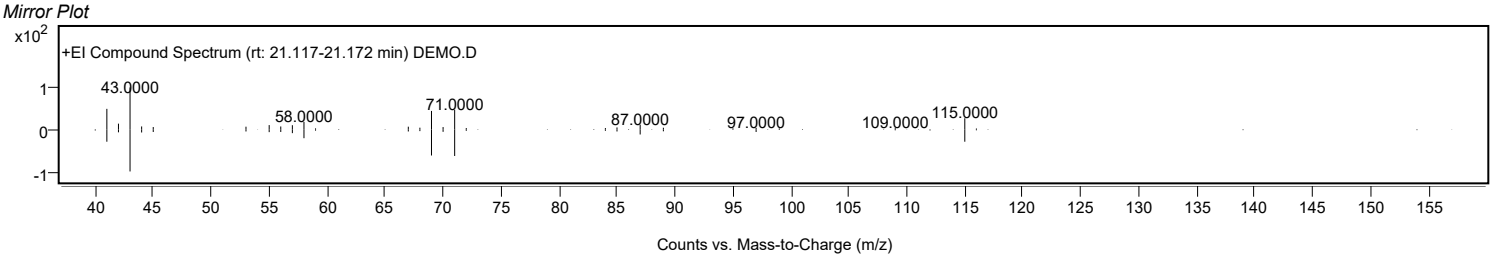
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			90.17			PWNose.xml

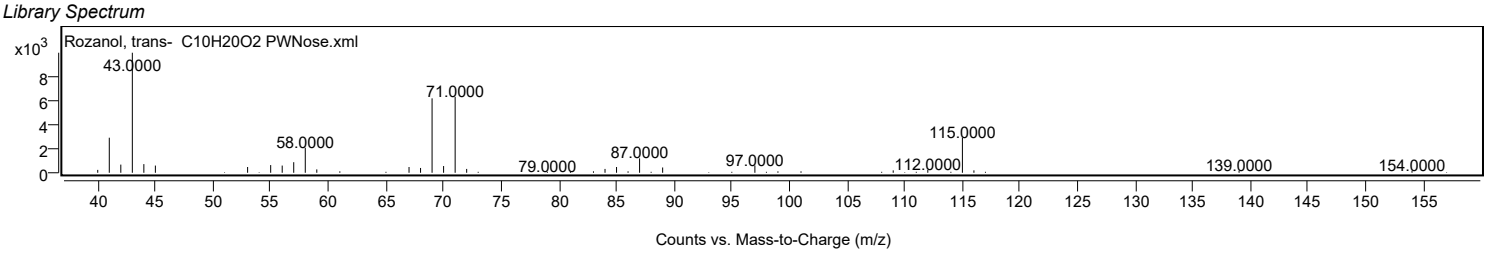
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 19: 1,5-Heptadiene, 3,4-dimethyl-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
1,5-Heptadiene, 3,4-dimethyl-	C9 H16	21.215			1000061-77-9	LibSearch	64.93	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		64.93			50		

Compound Discovery Report

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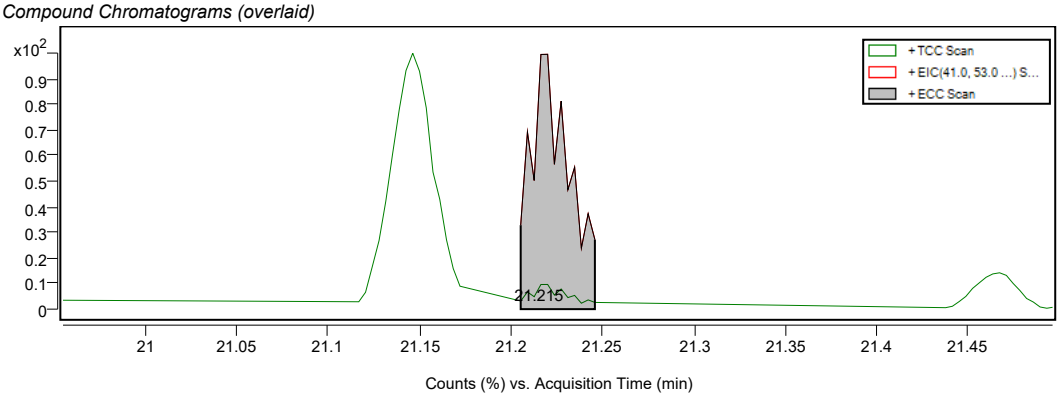
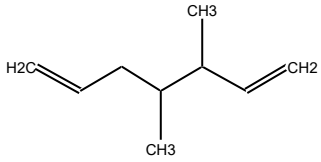
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
1,5-Heptadiene, 3,4-dimethyl-	C9H16		LibSearch	21.215	8.415		1000061-77-9	64.93		
2,6-Octadiene, 4-methyl-	C9H16		LibSearch	21.215	6.749		74498-94-5	63.12		
1,6-Heptadiene, 2-methyl-	C8H14		LibSearch	21.215	8.315		13643-06-6	62.58		
Cyclopentane, bromo-	C5H9Br		LibSearch	21.215	6.932		137-43-9	61.55		
Cyclopentane, nitro-	C5H9NO2		LibSearch	21.215	5.499		2562-38-1	61.13		
3-Methyl-3-nitrobut-1-ene	C5H9NO2		LibSearch	21.215	7.782		1809-67-2	60.87		
2-Butene, 1-bromo-3-methyl-	C5H9Br		LibSearch	21.215	7.882		870-63-3	60.20		
2,7-Nonadien-5-one, 4,6-dimethyl-	C11H18O		LibSearch	21.215	2.249		74630-80-1	59.89		
1,5-Heptadiene, 3,3-dimethyl-, (E)-	C9H16		LibSearch	21.215	7.399		67682-47-7	59.77		
2,6-Octadiene, 4,5-dimethyl-	C10H18		LibSearch	21.215	6.165		18476-57-8	59.05		
2-Methyl-4-bromo-1-butene	C5H9Br		LibSearch	21.215	8.182		20038-12-4	58.56		
4-Methyl-1,5-Heptadiene	C8H14		LibSearch	21.215	8.715		998-94-7	58.21		
Borane, ethylisopropylmethyl-	C6H15B		LibSearch	21.215			1000154-39-8	57.73		
4-Nonene, 2,3,3-trimethyl-, (E)-	C12H24		LibSearch	21.215	3.332		63830-67-1	57.72		
Cyclopentane, bromo-	C5H9Br		LibSearch	21.215	6.932		137-43-9	57.54		
Cyclopentane, nitro-	C5H9NO2		LibSearch	21.215	5.499		2562-38-1	57.40		
(Z)-4-Methyl-2-hexene	C7H14		LibSearch	21.215	10.199		3683-19-0	57.33		
1-Pentene, 3,3-dimethyl-	C7H14		LibSearch	21.215	10.832		3404-73-7	57.13		
1,5-Heptadiene, 3,6-dimethyl-	C9H16		LibSearch	21.215	7.432		34891-10-6	56.93		
2-Pentene, 4-methyl-, (E)-	C6H12		LibSearch	21.215	11.849		674-76-0	56.87		
3-Penten-1-ol, 4-methyl-	C6H12O		LibSearch	21.215	7.132		763-89-3	56.72		
Cyclopentanol, nitrate	C5H9NO3		LibSearch	21.215	4.232		21823-29-0	56.68		
Butanoate<3-methyl-2-butenyl 2-methyl->	C10H18O2		LibSearch	21.215	8.135		84254-80-8	56.44		
2-Methyl-4-bromo-1-butene	C5H9Br		LibSearch	21.215	8.182		20038-12-4	56.38		
1-Butene, 3,3-dimethyl-	C6H12		LibSearch	21.215	12.499		558-37-2	56.23		
4-Methyl-2-hexene,c&t	C7H14		LibSearch	21.215	10.199		3404-55-5	56.19		
2-Pentene, 2-methyl-	C6H12		LibSearch	21.215	11.165		625-27-4	56.16		
3-Methyl-3-chloro-1-butene	C5H9Cl		LibSearch	21.215	11.532		2190-48-9	56.11		
2-Butene, 2,3-dimethyl-	C6H12		LibSearch	21.215	11.549		563-79-1	56.10		
2-Pentene, 4-methyl-, (Z)-	C6H12		LibSearch	21.215	11.849		691-38-3	56.07		
6-Methyl-1,5-heptadiene	C8H14		LibSearch	21.215	8.015		7270-50-0	56.07		
2-Butene, 2,3-dimethyl-	C6H12		LibSearch	21.215	11.549		563-79-1	55.90		
Cyclopentane, bromo-	C5H9Br		LibSearch	21.215	6.932		137-43-9	55.86		
2-Hexene, 4-methyl-, (E)-	C7H14		LibSearch	21.215	10.199		3683-22-5	55.75		
2-Butene, 1-bromo-3-methyl-	C5H9Br		LibSearch	21.215	7.882		870-63-3	55.70		
2-Butene, 2,3-dimethyl-	C6H12		LibSearch	21.215	11.549		563-79-1	55.51		
1,6-Octadiene, 2,7-dimethyl-	C10H18		LibSearch	21.215	5.082		40195-09-3	55.50		
2-Hexene, 4-methyl-, (E)-	C7H14		LibSearch	21.215	10.199		3683-22-5	55.46		
Cyclopropane, 1,1,2-trimethyl-	C6H12		LibSearch	21.215	11.965		4127-45-1	55.45		
1,6-Octadiene, 3,5-dimethyl-, trans-	C10H18		LibSearch	21.215	6.465		74630-87-8	55.45		
4-Methyl-2-hexene,c&t	C7H14		LibSearch	21.215	10.199		3404-55-5	55.22		
1-Butene, 3,3-dimethyl-	C6H12		LibSearch	21.215	12.499		558-37-2	55.18		
1-Butene, 2,3-dimethyl-	C6H12		LibSearch	21.215	12.532		563-78-0	55.05		
Cyclopentane, bromo-	C5H9Br		LibSearch	21.215	6.932		137-43-9	55.02		
1-Butene, 3,3-dimethyl-	C6H12		LibSearch	21.215	12.499		558-37-2	55.00		
2-Pentene, 4-methyl-	C6H12		LibSearch	21.215	11.849		4461-48-7	54.97		
2-Propenoic acid, 2-methyl-, ethenyl ester	C6H8O2		LibSearch	21.215	8.849		4245-37-8	54.89		
2-Pentene, 2-methyl-	C6H12		LibSearch	21.215	11.165		625-27-4	54.75		
2-Pentene, 4-methyl-	C6H12		LibSearch	21.215	11.849		4461-48-7	54.74		
1-Pentene, 3,3-dimethyl-	C7H14		LibSearch	21.215	10.832		3404-73-7	54.69		

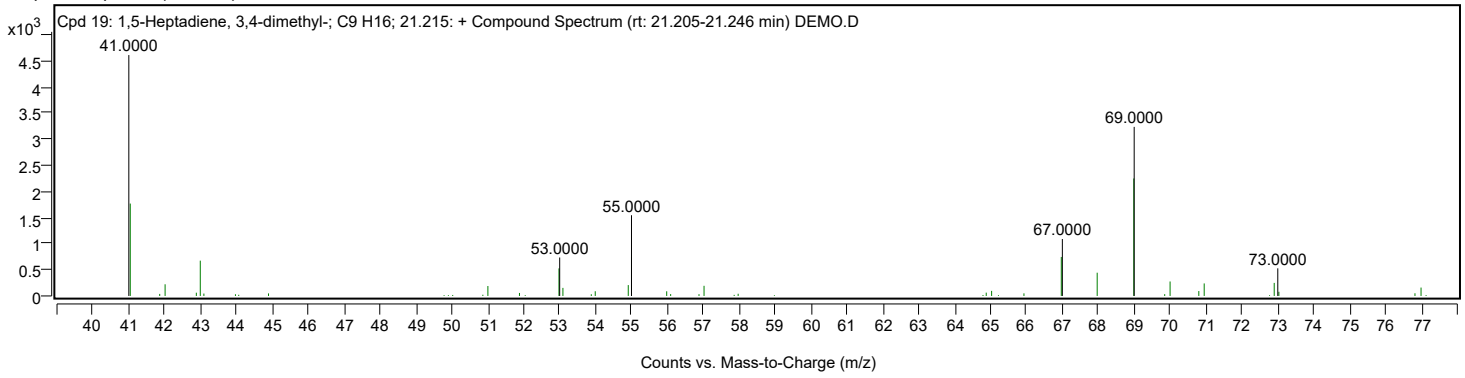
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



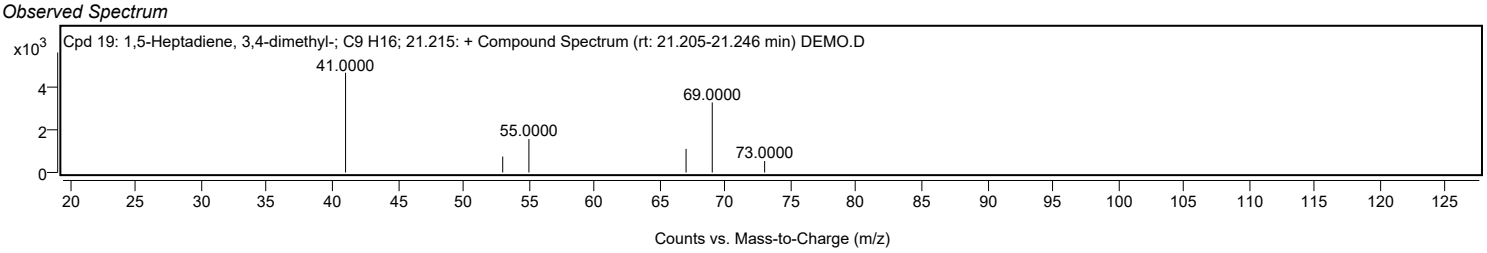
1,5-Heptadiene, 3,4-dimethyl-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			64.93			NIST.L

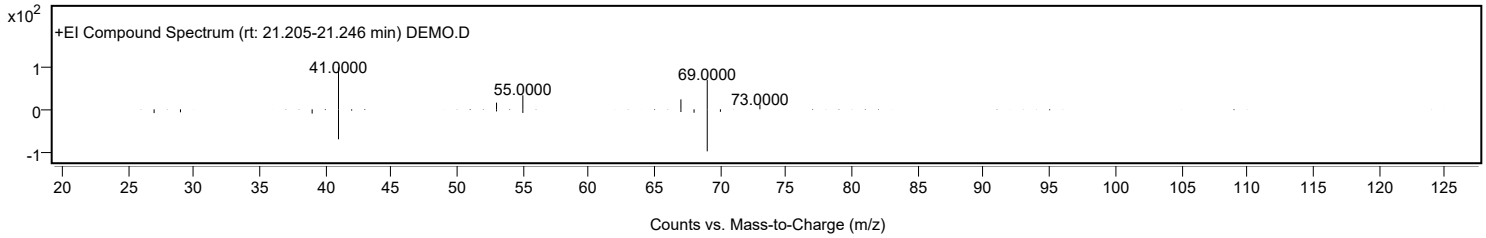
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			64.93			NIST.L

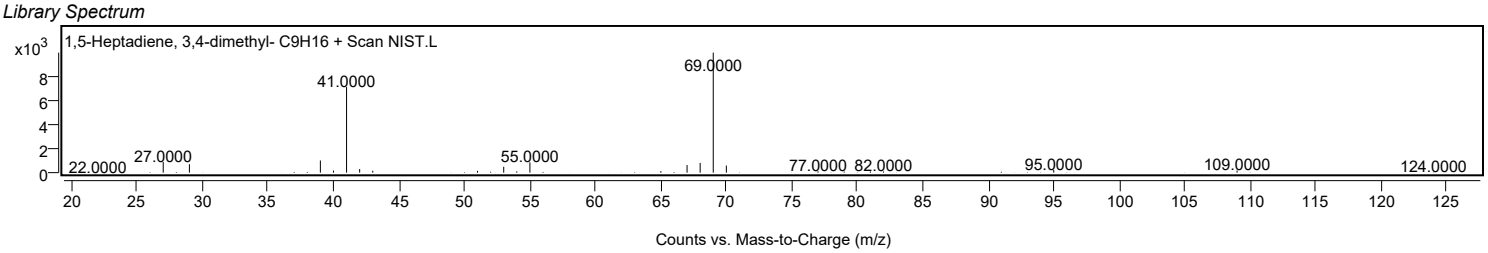
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 20: Linalyl acetate

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Linalyl acetate	C12 H20 O2	21.466			115-95-7	LibSearch	55.44	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		55.44			50		

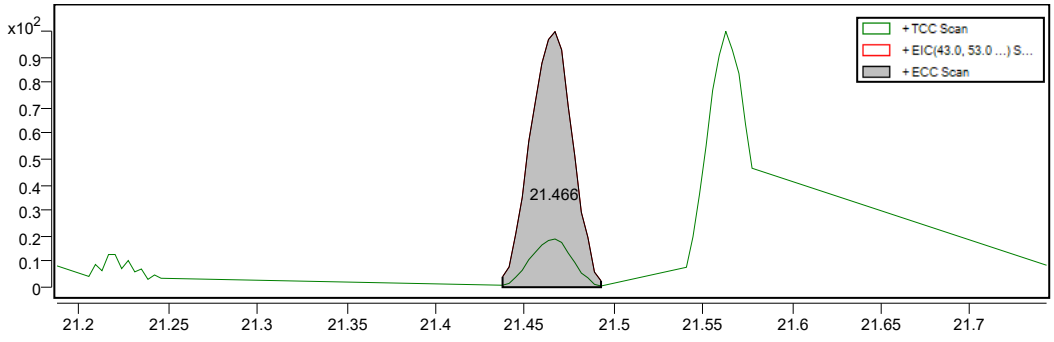
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

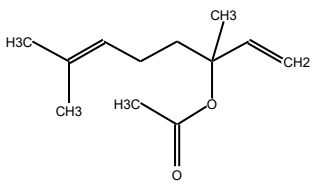
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Linalyl acetate	C12H20O2		LibSearch	21.466			115-95-7	55.44		
Linalyl acetate	C12H20O2		LibSearch	21.466	0.266		115-95-7	54.33		
trans-Ethyl-linalyl acetate	C13H22O2		LibSearch	21.466	-1.384		1000430-70-7	54.19		
Nona-1,6-dien-3-ol <3,7-dimethyl-> acetate	C13H22O2		LibSearch	21.466			61931-80-4	53.74		
Ocimene <(E)-, beta->	C10H16		LibSearch	21.466			3779-61-1	53.70		
Linalyl acetate	C12H20O2		LibSearch	21.466	0.266		115-95-7	52.85		
.beta.-Ocimene	C10H16		LibSearch	21.466	5.200		13877-91-3	52.82		
1,5-Dimethyl-1-vinyl-4-hexenyl butyrate	C14H24O2		LibSearch	21.466	-3.050		78-36-4	52.81		
Nonadien-1-yl acetate <3,6->	C11H18O2		LibSearch	21.466			76649-26-8	52.05		
Linalyl formate	C11H18O2		LibSearch	21.466			115-99-1	51.82		
Linalool acetate	C12H20O2		LibSearch	21.466	3.306		115-95-7	51.35		
Ocimenyl acetate, cis-	C12H20O2		LibSearch	21.466			72214-23-4	51.29		
1,3,7-Octatriene, 3,7-dimethyl-	C10H16		LibSearch	21.466	5.500		502-99-8	51.15		
1,6-Octadien-3-ol, 3,7-dimethyl-, formate	C11H18O2		LibSearch	21.466	0.300		115-99-1	51.07		
cis-Ethyl-linalyl acetate	C13H22O2		LibSearch	21.466	-1.384		1000430-70-6	50.75		
(-)-Isopinocampheol, acetate	C12H20O2		LibSearch	21.466	0.383		1000462-98-1	50.74		
1,3,6-Octatriene, 3,7-dimethyl-, (Z)-	C10H16		LibSearch	21.466	5.200		3338-55-4	50.42		
Ocimenyl acetate, trans-	C12H20O2		LibSearch	21.466			72214-23-4	50.39		
Carene <delta-3->	C10H16		LibSearch	21.466			13466-78-9	50.36		
1,2-Dihydropyridine, 1-(1-oxobutyl)-	C9H13NO		LibSearch	21.466	0.950		1000132-46-2	50.34		
Thujanol acetate<iso-3->	C12H20O2		LibSearch	21.466	2.716		62181-90-2	50.31		
Thujanol acetate<neo-3->	C12H20O2		LibSearch	21.466	2.426		0-00-0	50.06		
1,6-Octadien-3-ol, 3,7-dimethyl-, formate	C11H18O2		LibSearch	21.466	0.300		115-99-1	50.04		
Spiro[4.5]dec-1-ene	C10H16		LibSearch	21.466	3.200		697-27-8	49.97		
Thujanol acetate<neoiso-3->	C12H20O2		LibSearch	21.466	2.086		62181-91-3	49.88		
1,6-Octadien-3-ol, 3,7-dimethyl-, propanoate	C13H22O2		LibSearch	21.466	-1.384		144-39-8	49.88		
Nonadienol acetate<3E,6Z->	C11H18O2		LibSearch	21.466	1.416		211323-05-6	49.82		
Bicyclo[2.2.1]heptane, 7,7-dimethyl-2-methylene-	C10H16		LibSearch	21.466	5.750		471-84-1	49.76		
1,5-Dimethyl-1-vinyl-4-hexenyl butyrate	C14H24O2		LibSearch	21.466	-3.050		78-36-4	49.59		
Neobergamate	C12H20O2		LibSearch	21.466			1118-39-4	49.54		
Linalyl isobutyrate	C14H24O2		LibSearch	21.466	-1.984		78-35-3	49.52		
Linalyl acetate	C12H20O2		LibSearch	21.466	0.266		115-95-7	49.51		
1,3,6-Octatriene, 3,7-dimethyl-, (Z)-	C10H16		LibSearch	21.466	5.200		3338-55-4	49.35		
3,5-Methanocyclopentapyrazole, 3,3a,4,5,6,6a-hexahydro-3a,4,4-trimethyl-	C10H16N2		LibSearch	21.466			87143-58-6	49.31		
1,3,7-Octatriene, 3,7-dimethyl-	C10H16		LibSearch	21.466	5.500		502-99-8	49.25		
Acrylic acid, (5-cyclopropylidenepentyl) ester	C11H16O2		LibSearch	21.466	-0.167		1000156-23-5	49.22		
Linalool isobutyrate	C14H24O2		LibSearch	21.466			78-35-3	49.18		
trans-.beta.-Ocimene	C10H16		LibSearch	21.466	5.200		3779-61-1	49.14		
(+)-4-Carene	C10H16		LibSearch	21.466	6.150		29050-33-7	49.09		
Bicyclo[3.1.1]hept-2-ene, 3,6,6-trimethyl-	C10H16		LibSearch	21.466	5.666		4889-83-2	48.94		
Thujanol acetate<3->	C12H20O2		LibSearch	21.466	1.486		72747-24-1	48.91		
Oct-7-yn-1-ol, acetate	C10H16O2		LibSearch	21.466	1.800		1000506-59-0	48.91		
.beta.-Ocimene	C10H16		LibSearch	21.466	5.200		13877-91-3	48.89		
trans-.beta.-Ocimene	C10H16		LibSearch	21.466	5.200		3779-61-1	48.88		
4-Carene, (1S,3S,6R)-(-)-	C10H16		LibSearch	21.466	6.150		5208-50-4	48.87		
Linalyl acetate	C12H20O2		LibSearch	21.466	0.266		115-95-7	48.85		
Cyclohexene, 4-methylene-1-(1-methylethyl)-	C10H16		LibSearch	21.466	4.916		99-84-3	48.77		
1,3,6-Octatriene, 3,7-dimethyl-, (Z)-	C10H16		LibSearch	21.466	5.200		3338-55-4	48.61		
Ocimene <(Z)-, beta->	C10H16		LibSearch	21.466			3338-55-4	48.58		
Linalool butanoate	C14H24O2		LibSearch	21.466	-4.064		78-36-4	48.53		

Compound Chromatograms (overlaid)

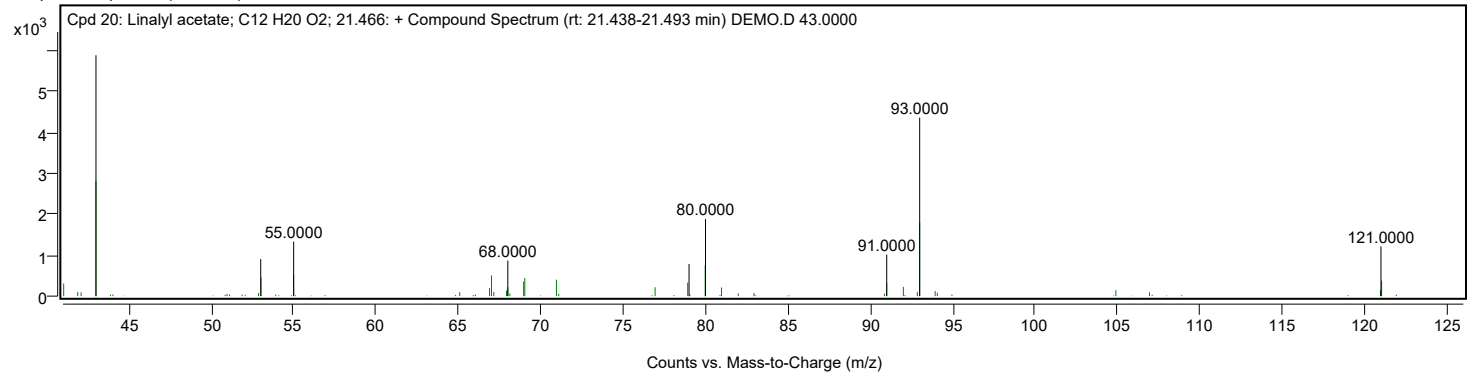


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



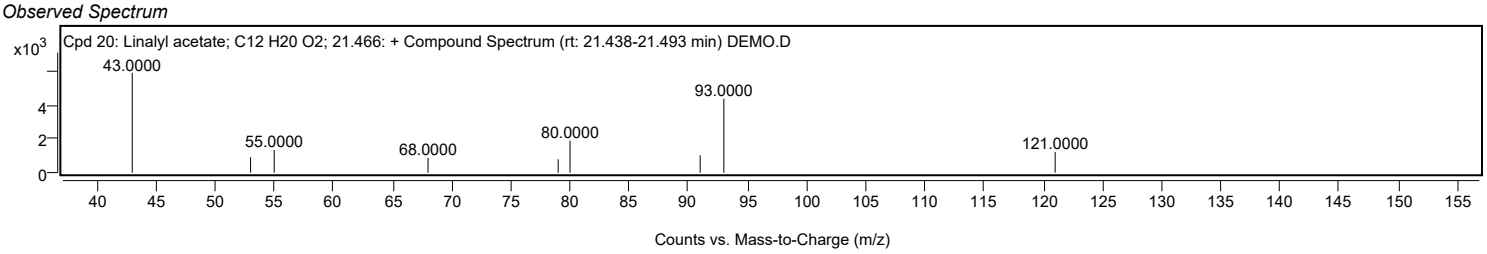
Linalyl acetate

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			55.44			PWNose.xml

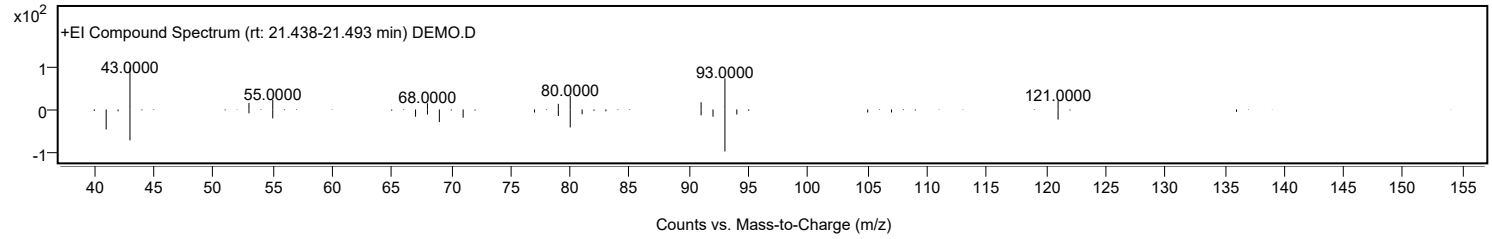
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			55.44			PWNose.xml

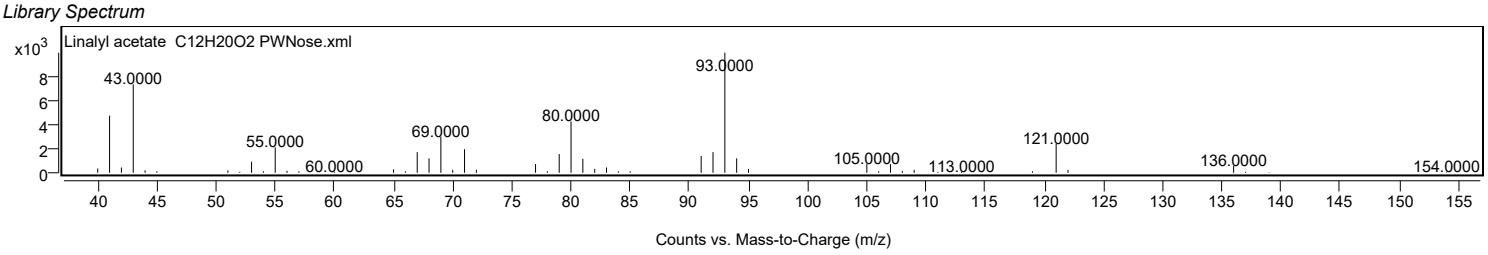
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 21: 2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-

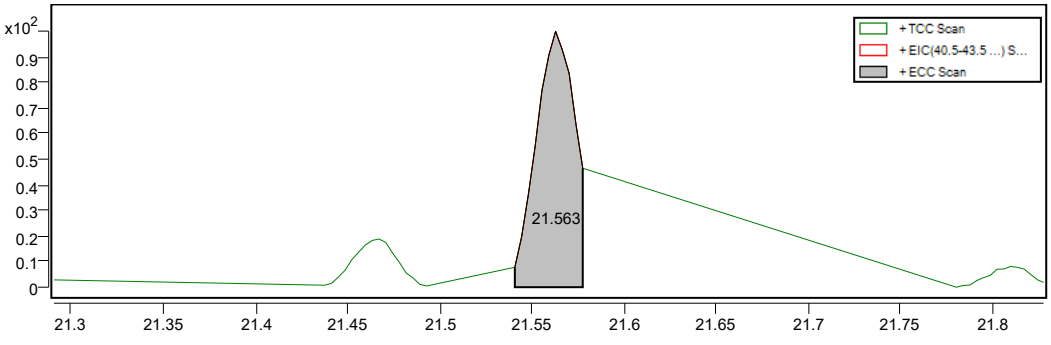
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-	C10 H18 O	21.563			106-25-2	LibSearch	83.84	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		83.84			50		

Compound ID Table

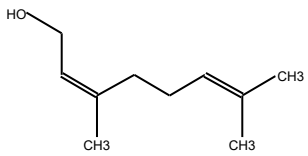
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-	C10H18O		LibSearch	21.563	1.097		106-25-2	83.84		
Geraniol	C10H18O		LibSearch	21.563			106-24-1	82.85		
Geraniol	C10H18O		LibSearch	21.563	3.613		106-24-1	81.82		
Lavandulol	C10H18O		LibSearch	21.563			58461-27-1	81.56		
Nerol	C10H18O		LibSearch	21.563			106-25-2	80.90		
Lavandulol	C10H18O		LibSearch	21.563	7.263		498-16-8	79.86		
Geranyl formate	C11H18O2		LibSearch	21.563	-0.920		105-86-2	78.00		
4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, (R)-	C10H18O		LibSearch	21.563	2.463		498-16-8	77.94		
2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-	C10H18O		LibSearch	21.563	1.097		106-25-2	77.76		
Neryl formate	C11H18O2		LibSearch	21.563	2.243		2142-94-1	77.73		
2,6-Octadien-1-ol, 3,7-dimethyl-	C10H18O		LibSearch	21.563	1.097		624-15-7	77.61		
Geraniol	C10H18O		LibSearch	21.563	1.097		106-24-1	76.97		
Geranyl formate	C11H18O2		LibSearch	21.563			105-86-2	76.74		
Nerol	C10H18O		LibSearch	21.563	4.593		106-25-2	76.58		
Geraniol	C10H18O		LibSearch	21.563	1.097		106-24-1	76.54		
4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, (R)-	C10H18O		LibSearch	21.563	2.463		498-16-8	76.43		
2,6-Octadien-1-ol, 3,7-dimethyl-	C10H18O		LibSearch	21.563	1.097		624-15-7	76.36		
4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, (R)-	C10H18O		LibSearch	21.563	2.463		498-16-8	76.25		
Geranyl formate	C11H18O2		LibSearch	21.563	1.453		105-86-2	75.76		
1-Hexyn-3-ol, 3,5-dimethyl-	C8H14O		LibSearch	21.563	7.530		107-54-0	75.66		
2,6-Octadiene, 4,5-dimethyl-	C10H18		LibSearch	21.563	6.513		18476-57-8	75.65		
4-Hexen-1-ol, 2-ethenyl-2,5-dimethyl-	C10H18O		LibSearch	21.563	2.413		50598-21-5	75.32		
*EU Geraniol	C10H18O		LibSearch	21.563			106-24-1	75.15		
1-Hexyn-3-ol, 3,5-dimethyl-	C8H14O		LibSearch	21.563	7.530		107-54-0	75.05		
4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-	C10H18O		LibSearch	21.563	2.463		58461-27-1	75.04		
2,6-Octadien-1-ol, 3,7-dimethyl-, formate, (Z)-	C11H18O2		LibSearch	21.563	-0.920		2142-94-1	74.87		
Nonadienal<2E,6Z->	C9H14O		LibSearch	21.563	7.923		557-48-2	74.73		
1,5-Heptadiene, 3,3-dimethyl-, (E)-	C9H16		LibSearch	21.563	7.747		67682-47-7	74.41		
Cyclopropanecarboxyllic acid, tridec-2-ynyl ester	C17H28O2		LibSearch	21.563	-10.070		1000299-38-2	73.92		
Oxirane, 2,2'-(1,4-butanediyl)bis-	C8H14O2		LibSearch	21.563	4.947		2426-07-5	73.90		
2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-	C10H18O		LibSearch	21.563	1.097		106-25-2	73.83		
Trifluoroacetyl-lavandulol	C12H17F3O2		LibSearch	21.563	3.163		28673-24-7	73.80		
Geraniol	C10H18O		LibSearch	21.563	1.097		106-24-1	73.72		
Nona-(2E,6E)-dienal	C9H14O		LibSearch	21.563			17587-33-6	73.60		
trans,cis-2,6-Nonadien-1-ol	C9H16O		LibSearch	21.563	1.980		28069-72-9	73.56		
1-Hexyn-3-ol, 3,5-dimethyl-	C8H14O		LibSearch	21.563	7.530		107-54-0	73.48		
Neryl formate	C11H18O2		LibSearch	21.563			2142-94-1	73.43		
1,5-Heptadiene, 3,3,6-trimethyl-	C10H18		LibSearch	21.563	6.463		35387-63-4	73.12		
1,5-Heptadiene, 3,4-dimethyl-	C9H16		LibSearch	21.563	8.763		1000061-77-9	73.06		
1,5-Heptadiene, 3,6-dimethyl-	C9H16		LibSearch	21.563	7.780		34891-10-6	73.04		
2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-	C10H18O		LibSearch	21.563	1.097		106-25-2	72.99		
1,6-Octadiene, 3,5-dimethyl-, trans-	C10H18		LibSearch	21.563	6.813		74630-87-8	72.92		
Geraniol	C10H18O		LibSearch	21.563	1.097		106-24-1	72.87		
Nonadienol<2E,6Z->	C9H16O		LibSearch	21.563	7.523		28069-72-9	72.80		
Nona-(2E,6Z)-dienol	C9H16O		LibSearch	21.563			28069-72-9	72.59		
6-Octen-1-ol, 7-methyl-3-methylene-	C10H18O		LibSearch	21.563	1.397		13066-51-8	72.35		
Cucumber alcohol	C9H16O		LibSearch	21.563			7786-44-9	71.99		
Dodecadien-1-al<2Z,6E->	C12H20O		LibSearch	21.563	-4.947		21662-13-5	71.99		
Allyl crotonate	C7H10O2		LibSearch	21.563			20474-93-5	71.74		
4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, (R)-	C10H18O		LibSearch	21.563	2.463		498-16-8	71.74		

Compound Chromatograms (overlaid)

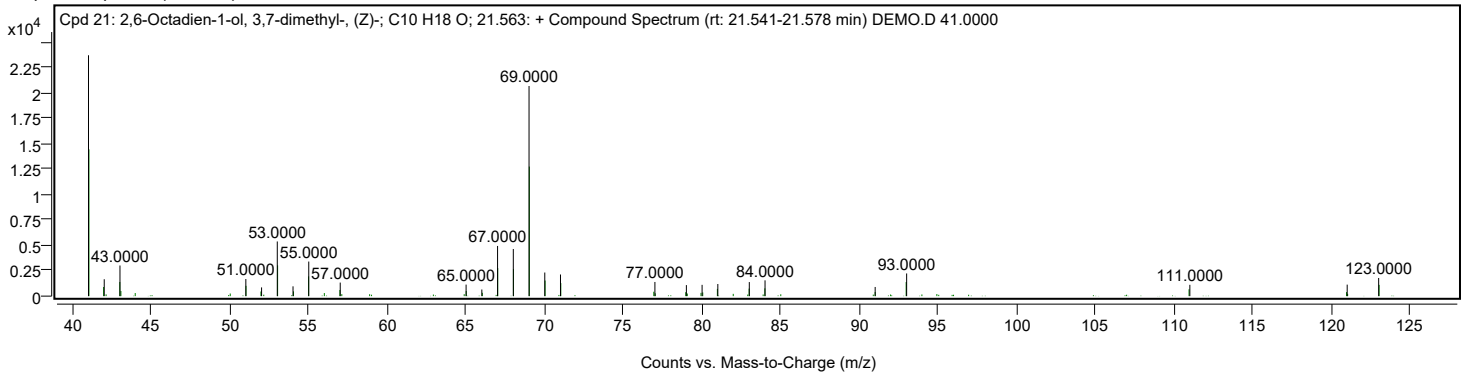


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



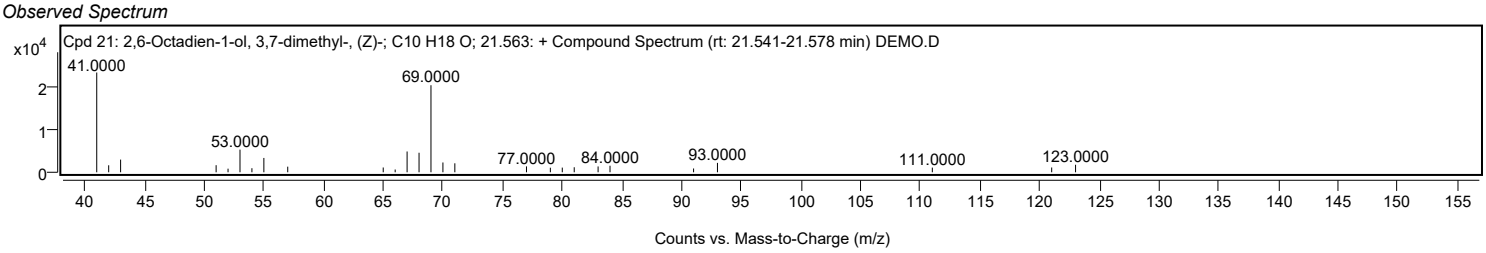
2,6-Octadien-1-ol, 3,7-dimethyl-, (Z)-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			83.84			NIST.L

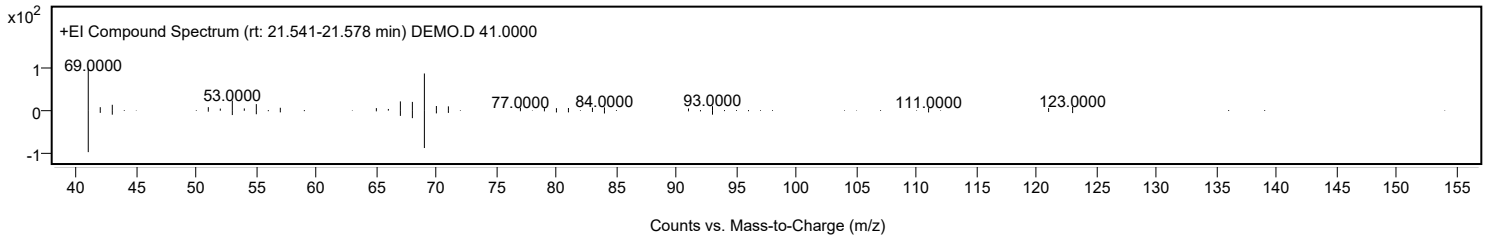
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			83.84			NIST.L

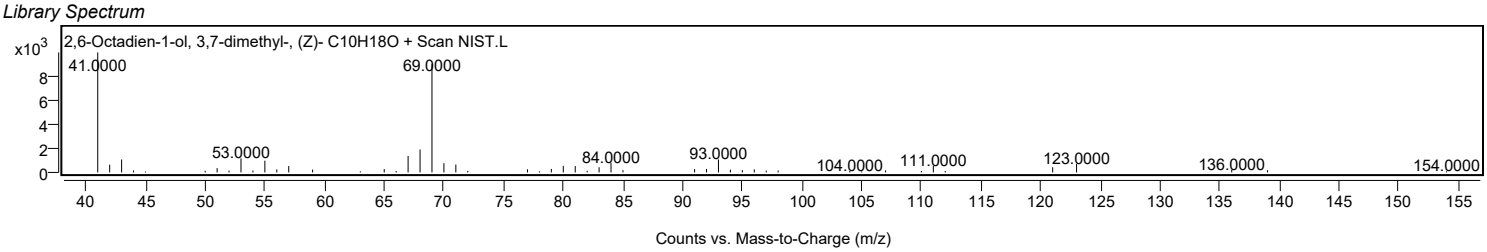
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 22: Carbonic acid, monoamide, N-isobutyl-, benzyl ester

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Carbonic acid, monoamide, N-isobutyl-, benzyl ester	C12 H17 N O2	21.811			1000420-28-2	LibSearch	62.11	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		62.11			50		

Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Carbonic acid, monoamide, N-isobutyl-, benzyl ester	C12H17NO2		LibSearch	21.811	-4.723		1000420-28-2	62.11		
Carbonic acid, monoamide, N-heptyl-, benzyl ester	C15H23NO2		LibSearch	21.811	-10.773		1010420-28-9	61.00		
Carbonic acid, monoamide, N-octyl-, benzyl ester	C16H25NO2		LibSearch	21.811	-12.423		1010420-29-0	60.96		
Carbonic acid, monoamide, N-butyl-, benzyl ester	C12H17NO2		LibSearch	21.811	-5.789		1000420-28-3	60.84		
Carbonic acid, monoamide, N-3-methylbutyl-, benzyl ester	C13H19NO2		LibSearch	21.811	-6.389		1000420-28-4	60.10		
Carbonic acid, monoamide, N-2-ethylhexyl-, benzyl ester	C16H25NO2		LibSearch	21.811	-11.356		1000420-28-8	59.85		
Carbonic acid, monoamide, N-pentyl-, benzyl ester	C13H19NO2		LibSearch	21.811	-7.456		1000420-28-5	59.81		
Carbonic acid, monoamide, N-decyl-, benzyl ester	C18H29NO2		LibSearch	21.811	-15.739		1000420-29-2	59.57		
Carbonic acid, monoamide, N-hexyl-, benzyl ester	C14H21NO2		LibSearch	21.811	-9.106		1000420-28-7	59.17		
Carbonic acid, monoamide, N-dodecyl-, benzyl ester	C20H33NO2		LibSearch	21.811	-19.056		1000420-29-4	59.01		
Carbonic acid, monoamide, N-propyl-, benzyl ester	C11H15NO2		LibSearch	21.811	-4.139		1000420-28-1	58.88		
Carbonic acid, monoamide, N-nonyl-, benzyl ester	C17H27NO2		LibSearch	21.811	-14.073		1000420-29-1	58.20		
Carbonic acid, monoamide, N-undecyl-, benzyl ester	C19H31NO2		LibSearch	21.811	-17.389		1000420-29-3	58.10		
Propanoic acid, phenylmethyl ester	C10H12O2		LibSearch	21.811	0.827		122-63-4	57.40		
Benzyl propanoate	C10H12O2		LibSearch	21.811			122-63-4	57.14		
Carbonic acid, monoamide, N-hexadecyl-, benzyl ester	C24H41NO2		LibSearch	21.811	-25.673		1000420-29-6	56.09		
Butanoic acid, 3-methyl-, phenylmethyl ester	C12H16O2		LibSearch	21.811	-1.423		103-38-8	56.06		
Carbonic acid, isobutyl 3-methylphenyl ester	C12H16O3		LibSearch	21.811	-2.923		1000357-83-1	55.66		
Propanoic acid, phenylmethyl ester	C10H12O2		LibSearch	21.811	0.827		122-63-4	55.15		
Propanoic acid, phenylmethyl ester	C10H12O2		LibSearch	21.811	0.827		122-63-4	55.04		
Carbamic acid, methyl-, phenylmethyl ester	C9H11NO2		LibSearch	21.811	-0.823		30379-59-0	54.90		
Carbonic acid, monoamide, N-octadecyl-, benzyl ester	C26H45NO2		LibSearch	21.811	-28.989		1000420-29-7	54.65		
Isovalerate <benzyl->	C12H16O2		LibSearch	21.811			103-38-8	54.48		
N-(3-Iodopropyl)carbamic acid, benzyl ester	C11H14INO2		LibSearch	21.811	-11.039		84792-78-9	54.33		
Propanoic acid, phenylmethyl ester	C10H12O2		LibSearch	21.811	0.827		122-63-4	54.16		
Benzyl propanoate	C10H12O2		LibSearch	21.811	3.521		122-63-4	53.73		
Glycine, N-benzyloxycarbonyl-, ethyl ester	C12H15NO4		LibSearch	21.811	-8.589		1000322-76-6	53.27		
Oxalic acid, isobutyl 2-methylphenyl ester	C13H16O4		LibSearch	21.811	-6.089		1000309-59-3	53.19		
Carbonic acid, butyl 3-methylphenyl ester	C12H16O3		LibSearch	21.811	-3.989		1000357-84-6	53.12		
Hydroxylamine, O-(phenylmethyl)-	C7H9NO		LibSearch	21.811	3.261		622-33-3	53.11		
Propanoic acid, phenylmethyl ester	C10H12O2		LibSearch	21.811	0.827		122-63-4	53.01		
Oxalic acid, butyl 2-methylphenyl ester	C13H16O4		LibSearch	21.811	-7.156		1000309-59-4	52.57		
Urea, (phenylmethoxy)-	C8H10N2O2		LibSearch	21.811	-4.473		2048-50-2	52.50		
Oxalic acid, heptyl 2-methylphenyl ester	C16H22O4		LibSearch	21.811	-12.139		1000309-59-7	52.42		
N-carbobenzyloxy-propan-3-ol-1-amine	C11H15NO3		LibSearch	21.811	-8.189		34637-22-4	52.32		
Glycine, N-benzyloxycarbonyl-, isobutyl ester	C14H19NO4		LibSearch	21.811	-10.823		1000322-76-7	52.26		
Benzeneacetic acid, phenylmethyl ester	C15H14O2		LibSearch	21.811	-8.739		102-16-9	51.96		
Propanoic acid, 2,2-dimethyl-, phenylmethyl ester	C12H16O2		LibSearch	21.811	-1.073		2094-69-1	51.90		
Butanoic acid, 3-methyl-, phenylmethyl ester	C12H16O2		LibSearch	21.811	-1.423		103-38-8	51.90		
Benzyl (1,2,3-thiadiazol-4-y)carbamate	C10H9N3O2S		LibSearch	21.811			1000443-04-2	51.84		
Carbamic acid, N-(3-oxo-4-isoxazolidinyl)-, benzyl ester	C11H12N2O4		LibSearch	21.811	-10.706		28832-02-2	51.50		
N-Benzyloxy-2-carbomethoxyaziridine	C11H13NO3		LibSearch	21.811	-4.023		53084-33-6	51.42		
Benzyl glycolate	C9H10O3		LibSearch	21.811	-1.556		30379-58-9	51.21		
Hydroxylamine, O-(phenylmethyl)-	C7H9NO		LibSearch	21.811	3.261		622-33-3	51.19		
Carbobenzyloxyglycine methyl ester	C11H13NO4		LibSearch	21.811	-6.923		1212-53-9	50.91		
N-Z-L-Homoserine lactone	C12H13NO4		LibSearch	21.811	-11.923		35677-89-5	50.40		
Propanoic acid, 2,2-dimethyl-, phenylmethyl ester	C12H16O2		LibSearch	21.811	-1.073		2094-69-1	50.25		
N-Z-L-Homoserine lactone	C12H13NO4		LibSearch	21.811	-11.923		35677-89-5	50.24		
L-Serine, N-[(phenylmethoxy)carbonyl]-	C11H13NO5		LibSearch	21.811	-13.056		1145-80-8	50.11		
Benzene, [(methylsulfinyl)methyl]-	C8H10OS		LibSearch	21.811	-0.923		824-86-2	49.99		

Compound Discovery Report

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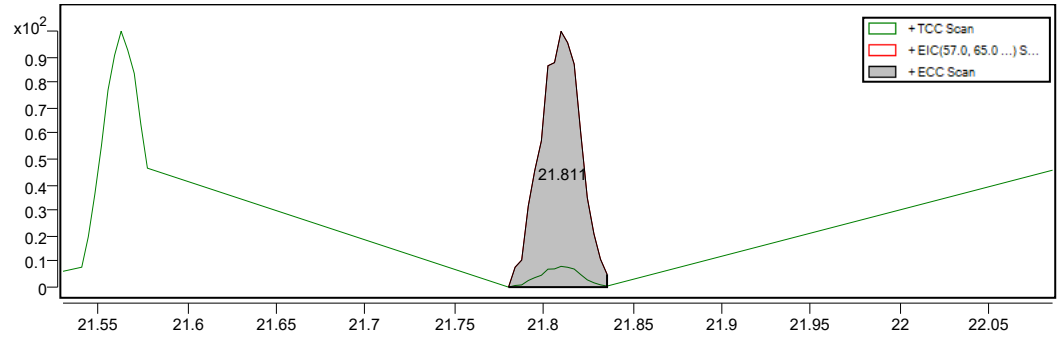
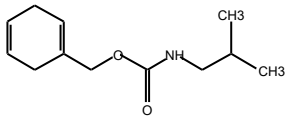
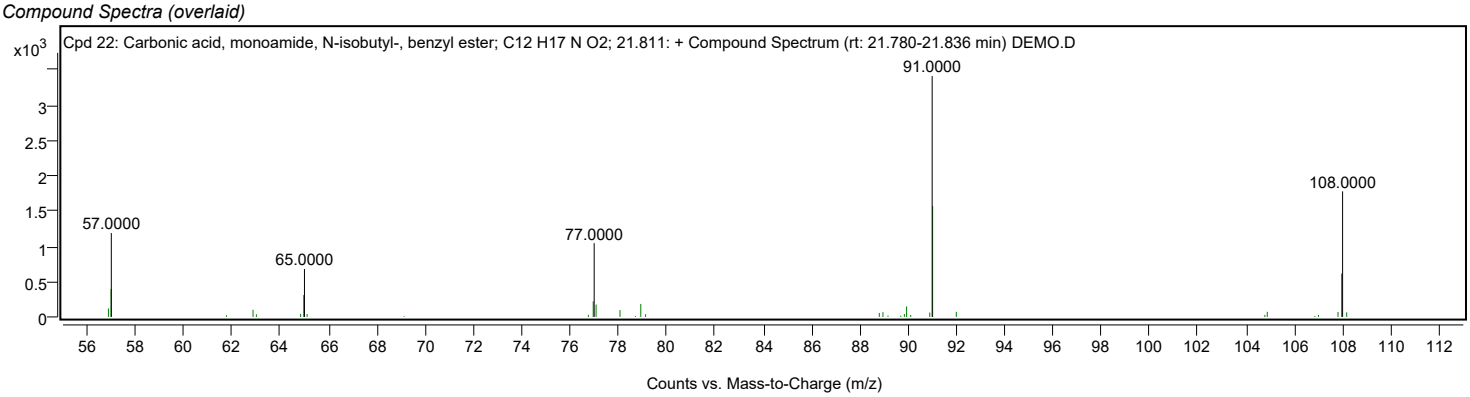
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



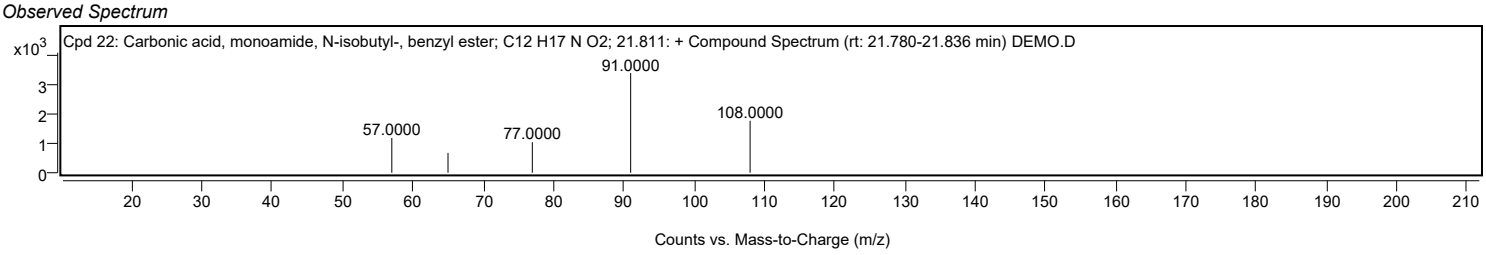
Carbonic acid, monoamide, N-isobutyl-, benzyl ester

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			62.11			NIST.L

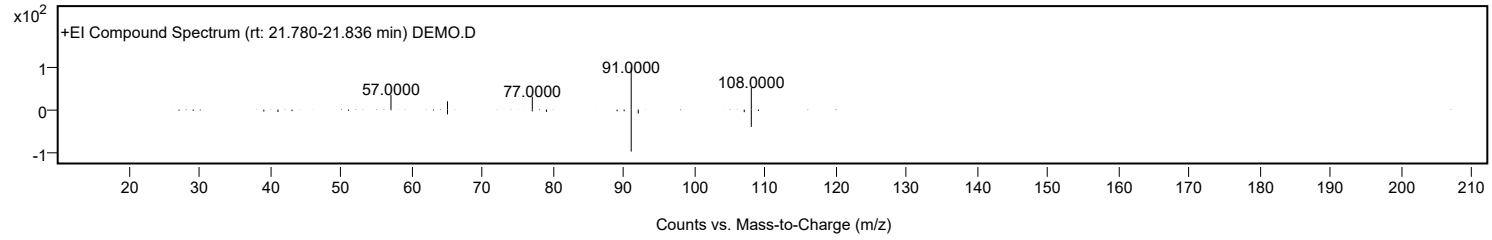
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			62.11			NIST.L

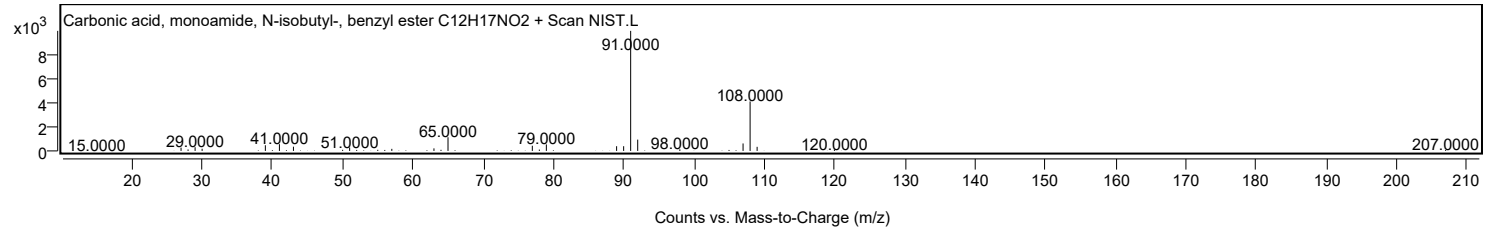
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 23: Citronellal <hydroxy->

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Citronellal <hydroxy->	C10 H20 O2	22.194			107-75-5	LibSearch	84.85	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		84.85			50		

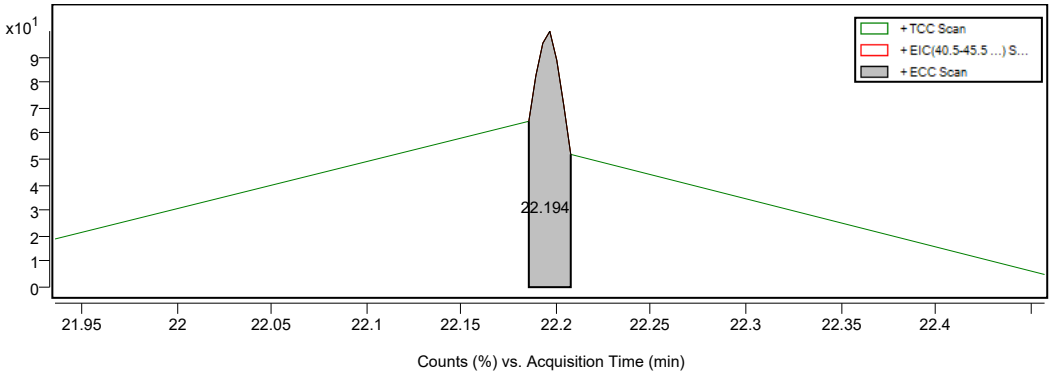
Compound Discovery Report

Agilent | Trusted Answers

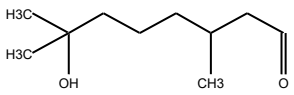
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Citronellal <hydroxy->	C10H20O2		LibSearch	22.194			107-75-5	84.85		
Hydroxy citronellal	C10H20O2		LibSearch	22.194	2.594		107-75-5	83.58		
Octanal, 7-hydroxy-3,7-dimethyl-	C10H20O2		LibSearch	22.194	1.678		107-75-5	80.55		
Octanal, 7-hydroxy-3,7-dimethyl-	C10H20O2		LibSearch	22.194	1.678		107-75-5	80.21		
Octanal, 7-hydroxy-3,7-dimethyl-	C10H20O2		LibSearch	22.194	1.678		107-75-5	76.12		
Octanal, 7-hydroxy-3,7-dimethyl-	C10H20O2		LibSearch	22.194	1.678		107-75-5	75.42		
*EU Hydroxy citronellal	C10H20O2		LibSearch	22.194			107-75-5	72.70		
1,8-Nonanediol, 8-methyl-	C10H22O2		LibSearch	22.194	-0.306		54725-73-4	69.93		
Heptanol<2,6-dimethyl-2->	C9H20O		LibSearch	22.194	14.714		13254-34-7	69.92		
Terpineol<cis-dihydro-alpha->	C10H20O		LibSearch	22.194	8.104		7322-63-6	68.80		
o-Menthan-8-ol	C10H20O		LibSearch	22.194	3.328		343855-44-7	68.78		
Vinyldimethylcarbinol	C5H10O		LibSearch	22.194			115-18-4	68.50		
6-Methylheptane-1,6-diol	C8H18O2		LibSearch	22.194	3.011		5392-57-4	68.03		
2-Hexanol, 2,5-dimethyl-, (S)-	C8H18O		LibSearch	22.194	8.128		3730-60-7	67.92		
Terpineol <trans-dihydro-alpha->	C10H20O		LibSearch	22.194			5114-00-1	67.86		
Terpineol<trans-dihydro-alpha->	C10H20O		LibSearch	22.194	8.864		5114-00-1	67.77		
Pentanol <3->	C5H12O		LibSearch	22.194			584-02-1	66.93		
2-Cyclobutyl-2-propanol	C7H14O		LibSearch	22.194	8.344		59383-67-4	66.84		
Cyclohexanemethanol, .alpha.,.alpha.,4-trimethyl-	C10H20O		LibSearch	22.194	3.328		498-81-7	66.50		
Terpineol <cis- dihydro- alpha->	C10H20O		LibSearch	22.194			7322-63-6	66.50		
Cyclohexanemethanol, .alpha.,.alpha.,4-trimethyl-	C10H20O		LibSearch	22.194	3.328		498-81-7	66.00		
2-Heptanol, 2,6-dimethyl-	C9H20O		LibSearch	22.194	6.478		13254-34-7	65.80		
Dimetol	C9H20O		LibSearch	22.194			13254-34-7	65.62		
2,3-Dimethyl-4-penten-2-ol	C7H14O		LibSearch	22.194	8.961		19781-52-3	65.51		
2-Nonanone, 9-hydroxy-	C9H18O2		LibSearch	22.194	0.611		25368-56-3	65.48		
Cyclohexanemethanol, 4-hydroxy-.alpha.,.alpha.,4-trimethyl-	C10H20O2		LibSearch	22.194	0.828		80-53-5	65.34		
Oxirane, (3-methylbutyl)-	C7H14O		LibSearch	22.194	9.811		53229-41-7	65.17		
2-Pentadecanone	C15H30O		LibSearch	22.194	-5.272		2345-28-0	65.17		
meso-3,4-Hexanediol	C6H14O2		LibSearch	22.194	6.494		22520-39-4	65.16		
Dihydromyrcenol	C10H20O		LibSearch	22.194	11.844		18479-58-8	65.11		
3-Pentadecanol	C15H32O		LibSearch	22.194	-5.722		53346-71-7	64.72		
Menthol <8-hydroxy-iso->	C10H20O2		LibSearch	22.194			91739-73-0	64.71		
Cyclohexanemethanol, .alpha.,.alpha.,4-trimethyl-, cis-	C10H20O		LibSearch	22.194	3.328		7322-63-6	64.69		
Coranol	C11H22O		LibSearch	22.194			83926-73-2	64.67		
2-Hexanone, 5-methyl-	C7H14O		LibSearch	22.194	9.044		110-12-3	64.62		
2-Methyl-2,3-pentanediol	C6H14O2		LibSearch	22.194	7.661		7795-80-4	64.42		
2-Hexadecanone	C16H32O		LibSearch	22.194	-6.939		18787-63-8	64.37		
2-Hexanone, 5-methyl-	C7H14O		LibSearch	22.194	9.044		110-12-3	64.05		
4-Octene-2,7-diol, 2,7-dimethyl-, Z-	C10H20O2		LibSearch	22.194	2.078		1000151-60-8	63.99		
2-Dodecanol, 2-methyl-	C13H28O		LibSearch	22.194	-1.222		1653-37-8	63.85		
2-Pentanol, 3-chloro-2-methyl-	C6H13ClO		LibSearch	22.194	8.028		74685-49-7	63.84		
2-Hexanone, 5-methyl-	C7H14O		LibSearch	22.194	9.044		110-12-3	63.74		
Decanone<2->	C10H20O		LibSearch	22.194	6.814		693-54-9	63.68		
3-Buten-2-ol, 2-methyl-	C5H10O		LibSearch	22.194	12.194		115-18-4	63.68		
2-Heptanol, 2-methyl-	C8H18O		LibSearch	22.194	7.061		625-25-2	63.50		
Hydroxy citronellol	C10H22O2		LibSearch	22.194	-0.636		107-74-4	63.44		
Cyclohexanemethanol, .alpha.,.alpha.,4-trimethyl-	C10H20O		LibSearch	22.194	3.328		498-81-7	63.25		
Cyclohexanemethanol, .alpha.,.alpha.,4-trimethyl-, trans-	C10H20O		LibSearch	22.194	3.328		5114-00-1	63.20		
6-Methyl-2-heptanol, methyl ether	C9H20O		LibSearch	22.194	7.794		1000365-52-0	63.15		
2-Decanol, methyl ether	C11H24O		LibSearch	22.194	3.428		1000333-83-9	63.03		

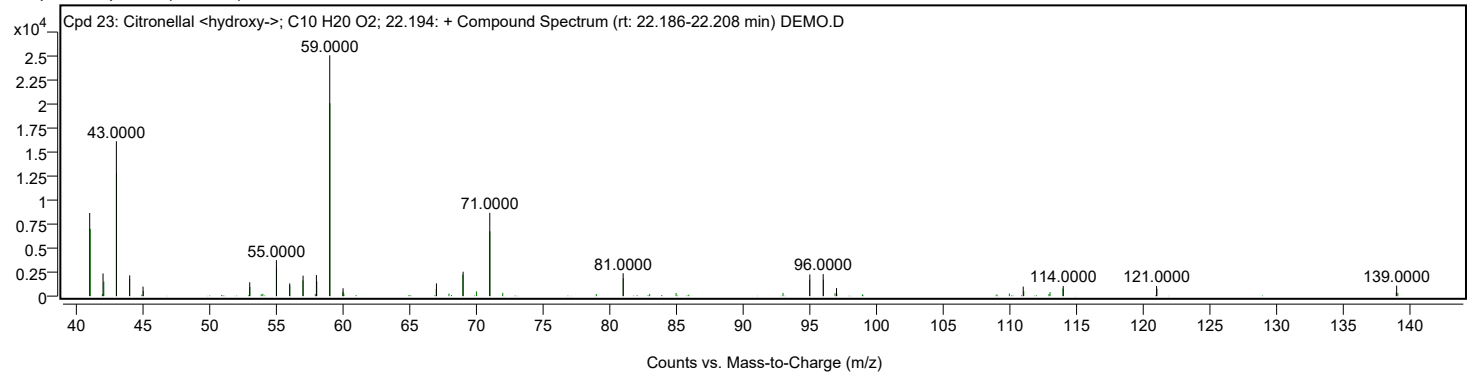
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



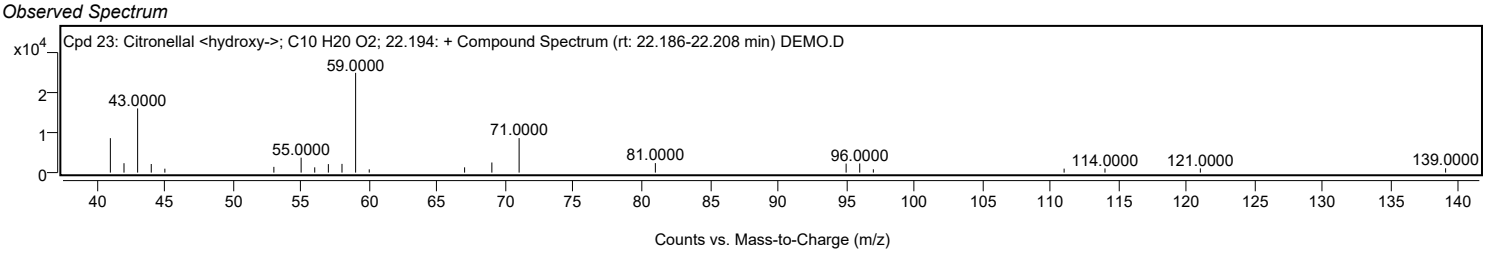
Citronellal <hydroxy->

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			84.85			PWNose.xml

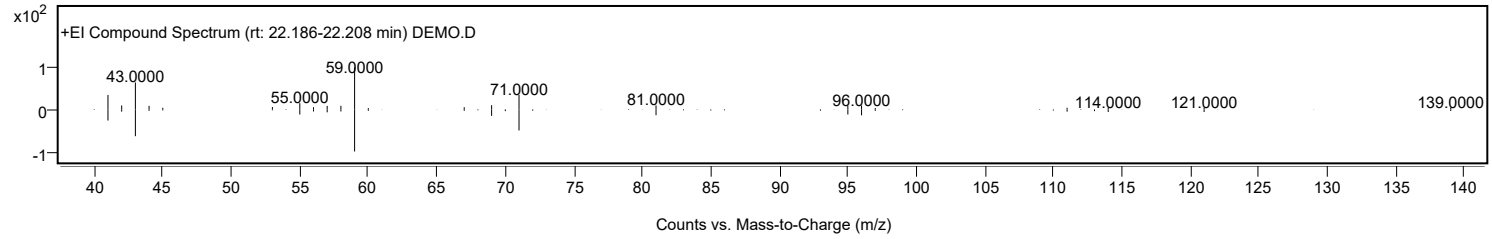
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			84.85			PWNose.xml

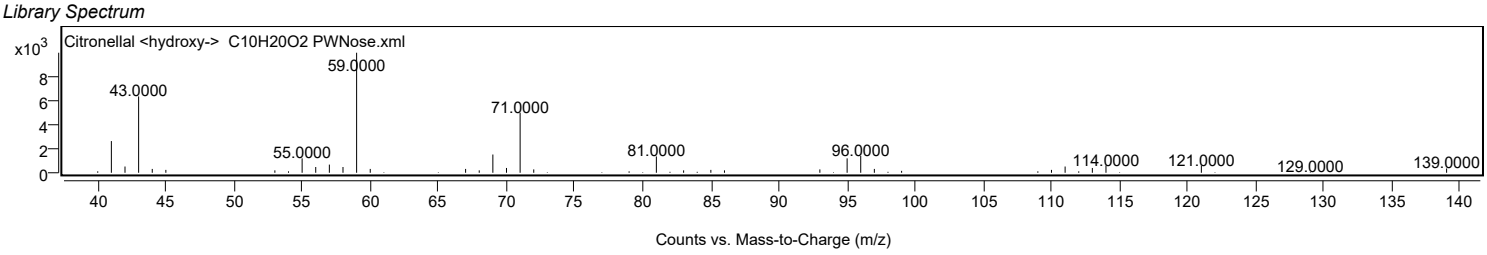
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 24: 3-Hexen-1-ol, propanoate, (Z)-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
3-Hexen-1-ol, propanoate, (Z)-	C9 H16 O2	22.482			33467-74-2	LibSearch	72.60	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		72.60			50		

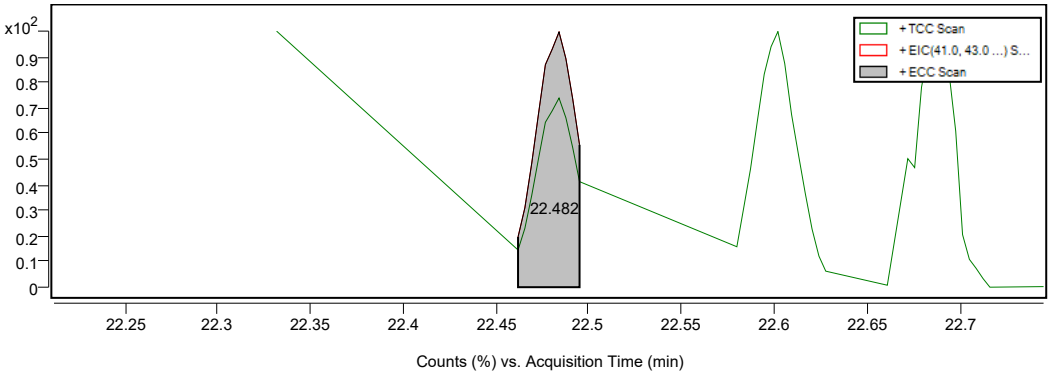
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

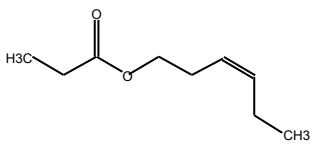
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
3-Hexen-1-ol, propanoate, (Z)-	C9H16O2		LibSearch	22.482	4.298		33467-74-2	72.60		
Hex-(3Z)-enol propanoate	C9H16O2		LibSearch	22.482			33467-74-2	71.96		
3-Hexen-1-ol, propanoate, (Z)-	C9H16O2		LibSearch	22.482	4.298		33467-74-2	71.65		
Hexenyl propionate<3Z->	C9H16O2		LibSearch	22.482	11.182		33467-74-2	70.73		
3-Hexen-1-ol, propanoate, (Z)-	C9H16O2		LibSearch	22.482	4.298		33467-74-2	69.81		
Hexenyl acetate<3E->	C8H14O2		LibSearch	22.482	14.642		3681-82-1	69.57		
3-Hexen-1-ol, acetate, (Z)-	C8H14O2		LibSearch	22.482	5.948		3681-71-8	68.97		
Hexenyl acetate<3Z->	C8H14O2		LibSearch	22.482	14.552		3681-71-8	68.67		
Hex-(3Z)-enyl acetate	C8H14O2		LibSearch	22.482			3681-71-8	68.07		
Octanoic acid, 3-hexenyl ester, (Z)-	C14H26O2		LibSearch	22.482	-3.985		61444-41-5	67.96		
(Z)-Hex-3-enyl isobutyl carbonate	C11H20O3		LibSearch	22.482	0.782		1000372-75-0	67.71		
Acetic acid, cyclohexyl ester	C8H14O2		LibSearch	22.482	5.032		622-45-7	67.44		
(E)-Hex-3-enyl isobutyl carbonate	C11H20O3		LibSearch	22.482	0.782		1000372-74-9	67.40		
Propanoic acid, 4-hexen-1-yl ester	C9H16O2		LibSearch	22.482	4.298		1000159-22-1	67.20		
4-Hexen-1-ol, acetate, (Z)-	C8H14O2		LibSearch	22.482	5.948		42125-17-7	66.84		
Hex-(3E)-enyl acetate	C8H14O2		LibSearch	22.482			3681-82-1	66.75		
cis-3-Hexenyl-.alpha.-methylbutyrate	C11H20O2		LibSearch	22.482	2.048		53398-85-9	66.57		
Hexenyl pyruvate<3Z->	C9H14O3		LibSearch	22.482	7.492		68133-76-6	66.31		
3-Hexen-1-ol, acetate, (Z)-	C8H14O2		LibSearch	22.482	5.948		3681-71-8	66.23		
Propanoic acid <2-oxo-, (3Z)-hexenyl-> ester	C9H14O3		LibSearch	22.482			68133-76-6	66.18		
Acetate <cyclohexyl->	C8H14O2		LibSearch	22.482			622-45-7	65.84		
4-Hexen-1-ol, acetate	C8H14O2		LibSearch	22.482	5.948		72237-36-6	65.79		
Hexenyl 2-methyl butanoate <(3Z)->	C11H20O2		LibSearch	22.482			53398-85-9	65.71		
cis-3-Hexenylpyruvate	C9H14O3		LibSearch	22.482	2.032		68133-76-6	65.51		
3-Hexenyl 2-methylbutyrate	C11H20O2		LibSearch	22.482			10094-41-4	65.36		
2-Hexen-1-ol, acetate, (E)-	C8H14O2		LibSearch	22.482	5.948		2497-18-9	65.35		
Acetic acid, cyclohexyl ester	C8H14O2		LibSearch	22.482	5.032		622-45-7	65.16		
2-Hexen-1-ol, propanoate, (E)-	C9H16O2		LibSearch	22.482	4.298		53398-80-4	64.98		
4-Hexen-1-ol, acetate	C8H14O2		LibSearch	22.482	5.948		72237-36-6	64.83		
3-Hexen-1-ol, acetate, (Z)-	C8H14O2		LibSearch	22.482	5.948		3681-71-8	64.70		
Acetic acid, cyclohexyl ester	C8H14O2		LibSearch	22.482	5.032		622-45-7	64.70		
Acetic acid, cyclohexyl ester	C8H14O2		LibSearch	22.482	5.032		622-45-7	64.56		
Formic acid, cyclohexyl ester	C7H12O2		LibSearch	22.482	5.065		4351-54-6	64.32		
(Z)-Hex-3-en-1-yl propyl carbonate	C10H18O3		LibSearch	22.482	1.382		1000372-80-5	64.19		
Cyclohexyl formate	C7H12O2		LibSearch	22.482	15.992		4351-54-6	64.18		
4-Hexen-1-ol, acetate	C8H14O2		LibSearch	22.482	5.948		72237-36-6	64.17		
3-Hexen-1-ol, acetate, (E)-	C8H14O2		LibSearch	22.482	5.948		3681-82-1	63.91		
Pyruvic acid, 3-hexenyl ester	C9H14O3		LibSearch	22.482	2.032		1000132-46-3	63.89		
3-Hexen-1-ol, acetate, (Z)-	C8H14O2		LibSearch	22.482	5.948		3681-71-8	63.71		
Formic acid, cyclohexyl ester	C7H12O2		LibSearch	22.482	5.065		4351-54-6	63.68		
Cyclohexanol formate	C7H12O2		LibSearch	22.482			4351-54-6	63.64		
(E)-Hex-3-en-1-yl propyl carbonate	C10H18O3		LibSearch	22.482	1.382		1000372-83-0	63.53		
Cyclohexanol acetate <cis-2-tert-butyl->	C12H22O2		LibSearch	22.482			20298-69-5	63.26		
cis-3-Hexenyl isovalerate	C11H20O2		LibSearch	22.482	2.048		35154-45-1	63.21		
cis-3-Hexenyl-.alpha.-methylbutyrate	C11H20O2		LibSearch	22.482	2.048		53398-85-9	63.01		
Hexenyl 2-methyl butanoate<3Z->	C11H20O2		LibSearch	22.482	5.412		53398-85-9	62.79		
Verdox	C12H22O2		LibSearch	22.482			88-41-5	62.75		
Cyclohexanol acetate<cis-2-tert-butyl->	C12H22O2		LibSearch	22.482	2.632		20298-69-5	62.73		
Cyclohexanol acetate<trans-2-tert-butyl->	C12H22O2		LibSearch	22.482	1.742		20298-70-8	62.73		
Cyclopentanol, 2-methyl-, acetate, trans-	C8H14O2		LibSearch	22.482	6.015		40991-94-4	62.51		

Compound Chromatograms (overlaid)

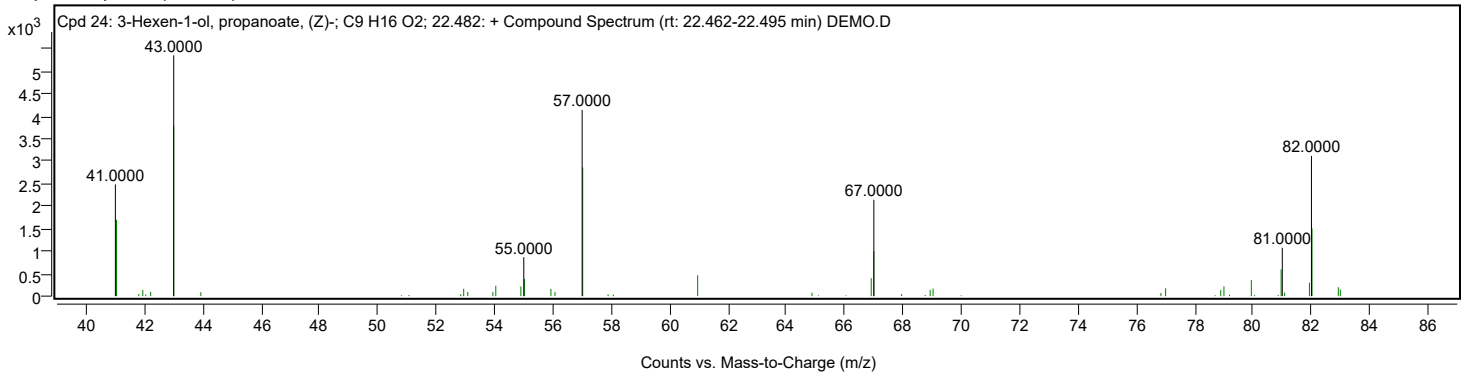


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



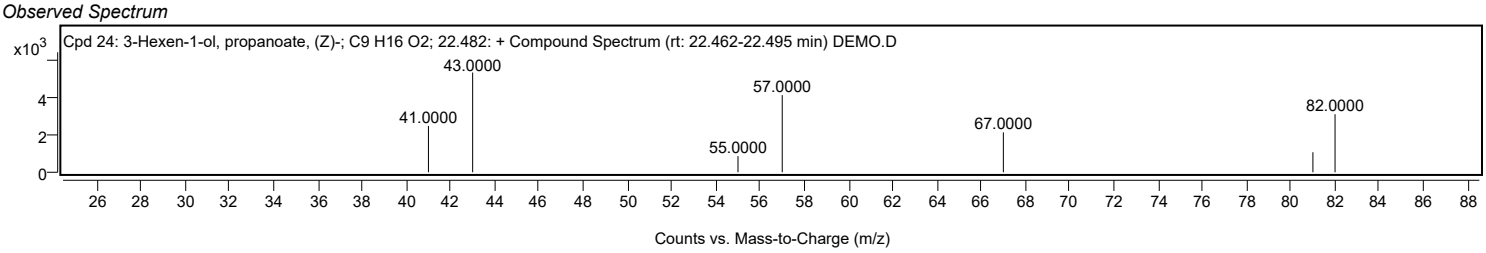
3-Hexen-1-ol, propanoate, (Z)-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			72.60			NIST.L

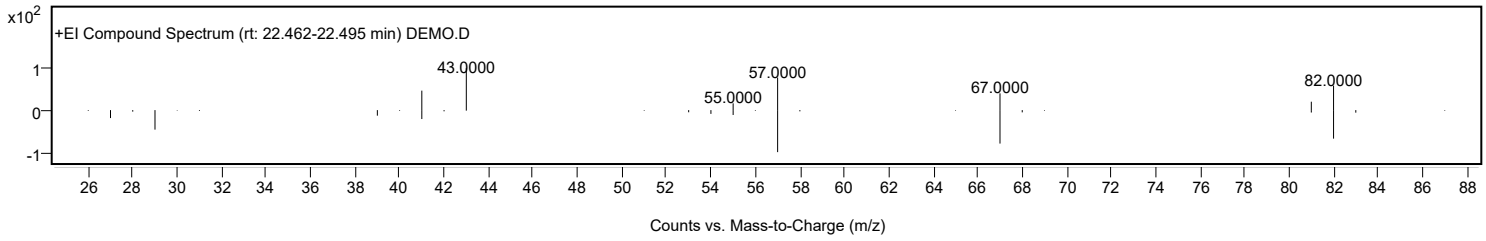
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			72.60			NIST.L

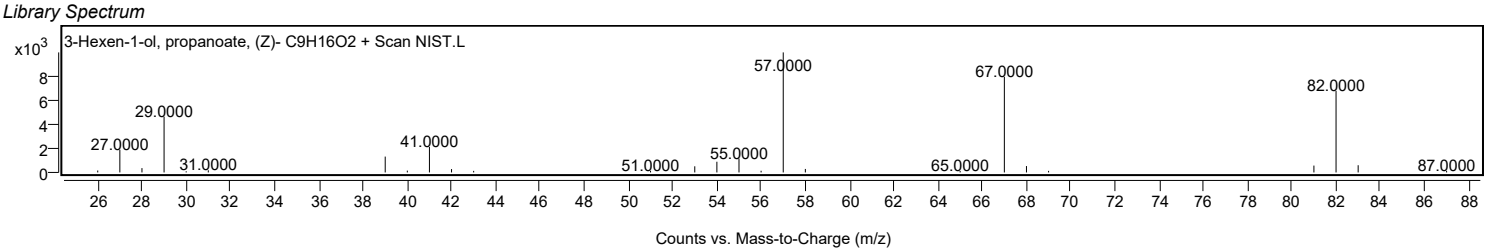
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 25: Benzenepropanol, .alpha.,.alpha.-dimethyl-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Benzenepropanol, .alpha.,.alpha.-dimethyl-	C11 H16 O	22.605			103-05-9	LibSearch	78.22	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		78.22			50		

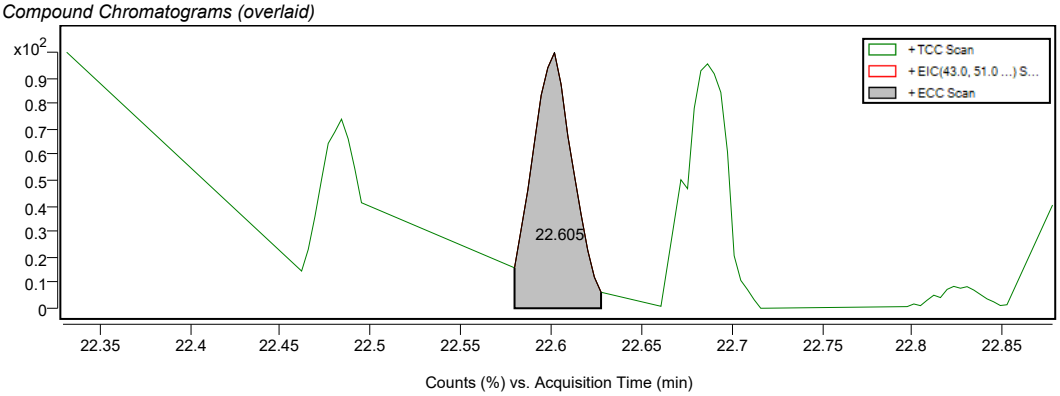
Compound Discovery Report

Agilent | Trusted Answers

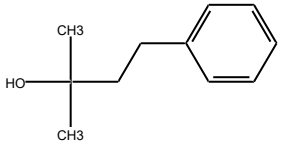
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Benzenepropanol, .alpha.,.alpha.-dimethyl-	C11H16O		LibSearch	22.605	1.222		103-05-9	78.22		
Phenylethyl dimethyl carbinol	C11H16O		LibSearch	22.605			103-05-9	73.17		
Benzenepropanol, .alpha.,.alpha.-dimethyl-	C11H16O		LibSearch	22.605	1.222		103-05-9	72.93		
Benzenepropanol, .alpha.,.alpha.-dimethyl-	C11H16O		LibSearch	22.605	1.222		103-05-9	69.86		
1,1-Dimethyl-3-phenylpropyl acetate	C13H18O2		LibSearch	22.605	-1.945		1010430-88-5	66.58		
Dimethylphenethylcarbinol acetate	C13H18O2		LibSearch	22.605			103-07-1	63.67		
1-Benzyl-2-methylpropyl acetate	C13H18O2		LibSearch	22.605	-1.212		1000429-24-0	63.35		
.alpha.,.alpha.-DIMETHYL-.gamma.-PHENYLETHYL ISOBUTYRATE	C15H22O2		LibSearch	22.605	-4.195		1000429-52-2	62.21		
1,1-Dimethyl-3-phenylpropyl butyrate	C15H22O2		LibSearch	22.605	-5.262		1000430-90-1	59.73		
Benzene, (3-chloro-3-methylbutyl)-	C11H15Cl		LibSearch	22.605	1.538		4830-95-9	55.99		
Benzenepropanenitrile	C9H9N		LibSearch	22.605	1.972		645-59-0	54.27		
Muguesia, anti-	C11H16O		LibSearch	22.605			56836-93-2	53.59		
Benzene, (3-methyl-3-butenyl)-	C11H14		LibSearch	22.605	3.305		6683-51-8	53.06		
Benzenepropanol, .alpha.,.alpha.-dimethyl-	C11H16O		LibSearch	22.605	1.222		103-05-9	52.74		
Benzenepropanenitrile	C9H9N		LibSearch	22.605	1.972		645-59-0	52.46		
Benzene, (3-methyl-3-butenyl)-	C11H14		LibSearch	22.605	3.305		6683-51-8	52.41		
Benzenepropanenitrile	C9H9N		LibSearch	22.605	1.972		645-59-0	51.60		
Muguesia, syn-	C11H16O		LibSearch	22.605			56836-93-2	51.03		
2-Azetidinecarbothioic acid, 1-(phenylmethyl)-, S-phenyl ester, (S)-	C17H17NOS		LibSearch	22.605	-17.178		127382-21-2	50.90		
1H-Benzimidazole, 1-ethyl-	C9H10N2		LibSearch	22.605	1.288		7035-68-9	50.47		
Benzenepropanenitrile	C9H9N		LibSearch	22.605	1.972		645-59-0	50.19		
1-Methylene-2-benzyloxy-cyclopropane	C11H12O		LibSearch	22.605	2.005		119819-29-3	49.37		
Benzene, (2-methyl-3-butenyl)-	C11H14		LibSearch	22.605	3.988		1647-06-9	49.22		
Benzene, (3-methyl-2-butenyl)-	C11H14		LibSearch	22.605	3.005		4489-84-3	47.50		
Benzene, (3-methyl-2-butenyl)-	C11H14		LibSearch	22.605	3.005		4489-84-3	47.03		
Benzene, 3-pentenyl-	C11H14		LibSearch	22.605	2.622		1745-16-0	46.92		
Benzene, (2-methyl-1-butenyl)-	C11H14		LibSearch	22.605	3.005		56253-64-6	45.80		
1-Methoxy-4-(2'-nitro-2'propenyl)benzene	C10H11NO3		LibSearch	22.605	-2.895		80255-23-8	45.49		
2-Amino-3-phenylpropionitrile	C9H10N2		LibSearch	22.605	-1.012		1000193-97-1	45.45		
Benzene, 3-pentenyl-, (E)-	C11H14		LibSearch	22.605	2.622		16091-23-9	45.45		
Ethyl-2-benzofuran	C10H10O		LibSearch	22.605	2.488		3131-63-3	45.43		
2,2-Dimethylindene, 2,3-dihydro-	C11H14		LibSearch	22.605	2.922		20836-11-7	45.09		
4-Benzyloxy-N-methylamphetamine	C17H21NO		LibSearch	22.605	-12.195		177079-66-2	44.80		
4-Aminopyrido[3,2-c]pyridazine	C7H6N4		LibSearch	22.605	-2.812		1000326-89-7	44.68		
1H-Indene, 2,3-dihydro-1,1-dimethyl-	C11H14		LibSearch	22.605	2.922		4912-92-9	44.58		
4-Carbamoyl-2-phenyl-2-oxazoline	C10H10N2O2		LibSearch	22.605	-6.428		99071-89-3	44.56		
Benzene, (1,1-dimethyl-2-propenyl)-	C11H14		LibSearch	22.605	4.322		18321-36-3	44.45		
Benzene, (2-methyl-1-methylenepropyl)-	C11H14		LibSearch	22.605	4.372		17498-71-4	44.41		
1H-Indene, 2,3-dihydro-1,1-dimethyl-	C11H14		LibSearch	22.605	2.922		4912-92-9	44.35		
Hydroxylamine, O-(phenylmethyl)-	C7H9NO		LibSearch	22.605	4.055		622-33-3	44.32		
trans-Rhubafuran	C12H16O		LibSearch	22.605			99343-91-6	43.91		
Benzene, (1,2-dimethyl-1-propenyl)-	C11H14		LibSearch	22.605	3.388		769-57-3	43.87		
4-Benzyloxy.beta.-methyl-.beta.-nitrostyrene	C16H15NO3		LibSearch	22.605	-14.412		7176-38-7	43.82		
2-Methyl-4-phenyl-2-butanol, TMS derivative	C14H24OSi		LibSearch	22.605	-0.578		1000098-08-3	43.82		
4-Ethyl-3-methyl-3-phenylpyrrolidine-2,5-dione (isomer 2)	C13H15NO2		LibSearch	22.605	-7.445		1000504-32-8	43.82		
Propanal benzyl isopropyl acetal	C13H20O2		LibSearch	22.605	-0.962		1010431-62-8	43.77		
Benzene, 1-methyl-2-(1-methyl-2-propenyl)-	C11H14		LibSearch	22.605	3.755		97664-19-2	43.63		
Oxalic acid, monoamide monohydrazide, N-benzyl-N''-(1-oxo-3-phenylprop-2-enyl)-	C18H17N3O3		LibSearch	22.605	-30.262		1000294-01-4	43.61		
N'-Benzyl-N,N-dimethylethylenediamine	C11H18N2		LibSearch	22.605	-1.378		103-55-9	43.59		
Benzene, (3-methyl-2-butenyl)-	C11H14		LibSearch	22.605	3.005		4489-84-3	43.50		

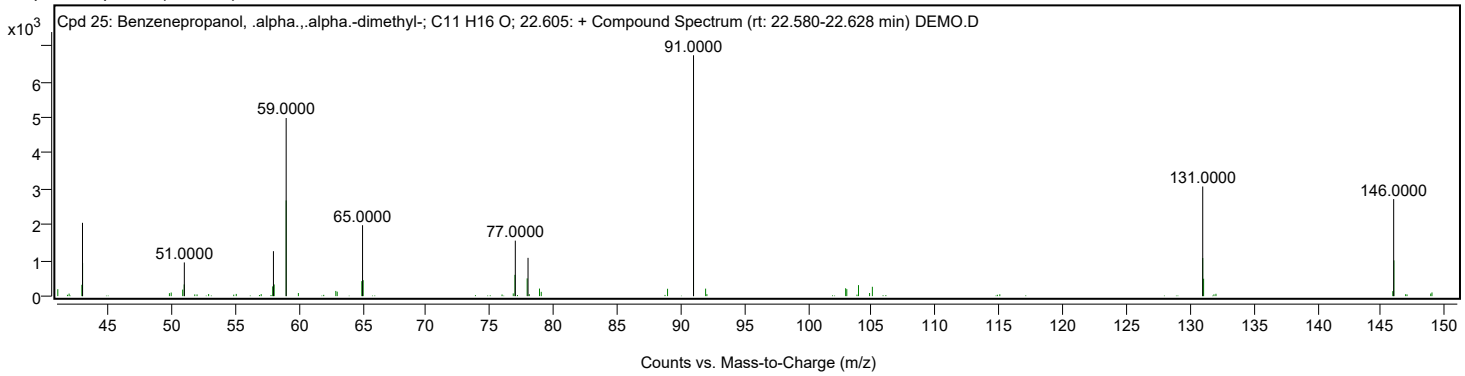
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



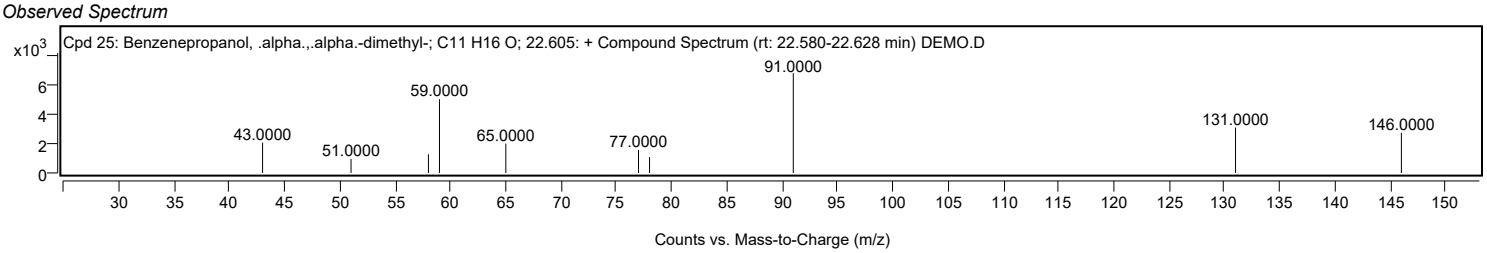
Benzenepropanol, .alpha.,.alpha.-dimethyl-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			78.22			NIST.L

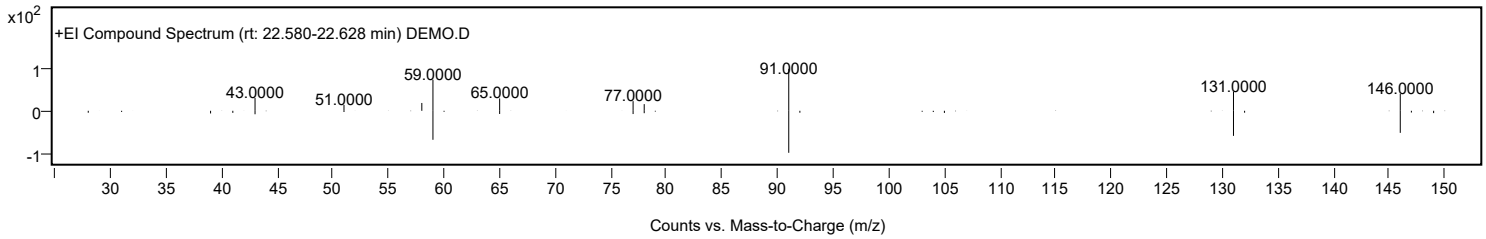
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			78.22			NIST.L

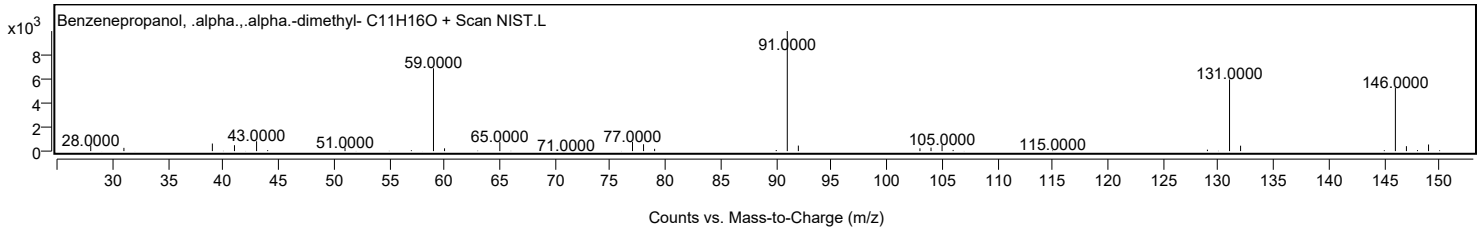
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 26: 5-methyl-2-(Z)-hepten-4-one

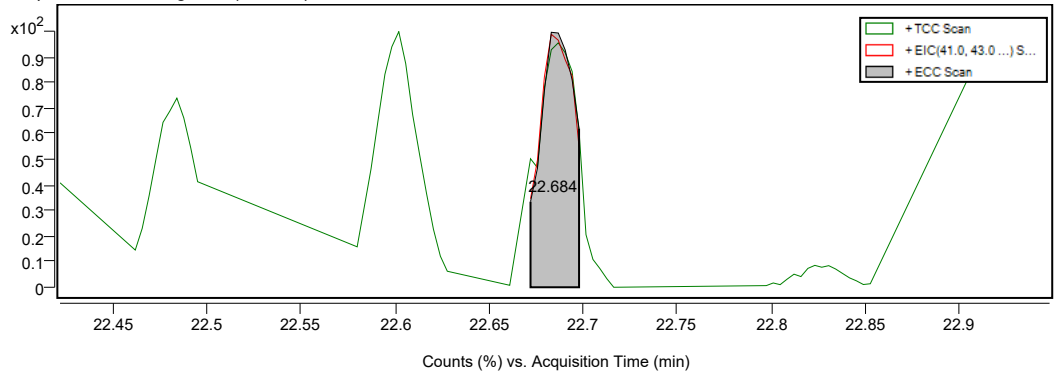
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
5-methyl-2-(Z)-hepten-4-one	C8 H14 O	22.684			24608-84-2	LibSearch	62.94	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		62.94			50		

Compound ID Table

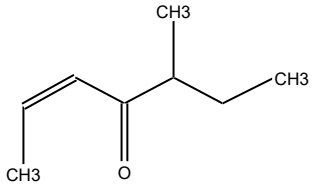
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
5-methyl-2-(Z)-hepten-4-one	C8H14O		LibSearch	22.684	7.750		24608-84-2	62.94		
D-Alanine, N-propargyloxycarbonyl-, dodecyl ester	C19H33NO4		LibSearch	22.684	-16.933		1000347-74-3	57.38		
4H-Pyran-4-one, 5-hydroxy-2-methyl-	C6H6O3		LibSearch	22.684	4.967		644-46-2	56.18		
D-Alanine, N-propargyloxycarbonyl-, tridecyl ester	C20H35NO4		LibSearch	22.684	-18.583		1000347-74-4	56.07		
Furan, 2,3-dihydro-3-(1-methylpropyl)-	C8H14O		LibSearch	22.684	8.250		56805-32-4	55.26		
Levetiracetam	C8H14N2O2		LibSearch	22.684	-3.383		102767-28-2	55.20		
1,3-Cyclopentanedione, 2-ethyl-	C7H10O2		LibSearch	22.684	4.300		823-36-9	55.10		
Etiracetam	C8H14N2O2		LibSearch	22.684	-3.383		33996-58-6	54.93		
(2,2,2-Trifluoroethoxy)ethene	C4H5F3O		LibSearch	22.684	17.367		1000306-54-7	53.66		
1,1,4,4-Tetrafluorobut-2-yne	C4H2F4		LibSearch	22.684	19.350		1010394-38-6	53.21		
Maltol propionate	C9H10O4		LibSearch	22.684	-0.466		68555-63-5	52.86		
Furan, 3-(1,1-dimethylethyl)-2,3-dihydro-	C8H14O		LibSearch	22.684	8.584		34314-82-4	52.78		
4-Hexen-3-one, 2,2-dimethyl-	C8H14O		LibSearch	22.684	8.084		20971-19-1	51.37		
N-t-Butylmethacrylamide	C8H15NO		LibSearch	22.684	4.367		6554-73-0	51.03		
3H-Pyrazol-3-one, 2,4-dihydro-4,4,5-trimethyl-	C6H10N2O		LibSearch	22.684	5.900		3201-20-5	50.58		
Levetiracetam	C8H14N2O2		LibSearch	22.684	-3.383		102767-28-2	50.32		
5-Formyl-3-methyluracil	C6H6N2O3		LibSearch	22.684	-1.716		107097-09-6	49.87		
Pyran-4-one <4H-, 2-methyl-, 3-(1-oxopropoxy)->	C9H10O4		LibSearch	22.684			68555-63-5	49.09		
Maltol propionate	C9H10O4		LibSearch	22.684	-4.306		68555-63-5	48.81		
Carbamic acid, N-methyl-N-(2-ethylhexyl)-, propargyl ester	C13H23NO2		LibSearch	22.684	-1.716		1010437-37-5	48.60		
Soman	C7H16FO2P		LibSearch	22.684			96-64-0	48.21		
Soman	C7H16FO2P		LibSearch	22.684			96-64-0	47.61		
1,3,5-Benzenetriol	C6H6O3		LibSearch	22.684	0.317		108-73-6	47.24		
Glycine, N-(trifluoroacetyl)-, butyl ester	C8H12F3NO3		LibSearch	22.684	2.384		764-16-9	46.70		
Glycine, N-(trifluoroacetyl)-, methyl ester	C5H6F3NO3		LibSearch	22.684	7.350		383-72-2	46.37		
Soman	C7H16FO2P		LibSearch	22.684			96-64-0	46.33		
1,3-Dioxacyclohex-4-en-6-one, 4-azidomethyl-2-t-butyl-	C9H13N3O3		LibSearch	22.684			1000195-54-4	46.31		
1,1-Dicyclopropylethanol	C8H14O		LibSearch	22.684	7.484		1000486-97-1	46.25		
2,4,6-Trihydroxybenzoic acid	C7H6O5		LibSearch	22.684	-7.516		83-30-7	46.25		
(2Z)-(2-Amino-1,3-thiazol-4-yl)[(2-tert-butoxy-1,1-dimethyl-2-oxoethoxy)imino]ethanoic acid	C13H19N3O5S		LibSearch	22.684	-20.383		86299-47-0	45.87		
1-Cyclpropylcarbonylpiperidine, 2,2,6,6-tetramethyl-	C13H23NO		LibSearch	22.684	-2.950		1000195-56-6	45.50		
Glycine, N-(trifluoroacetyl)-, butyl ester	C8H12F3NO3		LibSearch	22.684	2.384		764-16-9	45.15		
1,3,5-Benzenetriol	C6H6O3		LibSearch	22.684	0.317		108-73-6	44.37		
2-Methyl-2-octene	C9H18		LibSearch	22.684	7.667		16993-86-5	44.37		
Veloutone	C13H24O		LibSearch	22.684			65443-14-3	44.10		
5-Cyclopropyl-1,3,4-oxadiazol-2-ol	C5H6N2O2		LibSearch	22.684	5.200		1000445-07-9	44.08		
3H-Pyrazol-3-one, 2,4-dihydro-4,4,5-trimethyl-	C6H10N2O		LibSearch	22.684	5.900		3201-20-5	43.75		
Butanoic acid, 2-amino-4,4,4-trifluoro-3-oxo-, methyl ester	C5H6F3NO3		LibSearch	22.684	8.767		61141-67-1	43.71		
5(4H)-Oxazolone, 2-(1,1-dimethylethyl)-	C7H11NO2		LibSearch	22.684	3.550		81375-96-4	43.60		
Acetamide, N-butyl-2,2,2-trifluoro-	C6H10F3NO		LibSearch	22.684	8.484		400-59-9	43.33		
4-Cyclopentylmorpholine	C9H17NO		LibSearch	22.684	1.650		39198-78-2	43.31		
Acetamide, N-butyl-2,2,2-trifluoro-	C6H10F3NO		LibSearch	22.684	8.484		400-59-9	43.26		
1,3,5-Benzenetriol	C6H6O3		LibSearch	22.684	0.317		108-73-6	43.00		
Veloutone	C13H24O		LibSearch	22.684	2.054		65443-14-3	42.97		
2H-Pyran-2-one, 4-hydroxy-6-(2-oxopropyl)-	C8H8O4		LibSearch	22.684	-1.700		10310-07-3	42.53		
2-Hexene, 2,5,5-trimethyl-	C9H18		LibSearch	22.684	9.084		40467-04-7	41.79		
3,3-Dimethylbutyl methylphosphonofluoridate	C7H16FO2P		LibSearch	22.684			660-21-9	41.78		
Carbamic acid, N-methyl-N-octyl-, propargyl ester	C13H23NO2		LibSearch	22.684	-2.783		1000437-37-7	41.70		
Cyclopentyl-methyl-amine, N-trimethylacetyl-	C11H21NO		LibSearch	22.684	1.450		1342251-88-0	41.61		
Glycine, N-(trifluoroacetyl)-, 1-methylpropyl ester	C8H12F3NO3		LibSearch	22.684	3.450		39825-51-9	41.57		

Compound Chromatograms (overlaid)

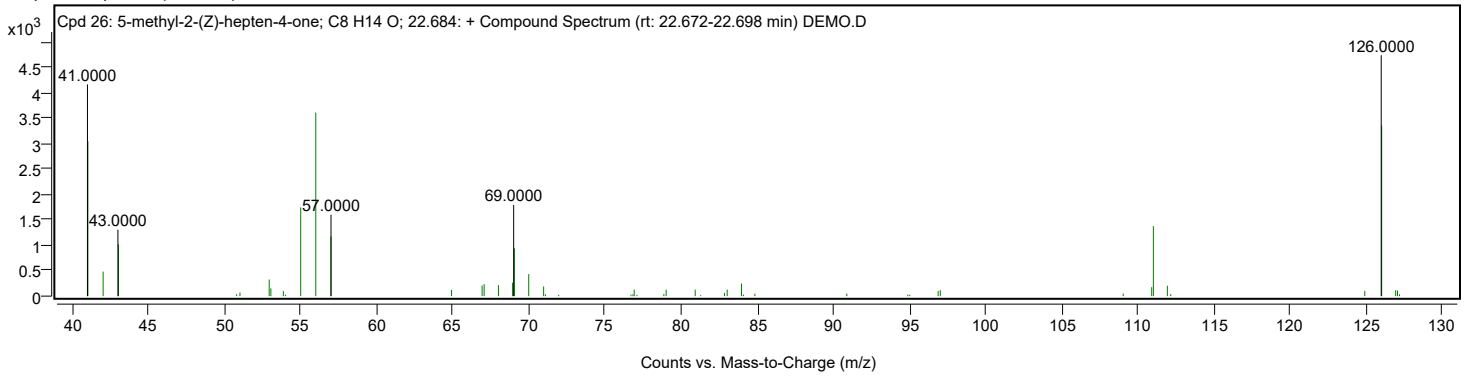


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



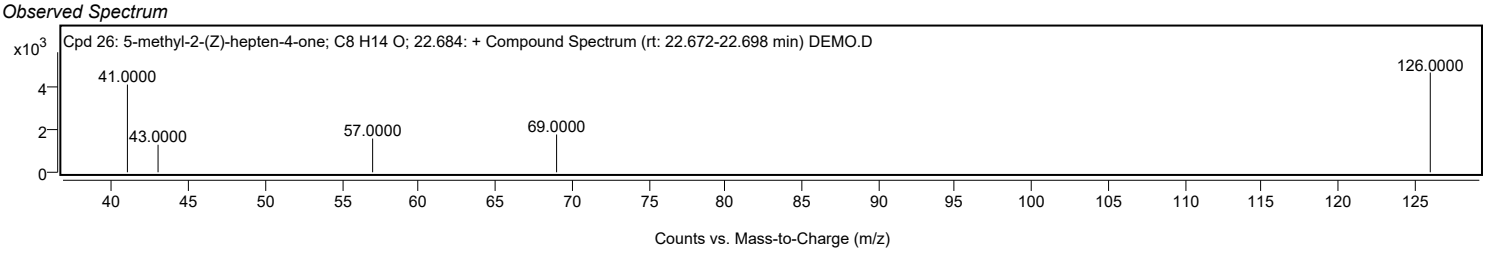
5-methyl-2-(Z)-hepten-4-one

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			62.94			NIST.L

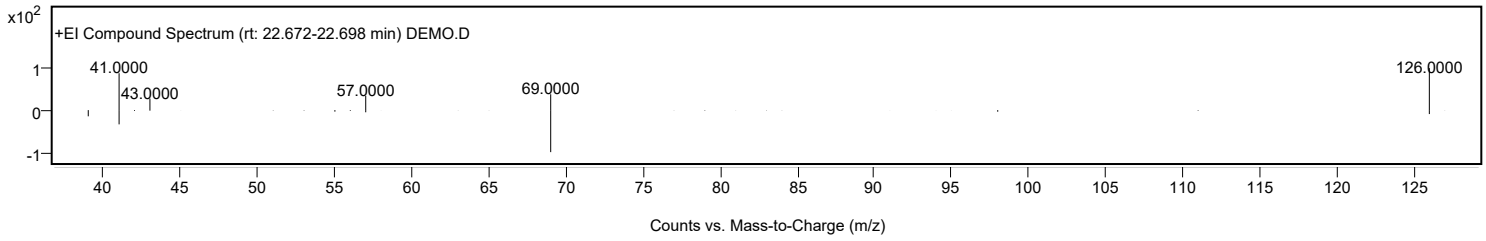
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			62.94			NIST.L

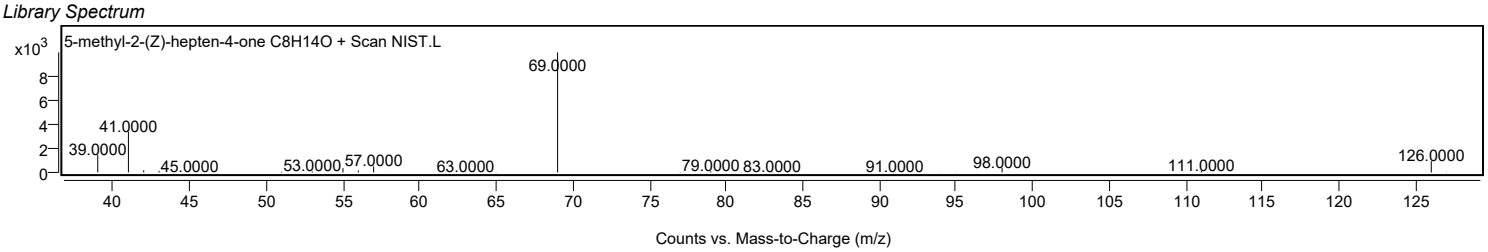
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 27: Cyclopentane, (1,1-dimethylethyl)-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Cyclopentane, (1,1-dimethylethyl)-	C9 H18	22.687			3875-52-3	LibSearch	61.77	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		61.77			50		

Compound Discovery Report

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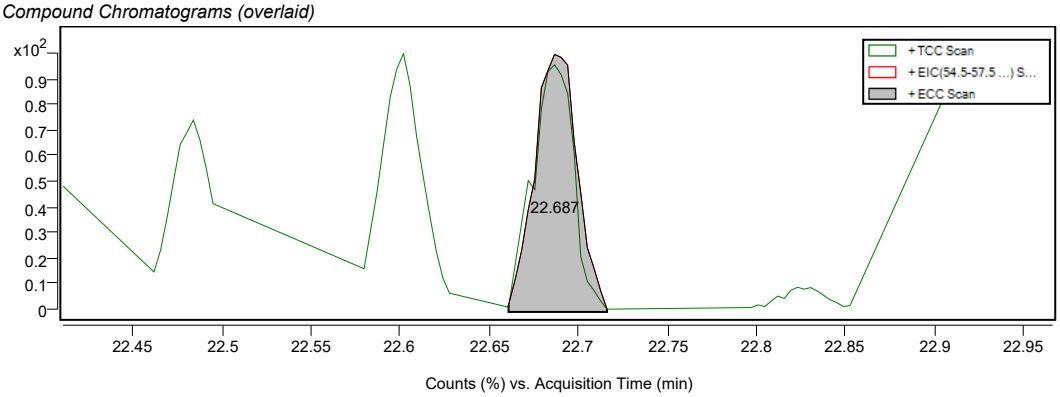
Compound ID Table

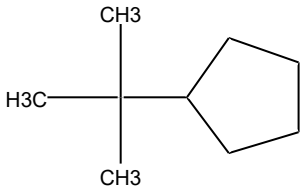
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Cyclopentane, (1,1-dimethylethyl)-	C9H18		LibSearch	22.687	8.120		3875-52-3	61.77		
2-Pyrrolidinone, 1-ethenyl-	C6H9NO		LibSearch	22.687	5.854		88-12-0	61.16		
1,3-Dimethyl-5-isobutylcyclohexane	C12H24		LibSearch	22.687	3.737		13131-76-5	60.43		
Cyclohexane, 1-ethyl-2,4-dimethyl-	C10H20		LibSearch	22.687	5.987		61142-69-6	59.57		
Cyclooctane, (1-methylpropyl)-	C12H24		LibSearch	22.687	1.787		16538-89-9	59.32		
2-Pyrrolidinone, 1-ethenyl-	C6H9NO		LibSearch	22.687	5.854		88-12-0	58.31		
Cyclooctane, butyl-	C12H24		LibSearch	22.687	0.704		16538-93-5	58.30		
2-Propenal	C3H4O		LibSearch	22.687	14.387		107-02-8	58.00		
Cyclohexane, 1,1,3-trimethyl-	C9H18		LibSearch	22.687	7.437		3073-66-3	57.31		
Cyclohexane, 1,1,3-trimethyl-	C9H18		LibSearch	22.687	7.437		3073-66-3	57.25		
2-Propenal	C3H4O		LibSearch	22.687	14.387		107-02-8	57.10		
Cyclohexane, 1-ethyl-1,3-dimethyl-, cis-	C10H20		LibSearch	22.687	5.770		62238-31-7	57.08		
Cyclohexane, 1,1,3-trimethyl-	C9H18		LibSearch	22.687	7.437		3073-66-3	56.88		
1H-1,2,4-Triazole-3-carboxaldehyde, 5-methyl-	C4H5N3O		LibSearch	22.687	2.487		56804-98-9	56.85		
Cyclohexane, 2-ethyl-1,3-dimethyl-	C10H20		LibSearch	22.687	5.987		7045-67-2	56.79		
1,1,4-Trimethylcyclohexane	C9H18		LibSearch	22.687	7.437		7094-27-1	56.06		
Cyclohexane, 1,3,5-trimethyl-	C9H18		LibSearch	22.687	7.637		1839-63-0	55.43		
Methane, isocyanato-	C2H3NO		LibSearch	22.687			624-83-9	55.17		
2-Pyrrolidinone, 1-ethenyl-	C6H9NO		LibSearch	22.687	5.854		88-12-0	55.14		
Cyclooctane, ethyl-	C10H20		LibSearch	22.687	4.020		13152-02-8	55.00		
2-Pyrrolidinone, 1-ethenyl-	C6H9NO		LibSearch	22.687	5.854		88-12-0	54.84		
Cyclohexane, 1,1,3-trimethyl-	C9H18		LibSearch	22.687	7.437		3073-66-3	54.68		
5-Undecene, 7-methyl-, (E)-	C12H24		LibSearch	22.687	3.387		74630-66-3	54.57		
Cyclohexane, 1-ethyl-1,4-dimethyl-, trans-	C10H20		LibSearch	22.687	5.770		62238-32-8	54.24		
2-Propenal	C3H4O		LibSearch	22.687	14.387		107-02-8	54.12		
Methane, isocyanato-	C2H3NO		LibSearch	22.687			624-83-9	54.10		
2-Propenal	C3H4O		LibSearch	22.687	14.387		107-02-8	54.05		
Cyclohexane, 1-ethyl-1,3-dimethyl-, trans-	C10H20		LibSearch	22.687	5.770		62238-29-3	53.85		
2-(Butyliden-2-one)tetrahydrofuran	C8H12O2		LibSearch	22.687	4.237		343270-50-8	53.58		
Cyclooctane, (1-methylpropyl)-	C12H24		LibSearch	22.687	1.787		16538-89-9	53.44		
Cyclohexane, 1,3,5-trimethyl-	C9H18		LibSearch	22.687	7.637		1839-63-0	53.28		
Cyclooctane, ethyl-	C10H20		LibSearch	22.687	4.020		13152-02-8	53.23		
Cyclohexane, 1-ethyl-1,4-dimethyl-, cis-	C10H20		LibSearch	22.687	5.770		62238-30-6	53.11		
Cyclohexane, 1,4-dimethyl-2-(2-methylpropyl)-, (1.alpha.,2.beta.,4.alpha.)-	C12H24		LibSearch	22.687	3.737		54411-17-5	52.97		
1,1,4-Trimethylcyclohexane	C9H18		LibSearch	22.687	7.437		7094-27-1	52.94		
Cyclohexane, 1,3,5-trimethyl-	C9H18		LibSearch	22.687	7.637		1839-63-0	52.79		
Undecane, 5-methylene-	C12H24		LibSearch	22.687	3.004		5698-48-6	52.76		
Cyclohexane, 1,3,5-trimethyl-, (1.alpha.,3.alpha.,5.alpha.)-	C9H18		LibSearch	22.687	7.637		1795-27-3	52.46		
5-Undecene, 7-methyl-, (Z)-	C12H24		LibSearch	22.687	3.387		74630-62-9	52.37		
4-Octene, 2,3,7-trimethyl-, [S-(E)]-	C11H22		LibSearch	22.687	7.187		52763-13-0	52.25		
Trans-1,4-diethylcyclohexane	C10H20		LibSearch	22.687	5.354		13990-93-7	52.08		
Cyclohexane, 1-ethyl-2,3-dimethyl-	C10H20		LibSearch	22.687	5.987		7058-05-1	51.98		
2-Pyrrolidinone, 1-(1-oxo-2-propenyl)-	C7H9NO2		LibSearch	22.687	1.937		2043-26-7	51.60		
Cyclohexane, 1,2-diethyl-, cis-	C10H20		LibSearch	22.687	5.354		824-43-1	51.57		
Cyclohexane, 1,3,5-trimethyl-, (1.alpha.,3.alpha.,5.alpha.)-	C9H18		LibSearch	22.687	7.637		1795-27-3	51.42		
Decane, 4-methylene-	C11H22		LibSearch	22.687	4.654		24949-41-5	50.77		
Cyclohexane, 1,1,2-trimethyl-	C9H18		LibSearch	22.687	7.437		7094-26-0	50.72		
Decane, 5-methyl-6-methylene-	C12H24		LibSearch	22.687	4.070		75029-95-7	50.72		
1-Decene, 2-methyl-	C11H22		LibSearch	22.687	4.654		13151-27-4	50.68		
Cyclohexane, 1,3,5-trimethyl-, (1.alpha.,3.alpha.,5.beta.)-	C9H18		LibSearch	22.687	7.637		1795-26-2	50.60		

Compound Chromatograms (overlaid)

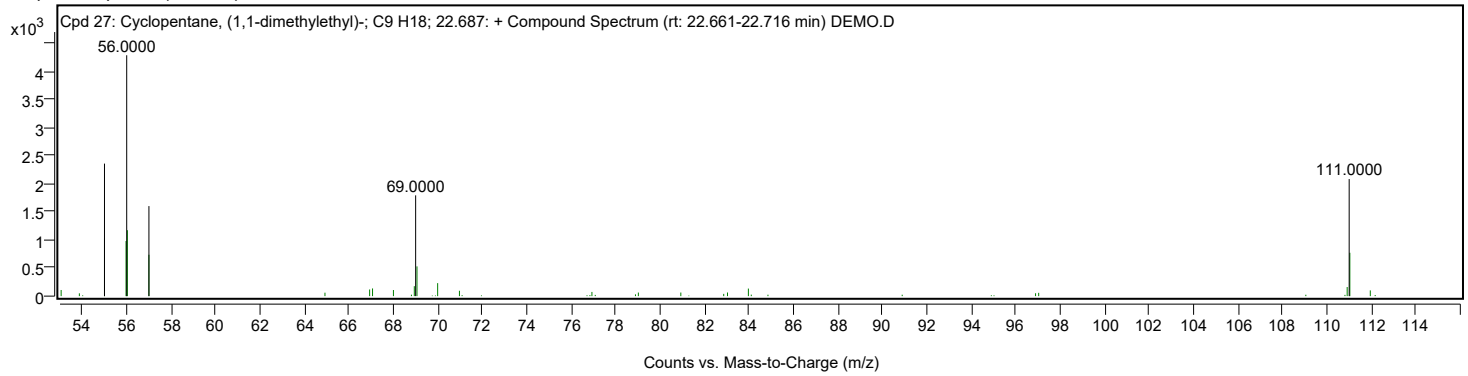


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



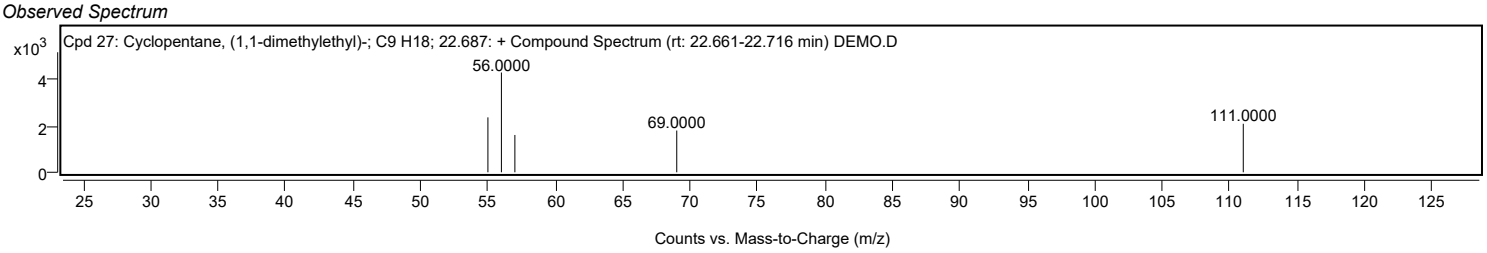
Cyclopentane, (1,1-dimethylethyl)-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			61.77			NIST.L

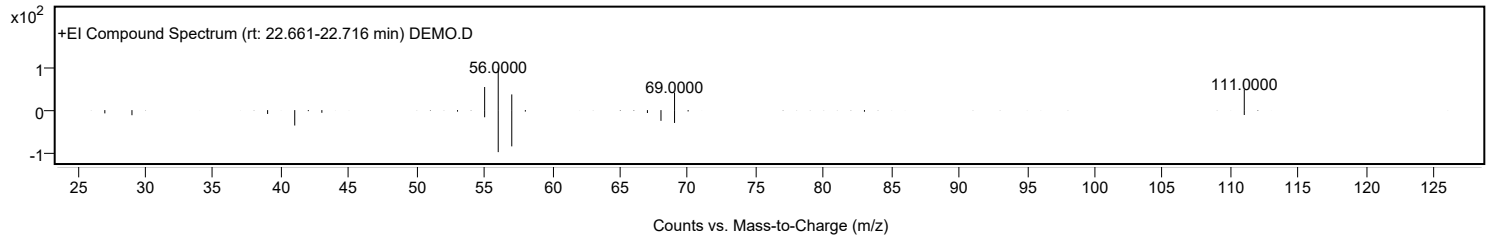
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			61.77			NIST.L

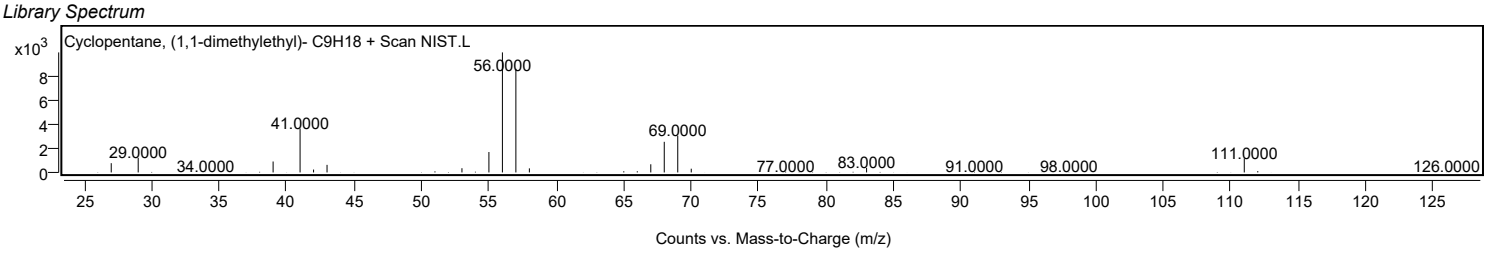
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 28: 2,3-Pentanedione

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
2,3-Pentanedione	C5 H8 O2	22.823			600-14-6	LibSearch	66.28	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		66.28			50		

Compound Discovery Report

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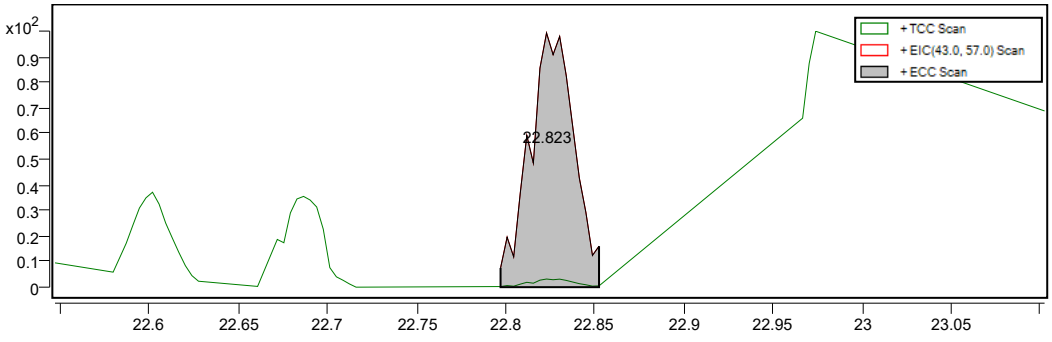
Compound ID Table

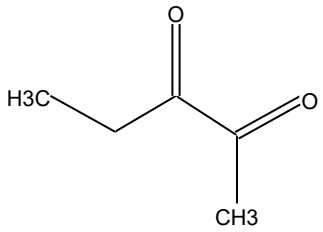
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
2,3-Pentanedione	C5H8O2		LibSearch	22.823	9.657		600-14-6	66.28		
anti-2-Acetoxyacetaldoxime	C4H7NO3		LibSearch	22.823	7.123		37858-07-4	62.74		
3-Buten-2-ol	C4H8O		LibSearch	22.823	13.307		598-32-3	58.57		
Pentandione<2,3->	C5H8O2		LibSearch	22.823	20.593		600-14-6	56.95		
Propylene carbonate	C4H6O3		LibSearch	22.823			108-32-7	54.08		
2-Butanone, 1-(acetyloxy)-	C6H10O3		LibSearch	22.823	7.473		1575-57-1	53.30		
Di-tert-butyl peroxide	C8H18O2		LibSearch	22.823	9.507		110-05-4	53.12		
Acetylpropionyl	C5H8O2		LibSearch	22.823			600-14-6	52.63		
2-Butanone, 1-(acetyloxy)-	C6H10O3		LibSearch	22.823	7.473		1575-57-1	51.53		
Butane, 1-propoxy-	C7H16O		LibSearch	22.823	9.607		3073-92-5	51.48		
Oxalic acid, butyl propyl ester	C9H16O4		LibSearch	22.823	1.990		1000309-25-6	50.73		
Butanenitrile, 2-hydroxy-3-methyl-	C5H9NO		LibSearch	22.823	8.457		10021-64-4	50.06		
Oxalic acid, isobutyl propyl ester	C9H16O4		LibSearch	22.823	3.057		1000309-25-5	48.84		
3-Buten-2-ol	C4H8O		LibSearch	22.823	13.307		598-32-3	48.20		
3-Buten-2-ol	C4H8O		LibSearch	22.823	13.307		598-32-3	47.84		
Propylene Carbonate	C4H6O3		LibSearch	22.823	8.240		108-32-7	47.49		
1-Propionylethyl acetate	C7H12O3		LibSearch	22.823	6.890		2983-05-3	46.48		
3-Buten-2-ol	C4H8O		LibSearch	22.823	13.307		598-32-3	45.89		
Sulfone, butyl isopropyl	C7H16O2S		LibSearch	22.823	3.490		31124-40-0	45.74		
3-Pentanone, 2-methyl-	C6H12O		LibSearch	22.823	11.323		565-69-5	45.70		
3,4-Hexanedione, 2,2,5-trimethyl-	C9H16O2		LibSearch	22.823	5.507		20633-03-8	45.49		
Propanoic acid, 1-methylethyl ester	C6H12O2		LibSearch	22.823	10.807		637-78-5	44.78		
Propanoic acid, 1-methylethyl ester	C6H12O2		LibSearch	22.823	10.807		637-78-5	44.71		
Acetyl valeryl	C7H12O2		LibSearch	22.823	6.340		96-04-8	44.49		
3-Pentanone, 2-methyl-	C6H12O		LibSearch	22.823	11.323		565-69-5	44.30		
Oxalic acid, heptyl propyl ester	C12H22O4		LibSearch	22.823	-2.993		1000309-26-0	43.44		
.alpha.-Amino-.gamma.-butyrolactone	C4H7NO2		LibSearch	22.823	5.657		1192-20-7	43.38		
Sulfurous acid, butyl propyl ester	C7H16O3S		LibSearch	22.823	0.490		1010309-16-9	43.33		
3-Buten-2-ol	C4H8O		LibSearch	22.823	13.307		598-32-3	43.30		
Butane, 1-propoxy-	C7H16O		LibSearch	22.823	9.607		3073-92-5	43.12		
Hexane, 4-ethyl-2,2-dimethyl-	C10H22		LibSearch	22.823	8.373		52896-99-8	43.01		
2-Pentanone, 4,4-dimethyl-	C7H14O		LibSearch	22.823	10.007		590-50-1	42.77		
Isopropyl ethyl ketone	C6H12O		LibSearch	22.823			565-69-5	42.73		
Pentane, 2,4-dimethyl-	C7H16		LibSearch	22.823	13.007		108-08-7	42.59		
3-Pentanone, 2-methyl-	C6H12O		LibSearch	22.823	11.323		565-69-5	42.19		
.alpha.-Amino-.gamma.-butyrolactone	C4H7NO2		LibSearch	22.823	5.657		1192-20-7	41.34		
Pentane, 1,3-epoxy-4-methyl-	C6H12O		LibSearch	22.823	11.757		15045-60-0	41.19		
Butane, 1-propoxy-	C7H16O		LibSearch	22.823	9.607		3073-92-5	40.90		
2-Pentanone, 4,4-dimethyl-	C7H14O		LibSearch	22.823	10.007		590-50-1	40.79		
Pentane, 2,4-dimethyl-	C7H16		LibSearch	22.823	13.007		108-08-7	40.40		
Pentane, 2,2,3,4-tetramethyl-	C9H20		LibSearch	22.823	11.107		1186-53-4	40.35		
tert-Butyl Hydroperoxide	C4H10O2		LibSearch	22.823	11.257		75-91-2	40.23		
Sulfurous acid, 2-propyl heptyl ester	C10H22O3S		LibSearch	22.823	-3.410		1000309-11-8	40.23		
2-Pentanone, 3-methyl-	C6H12O		LibSearch	22.823	11.323		565-61-7	39.60		
Pentane, 2,2-dimethyl-	C7H16		LibSearch	22.823	12.273		590-35-2	39.52		
Sulfurous acid, butyl 2-propyl ester	C7H16O3S		LibSearch	22.823	1.557		1010309-11-4	39.48		
Acetyl isovaleryl	C7H12O2		LibSearch	22.823			13706-86-0	39.38		
3-Hexanone	C6H12O		LibSearch	22.823	10.257		589-38-8	39.22		
(S)-(-)-1,2,4-Butanetriol, 4-acetate	C6H12O4		LibSearch	22.823	2.990		1000374-86-5	39.17		
3-Hexanone	C6H12O		LibSearch	22.823	10.257		589-38-8	39.16		

Compound Chromatograms (overlaid)

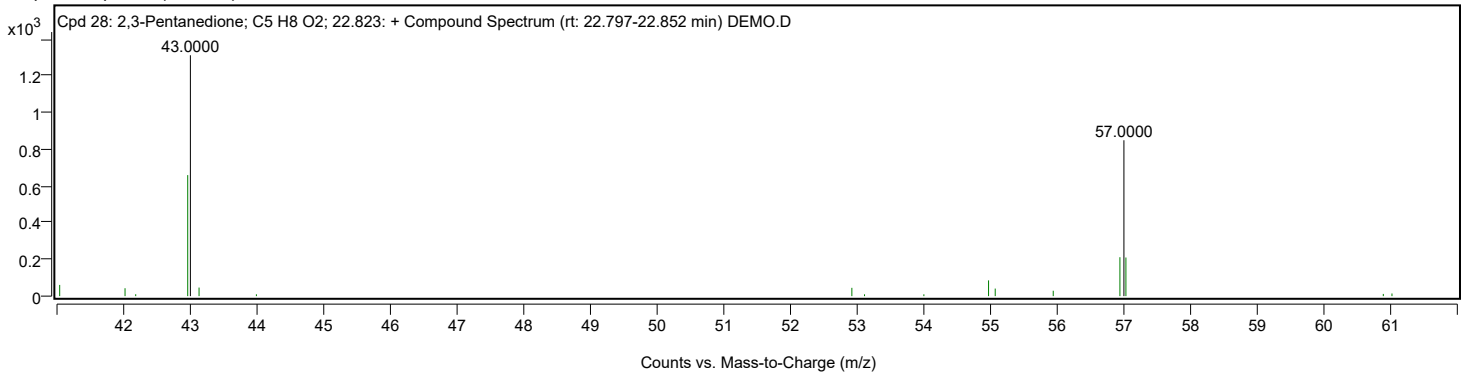


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



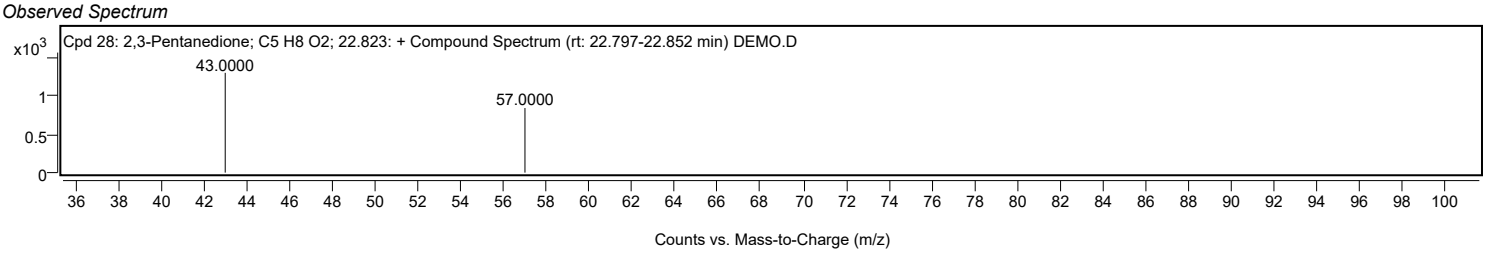
2,3-Pentanedione

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			66.28			NIST.L

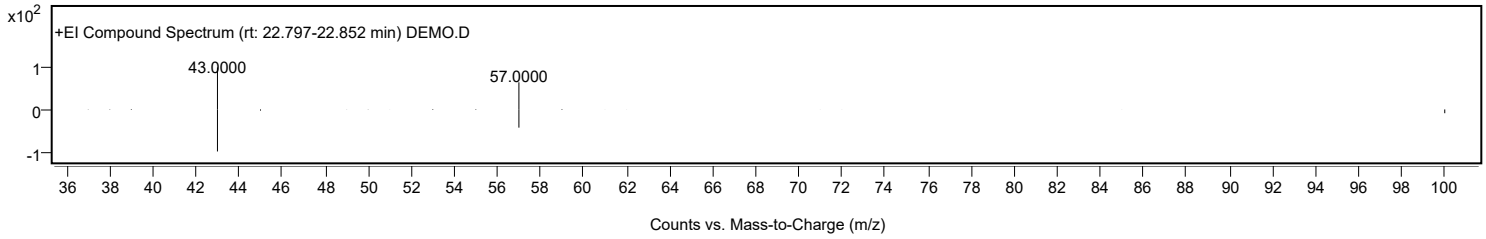
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			66.28			NIST.L

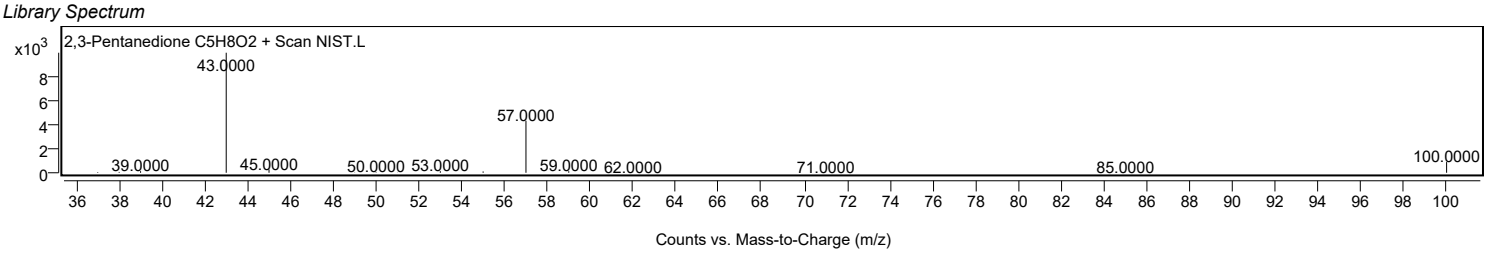
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 29: 6-Octen-1-ol, 3,7-dimethyl-, acetate

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
6-Octen-1-ol, 3,7-dimethyl-, acetate	C12 H22 O2	22.974			150-84-5	LibSearch	81.73	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		81.73			50		

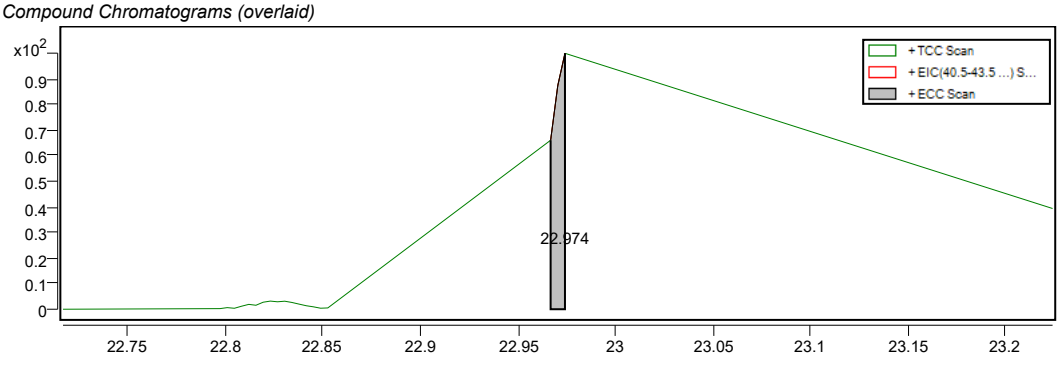
Compound Discovery Report

Agilent | Trusted Answers

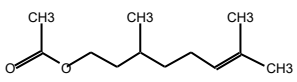
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
6-Octen-1-ol, 3,7-dimethyl-, acetate	C12H22O2		LibSearch	22.974	1.274		150-84-5	81.73		
Citronellyl acetate	C12H22O2		LibSearch	22.974	0.564		150-84-5	80.79		
Citronellyl acetate	C12H22O2		LibSearch	22.974			150-84-5	80.50		
6-Octen-1-ol, 3,7-dimethyl-, acetate	C12H22O2		LibSearch	22.974	1.274		150-84-5	78.44		
Citronellyl isobutyrate	C14H26O2		LibSearch	22.974			97-89-2	77.86		
Citronellol isobutanoate	C14H26O2		LibSearch	22.974	-5.096		97-89-2	77.71		
2,6-Octadiene, 2,6-dimethyl-	C10H18		LibSearch	22.974	6.557		2792-39-4	77.53		
Citronellyl isobutyrate	C14H26O2		LibSearch	22.974	-0.976		97-89-2	77.47		
6-Octen-1-ol, 3,7-dimethyl-, acetate	C12H22O2		LibSearch	22.974	1.274		150-84-5	76.63		
6-Octen-1-ol, 3,7-dimethyl-, acetate	C12H22O2		LibSearch	22.974	1.274		150-84-5	76.40		
Citronellyl butyrate	C14H26O2		LibSearch	22.974			141-16-2	75.71		
Citronellyl butyrate	C14H26O2		LibSearch	22.974	-2.043		141-16-2	75.23		
Citronellyl isobutyrate	C14H26O2		LibSearch	22.974	-0.976		97-89-2	75.21		
Citronellyl formate	C11H20O2		LibSearch	22.974			105-85-1	75.16		
6-Octen-1-ol, 3,7-dimethyl-, acetate	C12H22O2		LibSearch	22.974	1.274		150-84-5	75.04		
Citronellyl butyrate	C14H26O2		LibSearch	22.974	-2.043		141-16-2	75.03		
Citronellyl isobutyrate	C14H26O2		LibSearch	22.974	-0.976		97-89-2	74.96		
2-Butenoic acid, 3,7-dimethyl-6-octenyl ester	C14H24O2		LibSearch	22.974	-2.176		68039-38-3	74.64		
6-Octen-1-ol, 3,7-dimethyl-, formate	C11H20O2		LibSearch	22.974	1.307		105-85-1	74.58		
3,7-Dimethyloct-6-en-1-yl propyl carbonate	C14H26O3		LibSearch	22.974	-3.309		1000372-83-5	74.48		
Citronellyl butanoate	C14H26O2		LibSearch	22.974	-7.076		141-16-2	74.47		
Citronellyl formate	C11H20O2		LibSearch	22.974	4.054		105-85-1	74.03		
Citronellyl butyrate	C14H26O2		LibSearch	22.974	-2.043		141-16-2	73.74		
Citronellyl propionate	C13H24O2		LibSearch	22.974			141-14-0	73.66		
Citronellyl butyrate	C14H26O2		LibSearch	22.974	-2.043		141-16-2	73.50		
Cyclohexane, 1-methyl-4-(1-methylethenyl)-, cis-	C10H18		LibSearch	22.974	6.174		1879-07-8	73.30		
6-Octen-1-ol, 3,7-dimethyl-, formate	C11H20O2		LibSearch	22.974	1.307		105-85-1	73.19		
Hexanoic acid, 3,7-dimethyl-6-octenyl ester	C16H30O2		LibSearch	22.974	-5.359		10580-25-3	72.97		
3,7-Dimethyloct-6-enyl ethyl carbonate	C13H24O3		LibSearch	22.974	-1.659		1000373-78-1	72.83		
3,7-Dimethyloct-6-en-1-yl heptanoate	C17H32O2		LibSearch	22.974	-7.009		72934-17-9	72.54		
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-	C10H18		LibSearch	22.974	7.357		554-59-6	72.50		
6-Octen-1-ol, 3,7-dimethyl-, propanoate	C13H24O2		LibSearch	22.974	-0.393		141-14-0	72.21		
6-Octen-1-ol, 3,7-dimethyl-, propanoate	C13H24O2		LibSearch	22.974	-0.393		141-14-0	71.94		
Dec-(7Z)-enyl acetate	C12H22O2		LibSearch	22.974			13857-03-9	71.70		
Bicyclo[2.2.1]heptane, 1,7,7-trimethyl-	C10H18		LibSearch	22.974	7.141		464-15-3	71.55		
O-Trifluoroacetyl-menthol	C12H19F3O2		LibSearch	22.974	4.007		28587-50-0	71.54		
3,7-Dimethyloct-6-enyl isobutyl carbonate	C15H28O3		LibSearch	22.974	-3.893		1000372-79-6	71.40		
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-	C10H18		LibSearch	22.974	7.357		554-59-6	71.33		
Citronellyl propanoate	C13H24O2		LibSearch	22.974	-3.496		141-14-0	71.07		
Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate, (1.alpha.,2.alpha.,5.beta.)-	C12H22O2		LibSearch	22.974	1.241		2230-87-7	70.78		
Bicyclo[4.1.0]heptane, 3,7,7-trimethyl-	C10H18		LibSearch	22.974	7.357		554-59-6	70.60		
Menthyl acetate	C12H22O2		LibSearch	22.974			16409-45-3	70.23		
Citronellyl valerate	C15H28O2		LibSearch	22.974			7540-53-6	70.18		
Oct-7-enol <3,7-dimethyl->	C10H20O		LibSearch	22.974			141-25-3	70.16		
6-Octen-1-ol, 3,7-dimethyl-, propanoate	C13H24O2		LibSearch	22.974	-0.393		141-14-0	70.09		
6-Octen-1-ol, 3,7-dimethyl-, formate	C11H20O2		LibSearch	22.974	1.307		105-85-1	69.94		
Cyclohexanol, 5-methyl-2-(1-methylethyl)-, acetate, (1.alpha.,2.beta.,5.beta.)-	C12H22O2		LibSearch	22.974	1.241		20777-45-1	69.88		
6-Octen-1-ol, 3,7-dimethyl-, propanoate	C13H24O2		LibSearch	22.974	-0.393		141-14-0	69.87		
R(-)3,7-Dimethyl-1,6-octadiene	C10H18		LibSearch	22.974	7.541		10281-56-8	69.79		
Menthyl acetate	C12H22O2		LibSearch	22.974	1.241		89-48-5	69.52		

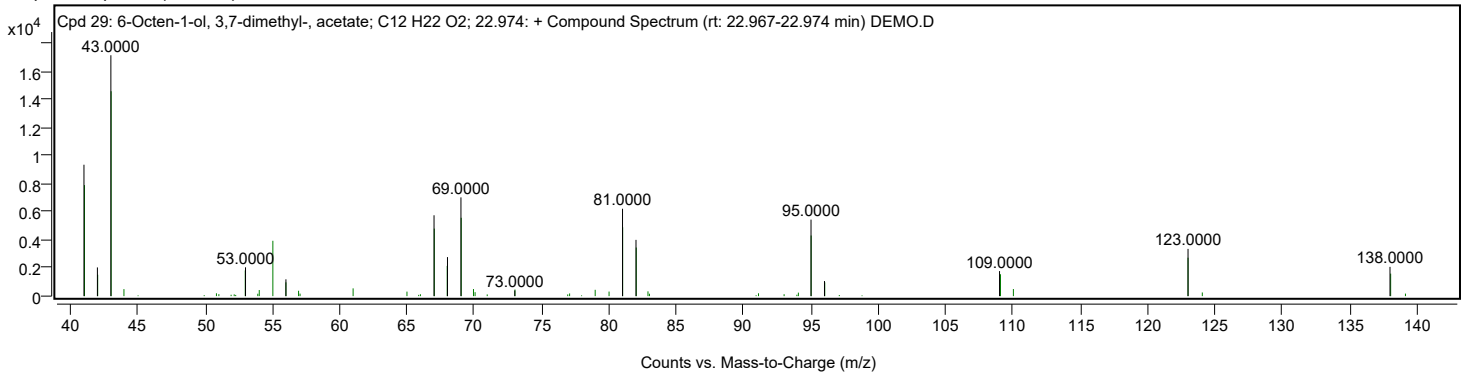
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



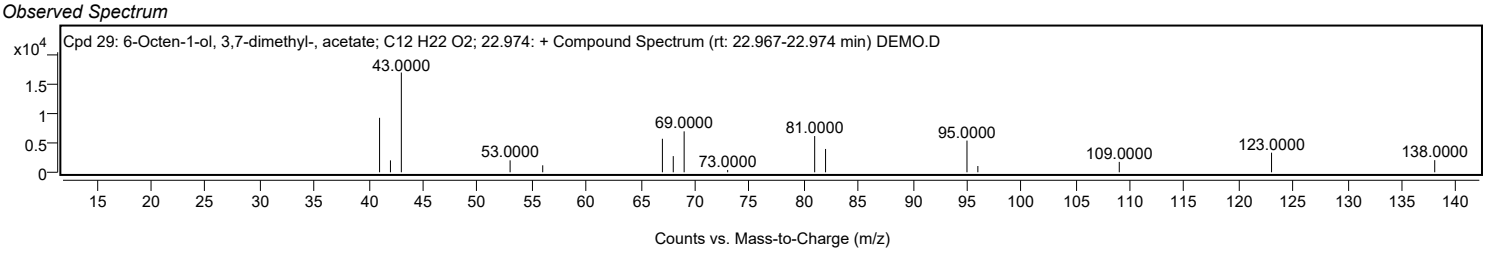
6-Octen-1-ol, 3,7-dimethyl-, acetate

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			81.73			NIST.L

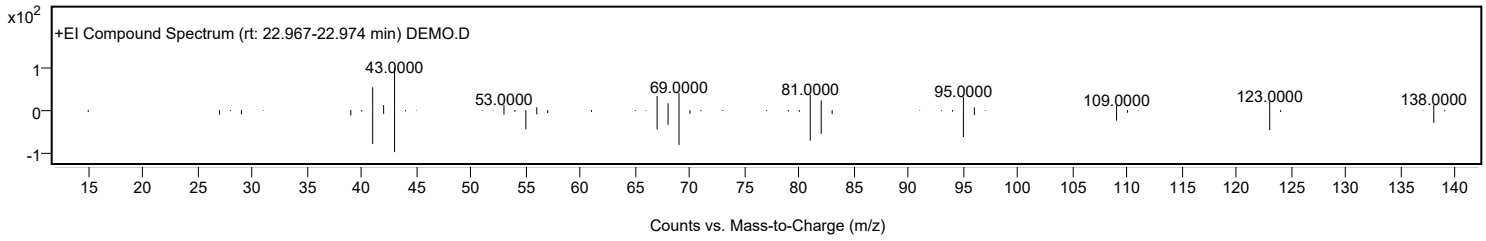
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			81.73			NIST.L

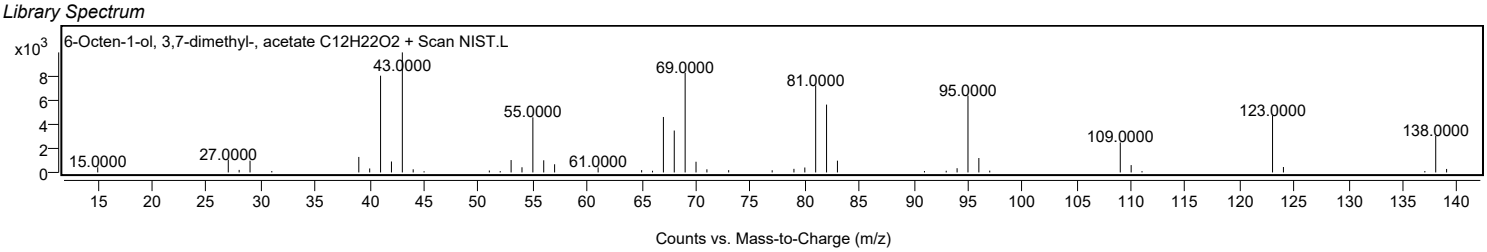
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 30: 2-Propanone, 1,1,1-trifluoro-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
2-Propanone, 1,1,1-trifluoro-	C3 H3 F3 O	23.397			421-50-1	LibSearch	57.33	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		57.33			50		

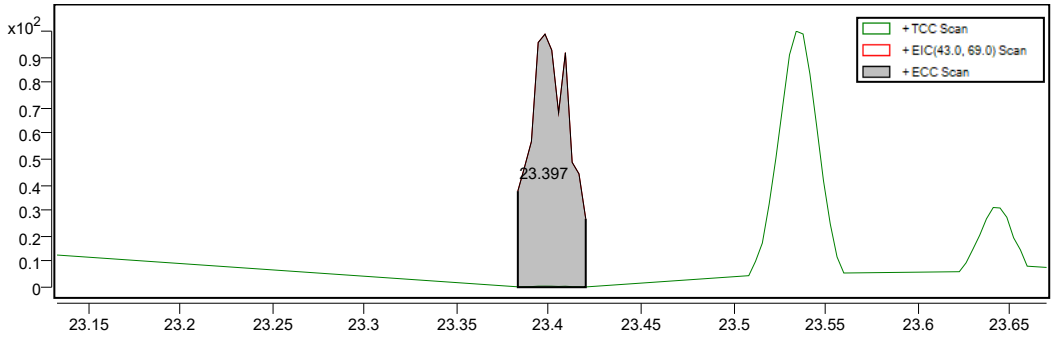
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

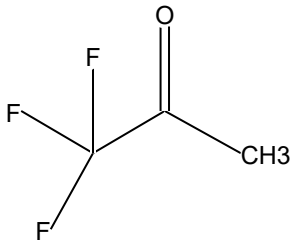
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
2-Propanone, 1,1,1-trifluoro-	C3H3F3O		LibSearch	23.397	18.564		421-50-1	57.33		
Acetyl cyanide	C3H3NO		LibSearch	23.397	11.714		631-57-2	52.62		
1-Oxo-1-[(trifluoromethyl)sulfinyl]ethane	C3H3F3O2S		LibSearch	23.397	10.714		1000461-17-1	52.54		
3-Butyn-2-ol, 2-methyl-	C5H8O		LibSearch	23.397	13.264		115-19-5	48.40		
Ethanone, 1-cyclopropyl-	C5H8O		LibSearch	23.397	12.464		765-43-5	46.59		
Ethanone, 1-cyclopropyl-	C5H8O		LibSearch	23.397	12.464		765-43-5	46.54		
1-Pentyn-3-ol, 3,4-dimethyl-	C7H12O		LibSearch	23.397	11.031		1482-15-1	45.52		
Ethanone, 1-cyclopropyl-	C5H8O		LibSearch	23.397	12.464		765-43-5	44.76		
3-Penten-2-one	C5H8O		LibSearch	23.397	12.364		625-33-2	44.02		
Ethanone, 1-cyclopropyl-	C5H8O		LibSearch	23.397	12.464		765-43-5	41.47		
Ethanone, 1-cyclopropyl-	C5H8O		LibSearch	23.397	12.464		765-43-5	41.26		
(3S)-(-)-3-Acetamidopyrrolidine	C6H12N2O		LibSearch	23.397	1.631		79286-74-1	41.05		
1-Pentyn-3-ol, 3,4-dimethyl-	C7H12O		LibSearch	23.397	11.031		1482-15-1	40.26		
(R)-(+)-2,2,2-Trifluoro-N-(3-pyrrolidinyl)acetamide	C6H9F3N2O		LibSearch	23.397	4.397		84424-06-6	38.92		
Diisopropylcyanamide	C7H14N2		LibSearch	23.397	8.681		3085-76-5	38.76		
Acetic acid, 3-mercapto-3-methylbutyl ester	C7H14O2S		LibSearch	23.397	5.014		1000314-31-4	37.87		
Isopropyl trifluoroacetate	C5H7F3O2		LibSearch	23.397	15.797		400-38-4	37.54		
Butane, 1,1-dichloro-3-methyl-	C5H10Cl2		LibSearch	23.397	10.064		625-66-1	36.48		
Propyl trifluoroacetate	C5H7F3O2		LibSearch	23.397	14.731		383-66-4	35.33		
Isopropyl trifluoroacetate	C5H7F3O2		LibSearch	23.397	15.797		400-38-4	33.20		
Hexyl 2-methyl-3-pentenoate	C12H22O2		LibSearch	23.397	2.287		58625-94-8	32.35		
4,5-Octanediol, 2,7-dimethyl-	C10H22O2		LibSearch	23.397	3.197		1000153-20-8	31.81		
Trifluoroacetic acid, 4-methylpentyl ester	C8H13F3O2		LibSearch	23.397	10.831		327-71-9	31.25		
Pentanoic acid, 2-hydroxy-4-methyl-, methyl ester	C7H14O3		LibSearch	23.397	7.014		40348-72-9	31.09		
4,8-Dimethyl-4-hydroxy-1-nonene	C11H22O		LibSearch	23.397	4.531		1000432-13-0	31.09		
Hexyl 2-methyl-3-pentenoate	C12H22O2		LibSearch	23.397			58625-94-8	30.59		
s-Tetrazine, 3,6-bis(diisopropylamino)-	C14H28N6		LibSearch	23.397	-5.236		19455-91-5	30.49		
Prenyl isobutyrate	C9H16O2		LibSearch	23.397	13.827		76649-23-5	30.36		
Ethanone, 1-cyclopentyl-	C7H12O		LibSearch	23.397	8.464		6004-60-0	30.31		
Prenyl isobutyrate	C9H16O2		LibSearch	23.397			76649-23-5	29.67		
Pentanal, 2,2-dimethyl-, hydrazone	C7H16N2		LibSearch	23.397	5.214		55724-26-0	29.21		
Methyl pentanoate <2-hydroxy-4-methyl->	C7H14O3		LibSearch	23.397			40348-72-9	28.77		
Methyl pentanoate<2-hydroxy-4-methyl->	C7H14O3		LibSearch	23.397	16.087		40348-72-9	28.74		
5-Bromo-n-amyl acetate	C7H13BrO2		LibSearch	23.397	3.714		15848-22-3	28.72		
1-Trifluoroacetoxy-2-methylpentane	C8H13F3O2		LibSearch	23.397	10.831		155089-96-6	28.57		
Pentanoic acid, 2-hydroxy-4-methyl-, methyl ester	C7H14O3		LibSearch	23.397	7.014		40348-72-9	28.45		
Pentanoic acid, 2-hydroxy-4-methyl-, (S)-	C6H12O3		LibSearch	23.397	5.531		13748-90-8	28.44		
.alpha.-Hydroxyisocaproic acid	C6H12O3		LibSearch	23.397	5.531		498-36-2	28.02		
4-Octanone, 5-hydroxy-2,7-dimethyl-	C10H20O2		LibSearch	23.397	3.647		6838-51-3	27.50		
6-Methyl-6-nitroheptan-2-one	C8H15NO3		LibSearch	23.397	2.564		142963-25-5	27.48		
Ethanone, 1-cyclopentyl-	C7H12O		LibSearch	23.397	8.464		6004-60-0	27.21		
Pentane, 2,2-dichloro-	C5H10Cl2		LibSearch	23.397	10.931		34887-14-4	27.16		
Pentanoic acid, 2-hydroxy-4-methyl-, methyl ester	C7H14O3		LibSearch	23.397	7.014		40348-72-9	26.92		
2-Pentanol, trifluoroacetate	C7H11F3O2		LibSearch	23.397	12.497		90991-71-2	26.88		
1-Trifluoroacetoxy-2-methylpentane	C8H13F3O2		LibSearch	23.397	10.831		155089-96-6	26.84		
2-Pentanone, 3-[(acetyloxy)methyl]-3,4-dimethyl-, (.+-.)-	C10H18O3		LibSearch	23.397	3.897		78641-04-0	26.81		
4-Pentenoic acid, 2-methyl-, hexyl ester	C12H22O2		LibSearch	23.397	1.614		1010406-10-9	26.21		
Propanoic acid, 2-methyl-, 3-methyl-2-butenyl ester	C9H16O2		LibSearch	23.397	6.664		76649-23-5	26.13		
6-Methyl-2,3-dihydropyran-2,4-dione	C6H6O3		LibSearch	23.397	3.597		541-98-0	25.59		
3-Methylpentyl acetate	C8H16O2		LibSearch	23.397	8.064		35897-13-3	25.58		

Compound Chromatograms (overlaid)

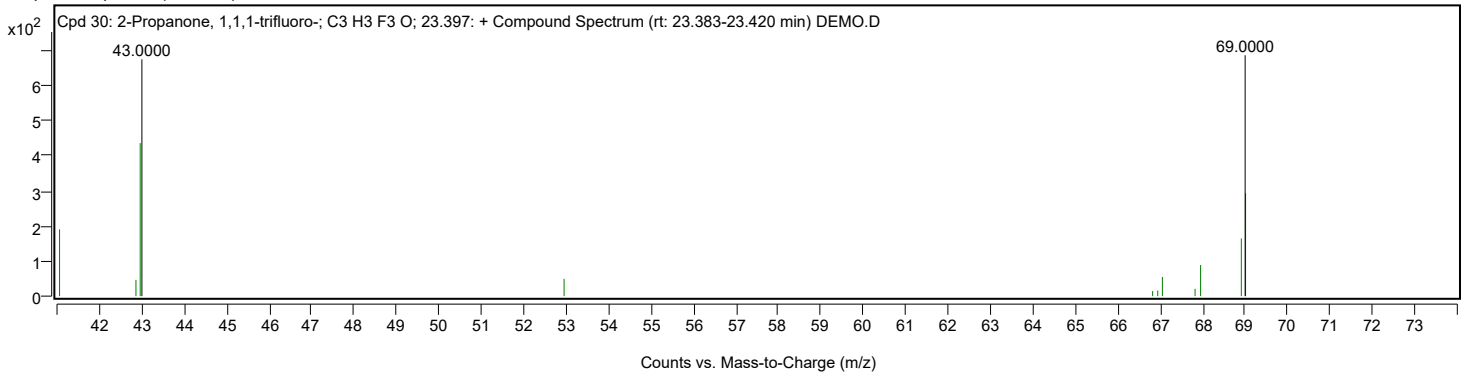


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



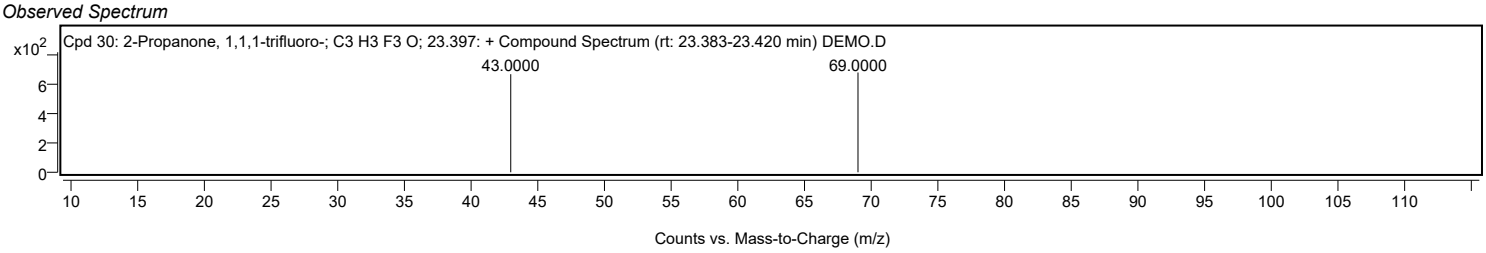
2-Propanone, 1,1,1-trifluoro-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			57.33			NIST.L

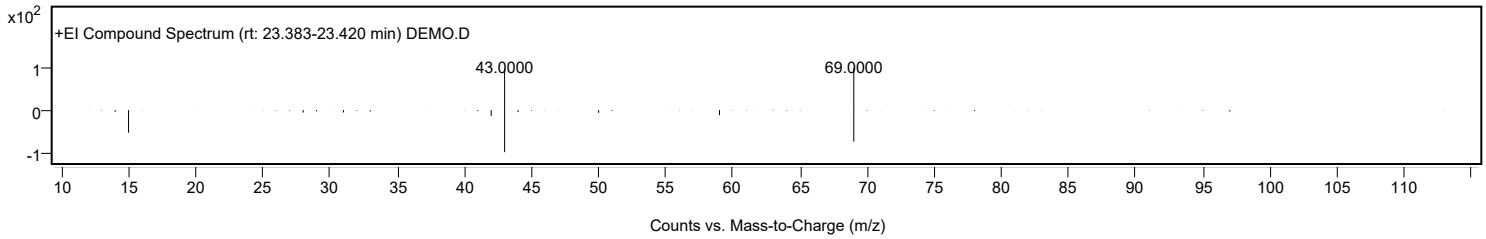
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			57.33			NIST.L

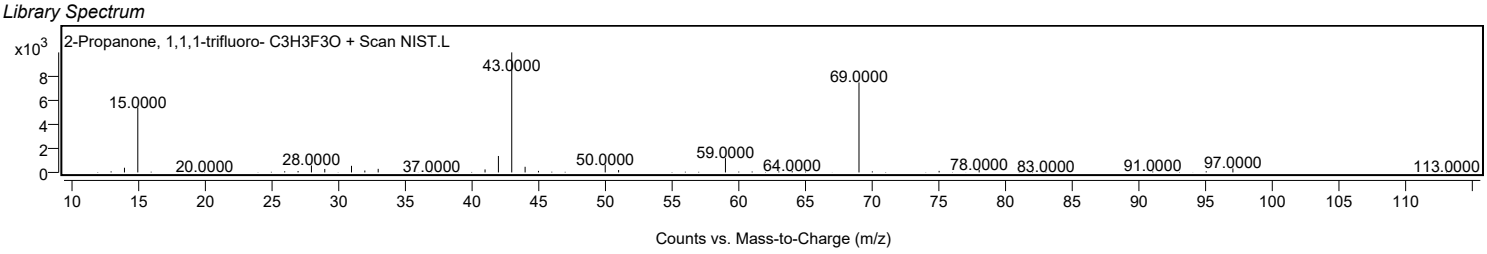
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 31: Herbanate isomer I

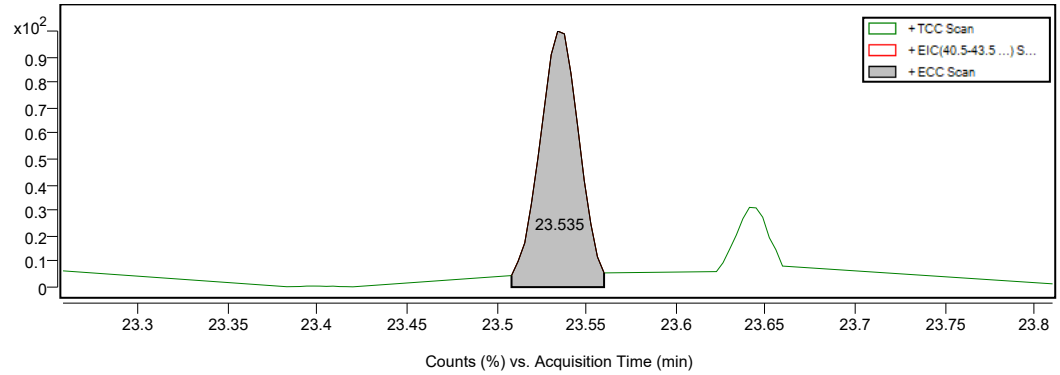
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Herbanate isomer I	C13 H20 O2	23.535			116126-82-0	LibSearch	95.14	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		95.14			50		

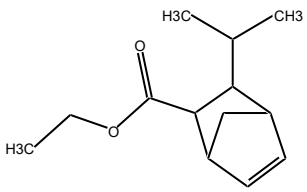
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Herbanate isomer I	C13H20O2		LibSearch	23.535			116126-82-0	95.14		
Herbanate isomer II	C13H20O2		LibSearch	23.535			116126-82-0	93.84		
Glutaric acid, ethyl hex-4-yn-3-yl ester	C13H20O4		LibSearch	23.535	-3.148		1010359-85-2	61.37		
Tricyclo[4.2.1.0<2,5>]non-3-ene	C9H12		LibSearch	23.535	11.152		7078-40-2	60.93		
Bicyclo[2.2.1]hept-5-ene-2-acetic acid, ethyl ester, endo-	C11H16O2		LibSearch	23.535	2.702		74876-17-8	59.99		
Norbornene-2-methanol<endo-5->	C8H12O		LibSearch	23.535	13.235		67671-06-1	59.25		
1H-Pyrrole, 1-phenyl-	C10H9N		LibSearch	23.535	2.685		635-90-5	59.12		
Norbornene-2-methanol<exo-5->	C8H12O		LibSearch	23.535	13.585		67671-05-0	58.63		
1H-Pyrrole, 1-phenyl-	C10H9N		LibSearch	23.535	2.685		635-90-5	58.31		
2-Propenoic acid, 3-bicyclo[2.2.1]hept-5-en-2-yl-	C10H12O2		LibSearch	23.535	1.069		15222-64-7	58.27		
Tricyclo[4.2.1.0(2,5)]non-7-ene, 3-(tert-butyl)-	C13H20		LibSearch	23.535	6.569		1000381-69-6	57.53		
Glutaric acid, ethyl non-5-yn-3-yl ester	C16H26O4		LibSearch	23.535	-8.131		1000359-79-7	57.48		
2,6-Dimethyl-4-oxatricyclo[5.2.1.0(2,6)]dec-8-en-3-ol	C11H16O2		LibSearch	23.535	3.752		1000190-92-8	57.37		
Norbornene-2-methanol <endo-5->	C8H12O		LibSearch	23.535			67671-06-1	57.36		
4,7-Methanoindene, 3a,4,5,6,7,7a-hexahydro-, endo-	C10H14		LibSearch	23.535	9.152		2825-86-7	57.17		
Tricyclo[6.2.1.0(2,7)]undec-9-ene, 4,5-divinyl-	C15H20		LibSearch	23.535	0.085		1000155-78-8	56.94		
5-Norbornene-2,3-diacetonitrile	C11H12N2		LibSearch	23.535	-2.048		101832-55-7	56.70		
Norbornene-2-methanol acetate<endo-5->	C10H14O2		LibSearch	23.535	7.415		16053-06-8	56.53		
Benzenepropanenitrile, .alpha.-methylene-	C10H9N		LibSearch	23.535	1.802		28769-48-4	56.47		
1H-Pyrrole, 1-phenyl-	C10H9N		LibSearch	23.535	2.685		635-90-5	56.34		
endo-N-Hydroxy-5-norbornene-2,3-dicarboximide	C9H9NO3		LibSearch	23.535	0.285		24183-94-6	56.31		
Norbornene-2-methanol acetate<exo-5->	C10H14O2		LibSearch	23.535	7.635		128435-13-2	56.13		
5-Exo-ethynyl-5-endo-norbornenol	C9H10O		LibSearch	23.535	6.335		106697-35-2	56.13		
Bicyclo[2.2.1]hept-2-ene, 5-ethenyl-	C9H12		LibSearch	23.535	8.969		3048-64-4	55.97		
4,7-Methano-1H-isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-, (3a.alpha.,4.alpha.,7.alpha.,7a.alpha.)-	C9H9NO2		LibSearch	23.535	3.585		6265-30-1	55.90		
But-3-yn-2-ol, 2-(bicyclo[2.2.1]hept-2-en-5-yl)-	C11H14O		LibSearch	23.535	3.985		17385-45-4	55.88		
Norbornene-2-methanol <exo-5->	C8H12O		LibSearch	23.535			67671-05-0	55.83		
Pentacyclo[8.2.1.1(4,7).0(2,9).0(3,8)]tetradec-5-ene	C14H18		LibSearch	23.535	4.419		1000436-82-6	55.76		
N-Acetyl-4-azatricyclo[5.2.1.0(2,6)]dec-8-ene-3,5-dione	C11H11NO3		LibSearch	23.535	-2.965		1000197-15-2	55.46		
3a,4,7,7a-Tetrahydro-4,7-methano-1H-isoindole-1,3(2H)-dione	C9H9NO2		LibSearch	23.535	3.585		3647-74-3	55.40		
4,7-Methano-1H-indene, 2,3,3a,4,7,7a-hexahydro-	C10H14		LibSearch	23.535	9.152		19398-83-5	55.38		
Bicyclo[2.2.1]hept-5-ene-2-carbonitrile	C8H9N		LibSearch	23.535	6.369		95-11-4	55.29		
Norbornene-2-methanol acetate <endo-5->	C10H14O2		LibSearch	23.535			16053-06-8	55.26		
Bicyclo[2.2.1]hept-2-ene, 5,6-bis(chloromethyl)-	C9H12Cl2		LibSearch	23.535	1.935		5992-56-3	55.04		
Bicyclo[2.2.1]hept-2-ene, 5-ethenyl-	C9H12		LibSearch	23.535	8.969		3048-64-4	54.95		
5-Allyl-2-norbornene	C10H14		LibSearch	23.535	7.302		31663-53-3	54.68		
4,7-Methano-1H-isoindole-1,3(2H)-dione, 3a,4,7,7a-tetrahydro-, (3a.alpha.,4.alpha.,7.alpha.,7a.alpha.)-	C9H9NO2		LibSearch	23.535	3.585		6265-30-1	54.68		
Glutaric acid, 2,6-dimethylnon-1-en-3-yn-5-yl ethyl ester	C18H28O4		LibSearch	23.535	-9.815		1000359-81-7	54.63		
Norbornene-2-methanol acetate <exo-5->	C10H14O2		LibSearch	23.535			42836-43-1	54.63		
3a,4,5,6,7,7a-Hexahydro-4,7-methanoindene	C10H14		LibSearch	23.535	9.152		4488-57-7	54.63		
Glutaric acid, ethyl 4-heptyl ester	C14H26O4		LibSearch	23.535	-4.515		1000359-45-2	54.59		
3-Oxabicyclo[4.1.0]heptane-7-carboxamide, 6-methyl-N-(1-naphthyl)-	C18H19NO2		LibSearch	23.535	-17.948		1000259-67-7	54.45		
1-Naphthalen-2-yl-3-phenylurea	C17H14N2O		LibSearch	23.535	-20.065		6299-42-9	54.42		
Glutaric acid, dec-9-enyl ethyl ester	C17H30O4		LibSearch	23.535	-10.398		1000405-10-3	54.36		
Bicyclo[2.2.1]hept-2-ene, 5-propyl-	C10H16		LibSearch	23.535	7.135		22094-80-0	54.34		
Bicyclo[2.2.1]hept-5-ene-2,2-dimethanol	C9H14O2		LibSearch	23.535	1.135		6707-12-6	54.19		
5-Norbornene-2-methanol	C8H12O		LibSearch	23.535	6.402		95-12-5	54.18		
4,7-Methanoindene, 3a,4,5,6,7,7a-hexahydro-, endo-	C10H14		LibSearch	23.535	9.152		2825-86-7	53.94		
Cyclobuta[1,2:3,4]dicyclopentene, 1,3a,3b,6,6a,6b-hexahydro-	C10H12		LibSearch	23.535	7.402		612-09-9	53.90		
bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 2-(2-oxopropyl)-, methyl ester	C12H16O3		LibSearch	23.535	-0.798		1000396-11-6	53.87		

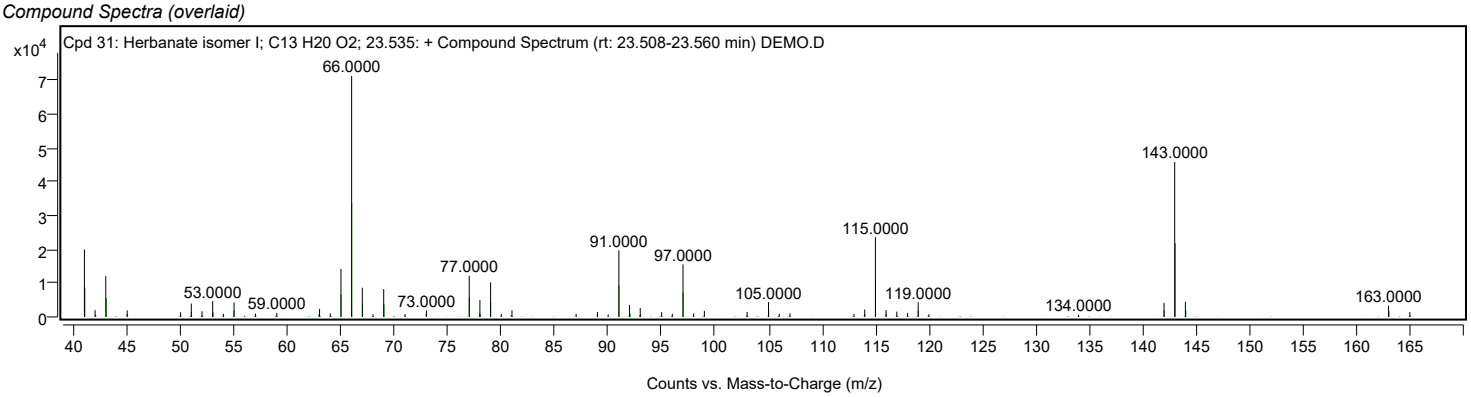
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



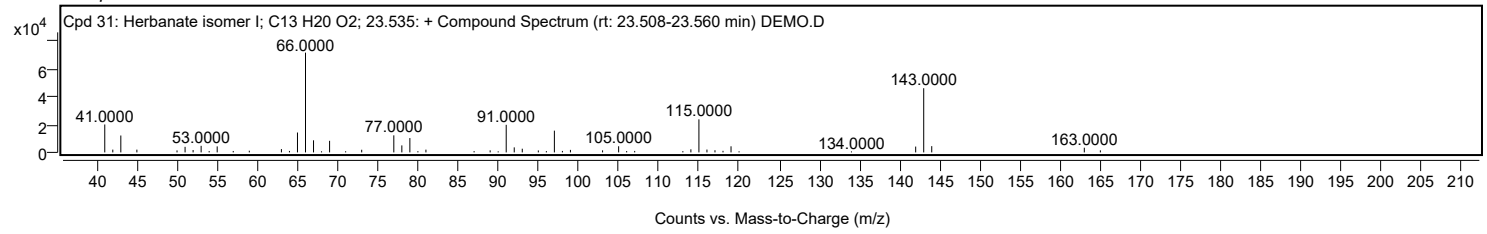
Herbanate isomer I

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			95.14			PWNose.xml

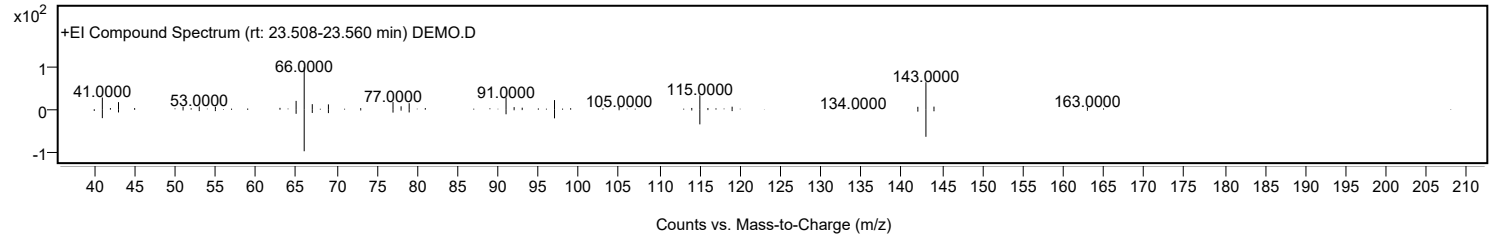
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			95.14			PWNose.xml

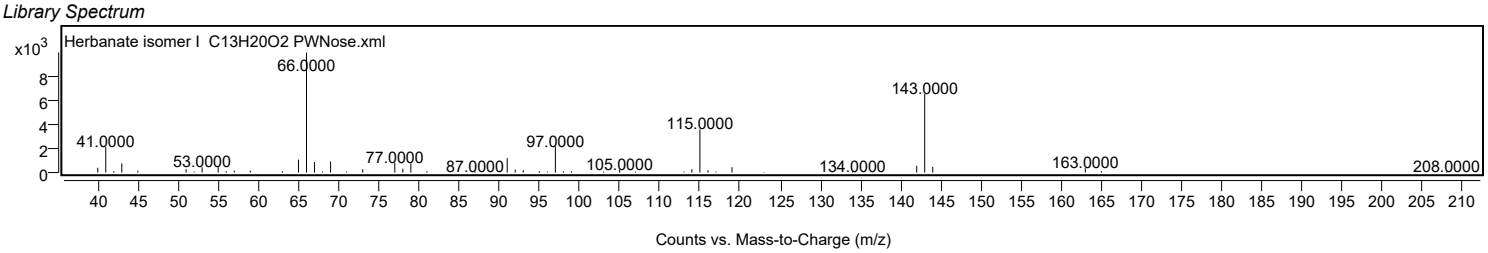
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 32: Herbanate isomer II

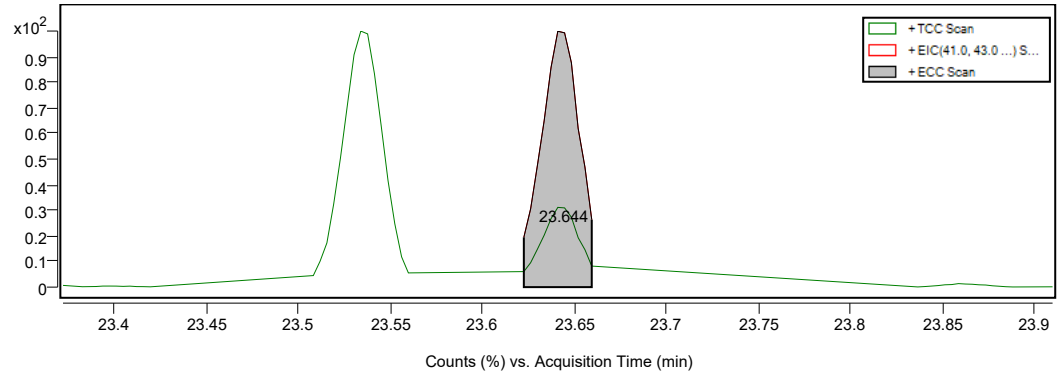
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Herbanate isomer II	C13 H20 O2	23.644			116126-82-0	LibSearch	90.41	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		90.41			50		

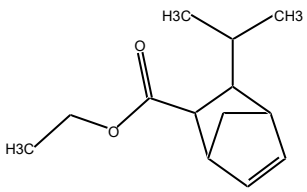
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Herbanate isomer II	C13H20O2		LibSearch	23.644			116126-82-0	90.41		
Herbanate isomer I	C13H20O2		LibSearch	23.644			116126-82-0	89.93		
Norbornene-2-methanol<endo-5->	C8H12O		LibSearch	23.644	13.344		67671-06-1	56.10		
Tricyclo[4.2.1.0<2,5>]non-3-ene	C9H12		LibSearch	23.644	11.261		7078-40-2	55.85		
Norbornene-2-methanol <endo-5->	C8H12O		LibSearch	23.644			67671-06-1	55.83		
Norbornene-2-methanol<exo-5->	C8H12O		LibSearch	23.644	13.694		67671-05-0	54.89		
5-Allyl-2-norbornene	C10H14		LibSearch	23.644	7.411		31663-53-3	54.20		
2-Bicyclo[2.2.1]hept-5-en-2-yl-ethanol	C9H14O		LibSearch	23.644	4.861		13080-91-6	54.11		
Norbornene-2-methanol acetate<endo-5->	C10H14O2		LibSearch	23.644	7.524		16053-06-8	54.03		
Bicyclo[2.2.1]hept-5-ene-2-acetic acid, ethyl ester, endo-	C11H16O2		LibSearch	23.644	2.811		74876-17-8	53.81		
2-Norbornen-5-ol, formate	C8H10O2		LibSearch	23.644	6.161		1000142-75-9	53.79		
Norbornene-2-methanol acetate <endo-5->	C10H14O2		LibSearch	23.644			16053-06-8	53.73		
Bicyclo[2.2.1]hept-2-ene, 5,6-bis(chloromethyl)-	C9H12Cl2		LibSearch	23.644	2.044		5992-56-3	53.71		
6-exo-Methylbicyclo[2.2.1]hept-2-ene-5-endo-carboxylic acid	C9H12O2		LibSearch	23.644	3.611		4397-23-3	53.58		
Norbornene-2-methanol acetate<exo-5->	C10H14O2		LibSearch	23.644	7.744		128435-13-2	53.15		
Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid	C8H10O2		LibSearch	23.644	4.628		120-74-1	53.06		
Norbornene-2-methanol <exo-5->	C8H12O		LibSearch	23.644			67671-05-0	52.89		
4,7-Methanoindene, 3a,4,5,6,7,7a-hexahydro-, endo-	C10H14		LibSearch	23.644	9.261		2825-86-7	52.76		
Pentacyclo[8.2.1.1(4,7).0(2,9).0(3,8)]tetradec-5-ene	C14H18		LibSearch	23.644	4.528		1000436-82-6	52.62		
Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid	C8H10O2		LibSearch	23.644	4.628		120-74-1	52.60		
Bicyclo[2.2.1]hept-2-ene, 5-ethenyl-	C9H12		LibSearch	23.644	9.078		3048-64-4	52.46		
Norbornen-2-ol acetate<endo-5->	C9H12O2		LibSearch	23.644	12.424		99295-40-6	52.41		
Norbornene-2-methanol acetate <exo-5->	C10H14O2		LibSearch	23.644			42836-43-1	52.39		
4,7-Methanoindene, 3a,4,5,6,7,7a-hexahydro-, endo-	C10H14		LibSearch	23.644	9.261		2825-86-7	52.12		
Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid	C8H10O2		LibSearch	23.644	4.628		120-74-1	52.11		
Bicyclo[2.2.1]hept-2-ene, 5-ethenyl-	C9H12		LibSearch	23.644	9.078		3048-64-4	51.94		
bicyclo[2.2.1]hept-5-ene-2-carboxylic acid, 2-(2-oxopropyl)-, methyl ester	C12H16O3		LibSearch	23.644	-0.689		1000396-11-6	51.85		
Norbornen-2-ol acetate<exo-5->	C9H12O2		LibSearch	23.644	12.594		5257-37-4	51.82		
4,7-Methano-1H-indene, 2,3,3a,4,7,7a-hexahydro-	C10H14		LibSearch	23.644	9.261		19398-83-5	51.78		
Norbornene	C7H10		LibSearch	23.644	21.144		498-66-8	51.72		
5-Norbornene-2-methanol	C8H12O		LibSearch	23.644	6.511		95-12-5	51.71		
Norbornene	C7H10		LibSearch	23.644			498-66-8	51.67		
Bicyclo[2.2.1]hept-2-ene, 5-propyl-	C10H16		LibSearch	23.644	7.244		22094-80-0	51.63		
5-Ethyl bicyclo[2.2.1]-2-heptene	C9H14		LibSearch	23.644	8.911		15403-89-1	51.63		
Spiro[bicyclo[2.2.1]hept-5-ene-2,1'-cyclopropane]	C9H12		LibSearch	23.644	9.011		6572-50-5	51.54		
But-3-yn-2-ol, 2-(bicyclo[2.2.1]hept-2-en-5-yl)-	C11H14O		LibSearch	23.644	4.094		17385-45-4	51.52		
Norbornen-2-ol<endo-5->	C7H10O		LibSearch	23.644	17.794		106928-44-3	51.50		
Bicyclo[2.2.1]hept-2-ene, 5-ethenyl-	C9H12		LibSearch	23.644	9.078		3048-64-4	51.22		
5-Exo-ethynyl-5-endo-norbornenol	C9H10O		LibSearch	23.644	6.444		106697-35-2	51.19		
3a,4,5,6,7,7a-Hexahydro-4,7-methanoindene	C10H14		LibSearch	23.644	9.261		4488-57-7	51.02		
Benzene, (2-cyclopenten-1-ylmethyl	C12H14		LibSearch	23.644	1.711		55969-86-3	51.02		
5-Norbornene-2,3-diacetonitrile	C11H12N2		LibSearch	23.644	-1.939		101832-55-7	50.84		
Cyclopropane, (R,R)-1-((Z),(Z)-hexa-1',3'-dienyl)-2-ethenyl-	C11H16		LibSearch	23.644	5.578		77210-41-4	50.82		
Bicyclo[2.2.1]hept-5-ene-2-carboxylic acid	C8H10O2		LibSearch	23.644	4.628		120-74-1	50.71		
2-Methylbicyclo[2.2.1]-5-heptene-2-carboxylic acid	C9H12O2		LibSearch	23.644	3.394		825-03-6	50.57		
Norbornen-2-ol acetate <endo-5->	C9H12O2		LibSearch	23.644			99295-40-6	50.47		
Norbornen-2-ol<exo-5->	C7H10O		LibSearch	23.644	17.594		71030-14-3	50.32		
11-Chlorohexacyclo[6.6.1.1(3,6).1(10,13).0(2,7).0(9,14)]heptadec-4-ene (isomer 2)	C17H21Cl		LibSearch	23.644	-2.606		1000436-29-0	50.30		
Bicyclo[3.2.0]hept-2-ene, cis-	C7H10		LibSearch	23.644	11.578		1000155-54-0	50.25		
Tetracyclo[3,3,1,0(2,4),0(6,8)]nonane	C9H12		LibSearch	23.644	12.594		24506-61-4	50.03		

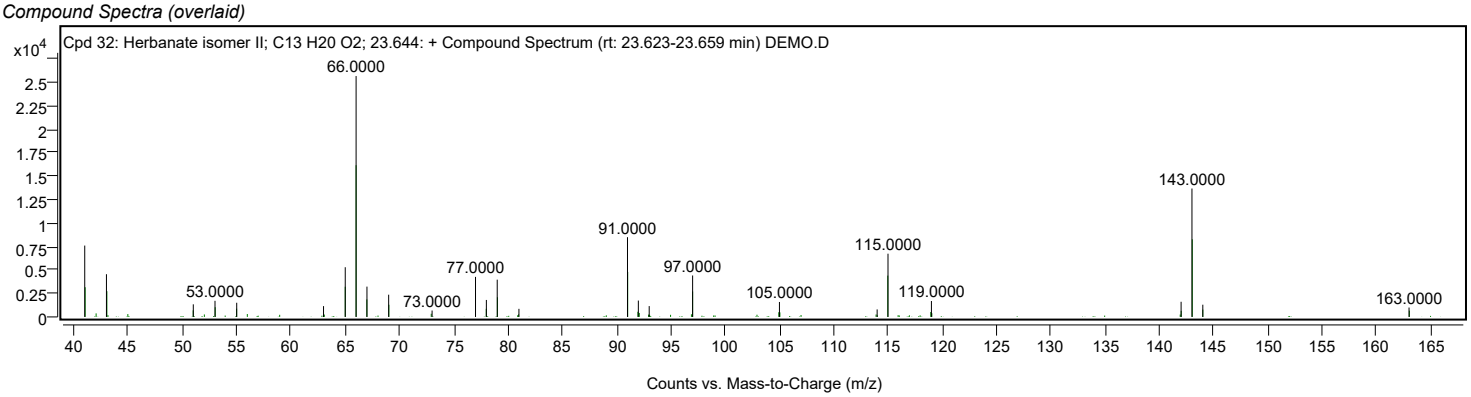
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



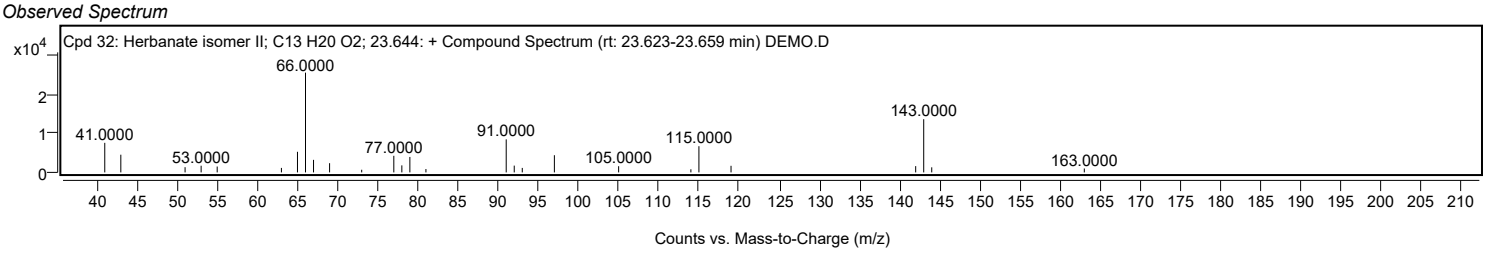
Herbanate isomer II

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			90.41			PWNose.xml

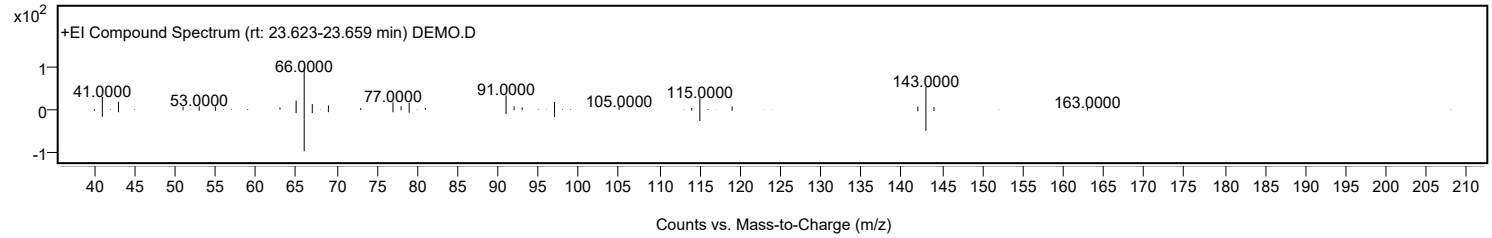
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			90.41			PWNose.xml

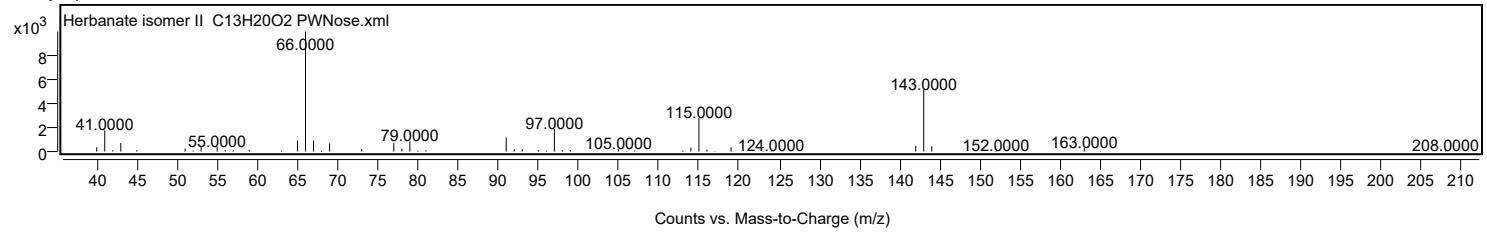
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 33: Cyclopropyl 2-(5'-methyl-2'-furyl)cyclopropyl ketone

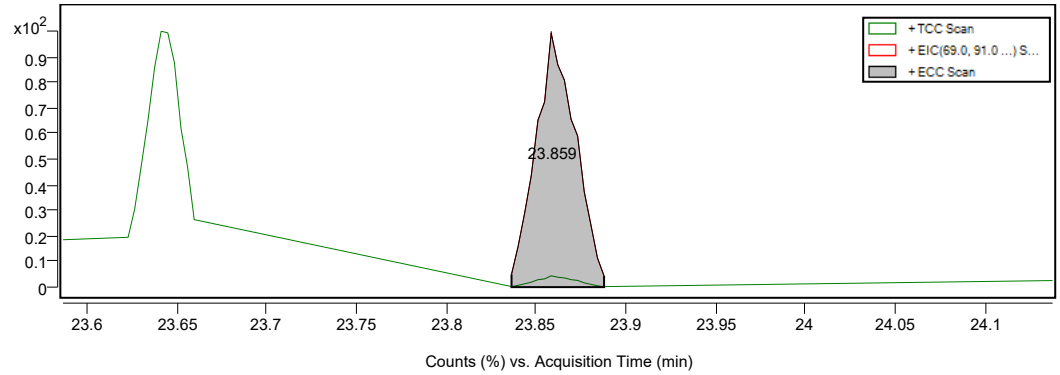
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Cyclopropyl 2-(5'-methyl-2'-furyl)cyclopropyl ketone	C12 H14 O2	23.859			1000139-92-9	LibSearch	44.09	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		44.09			50		

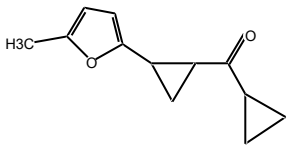
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Cyclopropyl 2-(5'-methyl-2'-furyl)cyclopropyl ketone	C12H14O2		LibSearch	23.859	0.026		1000139-92-9	44.09		
Damascenone <(Z)-beta->	C13H18O		LibSearch	23.859			59739-63-8	41.53		
Damascenone<(Z)-beta->	C13H18O		LibSearch	23.859	0.969		59739-63-8	41.44		
2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-	C13H18O		LibSearch	23.859	-0.141		23696-85-7	39.01		
2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (E)-	C13H18O		LibSearch	23.859	-0.141		23726-93-4	38.89		
2-Propenoic acid, 2-methyl-, 3-(trimethoxysilyl)propyl ester	C10H20O5Si		LibSearch	23.859	2.409		2530-85-0	38.76		
2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (E)-	C13H18O		LibSearch	23.859	-0.141		23726-93-4	38.36		
Cyclopropanecarboxylic acid, 4-isopropylphenyl ester	C13H16O2		LibSearch	23.859	-1.291		1000331-01-9	37.23		
Phenylacetic acid, 3-methylbut-2-enyl ester	C13H16O2		LibSearch	23.859	-1.841		151091-17-7	37.23		
Cyclopropanecarboxylic acid, [1-[(2-methoxyphenyl)methyl]-1H-1,3-benzimidazol-2-yl]methyl ester	C20H20N2O3		LibSearch	23.859	-21.108		1010337-33-6	37.13		
Crotonic acid, o-formylphenyl ester	C11H10O3		LibSearch	23.859	-2.291		114636-69-0	37.04		
Ethanone, 1-cyclopropyl-2-phenyl-	C11H12O		LibSearch	23.859	1.709		14113-94-1	36.84		
Damascenone<(E)-beta->	C13H18O		LibSearch	23.859	-0.011		23726-93-4	36.59		
2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (E)-	C13H18O		LibSearch	23.859	-0.141		23726-93-4	36.51		
2-propenoic acid, 2-methyl-, 2-formylphenyl ester	C11H10O3		LibSearch	23.859	-1.608		1000400-21-1	36.02		
2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-, (E)-	C13H18O		LibSearch	23.859	-0.141		23726-93-4	35.33		
2-Buten-1-one, 1-(2,6,6-trimethyl-1,3-cyclohexadien-1-yl)-	C13H18O		LibSearch	23.859	-0.141		23696-85-7	35.11		
Damascenone <(E)-, beta->	C13H18O		LibSearch	23.859			23726-93-4	35.05		
7,8-Dihydroyangonin	C15H16O4		LibSearch	23.859	-11.574		3155-52-0	34.91		
2-Methoxybenzyl alcohol, trifluoroacetate	C10H9F3O3		LibSearch	23.859	4.142		1000365-18-8	33.32		
Phenylacetic acid, 3-methylbut-2-enyl ester	C13H16O2		LibSearch	23.859	-1.841		151091-17-7	33.01		
Benzeneacetic acid <3,7-dimethyl-, 2,6-octadienyl-> ester	C18H24O2		LibSearch	23.859			71648-43-6	31.20		
2-Propenoic acid, 2-methyl-, 3-(trimethoxysilyl)propyl ester	C10H20O5Si		LibSearch	23.859	2.409		2530-85-0	30.55		
1-Formyl-2,2,6-trimethyl-3-cis-(3-methylbut-2-enyl)-5-cyclohexene	C15H24O		LibSearch	23.859	-3.124		1000144-10-1	30.27		
Benzeneethanol, .alpha.-(2-methylpropyl)-	C12H18O		LibSearch	23.859	0.709		7779-78-4	29.96		
Geranyl phenylacetate	C18H24O2		LibSearch	23.859	-9.891		102-22-7	28.74		
Glutaric acid, 3-methylbut-2-en-1-yl 2-isopropylphenyl ester	C19H26O4		LibSearch	23.859	-13.741		1000391-91-5	28.56		
Nonanamide, 2,2,3,3,4,4,5,5,6,6,7,7,8,8,9,9,9-heptadecafluoro-N-[3-(trimethoxysilyl)propyl]-	C15H16F17NO4Si		LibSearch	23.859	8.642		1010460-79-6	28.53		
Duprezianen-3-one <2-epi-beta->	C15H22O		LibSearch	23.859			288252-79-9	28.46		
Cyclopropanecarboxylic acid, benzyl ester	C11H12O2		LibSearch	23.859	1.176		20121-75-9	28.05		
Duprezianen-3-one<2-epi-beta->	C15H22O		LibSearch	23.859	-10.561		288252-79-9	27.88		
benzoic acid, 4-[(2-methyl-1-oxo-2-propen-1-yl)oxy]-, methyl ester	C12H12O4		LibSearch	23.859	-2.908		1000400-77-3	27.53		
2,4-Dimethylphenyl heptafluorobutyrate	C12H9F7O2		LibSearch	23.859	6.492		1000453-60-4	27.44		
Benzyl but-2-enoate	C11H12O2		LibSearch	23.859	1.076		1000144-08-9	26.93		
Neryl phenylacetate	C18H24O2		LibSearch	23.859	-9.891		1000109-59-4	26.65		
Propanenitrile, 3-phenyl-2-(methylamino)	C10H12N2		LibSearch	23.859	-0.674		58626-96-3	26.12		
Oxalic acid, isohexyl 2-isopropylphenyl ester	C17H24O4		LibSearch	23.859	-9.608		1000309-56-5	26.10		
Geranyl phenylacetate	C18H24O2		LibSearch	23.859	-9.891		102-22-7	26.03		
Glutaric acid, 3-methylbut-2-en-1-yl 4-acetylphenyl ester	C18H22O5		LibSearch	23.859	-15.424		1000392-03-3	26.03		
3-Buten-2-one, 3-methyl-1-phenyl-	C11H12O		LibSearch	23.859	2.292		55956-30-4	25.62		
benzoic acid, 4-[(2-methyl-1-oxo-2-propen-1-yl)oxy]-, ethyl ester	C13H14O4		LibSearch	23.859	-4.574		1000401-06-0	25.40		
Benzyl crotonate	C11H12O2		LibSearch	23.859	1.076		1000429-17-6	25.36		
2,4,4-Trimethyl-3-hydroxymethyl-5a-(3-methyl-but-2-enyl)-cyclohexene	C15H26O		LibSearch	23.859	-4.024		1000144-10-5	24.57		
6-Bromohexanoic acid, 4-isopropylphenyl ester	C15H21BrO2		LibSearch	23.859	-9.508		1000331-04-0	24.46		
1-Formyl-2,2,6-trimethyl-3-trans-(3-methyl-but-2-enyl)-5-cyclohexene	C15H24O		LibSearch	23.859	-3.124		1000144-09-9	24.45		
3-Methyl-6-hepten-1-yn-3-ol	C8H12O		LibSearch	23.859	8.926		51193-99-8	23.48		
3-(5-Benzyloxy-3-methylpent-3-enyl)-2,2-dimethyloxirane	C17H24O2		LibSearch	23.859	-7.391		1000192-21-5	23.18		
Benzeneethanol, .alpha.-(2-methylpropyl)-	C12H18O		LibSearch	23.859	0.709		7779-78-4	23.14		
1-Benzyl-3-(4-chloro-phenyl)-1-(1-cyclopropyl-ethyl)-urea	C19H21ClN2O		LibSearch	23.859	-19.974		1000297-05-8	22.82		
Benzeneacetic acid, 2-ethylcyclohexyl ester	C16H22O2		LibSearch	23.859	-7.491		1000282-63-9	22.75		

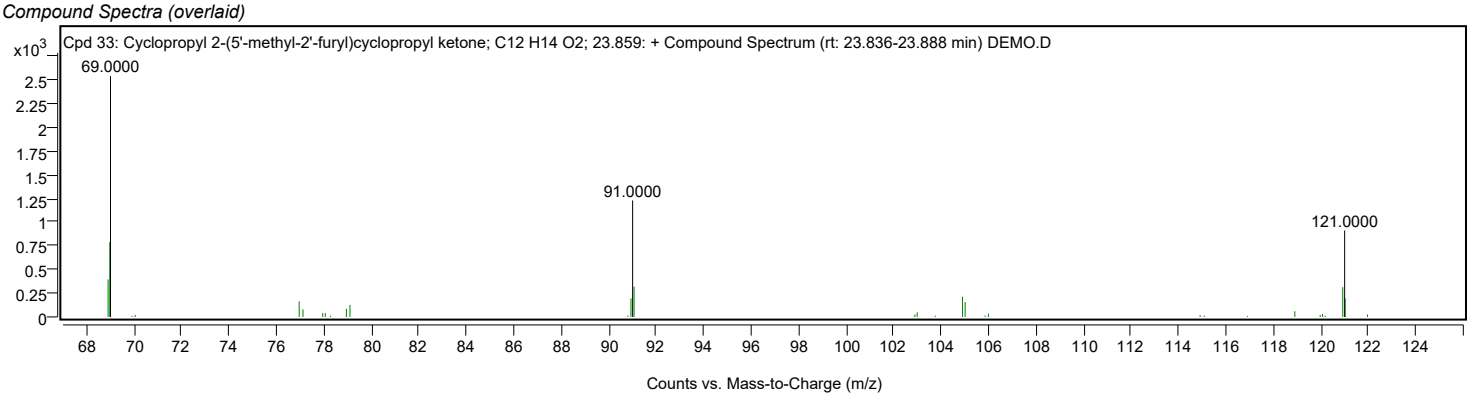
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



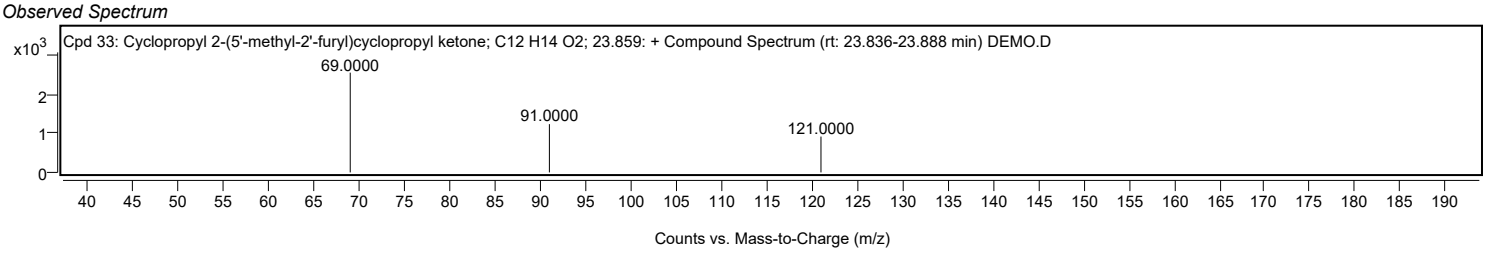
Cyclopropyl 2-(5'-methyl-2'-furyl)cyclopropyl ketone

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			44.09			NIST.L

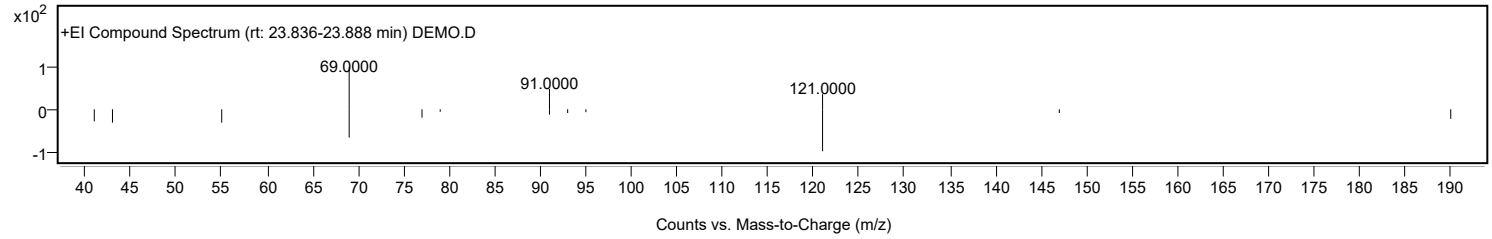
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			44.09			NIST.L

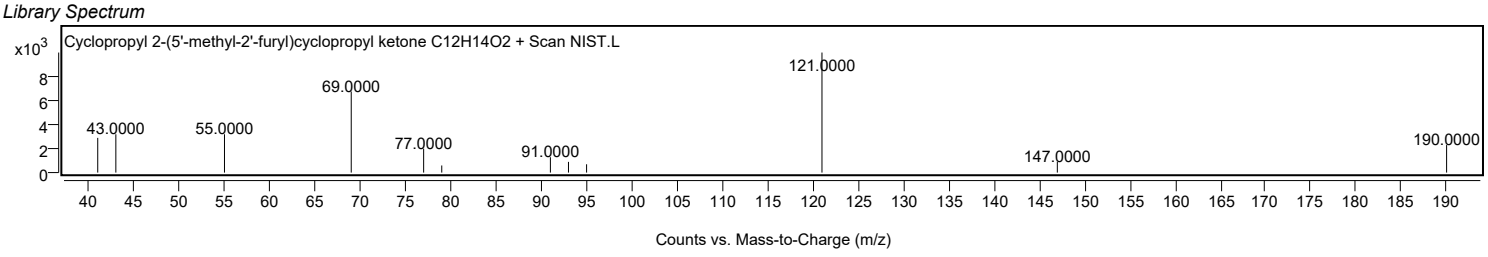
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 34: (5Z)-3-Methyl-1,5-heptadiene

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
(5Z)-3-Methyl-1,5-heptadiene	C8 H14	24.389			50763-51-4	LibSearch	44.90	Chrom Decon	NIST.L

Compound Discovery Report

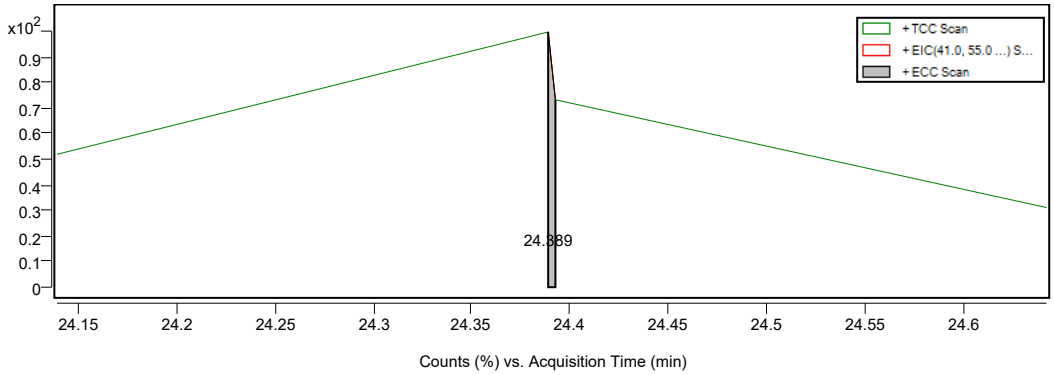
Agilent | Trusted Answers

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		44.90			50		

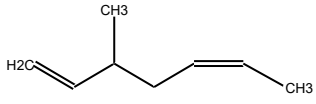
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
(5Z)-3-Methyl-1,5-heptadiene	C8H14		LibSearch	24.389	11.889		50763-51-4	44.90		
1,5-Heptadiene, 3-methyl-, (E)-	C8H14		LibSearch	24.389	11.889		50592-72-8	44.48		
1,5-Hexadiene, 2,4-dimethyl-	C8H14		LibSearch	24.389	12.556		68701-71-3	43.49		
2-Methyl-1,5-heptadiene (c,t)	C8H14		LibSearch	24.389	11.189		6766-54-7	42.95		
5-Cyano-1-pentene	C6H9N		LibSearch	24.389	10.172		5048-19-1	42.63		
1,5-Heptadiene, 2-methyl-, (E)-	C8H14		LibSearch	24.389	11.189		41044-63-7	41.63		
1,5-Heptadiene, 3-methyl-	C8H14		LibSearch	24.389	11.889		4894-62-6	41.36		
1,5-Heptadiene, 3-methyl-, (E)-	C8H14		LibSearch	24.389	11.889		50592-72-8	41.09		
1,5-Heptadiene, 2-methyl-, (Z)-	C8H14		LibSearch	24.389	11.189		41044-64-8	40.60		
2-Methyl-1,5-heptadiene (c,t)	C8H14		LibSearch	24.389	11.189		6766-54-7	39.97		
5,10-Pentadecadienal, (Z,Z)-	C15H26O		LibSearch	24.389	-4.228		64275-49-6	38.00		
1,5-Hexadiene, 2,5-dimethyl-	C8H14		LibSearch	24.389	11.872		627-58-7	36.74		
5,10-Pentadecadienal, (E,E)-	C15H26O		LibSearch	24.389	-4.228		64275-42-9	36.30		
Zinc, bis(2-methyl-2-propenyl)-	C8H14Zn		LibSearch	24.389			15961-33-8	36.15		
1,5-Hexadiene, 2,5-dimethyl-	C8H14		LibSearch	24.389	11.872		627-58-7	36.02		
1,4-Hexadiene, 2,5-dimethyl-	C8H14		LibSearch	24.389	11.572		927-97-9	35.34		
1,4-Heptadiene, 3,3,6-trimethyl-	C10H18		LibSearch	24.389	9.972		74498-89-8	34.05		
Cyclohexanemethanol, .alpha.-propyl-	C10H20O		LibSearch	24.389	3.706		4352-42-5	32.36		
2,7-Octadiene, 4-methyl-	C9H16		LibSearch	24.389	10.222		1000061-78-0	31.97		
Borane, ethylisopropylmethyl-	C6H15B		LibSearch	24.389			1000154-39-8	31.05		
4-(Chloromethyl)oxolan-2-one	C5H7ClO2		LibSearch	24.389	5.872		1000486-88-0	30.48		
1,6-Heptadiene, 3-methyl-	C8H14		LibSearch	24.389	12.172		50871-05-1	29.34		
1,6-Octadiene, 3,7-dimethyl-, (S)-	C10H18		LibSearch	24.389	8.956		10281-55-7	29.30		
Pinocamphone<cis->	C10H16O		LibSearch	24.389	9.819		15358-88-0	29.19		
3-(Chloromethyl)oxolan-2-one	C5H7ClO2		LibSearch	24.389	5.872		1000486-88-1	29.17		
Thiophene, tetrahydro-, 1,1-dioxide	C4H8O2S		LibSearch	24.389			126-33-0	28.91		
Citronellene <beta->	C10H18		LibSearch	24.389			2436-90-0	28.45		
6-Hepten-1-ol, 5-methyl-	C8H16O		LibSearch	24.389	7.972		26799-28-0	28.39		
Citronellene<beta->	C10H18		LibSearch	24.389	18.239		2436-90-0	28.07		
6-Oxabicyclo[3.1.0]hexane	C5H8O		LibSearch	24.389	14.206		285-67-6	27.75		
Borane, butyldiethyl-	C8H19B		LibSearch	24.389			40218-56-2	27.57		
1,6-Octadiene, 5,7-dimethyl-, (R)-	C10H18		LibSearch	24.389	8.956		85006-04-8	27.02		
3-Hepten-1-ol	C7H14O		LibSearch	24.389	8.256		10606-47-0	26.98		
Oxazirane, 2-(dimethylethyl)-3-methoxy-	C6H13NO2		LibSearch	24.389	10.839		103202-91-1	26.87		
.alpha.-CITRONELLENE	C10H18		LibSearch	24.389	9.256		6874-35-7	26.81		
Propanal, di-2-propenylhydrazone	C9H16N2		LibSearch	24.389	5.039		75268-09-6	26.78		
1,9-Decadiene	C10H18		LibSearch	24.389	7.806		1647-16-1	26.76		
Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-, [1R-(1.alpha.,2.beta.,5.alpha.)]-	C10H18		LibSearch	24.389	8.772		4795-86-2	26.74		
6-Oxabicyclo[3.1.0]hexane	C5H8O		LibSearch	24.389	14.206		285-67-6	26.36		
R(-)3,7-Dimethyl-1,6-octadiene	C10H18		LibSearch	24.389	8.956		10281-56-8	26.03		
2-Propenoic acid, 5-methyl-2-(1-methylethyl)cyclohexyl ester	C13H22O2		LibSearch	24.389	1.156		82277-50-7	26.03		
Pentylenetetrazol	C6H10N4		LibSearch	24.389			54-95-5	26.02		
1,8-Nonadiene	C9H16		LibSearch	24.389	9.456		4900-30-5	26.00		
1-Pentene, 3-methyl-	C6H12		LibSearch	24.389	15.322		760-20-3	25.93		
4-Nonene, 1-bromo-, (E)-	C9H17Br		LibSearch	24.389	4.056		16695-35-5	25.91		
3-Hexene, (E)-	C6H12		LibSearch	24.389	13.956		13269-52-8	25.87		
Undecenol <10->	C11H22O		LibSearch	24.389			112-43-6	25.78		
2H-Pyran, 2-(tert-butylthio)tetrahydro-	C9H18OS		LibSearch	24.389	3.822		1927-53-3	25.75		
Bicyclo[3.1.1]heptane, 2,6,6-trimethyl-, [1R-(1.alpha.,2.alpha.,5.alpha.)]-	C10H18		LibSearch	24.389	8.772		4863-59-6	25.59		
1,6-Heptadiene, 3,3-dimethyl-	C9H16		LibSearch	24.389	10.856		68701-61-1	25.53		

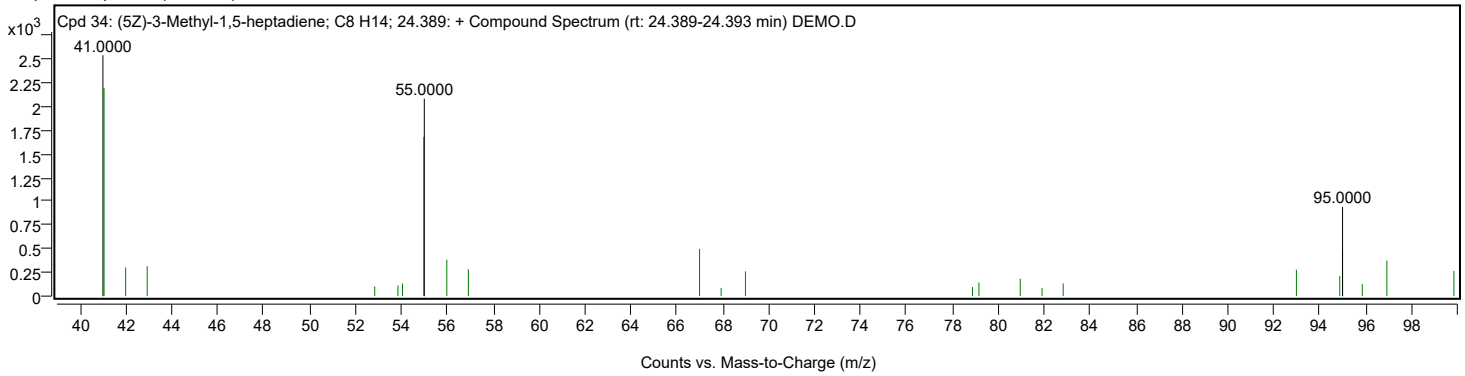
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



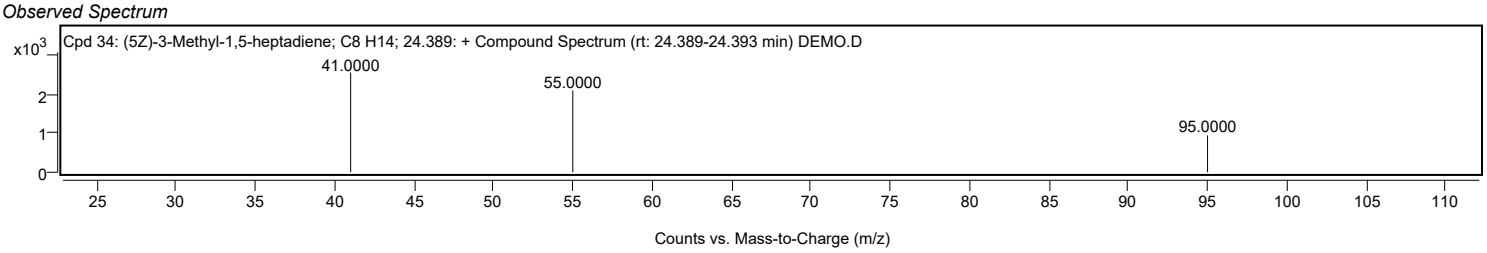
(5Z)-3-Methyl-1,5-heptadiene

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			44.90			NIST.L

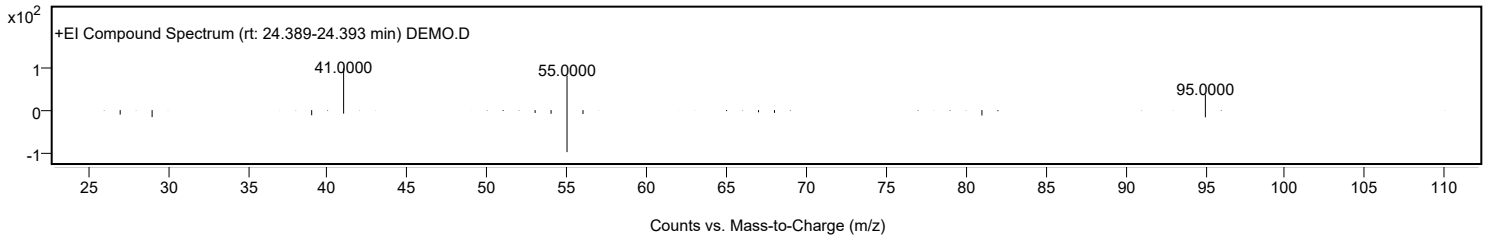
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			44.90			NIST.L

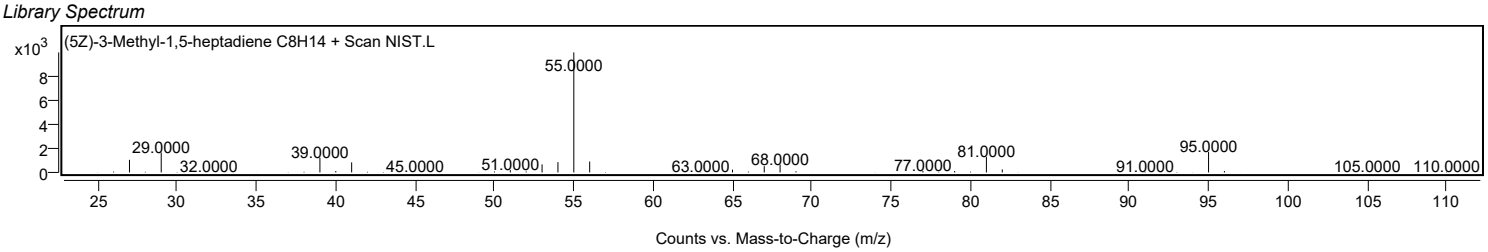
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 35: 3-Methylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
3-Methylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester	C15 H10 Cl2 O3	24.796			1010331-26-9	LibSearch	62.68	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		62.68			50		

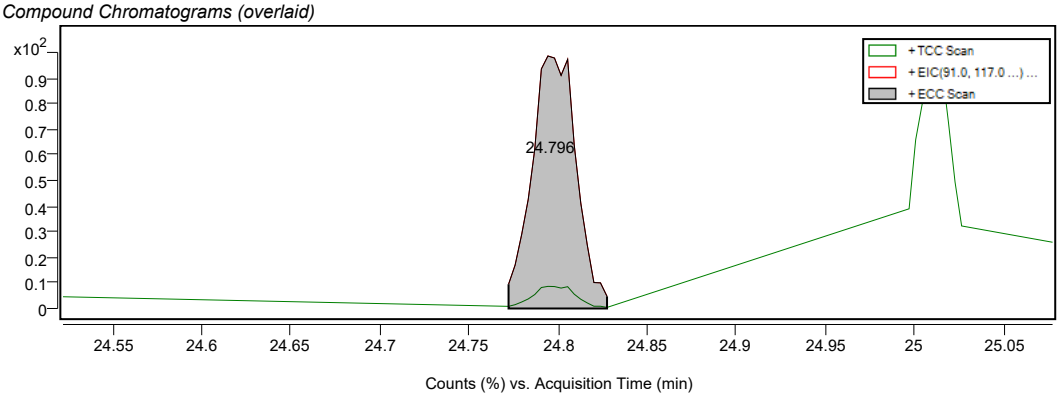
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
3-Methylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester	C15H10Cl2O3		LibSearch	24.796	-15.354		1010331-26-9	62.68		
1,3-Benzenediol, O,O'-di(2-methylbenzoyl)-	C22H18O4		LibSearch	24.796	-22.104		1000330-74-0	62.39		
3-(4-Methylbenzoyl)-2-thioxo-4-thiazolyl 4-methylbenzoate	C19H15NO3S2		LibSearch	24.796	-27.038		299929-13-8	62.26		
2-Methyl-2-(4-methylbenzoyl)malononitrile	C12H10N2O		LibSearch	24.796	-5.988		1000326-92-9	62.26		
2-Methylbenzoic acid, 2,3-dichlorophenyl ester	C14H10Cl2O2		LibSearch	24.796	-10.321		1000331-28-3	62.07		
2-Methylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester	C15H10Cl2O3		LibSearch	24.796	-15.354		1000331-28-4	61.76		
1,2-Benzenediol, o-(2-methylbenzoyl)-	C14H12O3		LibSearch	24.796	-8.004		1000325-95-2	61.62		
4-Methylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester	C15H10Cl2O3		LibSearch	24.796	-15.354		1000331-36-6	61.58		
1,2-Benzenediol, O-(5-chlorovaleryl)-O-(2-methylbenzoyl)-	C19H19ClO4		LibSearch	24.796	-19.371		1000329-74-2	61.53		
p-Toluic acid, 5-fluoro-2-nitrophenyl ester	C14H10FNO4		LibSearch	24.796	-10.504		1000292-64-6	61.26		
o-Toluic acid, 4-cyanophenyl ester	C15H11NO2		LibSearch	24.796	-8.954		1010307-45-8	61.16		
4-Methylbenzoic acid, 2,3-dichlorophenyl ester	C14H10Cl2O2		LibSearch	24.796	-10.321		1000331-36-5	60.97		
1,2-Benzenediol, O,O'-di(2-methylbenzoyl)-	C22H18O4		LibSearch	24.796	-22.104		1000325-95-5	60.78		
m-Toluic acid, 4-cyanophenyl ester	C15H11NO2		LibSearch	24.796	-8.954		1000307-56-9	60.65		
Benzoic acid, 3-methyl-, pentafluorophenyl ester	C14H7F5O2		LibSearch	24.796	-2.238		1000355-70-7	60.54		
o-Toluic acid, 4-nitrophenyl ester	C14H11NO4		LibSearch	24.796	-10.921		1000307-46-0	60.33		
4-Methylbenzoic acid, pentafluorophenyl ester	C14H7F5O2		LibSearch	24.796	-2.238		1000354-15-1	60.18		
p-Toluic acid, 3,5-difluorophenyl ester	C14H10F2O2		LibSearch	24.796	-3.488		1000292-64-0	60.15		
4-Methylbenzoic acid, 2-fluorophenyl ester	C14H11FO2		LibSearch	24.796	-3.904		1000325-59-8	60.14		
1,2-Benzenediol, o-(2,2,3,3,4,4,4-heptafluorobutyryl)-o'-(4-methylbenzoyl)-	C18H11F7O4		LibSearch	24.796	-6.588		1000325-97-7	60.08		
m-Toluic acid, 4-nitrophenyl ester	C14H11NO4		LibSearch	24.796	-10.921		1000307-57-1	60.03		
3-Methylbenzoic acid, 3-fluorophenyl ester	C14H11FO2		LibSearch	24.796	-3.904		1000331-26-2	59.98		
1,2-Benzenediol, O-(4-methylbenzoyl)-O'-propoxycarbonyl-	C18H18O5		LibSearch	24.796	-15.238		1010329-75-8	59.97		
p-Toluic acid, 3,4-dichlorophenyl ester	C14H10Cl2O2		LibSearch	24.796	-10.321		1000307-76-9	59.87		
3-Methylbenzoic acid, 2,3-dichlorophenyl ester	C14H10Cl2O2		LibSearch	24.796	-10.321		1000331-26-8	59.81		
o-Toluic acid, 3,4-dichlorophenyl ester	C14H10Cl2O2		LibSearch	24.796	-10.321		1000307-45-9	59.64		
1,2-Benzenediol, o-(4-methylbenzoyl)-	C14H12O3		LibSearch	24.796	-8.004		1000325-98-1	59.52		
1,3-Benzenediol, o-(2-bromopropionyl)-o'-(3-methylbenzoyl)-	C17H15BrO4		LibSearch	24.796	-16.188		1000330-83-0	59.38		
1,3-Benzenediol, O-methoxycarbonyl-O'-(4-methylbenzoyl)-	C16H14O5		LibSearch	24.796	-11.921		1010345-55-0	59.14		
1,2-Benzenediol, O-methoxycarbonyl-O'-(4-methylbenzoyl)-	C16H14O5		LibSearch	24.796	-11.921		1000329-75-7	58.90		
1,2-Benzenediol, o-(3-methylbenzoyl)-	C14H12O3		LibSearch	24.796	-8.004		1000325-96-4	58.89		
3-Methylbenzoic acid, 3-chlorophenyl ester	C14H11ClO2		LibSearch	24.796	-7.321		1010325-71-2	58.82		
3-Methylbenzoic acid, 2-fluorophenyl ester	C14H11FO2		LibSearch	24.796	-3.904		1000325-70-9	58.69		
4-Methylbenzoic acid, 3-chlorophenyl ester	C14H11ClO2		LibSearch	24.796	-7.321		1000325-60-1	58.62		
o-Toluic acid, 4-chlorophenyl ester	C14H11ClO2		LibSearch	24.796	-7.321		1000307-45-5	58.49		
2-Methylbenzoic acid, 4-chloro-2-methylphenyl ester	C15H13ClO2		LibSearch	24.796	-9.204		1010331-28-1	58.04		
p-Toluic acid, 2-chlorophenyl ester	C14H11ClO2		LibSearch	24.796	-7.321		1000292-64-3	57.83		
1,2-Benzenediol, o-(2-bromopropionyl)-o'-(3-methylbenzoyl)-	C17H15BrO4		LibSearch	24.796	-16.188		1000325-96-8	57.75		
1,3-Benzenediol, O-(4-methylbenzoyl)-O'-propoxycarbonyl-	C18H18O5		LibSearch	24.796	-15.238		1000345-55-1	57.52		
2-Methylbenzoic acid, 2-fluorophenyl ester	C14H11FO2		LibSearch	24.796	-3.904		1000325-60-5	57.52		
Benzene, 1,1'-(1,1,2,2-tetramethyl-1,2-ethanediyl)bis-	C18H22		LibSearch	24.796	-5.121		1889-67-4	57.51		
p-Toluic acid, 4-chlorophenyl ester	C14H11ClO2		LibSearch	24.796	-7.321		1010307-76-5	57.40		
p-Toluic acid, 2-bromo-4-fluorophenyl ester	C14H10BrFO2		LibSearch	24.796	-9.238		1000292-64-4	57.19		
Benzoic acid, 4-methyl-, phenyl ester	C14H12O2		LibSearch	24.796	-4.321		1900-85-2	57.17		
Benzamide, N-(3-nitrophenyl)-4-methyl-	C14H12N2O3		LibSearch	24.796	-14.804		1000306-96-2	57.15		
2-Methylbenzoic acid, 3-chlorophenyl ester	C14H11ClO2		LibSearch	24.796	-7.321		1000325-60-8	57.11		
3-Methylbenzoic acid, 2,4,6-trichlorophenyl ester	C14H9Cl3O2		LibSearch	24.796	-13.321		1000325-71-4	56.98		
2-Methylbenzoic acid, 4-isopropylphenyl ester	C17H18O2		LibSearch	24.796	-8.454		1000331-28-2	56.94		
1,3-Benzenediol, O-(2,6-difluorobenzoyl)-O'-(2-methylbenzoyl)-	C21H14F2O4		LibSearch	24.796	-19.371		1000345-52-6	56.89		

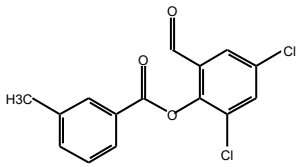
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
4-Methylbenzoic acid, 2,5-dichlorophenyl ester	C14H10Cl2O2		LibSearch	24.796	-10.321		1000325-60-2	56.59		

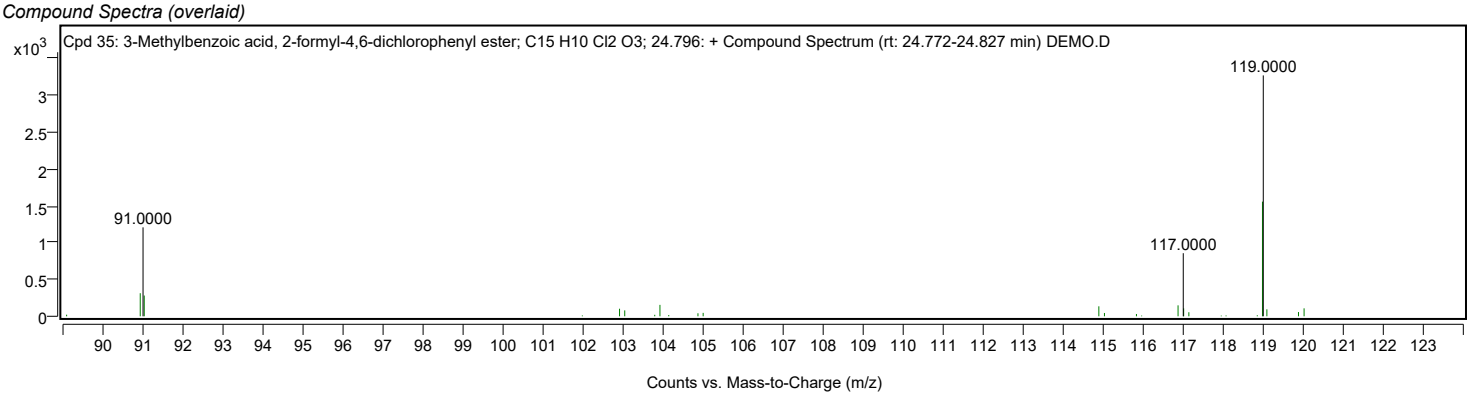
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



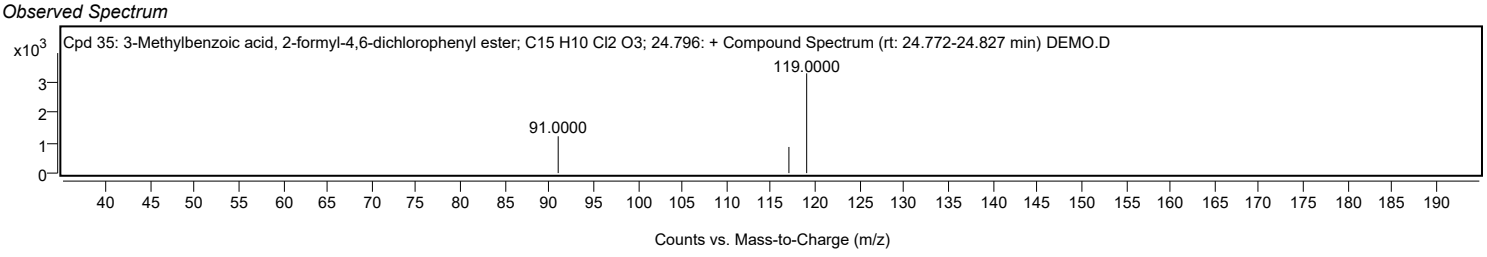
3-Methylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			62.68			NIST.L

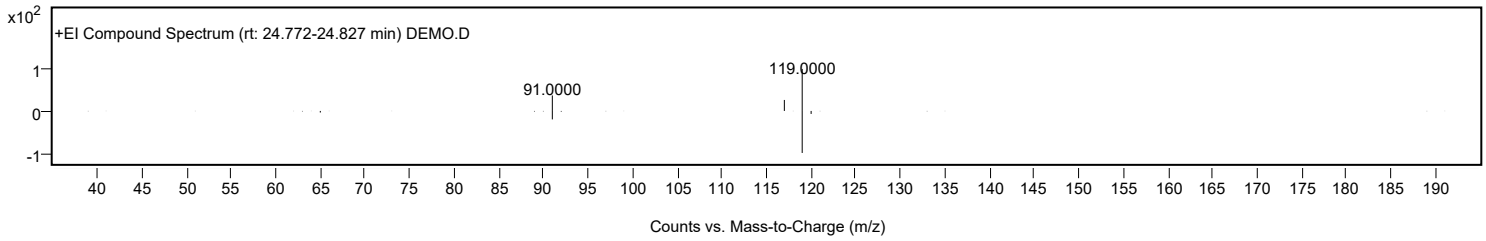
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			62.68			NIST.L

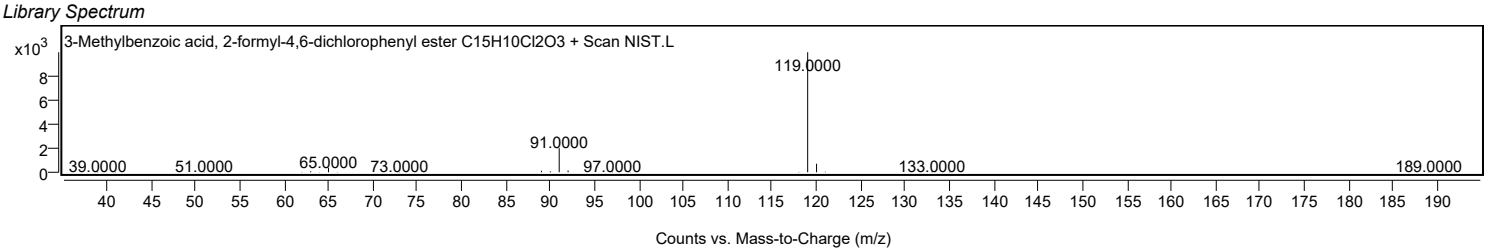
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 36: 2(3H)-Furanone, 5-hexyldihydro-

Compound Discovery Report

Agilent | Trusted Answers

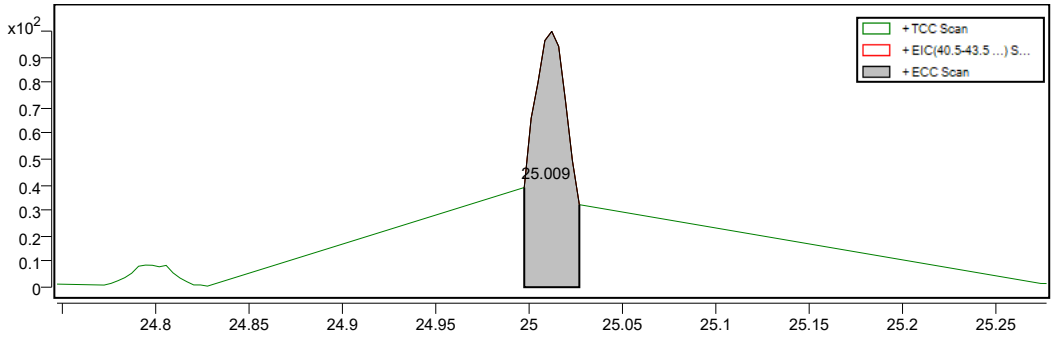
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
2(3H)-Furanone, 5-hexyldihydro-	C10 H18 O2	25.009			706-14-9	LibSearch	81.73	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		81.73			50		

Compound ID Table

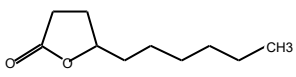
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
2(3H)-Furanone, 5-hexyldihydro-	C10H18O2		LibSearch	25.009	1.959		706-14-9	81.73		
Heptalactone<gamma->	C7H12O2		LibSearch	25.009	11.629		105-21-5	80.47		
2-Propyltetrahydropyran	C8H16O		LibSearch	25.009	8.875		3857-17-8	80.21		
2(3H)-Furanone, dihydro-5-propyl-	C7H12O2		LibSearch	25.009	6.925		105-21-5	80.15		
2(3H)-Furanone, 5-acetyldihydro-	C6H8O3		LibSearch	25.009	6.309		29393-32-6	79.89		
Oxetane, 2-ethyl-3-methyl-	C6H12O		LibSearch	25.009	13.509		53778-62-4	79.72		
2(3H)-Furanone, dihydro-5-propyl-	C7H12O2		LibSearch	25.009	6.925		105-21-5	79.19		
2-Propyltetrahydropyran	C8H16O		LibSearch	25.009	8.875		3857-17-8	79.03		
5-Hydroxypentanal	C5H10O2		LibSearch	25.009	9.192		4221-03-8	78.98		
Heptalactone <gamma->	C7H12O2		LibSearch	25.009			105-21-5	78.86		
2(3H)-Furanone, dihydro-5-propyl-	C7H12O2		LibSearch	25.009	6.925		105-21-5	78.46		
Furan, tetrahydro-2,4-dimethyl-, trans-	C6H12O		LibSearch	25.009	13.159		39168-02-0	78.34		
Furan, tetrahydro-2,4-dimethyl-, cis-	C6H12O		LibSearch	25.009	13.159		39168-01-9	77.82		
Hexane, 3-iodo-	C6H13I		LibSearch	25.009	8.875		31294-91-4	77.53		
2(3H)-Furanone, dihydro-5-pentyl-	C9H16O2		LibSearch	25.009	3.609		104-61-0	77.27		
Hexane <2-methyl->	C7H16		LibSearch	25.009			591-76-4	76.94		
2(3H)-Furanone, dihydro-5-propyl-	C7H12O2		LibSearch	25.009	6.925		105-21-5	76.91		
2(3H)-Furanone, 5-acetyldihydro-	C6H8O3		LibSearch	25.009	6.309		29393-32-6	76.76		
2H-Pyran, 2-(bromomethyl)tetrahydro-	C6H11BrO		LibSearch	25.009	7.242		34723-82-5	76.73		
2-Furanmethanol, tetrahydro-5-methyl-, trans-	C6H12O2		LibSearch	25.009	9.125		54774-28-6	76.58		
2(3H)-Furanone, 5-ethyldihydro-	C6H10O2		LibSearch	25.009	8.575		695-06-7	76.34		
Hexane, 2-bromo-	C6H13Br		LibSearch	25.009	10.842		3377-86-4	76.20		
Valeric anhydride	C10H18O3		LibSearch	25.009			2082-59-9	76.20		
2(3H)-Furanone, dihydro-5-propyl-	C7H12O2		LibSearch	25.009	6.925		105-21-5	76.16		
2(3H)-Furanone, 5-butyldihydro-	C8H14O2		LibSearch	25.009	5.275		104-50-7	76.04		
Hexane, 3-bromo-	C6H13Br		LibSearch	25.009	10.842		3377-87-5	75.99		
2H-Pyran-2-methanol, tetrahydro-	C6H12O2		LibSearch	25.009	8.142		100-72-1	75.88		
2(3H)-Furanone, 5-ethyldihydro-	C6H10O2		LibSearch	25.009	8.575		695-06-7	75.82		
Octalactone <gamma->	C8H14O2		LibSearch	25.009			104-50-7	75.82		
2(3H)-Furanone, 5-hexyldihydro-	C10H18O2		LibSearch	25.009	1.959		706-14-9	75.75		
1,5-Heptadien-4-ol, 3,3,6-trimethyl-	C10H18O		LibSearch	25.009	7.209		27644-04-8	75.69		
Hexane, 2-bromo-	C6H13Br		LibSearch	25.009	10.842		3377-86-4	75.67		
2-Heptene, 2-methoxy-	C8H16O		LibSearch	25.009	10.392		61142-43-6	75.59		
Hexalactone<gamma->	C6H10O2		LibSearch	25.009	15.679		695-06-7	75.49		
Hexane, 3-bromo-	C6H13Br		LibSearch	25.009	10.842		3377-87-5	75.46		
Hexalactone <gamma->	C6H10O2		LibSearch	25.009			695-06-7	75.40		
Sulfurous acid, isohexyl hexyl ester	C12H26O3S		LibSearch	25.009	-4.541		1000309-12-8	75.15		
Decalactone <gamma->	C10H18O2		LibSearch	25.009			706-14-9	74.97		
2-Pentanone, 3-ethyl-3-methyl-	C8H16O		LibSearch	25.009	10.542		19780-65-5	74.71		
2(3H)-Furanone, dihydro-5-propyl-	C7H12O2		LibSearch	25.009	6.925		105-21-5	74.59		
Valeric anhydride	C10H18O3		LibSearch	25.009	3.025		2082-59-9	74.30		
5-Methylhexane-2,4-dione, enol	C7H12O2		LibSearch	25.009	9.775		1000202-24-1	74.28		
Octalactone<gamma->	C8H14O2		LibSearch	25.009	6.989		104-50-7	74.10		
2-Methylbutanoic anhydride	C10H18O3		LibSearch	25.009	5.175		1468-39-9	74.07		
Hexane, 2-methyl-	C7H16		LibSearch	25.009	14.125		591-76-4	74.02		
Artemisia alcohol	C10H18O		LibSearch	25.009	14.249		57590-19-9	73.88		
2(3H)-Furanone, 5-ethyldihydro-	C6H10O2		LibSearch	25.009	8.575		695-06-7	73.87		
Hexane, 3-bromo-	C6H13Br		LibSearch	25.009	10.842		3377-87-5	73.84		
Nonalactone<gamma->	C9H16O2		LibSearch	25.009	2.229		104-61-0	73.80		
Furfuryl alcohol, tetrahydro-5-methyl-, cis-	C6H12O2		LibSearch	25.009	9.125		16015-08-0	73.55		

Compound Chromatograms (overlaid)

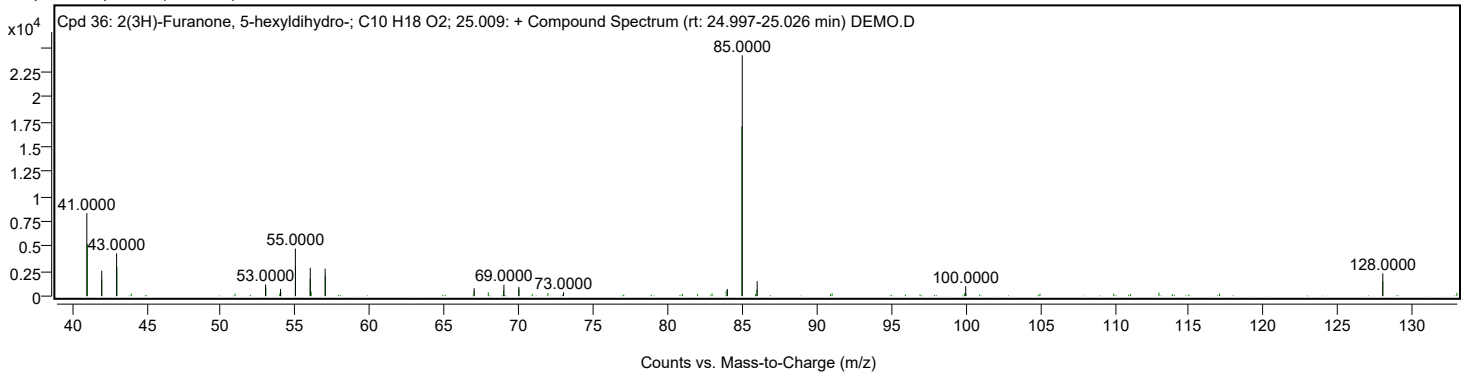


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



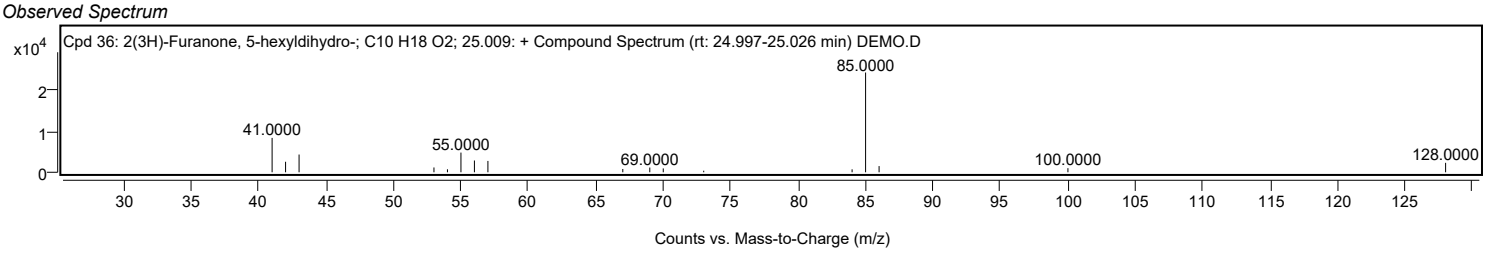
2(3H)-Furanone, 5-hexyldihydro-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			81.73			NIST.L

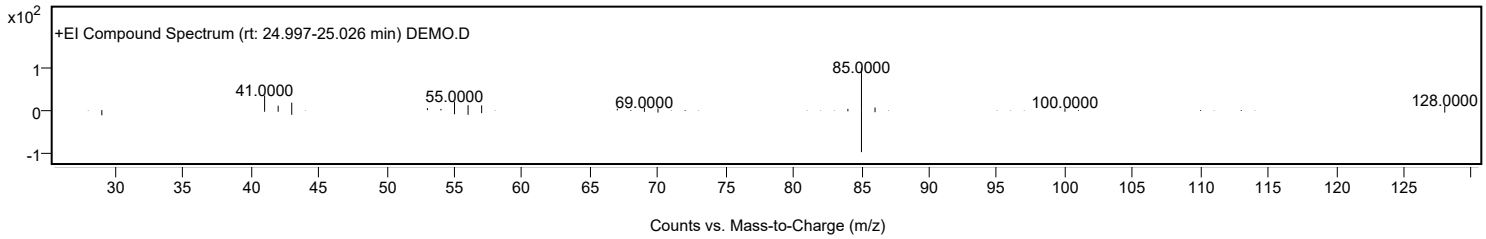
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			81.73			NIST.L

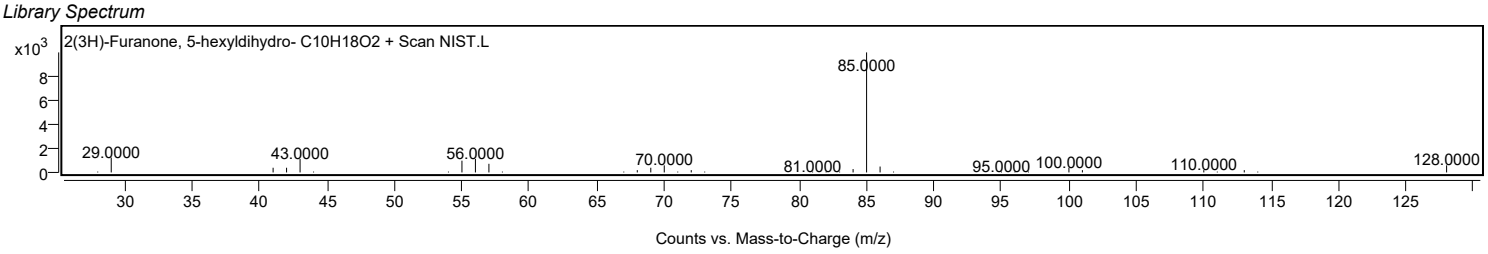
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 37: 2-Butanone, 3-methyl-1-phenyl-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
2-Butanone, 3-methyl-1-phenyl-	C11 H14 O	25.295			2893-05-2	LibSearch	42.30	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		42.30			30		

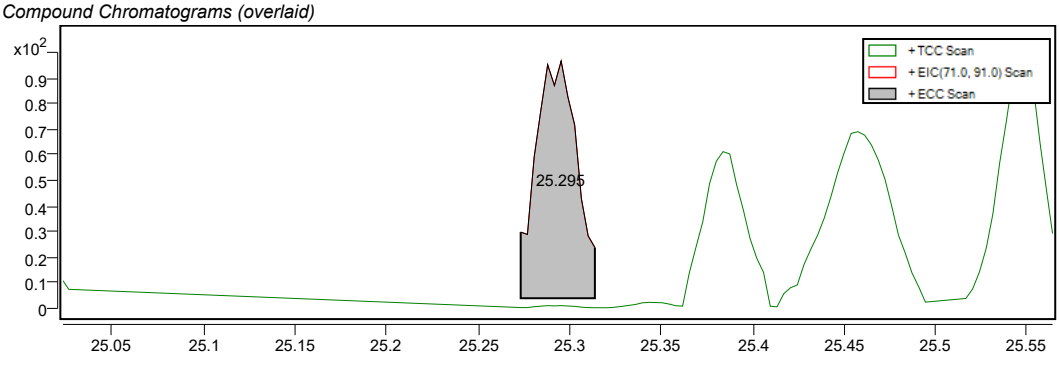
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

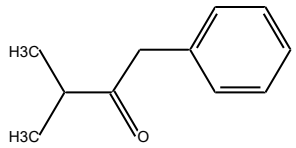
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
2-Butanone, 3-methyl-1-phenyl-	C11H14O		LibSearch	25.295	4.245		2893-05-2	42.30		
2-Butanone, 3-methyl-1-phenyl-	C11H14O		LibSearch	25.295	4.245		2893-05-2	39.22		
2-Pentanone, 1-phenyl-	C11H14O		LibSearch	25.295	3.178		6683-92-7	34.29		
2-Butanone, 3-methyl-1-phenyl-	C11H14O		LibSearch	25.295	4.245		2893-05-2	33.04		
Phenethyl butyrate <alpha,alpha-dimethyl->	C14H20O2		LibSearch	25.295			10094-34-5	33.02		
Benzyl mercaptan, S-(2-methylpropionyl)-	C11H14OS		LibSearch	25.295	0.062		61915-58-0	29.55		
Benzene, (2,2-dimethylbutyl)-	C12H18		LibSearch	25.295	5.195		28080-86-6	26.69		
Propanoic acid, 2-chloro-, 1-methylbutyl ester	C8H15ClO2		LibSearch	25.295	7.628		88736-64-5	25.91		
Isobutyrate dimethyl benzyl carbinyl	C14H20O2		LibSearch	25.295			59354-71-1	23.07		
5-Nonen-4-one, 9-phenyl-, (E)-	C15H20O		LibSearch	25.295	-3.588		55282-85-4	22.34		
Benzenepropanol, .alpha.-1-propenyl-	C12H16O		LibSearch	25.295	0.945		80227-73-2	22.30		
Guanidine, 2-benzyl-1,3-dimethyl-	C10H15N3		LibSearch	25.295	-2.738		55-73-2	20.12		
Butanamide, N-[[5-(4-pyridinyl)-2H-1,2,3,4-tetrazol-2-yl]methyl]-	C11H14N6O		LibSearch	25.295			1000362-24-9	19.82		
2-Ethylbutyric acid, 1-phenylpropyl ester	C15H22O2		LibSearch	25.295	-1.838		1000370-19-4	19.41		
Mefranal	C12H16O		LibSearch	25.295	-0.305		55066-49-4	19.06		
Mefranal	C12H16O		LibSearch	25.295			55066-49-4	18.95		
Neopentyl-.beta.-phenylpropionate	C14H20O2		LibSearch	25.295	-0.905		28048-96-6	17.30		
Neopentyl-.beta.-phenylpropionate	C14H20O2		LibSearch	25.295	-0.905		28048-96-6	16.95		
Perillyl butyrate	C14H22O2		LibSearch	25.295	-1.088		1000428-74-6	13.31		
Dithiocarbamic acid, N,N-dipentyl-S-methyl-	C12H25NS2		LibSearch	25.295	-6.372		1010490-87-8	12.82		
Dithiocarbamic acid, N,N-(3-methylbutyl)-S-methyl-	C12H25NS2		LibSearch	25.295	-4.238		1000490-88-0	12.80		
Propionamide, N-allyl-N-methyl-3-phenyl-	C13H17NO		LibSearch	25.295	-1.055		1000446-22-0	12.63		
Perillyl isobutyrate	C14H22O2		LibSearch	25.295	-0.022		1000429-32-1	12.21		
1,2,4,5-Tetrazine, 1,4-diacetylhexahydro-2,5-bis(3-phenylpropyl)-	C24H32N4O2		LibSearch	25.295	-31.138		35029-01-7	9.19		
Silane, diethyldi(1-phenylpropoxy)-	C22H32O2Si		LibSearch	25.295	-12.955		1000363-27-9	5.90		
3,6-methanonaphth[2,3-b]oxirene-2,7-dione, 4-bromooctahydro-5-hydroxy-	C11H11BrO4		LibSearch	25.295	-4.705		1000397-26-5	5.27		
2-(3-Benzyloxy-4-methoxyphenyl)-3,7-dimethoxy-4H-chromen-4-one	C25H22O6		LibSearch	25.295	-31.005		97257-15-3	5.09		
Cyperanic acid	C15H22O4		LibSearch	25.295	-10.288		117869-89-3	4.75		
17-O-Methyl testosterone ether	C20H30O2		LibSearch	25.295	-9.505		13990-32-4	4.60		
Silane, diethyldi(3-phenylpropoxy)-	C22H32O2Si		LibSearch	25.295	-15.088		1000363-15-8	4.58		

Compound Chromatograms (overlaid)

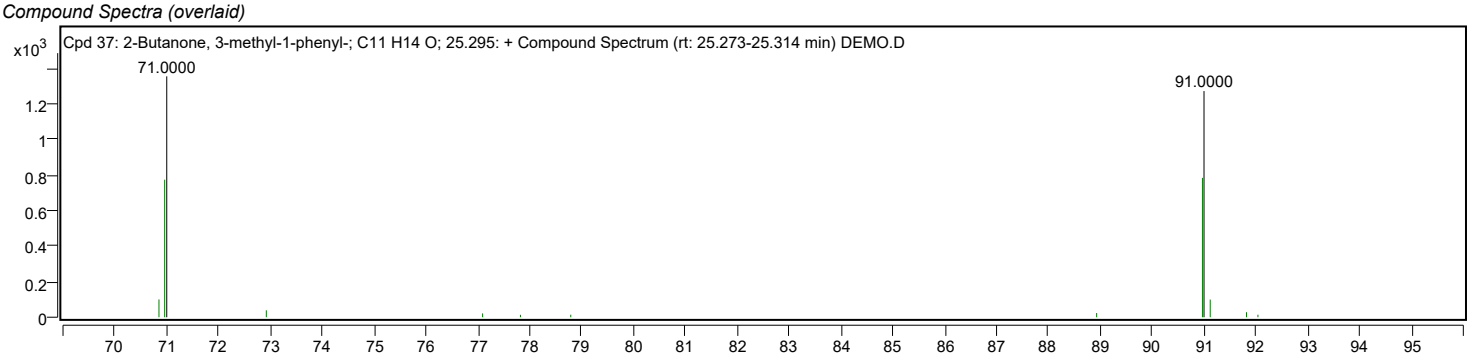


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



Counts vs. Mass-to-Charge (m/z)

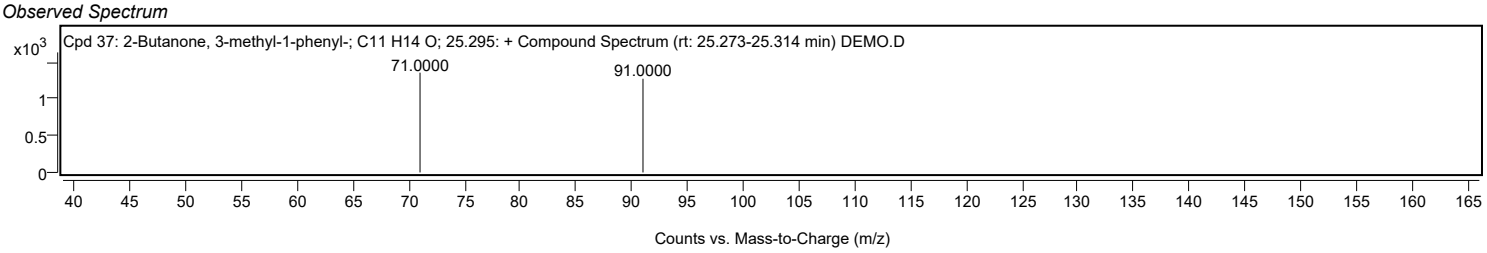
2-Butanone, 3-methyl-1-phenyl-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			42.30			NIST.L

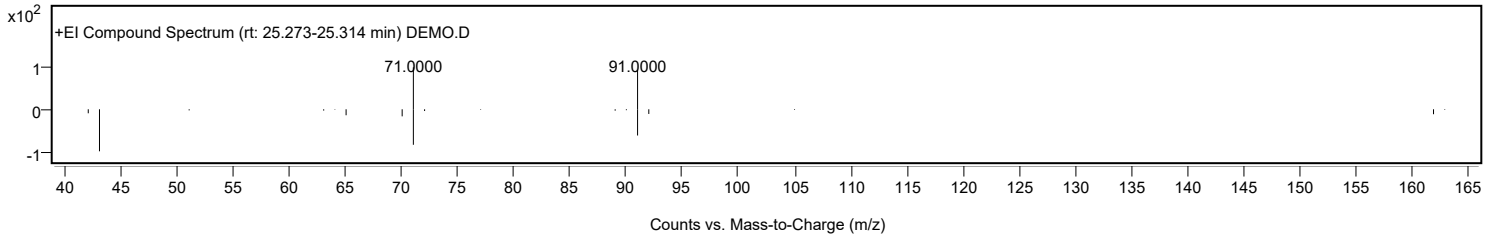
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			42.30			NIST.L

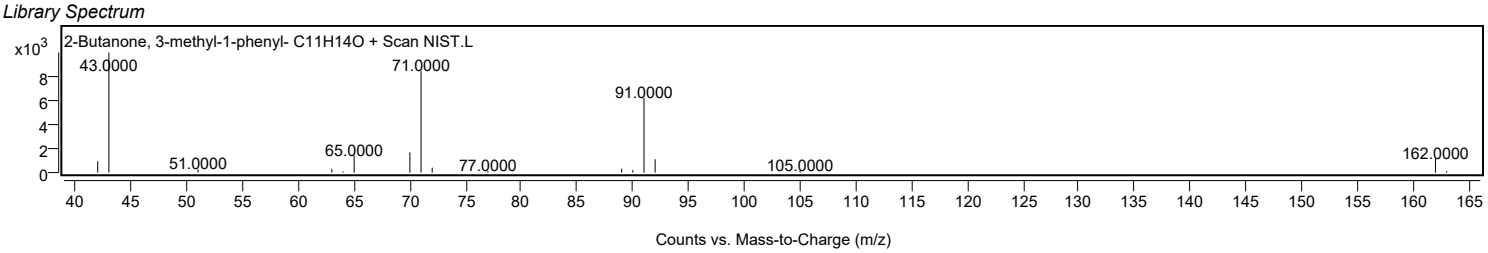
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 38: D-Alanine, N-(4-anisoyl)-, isohexyl ester

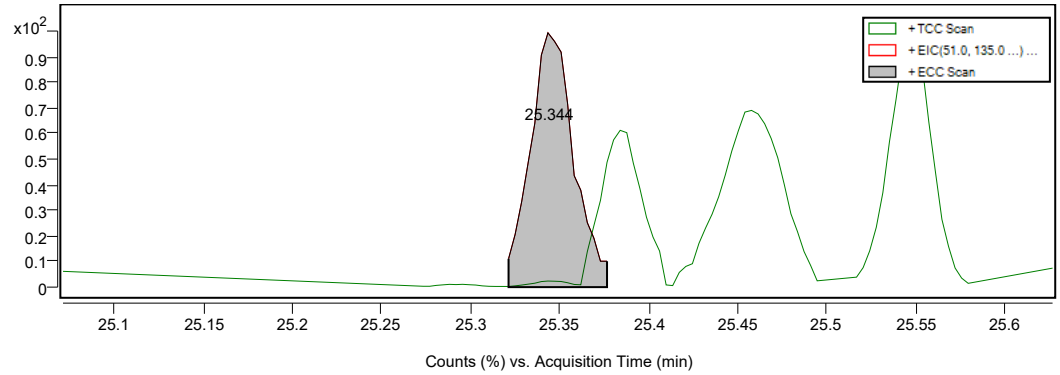
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
D-Alanine, N-(4-anisoyl)-, isohexyl ester	C17 H25 N O4	25.344			1000348-49-0	LibSearch	69.01	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		69.01			50		

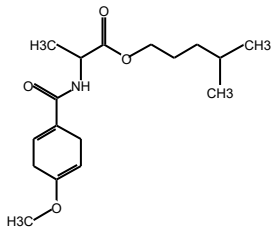
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
D-Alanine, N-(4-anisoyl)-, isohexyl ester	C17H25NO4		LibSearch	25.344	-13.273		1000348-49-0	69.01		
D-Alanine, N-(4-anisoyl)-, hexyl ester	C17H25NO4		LibSearch	25.344	-14.339		1010348-49-1	67.62		
D-Alanine, N-(4-anisoyl)-, pentyl ester	C16H23NO4		LibSearch	25.344	-12.673		1000348-48-9	67.39		
D-Alanine, N-(4-anisoyl)-, butyl ester	C15H21NO4		LibSearch	25.344	-11.023		1000348-48-8	67.38		
D-Alanine, N-(4-anisoyl)-, ethyl ester	C13H17NO4		LibSearch	25.344	-7.706		1000348-48-5	66.93		
D-Alanine, N-(4-anisoyl)-, octyl ester	C19H29NO4		LibSearch	25.344	-17.656		1000348-49-2	66.75		
D-Alanine, N-(4-anisoyl)-, decyl ester	C21H33NO4		LibSearch	25.344	-20.956		1000348-49-4	66.36		
D-Alanine, N-(4-anisoyl)-, isobutyl ester	C15H21NO4		LibSearch	25.344	-9.956		1000348-48-7	66.31		
D-Alanine, N-(4-anisoyl)-, undecyl ester	C22H35NO4		LibSearch	25.344	-22.623		1000348-49-5	65.70		
D-Alanine, N-(4-anisoyl)-, nonyl ester	C20H31NO4		LibSearch	25.344	-19.306		1000348-49-3	65.24		
D-Alanine, N-(4-anisoyl)-, propyl ester	C14H19NO4		LibSearch	25.344	-9.373		1000348-48-6	65.22		
D-Alanine, N-(4-anisoyl)-, tridecyl ester	C24H39NO4		LibSearch	25.344	-25.939		1000348-49-7	65.18		
D-Alanine, N-(4-anisoyl)-, dodecyl ester	C23H37NO4		LibSearch	25.344	-24.273		1000348-49-6	65.06		
D-Alanine, N-(4-anisoyl)-, pentadecyl ester	C26H43NO4		LibSearch	25.344	-29.239		1000348-49-8	64.17		
D-Alanine, N-(3-anisoyl)-, isohexyl ester	C17H25NO4		LibSearch	25.344	-13.273		1000354-04-5	63.23		
3,4-Methylenedioxyphenyl acetone	C10H10O3		LibSearch	25.344	0.794		4676-39-5	63.22		
l-Alanine, N-(O-anisoyl)-, methyl ester	C12H15NO4		LibSearch	25.344	-6.056		1010299-75-1	62.70		
D-Alanine, N-(3-anisoyl)-, nonyl ester	C20H31NO4		LibSearch	25.344	-19.306		1000354-04-8	61.05		
D-Alanine, N-(4-anisoyl)-, hexadecyl ester	C27H45NO4		LibSearch	25.344	-30.906		1000348-49-9	60.72		
1,3-Benzodioxole, 5-(2,2-dimethylethyl)-	C11H14O2		LibSearch	25.344	2.477		28140-80-9	60.29		
3,4-Methylenedioxyphenyl acetone	C10H10O3		LibSearch	25.344	0.794		4676-39-5	60.12		
D-Alanine, N-(3-anisoyl)-, butyl ester	C15H21NO4		LibSearch	25.344	-11.023		1000354-04-3	60.00		
D-Alanine, N-(4-anisoyl)-, heptadecyl ester	C28H47NO4		LibSearch	25.344	-32.556		1000348-50-0	59.44		
D-Alanine, N-(3-anisoyl)-, octyl ester	C19H29NO4		LibSearch	25.344	-17.656		1000354-04-7	59.43		
3,4-Methylenedioxyphenyl acetone	C10H10O3		LibSearch	25.344	0.794		4676-39-5	59.18		
3,4-Methylenedioxyphenyl acetone	C10H10O3		LibSearch	25.344	0.794		4676-39-5	58.93		
l-Alanine, N-(p-anisoyl)-, methyl ester	C12H15NO4		LibSearch	25.344	-6.056		1000299-66-8	58.87		
D-Alanine, N-(3-anisoyl)-, pentyl ester	C16H23NO4		LibSearch	25.344	-12.673		1000354-04-4	58.48		
D-Alanine, N-(3-anisoyl)-, heptyl ester	C18H27NO4		LibSearch	25.344	-15.989		1000354-04-6	58.47		
D-Alanine, N-(3-anisoyl)-, tridecyl ester	C24H39NO4		LibSearch	25.344	-25.939		1010354-05-1	58.29		
D-Alanine, N-(3-anisoyl)-, undecyl ester	C22H35NO4		LibSearch	25.344	-22.623		1000354-04-9	58.04		
D-Alanine, N-(4-anisoyl)-, tetradecyl ester	C25H41NO4		LibSearch	25.344	-27.589		1000354-06-5	58.02		
l-Alanine, N-(m-anisoyl)-, heptyl ester	C18H27NO4		LibSearch	25.344	-15.989		1000313-96-5	57.74		
3,4-Methylenedioxyphenyl acetone	C10H10O3		LibSearch	25.344	0.794		4676-39-5	57.16		
l-Alanine, N-(m-anisoyl)-, octyl ester	C19H29NO4		LibSearch	25.344	-17.656		1000313-96-6	57.07		
D-Alanine, N-(3-anisoyl)-, dodecyl ester	C23H37NO4		LibSearch	25.344	-24.273		1000354-05-0	57.02		
l-Alanine, N-(m-anisoyl)-, nonyl ester	C20H31NO4		LibSearch	25.344	-19.306		1000313-96-7	56.71		
D-Alanine, N-(3-anisoyl)-, pentadecyl ester	C26H43NO4		LibSearch	25.344	-29.239		1000354-05-3	55.94		
l-Alanine, N-(m-anisoyl)-, decyl ester	C21H33NO4		LibSearch	25.344	-20.956		1000313-96-8	55.88		
l-Alanine, N-(m-anisoyl)-, isobutyl ester	C15H21NO4		LibSearch	25.344	-9.956		1000313-96-3	55.52		
l-Alanine, N-(m-anisoyl)--, propyl ester	C14H19NO4		LibSearch	25.344	-9.373		1000313-96-2	55.45		
D-Alanine, N-(3-anisoyl)-, tetradecyl ester	C25H41NO4		LibSearch	25.344	-27.589		1000354-05-2	53.97		
1H-Pyrazole-5-carboxamide, 3-cyclopropyl-N-(1-methylpropyl)-	C11H17N3O		LibSearch	25.344	-7.073		1000351-60-3	53.37		
D-Alanine, N-(3-anisoyl)-, hexadecyl ester	C27H45NO4		LibSearch	25.344	-30.906		1000354-05-4	53.03		
Sarcosine, N-(4-methoxybenzoyl)-, isohexyl ester	C17H25NO4		LibSearch	25.344	-11.006		1000321-42-3	52.85		
l-Alanine, N-(m-anisoyl)-, methyl ester	C12H15NO4		LibSearch	25.344	-6.056		1010299-70-6	51.14		
Benzamide, 2-methoxy-N-(2-butyl)-N-(2-ethylhexyl)-	C20H33NO2		LibSearch	25.344	-12.123		1000464-25-9	50.65		
l-Alanine, N-(m-anisoyl)-, pentyl ester	C16H23NO4		LibSearch	25.344	-12.673		1000313-96-4	50.27		
2,5-Bis(2-methylpropyl)-3,6-dimethylpyrazine	C14H24N2		LibSearch	25.344	-1.139		10132-41-9	48.65		
l-Alanine, N-(m-anisoyl)-, undec-10-enyl ester	C22H33NO4		LibSearch	25.344	-22.456		1000313-96-9	48.60		

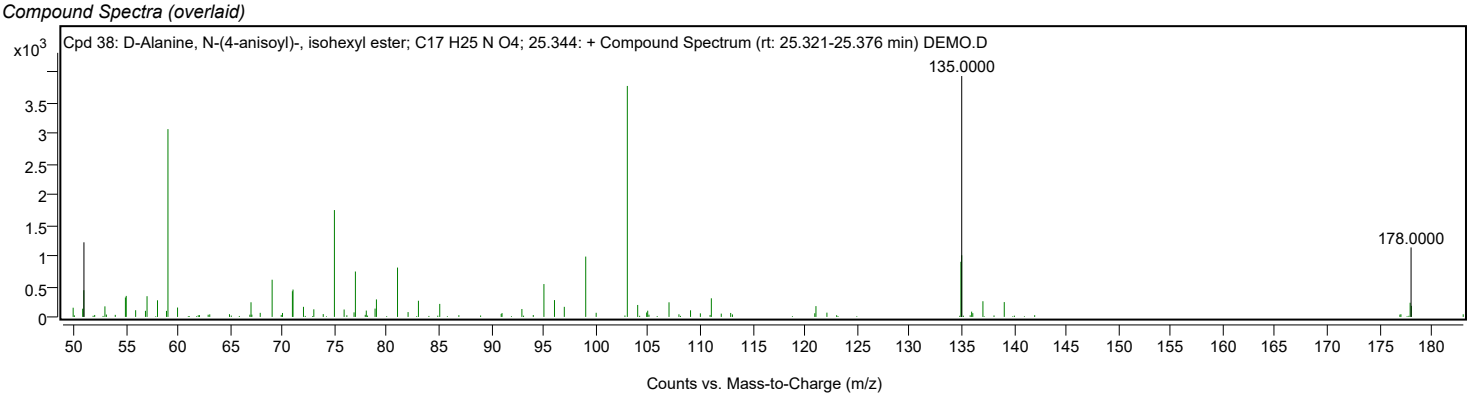
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



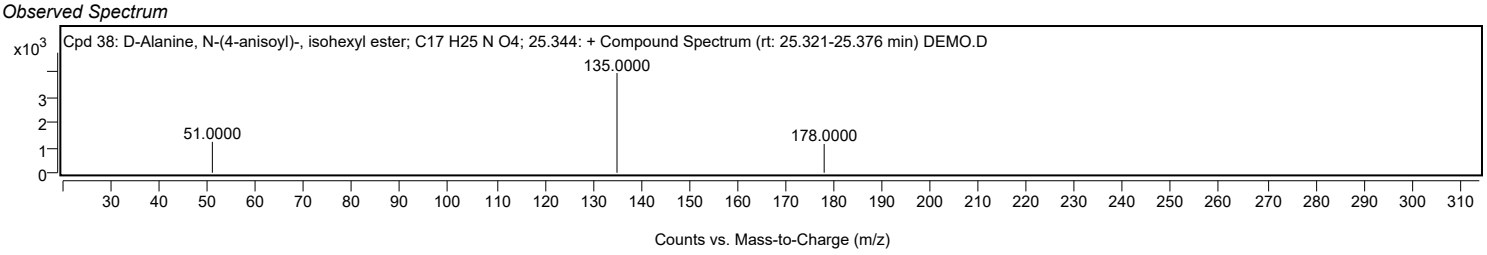
D-Alanine, N-(4-anisoyl)-, isohexyl ester

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			69.01			NIST.L

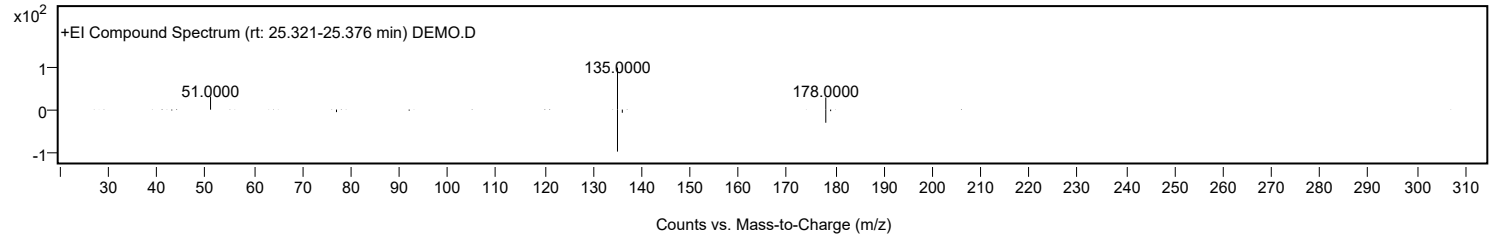
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			69.01			NIST.L

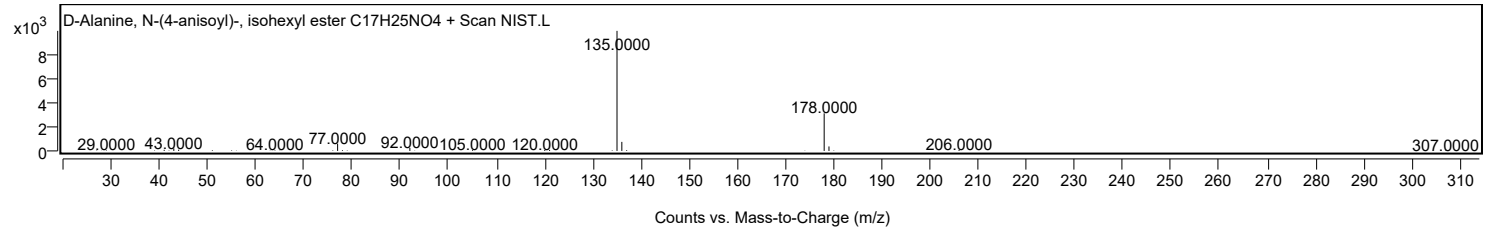
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 39: Hydroxycitronellal <diethyl-> acetal

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Hydroxycitronellal <diethyl-> acetal	C14 H30 O3	25.386			7779-94-4	LibSearch	89.78	Chrom Decon	PWNose.xml

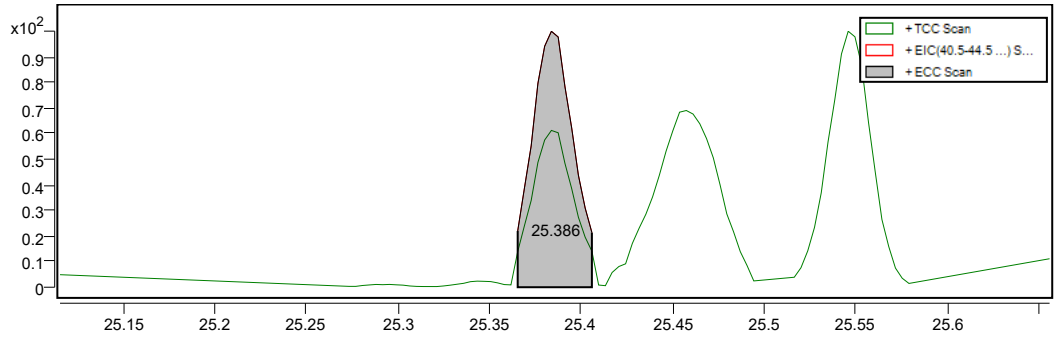
Compound Discovery Report

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		89.78			50		

Compound ID Table

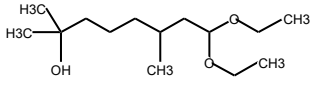
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Hydroxycitronellal <diethyl-> acetal	C14H30O3		LibSearch	25.386			7779-94-4	89.78		
Hydroxycitronellal diethyl acetal	C14H30O3		LibSearch	25.386	-0.080		1000431-48-9	89.63		
Hydroxy citronellal<diethyl acetal->	C14H30O3		LibSearch	25.386	-4.754		7779-94-4	84.79		
Hexenal<diethyl acetal-(3Z-)->	C10H20O2		LibSearch	25.386	14.246		73545-18-3	66.16		
Hexenal<diethyl acetal-(3E)->	C10H20O2		LibSearch	25.386	14.376		51795-75-6	66.15		
Hexenal <diethyl acetal-(3E)->	C10H20O2		LibSearch	25.386			51795-75-6	66.14		
2-Diethoxymethyl-3-methyl-butan-1-ol	C10H22O3		LibSearch	25.386	5.103		1000194-34-9	64.77		
Hex-3-enal <cis-, diethyl-> acetal	C10H20O2		LibSearch	25.386			73545-18-3	64.40		
4-Decene, 1,1-diethoxy-, (Z)	C14H28O2		LibSearch	25.386			73545-19-4	63.59		
2-Dimethylsilyloxytridecane	C15H34OSi		LibSearch	25.386	-0.914		1000278-83-1	62.74		
Heptanal, diethyl acetal-	C11H24O2		LibSearch	25.386			688-82-4	62.30		
Decenal<4E->,diethyl acetal	C14H28O2		LibSearch	25.386	-2.344		0-00-0	62.23		
Heptanal, diethyl acetal-	C11H24O2		LibSearch	25.386	10.126		688-82-4	61.88		
2-Dimethylsilyloxytetradecane	C16H36OSi		LibSearch	25.386	-2.564		1000278-84-3	61.81		
cis-3-Hexenal diethyl acetal	C10H20O2		LibSearch	25.386	6.870		73545-18-3	61.66		
Decenal<4Z->, diethyl acetal	C14H28O2		LibSearch	25.386	-1.664		73545-19-4	61.63		
Heptenal<4E->, diethyl acetal	C11H22O2		LibSearch	25.386	10.126		18492-66-5	61.37		
Octane, 1,1-diethoxy-	C12H26O2		LibSearch	25.386	3.686		54889-48-4	61.35		
Heptenal<4Z->, diethyl acetal	C11H22O2		LibSearch	25.386	10.496		18492-65-4	61.11		
Heptenal <4Z->, diethyl acetal	C11H22O2		LibSearch	25.386			18492-65-4	61.05		
4-Decene, 1,1-diethoxy-, (E)	C14H28O2		LibSearch	25.386			73545-19-4	60.78		
1-Butene, 4,4-diethoxy-2-methyl-	C9H18O2		LibSearch	25.386	9.203		54340-95-3	60.67		
Silane, (chloromethyl)ethoxydimethyl-	C5H13ClOSi		LibSearch	25.386	13.236		13508-53-7	60.66		
2-(2,2-Diethoxyethyl)furan	C10H16O3		LibSearch	25.386	4.936		1000411-31-4	60.54		
Hexadecanoic acid, 3-hydroxy-, methyl ester	C17H34O3		LibSearch	25.386	-8.630		51883-36-4	60.49		
Heptenal <4E->, diethyl acetal	C11H22O2		LibSearch	25.386			18492-66-5	60.39		
Methyl 3-hydroxytetradecanoate	C15H30O3		LibSearch	25.386	-5.314		55682-83-2	60.27		
Butyraldehyde <3-methyl-, diethyl-> acetal	C9H20O2		LibSearch	25.386			3842-03-3	60.23		
cis-3-Hexenal diethyl acetal	C10H20O2		LibSearch	25.386	6.870		73545-18-3	60.20		
Methyl 3-hydroxytetradecanoate	C15H30O3		LibSearch	25.386	-5.314		55682-83-2	60.04		
Octadecanoic acid, 3-hydroxy-, methyl ester	C19H38O3		LibSearch	25.386	-11.930		2420-36-2	59.90		
Butane, 1,1-diethoxy-3-methyl-	C9H20O2		LibSearch	25.386	9.736		3842-03-3	59.78		
Alpinal diethyl acetal	C13H28O2		LibSearch	25.386	4.503		1000430-79-8	59.62		
Octane, 1,1-diethoxy-	C12H26O2		LibSearch	25.386	3.686		54889-48-4	59.51		
7-Diethoxymethylbicyclo[3.2.0]heptan-2-one	C12H20O3		LibSearch	25.386	1.070		1010192-95-9	59.42		
Decane, 1,1-diethoxy-	C14H30O2		LibSearch	25.386	0.370		34764-02-8	59.02		
Heptane, 1,1-diethoxy-	C11H24O2		LibSearch	25.386	5.353		688-82-4	59.00		
Dimethyl(1-cyclopentylethoxy)silane	C9H20OSi		LibSearch	25.386	8.320		1000278-72-3	58.72		
Butane, 1,1-diethoxy-3-methyl-	C9H20O2		LibSearch	25.386	9.736		3842-03-3	58.43		
Citronellal <hydroxy-> dimethyl acetal	C12H26O3		LibSearch	25.386			141-92-4	58.23		
Butane, 1,1-diethoxy-3-methyl-	C9H20O2		LibSearch	25.386	9.736		3842-03-3	58.01		
Silane, (chloromethyl)ethoxydimethyl-	C5H13ClOSi		LibSearch	25.386	13.236		13508-53-7	57.94		
Butane, 1,1-diethoxy-3-methyl-	C9H20O2		LibSearch	25.386	9.736		3842-03-3	57.90		
Formic acid, TBDMS derivative	C7H16O2Si		LibSearch	25.386	11.936		1000366-59-6	57.73		
Nonane, 1,1-diethoxy-	C13H28O2		LibSearch	25.386	2.036		54815-13-3	57.67		
Decane, 1,1-diethoxy-	C14H30O2		LibSearch	25.386	0.370		34764-02-8	57.55		
Silane, (chloromethyl)ethoxydimethyl-	C5H13ClOSi		LibSearch	25.386	13.236		13508-53-7	57.24		
Acrolein, 3-ethoxy-, diethyl acetal	C9H18O3		LibSearch	25.386	7.270		5444-80-4	56.65		
cis-4-Hepten-1-al diethyl acetal	C11H22O2		LibSearch	25.386	5.220		18492-65-4	56.61		
1-Butene, 4,4-diethoxy-2-methyl-	C9H18O2		LibSearch	25.386	9.203		54340-95-3	56.35		

Compound Chromatograms (overlaid)

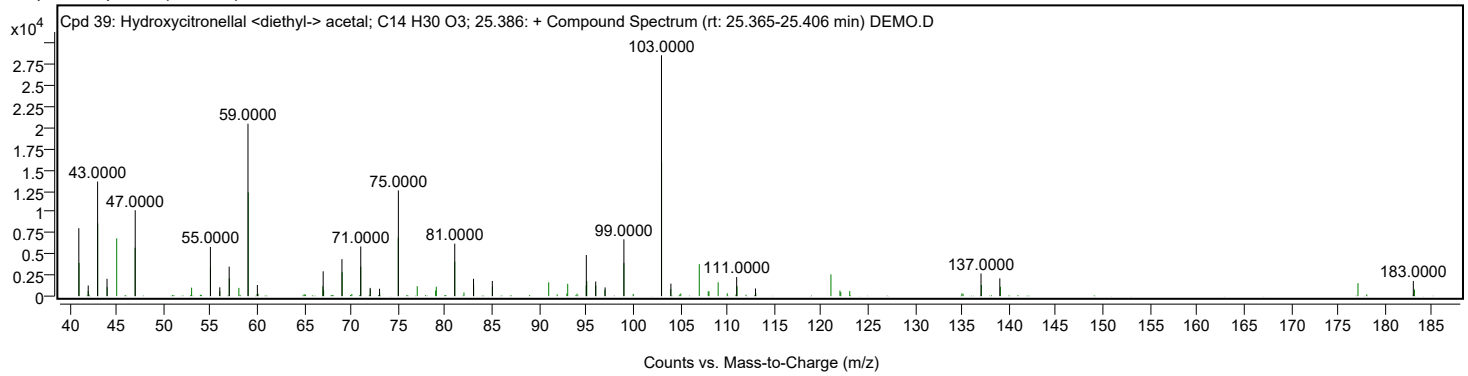


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



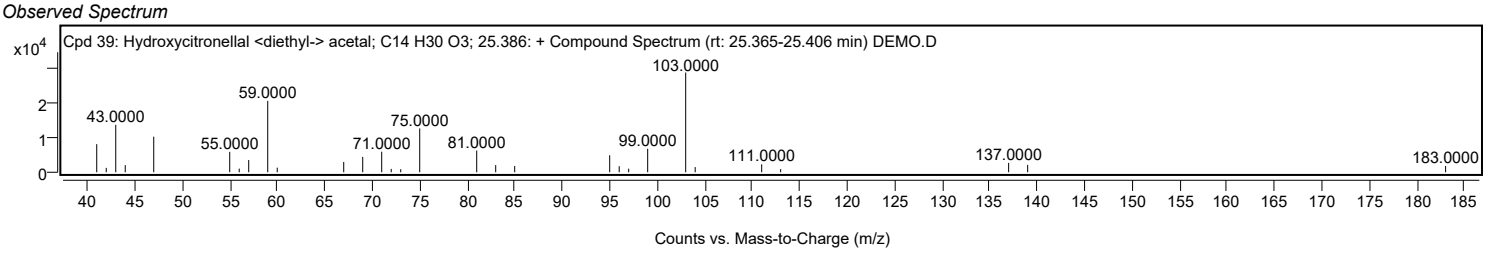
Hydroxycitronellal <diethyl-> acetal

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			89.78			PWNose.xml

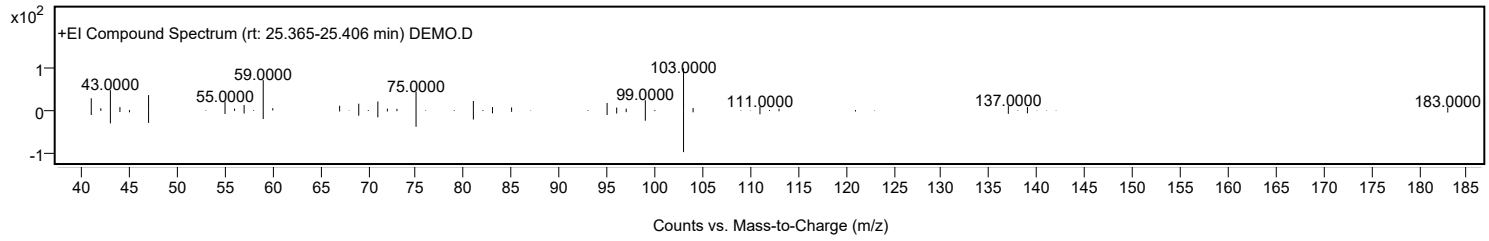
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			89.78			PWNose.xml

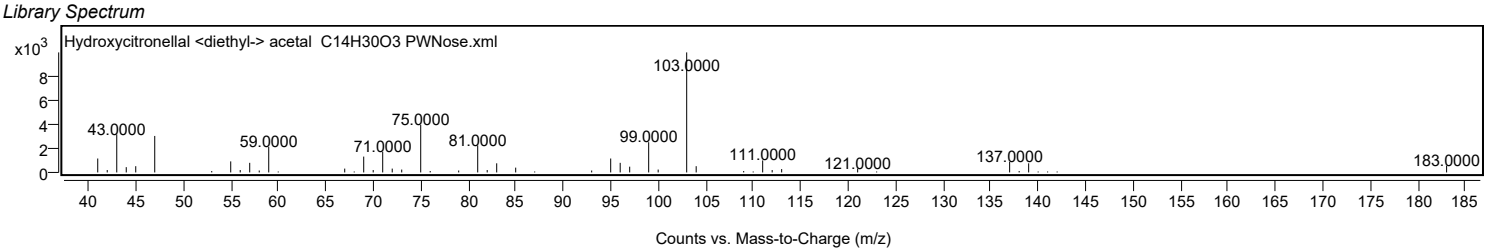
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 40: benzamide, N-[4-[[2-[4-[(butylsulfonyl)amino]phenoxy]-1-oxotetradecyl]amino]-2-hydroxyphenyl]-

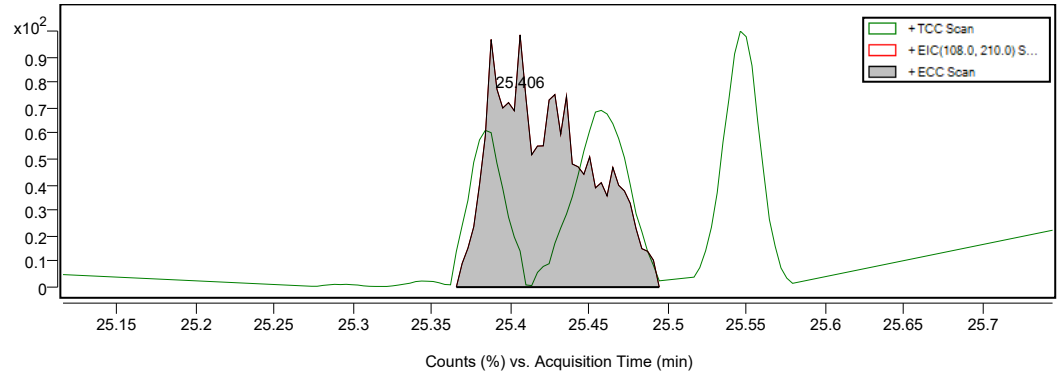
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
benzamide, N-[4-[[2-[4-[(butylsulfonyl)amino]phenoxy]-1-oxotetradecyl]amino]-2-hydroxyphenyl]-	C37 H51 N3 O6 S	25.406			1000403-01-5	LibSearch	9.67	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		9.67			1		

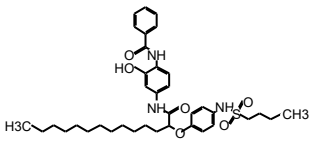
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
benzamide, N-[4-[[2-[4-[(butylsulfonyl)amino]phenoxy]-1-oxotetradecyl]amino]-2-hydroxyphenyl]-	C37H51N3O6S		LibSearch	25.406	-69.494		1000403-01-5	9.67		

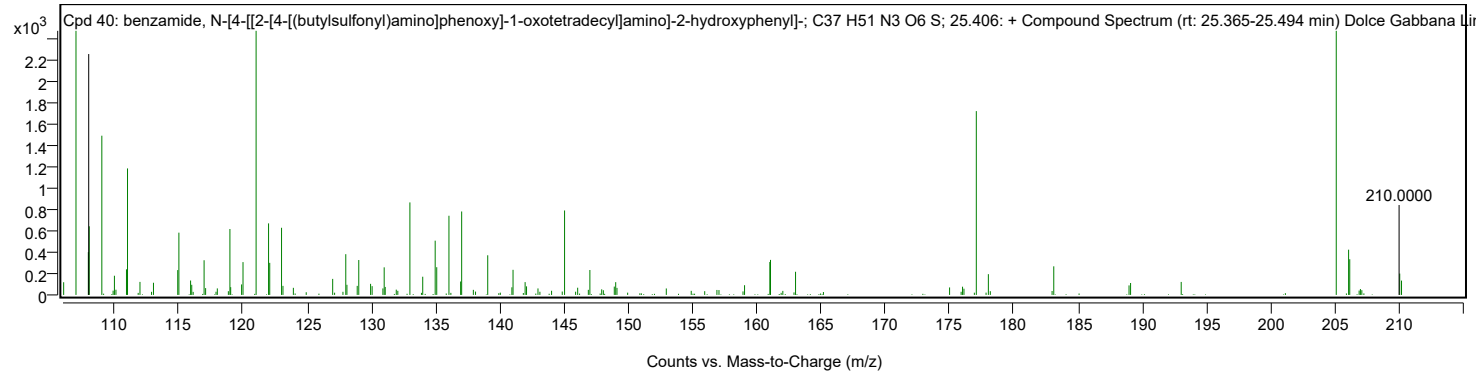
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



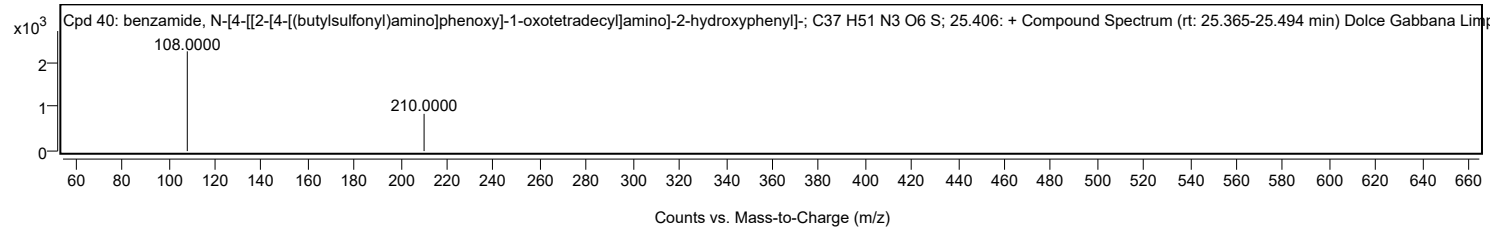
benzamide, N-[4-[[2-[4-[(butylsulfonyl)amino]phenoxy]-1-oxotetradecyl]amino]-2-hydroxyphenyl]-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			9.67			NIST.L

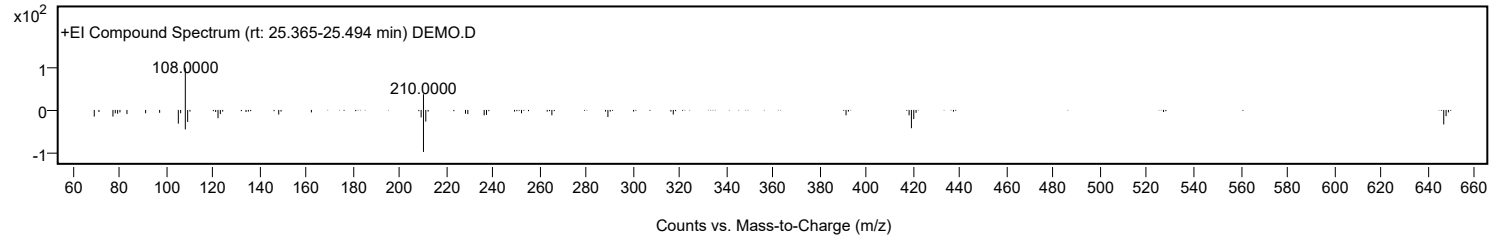
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			9.67			NIST.L

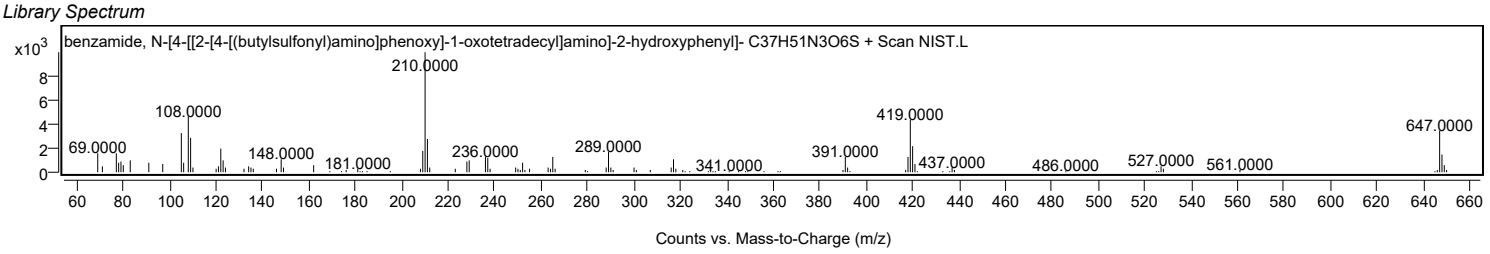
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 41: Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-, methylcarbamate

Compound Discovery Report

Agilent | Trusted Answers

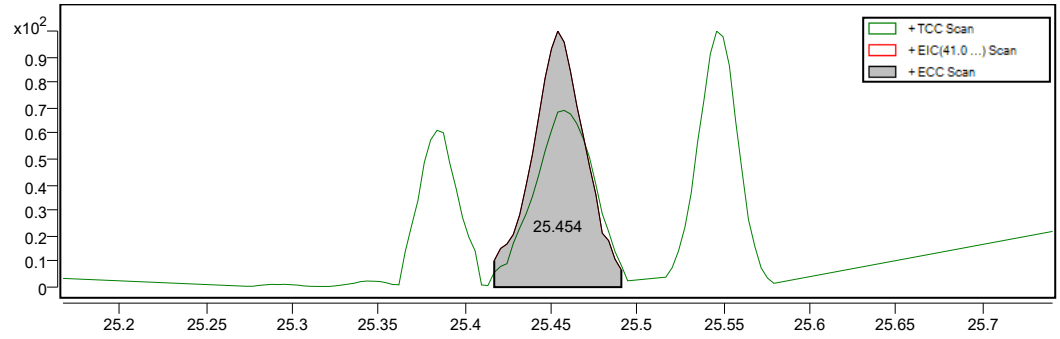
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-, methylcarbamate	C17 H27 N O2	25.454			1918-11-2	LibSearch	84.98	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		84.98			50		

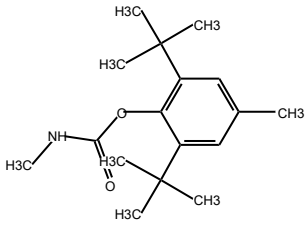
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-, methylcarbamate	C17H27NO2		LibSearch	25.454	-8.313		1918-11-2	84.98		
BHT	C15H24O		LibSearch	25.454			128-37-0	84.65		
Butylated Hydroxytoluene	C15H24O		LibSearch	25.454	-2.346		128-37-0	81.82		
Butylated Hydroxytoluene	C15H24O		LibSearch	25.454	-2.346		128-37-0	81.77		
Butylated Hydroxytoluene	C15H24O		LibSearch	25.454	-2.346		128-37-0	80.71		
Butylated Hydroxytoluene	C15H24O		LibSearch	25.454	-2.346		128-37-0	80.34		
Phenol, 4,6-di(1,1-dimethylethyl)-2-methyl-	C15H24O		LibSearch	25.454	-2.346		616-55-7	78.63		
Butylated Hydroxytoluene	C15H24O		LibSearch	25.454	-2.346		128-37-0	78.08		
Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-, methylcarbamate	C17H27NO2		LibSearch	25.454	-8.313		1918-11-2	77.81		
Butylated Hydroxytoluene	C15H24O		LibSearch	25.454	-2.346		128-37-0	77.70		
Phenol, 4,6-di(1,1-dimethylethyl)-2-methyl-	C15H24O		LibSearch	25.454	-2.346		616-55-7	75.13		
2,4,6-Tris(1,1-dimethylethyl)-4-methylcyclohexa-2,5-dien-1-one	C19H32O		LibSearch	25.454	-4.713		19687-22-0	75.00		
Phenol, 2,4,6-tris(1-methylethyl)-	C15H24O		LibSearch	25.454	-1.963		2934-07-8	73.88		
Butylated hydroxytoluene	C15H24O		LibSearch	25.454	-3.976		128-37-0	72.35		
Propanoic acid, 2-methyl-3-[4-t-butyl]phenyl-	C14H20O2		LibSearch	25.454	-3.063		1000131-87-0	71.41		
2,6-Di-t-butyl-4-methylphenol acetate(ester)	C17H26O2		LibSearch	25.454	-4.996		29311-34-0	69.17		
2H-1-Benzopyran, 6,7-dimethoxy-2,2-dimethyl-	C13H16O3		LibSearch	25.454	-2.046		644-06-4	66.64		
4,6-di-tert-Butyl-m-cresol	C15H24O		LibSearch	25.454	-2.346		497-39-2	66.46		
2,6-Bis(1,1-dimethylethyl)-4-methyl-4-isopropylcyclohexa-2,5-dien-1-one	C18H30O		LibSearch	25.454	-3.396		4278-82-4	65.33		
Cyclopropanecarboxylic acid, 1-hydroxy-, (2,6-di-t-butyl-4-methylphenyl) ester	C19H28O3		LibSearch	25.454	-10.846		108546-75-4	64.87		
Phenol, 2,4-bis(1,1-dimethylpropyl)-	C16H26O		LibSearch	25.454	-3.779		120-95-6	64.31		
2H-1-Benzopyran, 6,7-dimethoxy-2,2-dimethyl-	C13H16O3		LibSearch	25.454	-2.046		644-06-4	63.14		
Phenol, 2,4-bis(1,1-dimethylpropyl)-	C16H26O		LibSearch	25.454	-3.779		120-95-6	62.66		
Phenol, 2,4-bis(1,1-dimethylpropyl)-	C16H26O		LibSearch	25.454	-3.779		120-95-6	61.88		
Ethyl 4-acetyl-3,5-dimethylbenzoate	C13H16O3		LibSearch	25.454	-3.463		1000431-98-6	61.68		
Ageratochromene	C13H16O3		LibSearch	25.454	-9.706		644-06-4	61.52		
Trimethyl-3,4-methylenedioxychromane	C13H16O3		LibSearch	25.454	-2.796		1000378-97-7	60.99		
Benzo[b]dihydropyran, 6-hydroxy-4,4,5,7,8-pentamethyl-	C14H20O2		LibSearch	25.454	-5.379		50442-70-1	59.98		
1-(Hydroxy-phenyl-methyl)-2-methyl-cyclopropanecarboxylic acid, 2,6-di-t-butyl-4-methyl-phenyl ester	C27H36O3		LibSearch	25.454	-24.513		108546-86-7	59.61		
Ethanone, 1-(5,6,7,8-tetrahydro-2,8,8-trimethyl-4H-cyclohepta[b]furan-5-yl)-	C14H20O2		LibSearch	25.454	-1.746		71596-88-8	59.55		
2,4-Di-tert-amylphenol, acetate	C18H28O2		LibSearch	25.454	-6.429		1000467-03-0	59.49		
Propanoic acid, 2,2-dimethyl-, 2,6-bis(1,1-dimethylethyl)-4-methylphenyl ester	C20H32O2		LibSearch	25.454	-8.563		54644-43-8	59.18		
4-Phenyl-3-buten-2-ol, (E)-, TMS derivative	C13H20OSi		LibSearch	25.454	3.454		76987-16-1	59.12		
1,3-Dioxolane, 2-(2,4-dimethylphenyl)-2,4,5-trimethyl-, (2.alpha.,4.alpha.,5.beta.)-	C14H20O2		LibSearch	25.454	-1.779		74752-98-0	58.89		
5H,6H,7H-pyrrolo[3,4-b]pyridine-5,7-dione, TMS derivative	C10H12N2O2Si		LibSearch	25.454	0.354		1000485-20-1	58.88		
2,4-Di-tert-amylphenol, O-isopropyloxycarbonyl-	C20H32O3		LibSearch	25.454	-9.946		1000487-38-5	57.76		
Silane, methyltriisopropoxy-	C10H24O3Si		LibSearch	25.454	9.437		1000416-18-8	57.50		
1-Phenyl-1-hepten-3-ol, (E)-, TMS derivative	C16H26OSi		LibSearch	25.454	-1.513		1010164-85-1	57.18		
Benzenamine, N,N-diethyl-4-(2-nitroethenyl)-	C12H16N2O2		LibSearch	25.454	-3.596		64462-51-7	57.16		
Succinic acid, di(2-ethylphenyl) ester	C20H22O4		LibSearch	25.454	-16.629		1000389-95-7	57.06		
Silane, dodecyltripropoxy-	C21H46O3Si		LibSearch	25.454	-11.979		1610355-28-6	56.89		
1-Aminocyclopropanecarboxylic acid, 2,6-di-t-butyl-4-methyl-phenyl ester	C19H29NO2		LibSearch	25.454	-11.963		1000193-63-3	56.64		
Cyclopropanecarboxylic acid, 1-(hydroxyphenylmethyl)-2-phenyl-, 2,6-bis(1,1-dimethylethyl)-4-methylphenyl ester	C32H38O3		LibSearch	25.454	-34.079		108546-90-3	56.63		
Hexyltripropoxysilane	C15H34O3Si		LibSearch	25.454	-2.046		19763-34-9	56.34		
Xylazine	C12H16N2S		LibSearch	25.454	-7.363		7361-61-7	55.63		
1-(4-Butoxy-2,6-dimethylphenyl)ethanone	C14H20O2		LibSearch	25.454	-3.596		1000190-22-9	55.28		
1-Ethyl-1-(2-phenylethoxy)-1-silacyclopentane	C14H22OSi		LibSearch	25.454	0.037		1000279-36-8	54.96		
Xylazine	C12H16N2S		LibSearch	25.454	-7.363		7361-61-7	54.73		
Propanamide, 3-(4-ethoxyphenyl)-N-(3-trifluoromethylphenyl)-3-oxo-	C19H18F3NO3		LibSearch	25.454	-16.829		1000271-49-2	54.63		
Atropic acid, TMS derivative	C12H16O2Si		LibSearch	25.454	3.204		1000484-83-7	54.46		

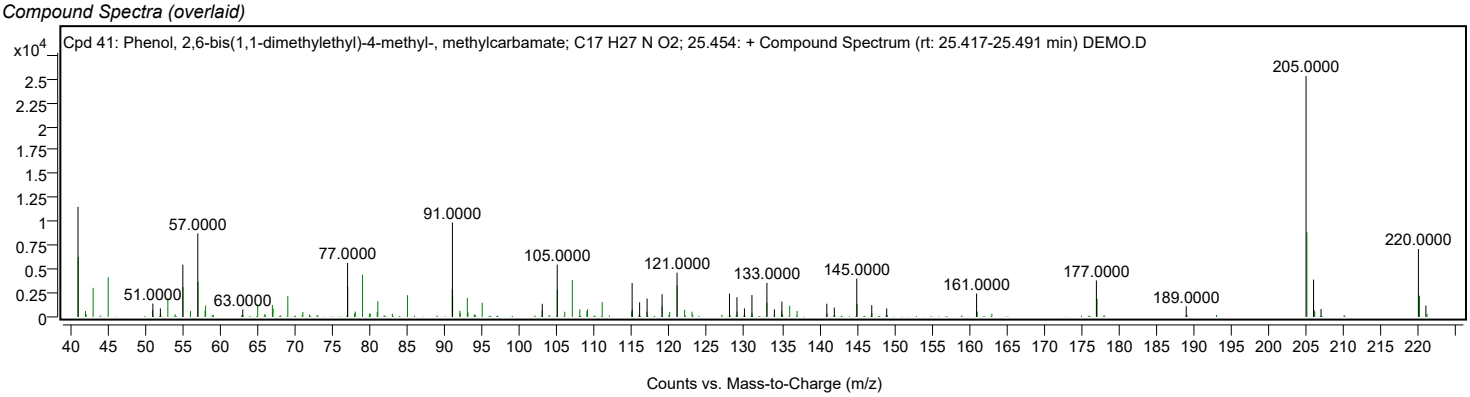
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



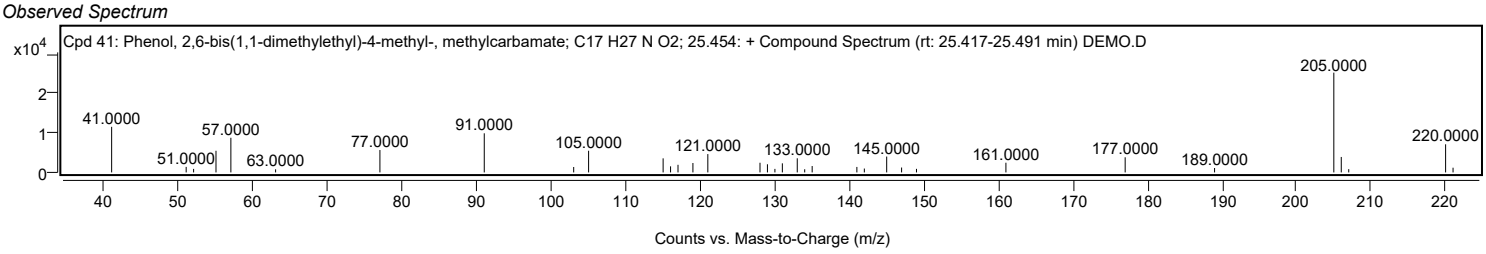
Phenol, 2,6-bis(1,1-dimethylethyl)-4-methyl-, methylcarbamate

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			84.98			NIST.L

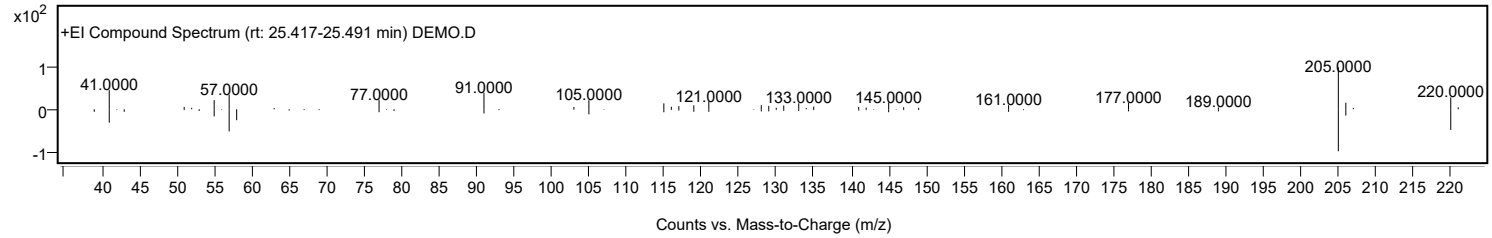
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			84.98			NIST.L

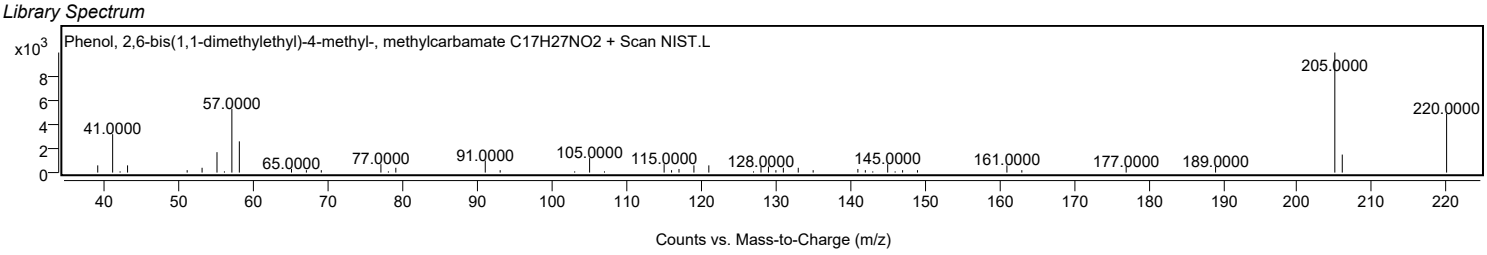
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 42: Tricyclo[4.3.0.0(3,8)]nonan-7-one

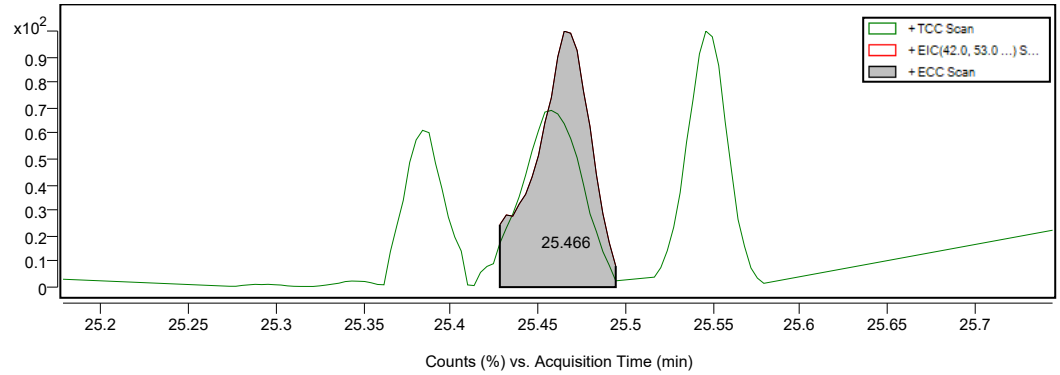
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Tricyclo[4.3.0.0(3,8)]nonan-7-one	C9 H12 O	25.466			103001-16-7	LibSearch	48.61	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		48.61			50		

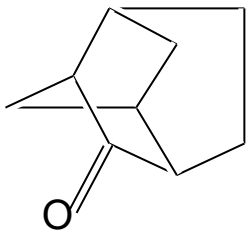
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Tricyclo[4.3.0.0(3,8)]nonan-7-one	C9H12O		LibSearch	25.466	7.883		103001-16-7	48.61		
(1R,5S)-rel-3-Ethyl-2,4-dioxa-3-phosphabicyclo[3.3.1]nonane 3-oxide	C8H15O3P		LibSearch	25.466			1000487-19-8	47.94		
Bicyclo[3.3.1]non-2-en-9-one	C9H12O		LibSearch	25.466	6.549		4844-11-5	45.91		
Methyl pentyl methylphosphonate	C7H17O3P		LibSearch	25.466			170082-80-1	45.72		
Butyl methyl methylphosphonate	C6H15O3P		LibSearch	25.466			683-32-9	45.58		
Methyl propyl methylphosphonate	C5H13O3P		LibSearch	25.466			683-25-0	45.24		
Isopropyl methyl methylphosphonate	C5H13O3P		LibSearch	25.466			690-64-2	45.06		
Linalool, methyl ether	C11H20O		LibSearch	25.466	7.449		1000352-63-6	45.04		
4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-	C10H18O		LibSearch	25.466	6.366		58461-27-1	44.95		
Hexyl methyl methylphosphonate	C8H19O3P		LibSearch	25.466			133736-02-4	44.94		
Succinic acid, di(neryl) ester	C24H38O4		LibSearch	25.466	-19.234		1000391-24-4	44.75		
Cyclohexane, 1-methylene-4-(1-methylethenyl)-	C10H16		LibSearch	25.466	8.583		499-97-8	44.51		
Butanoic acid, 3-methyl-, 1-ethenyl-1,5-dimethyl-4-hexenyl ester	C15H26O2		LibSearch	25.466	0.366		1118-27-0	44.38		
Mentha-1(7),8-diene <p->	C10H16		LibSearch	25.466			499-97-8	44.25		
Succinic acid, 3-methylbut-2-en-1-yl neryl ester	C19H30O4		LibSearch	25.466	-11.201		1000391-23-7	44.17		
Cyclohexane, 1-methylene-4-(1-methylethenyl)-	C10H16		LibSearch	25.466	8.583		499-97-8	44.10		
Lavandulol	C10H18O		LibSearch	25.466	11.166		498-16-8	44.06		
3,7-Dimethyl-1-phenylsulfonyl-2,6-octadiene	C16H22O2S		LibSearch	25.466	-10.617		1000432-27-5	44.03		
1-Bromo-3,7-dimethyl-2,6-octadiene	C10H17Br		LibSearch	25.466	4.099		35719-26-7	43.92		
Glutaric acid, di(neryl) ester	C25H40O4		LibSearch	25.466	-20.884		1000405-08-3	43.92		
Butanoic acid, 3-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (Z)-	C15H26O2		LibSearch	25.466	-0.967		3915-83-1	43.88		
4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, (R)-	C10H18O		LibSearch	25.466	6.366		498-16-8	43.83		
4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, (R)-	C10H18O		LibSearch	25.466	6.366		498-16-8	43.82		
Lavandulol	C10H18O		LibSearch	25.466			58461-27-1	43.81		
Heptyl methyl methylphosphonate	C9H21O3P		LibSearch	25.466			170275-60-2	43.55		
4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, (R)-	C10H18O		LibSearch	25.466	6.366		498-16-8	43.49		
Carbamic acid, N-phenyl-, 1,5-dimethyl-1-vinyl-4-hexenyl ester	C17H23NO2		LibSearch	25.466	-8.601		118723-77-6	43.49		
Isopropyl methyl methylphosphonate	C5H13O3P		LibSearch	25.466			690-64-2	43.32		
Neryl isovalerate	C15H26O2		LibSearch	25.466			3915-83-1	43.32		
3-Benzylsulfonyl-2,6,6-trimethylbicyclo(3.1.1)heptane	C17H24O2S		LibSearch	25.466	-10.834		1000242-12-7	42.93		
Geranyl isovalerate	C15H26O2		LibSearch	25.466	-0.967		109-20-6	42.83		
Cyclohexyl methyl methylphosphonate	C8H17O3P		LibSearch	25.466			7040-52-0	42.76		
1,3-Cyclohexadiene, 5-butyl-	C10H16		LibSearch	25.466	8.083		30168-57-1	42.60		
Butanoic acid, 2-methyl-, 3,7-dimethyl-2,6-octadienyl ester, (Z)-	C15H26O2		LibSearch	25.466	-0.967		51117-19-2	42.42		
p-Menth-2-en-7-ol, cis-	C10H18O		LibSearch	25.466	5.449		19898-86-3	42.41		
4-Oxatricyclo[5.2.1.0(2,6)]decan-8-ol	C9H14O2		LibSearch	25.466	7.833		1000192-17-9	42.32		
Adamantane	C10H16		LibSearch	25.466	10.799		281-23-2	42.27		
Linalyl methyl-ethyl-acetate	C15H26O2		LibSearch	25.466	0.366		1000430-70-9	42.11		
Butanoic acid, 3-methyl-, 1-ethenyl-1,5-dimethyl-4-hexenyl ester	C15H26O2		LibSearch	25.466	0.366		1118-27-0	42.09		
Succinic acid, di(geranyl) ester	C24H38O4		LibSearch	25.466	-19.234		1000391-21-7	42.06		
Neryl isovalerate	C15H26O2		LibSearch	25.466	-6.714		3915-83-1	41.95		
Geranyl isovalerate	C15H26O2		LibSearch	25.466			109-20-6	41.94		
Linalyl isovalerate	C15H26O2		LibSearch	25.466			1118-27-0	41.90		
Lavandulyl <2-methyl-> butyrate	C15H26O2		LibSearch	25.466			17609-96-0	41.58		
Nerol, methyl ether	C11H20O		LibSearch	25.466	6.116		1000352-64-1	41.56		
(.+/-.)-Lavandulol, methyl ether	C11H20O		LibSearch	25.466	7.483		1000352-62-7	41.54		
Pentanoic acid, 3,7-dimethyl-2,6-octadienyl ester, (E)-	C15H26O2		LibSearch	25.466	-2.034		10402-47-8	41.54		
p-Menth-2-en-7-ol, trans-	C10H18O		LibSearch	25.466	5.449		19898-87-4	41.46		
Epoxy-ocimene<Z->	C10H16O		LibSearch	25.466	12.746		33281-83-3	41.40		
4-Methyl-6-(tetrahydropyran-2-yloxy)hex-4-enal	C12H20O3		LibSearch	25.466	-1.451		64218-01-5	41.36		

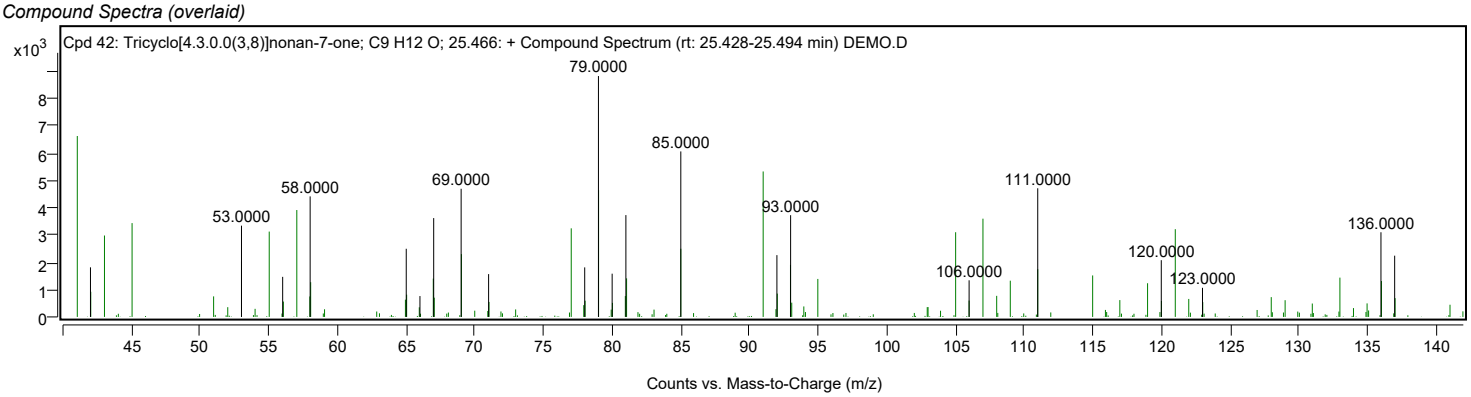
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



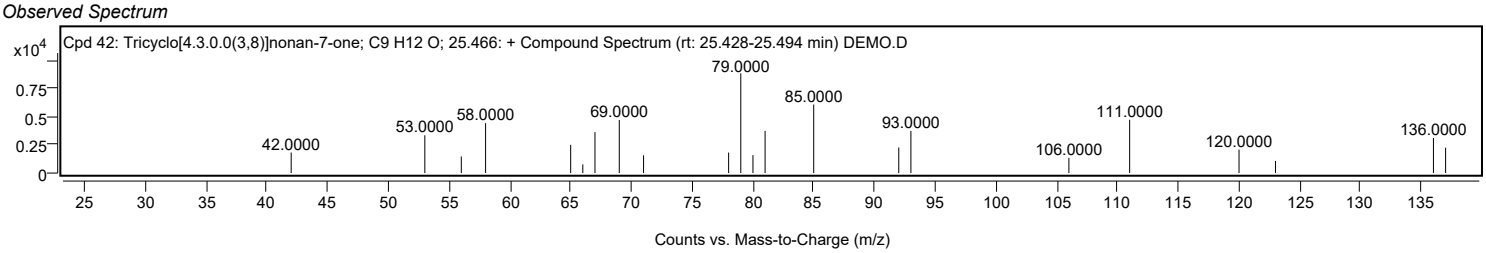
Tricyclo[4.3.0.0(3,8)]no nan-7-one

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			48.61			NIST.L

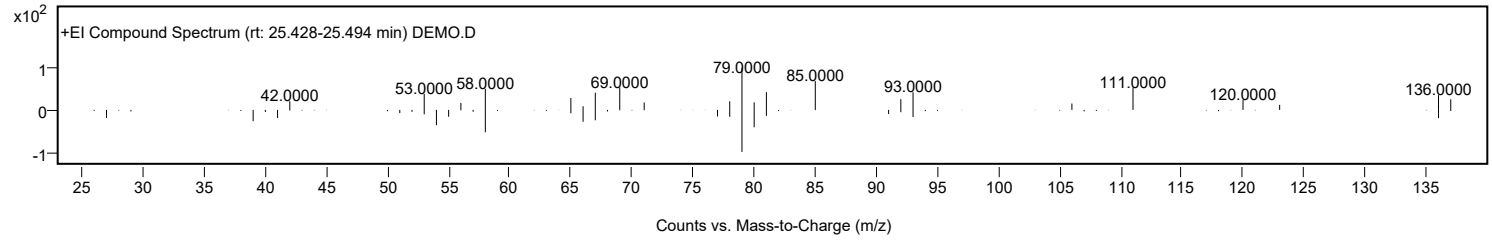
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			48.61			NIST.L

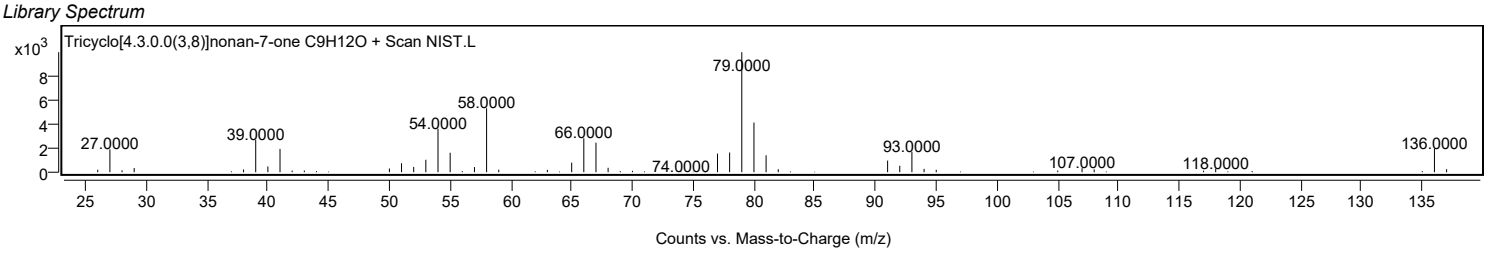
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 43: 4-Amino-5-o-tolyl-4H-[1,2,4]triazole-3-thiol, 2TMS

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
4-Amino-5-o-tolyl-4H-[1,2,4]triazole-3-thiol, 2TMS	C15 H26 N4 S Si2	25.476			1000509-47-9	LibSearch	1.70	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		1.70			4		

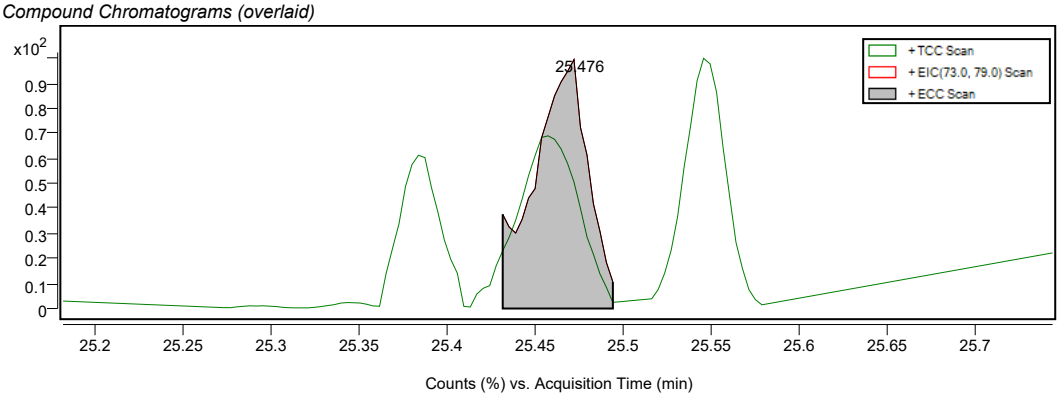
Compound Discovery Report

Agilent | Trusted Answers

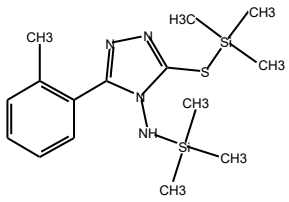
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
4-Amino-5-o-tolyl-4H-[1,2,4]triazole-3-thiol, 2TMS	C15H26N4SSi2		LibSearch	25.476	-12.624		1000509-47-9	1.70		
4-Amino-5-benzyl-4H-1,2,4-triazol-3-yl hydrosulfide, 2 TMS derivative	C15H26N4SSi2		LibSearch	25.476	-12.391		1000476-91-2	1.53		
7-(Trimethylsilyl)oxycoumarin-3-carboxylic acid, trimethylsilyl ester	C16H22O5Si2		LibSearch	25.476	-10.141		1000454-71-9	1.52		
3-Deazaadenine, 3TMS	C15H30N4Si3		LibSearch	25.476	-3.891		1010499-66-0	1.28		

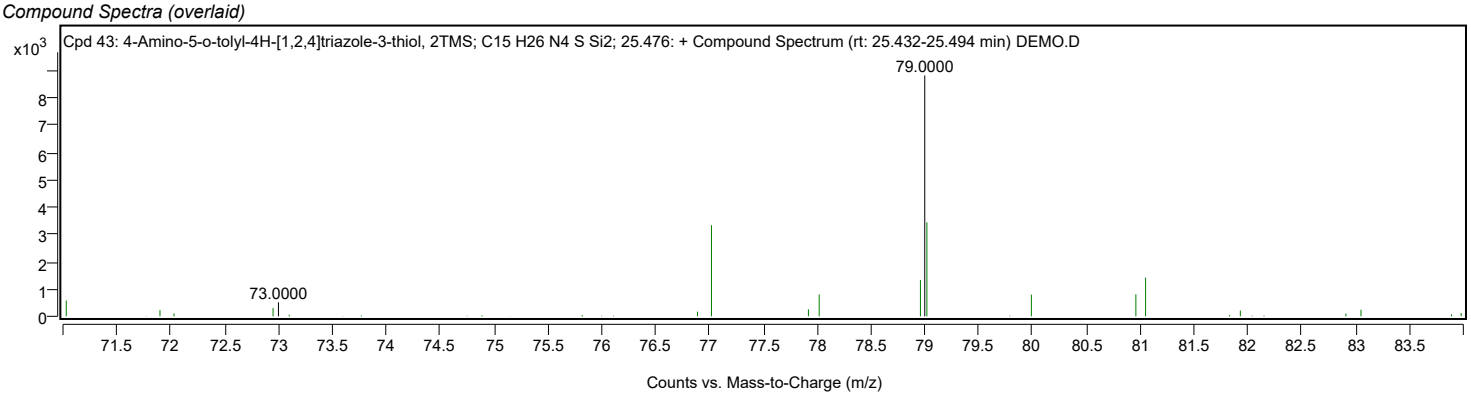
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



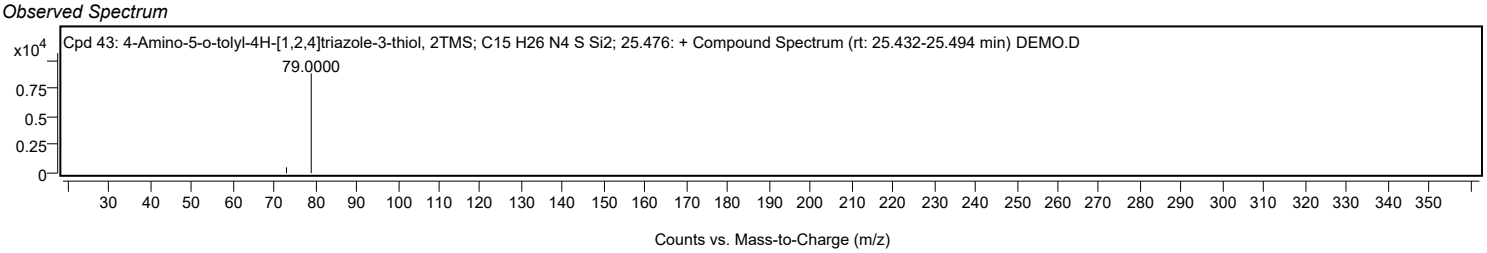
4-Amino-5-o-tolyl-4H-[1,2,4]triazole-3-thiol, 2TMS

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			1.70			NIST.L

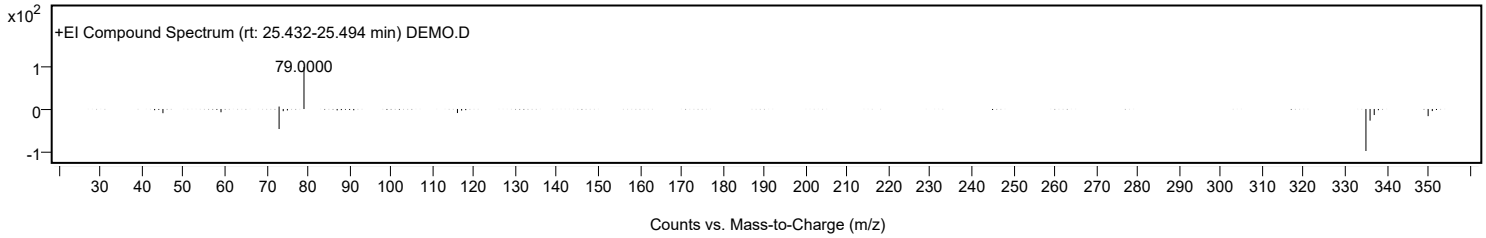
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			1.70			NIST.L

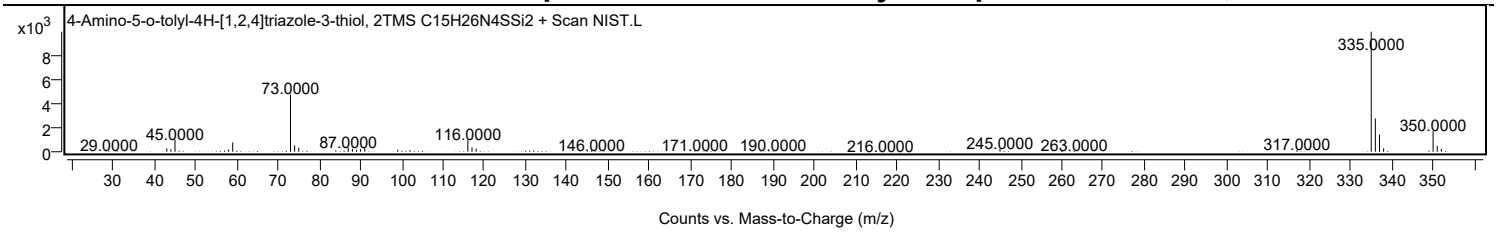
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 44: Caryophyllene<Z->

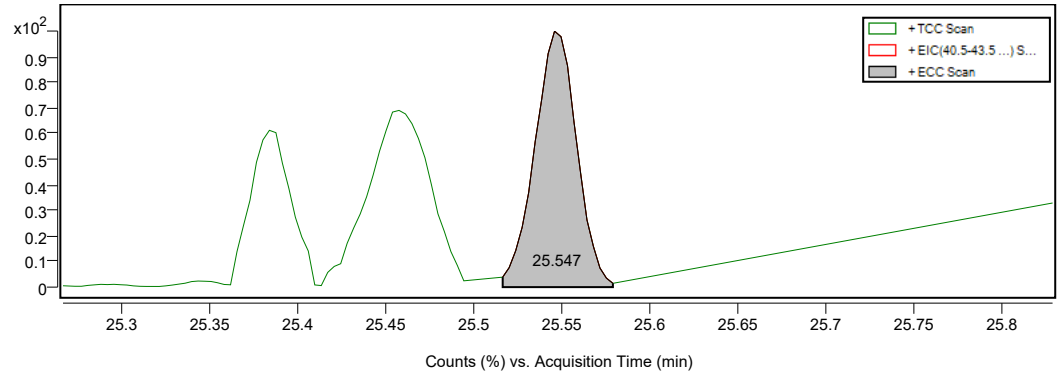
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Caryophyllene<Z->	C15 H24	25.547			118-65-0	LibSearch	79.00	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		79.00			50		

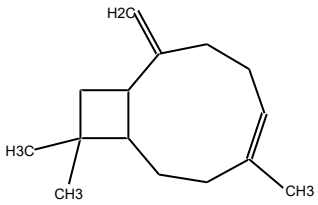
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Caryophyllene<Z->	C15H24		LibSearch	25.547	0.597		118-65-0	79.00		
Cyclohexane, 1,2-diethenyl-4-(1-methylethylidene)-, cis-	C13H20		LibSearch	25.547	4.197		34528-95-5	77.42		
Caryophyllene <(Z)->	C15H24		LibSearch	25.547			118-65-0	76.67		
1,4-Methanocycloocta[d]pyridazine, 1,4,4a,5,6,9,10,10a-octahydro-11,11-dimethyl-, (1.alpha.,4.alpha.,4a.alpha.,10a.alpha.)-	C13H20N2		LibSearch	25.547			1000221-85-9	76.39		
Caryophyllene(E-)	C15H24		LibSearch	25.547	0.187		87-44-5	76.25		
Bicyclo[2.2.1]heptane, 2-cyclopropylidene-1,7,7-trimethyl-	C13H20		LibSearch	25.547	4.697		1000159-45-7	75.83		
Icosa-9,11-diyne	C20H34		LibSearch	25.547	-8.519		28393-07-9	75.39		
Bicyclo[5.2.0]nonane, 4-methylene-2,8,8-trimethyl-2-vinyl-	C15H24		LibSearch	25.547	2.097		1000159-38-2	75.35		
Longipinene<beta->	C15H24		LibSearch	25.547	0.907		41432-70-6	75.29		
Sesquisabinene	C15H24		LibSearch	25.547	-1.503		58319-04-3	75.17		
.alpha.-Farnesene	C15H24		LibSearch	25.547	1.247		502-61-4	75.05		
Aromadendrane<dehydro->	C15H24		LibSearch	25.547	-1.613		85048-01-7	74.38		
Longipinene <beta->	C15H24		LibSearch	25.547			41432-70-6	74.25		
Caryophyllene	C15H24		LibSearch	25.547	0.647		87-44-5	74.16		
Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-	C15H24		LibSearch	25.547	0.647		13877-93-5	74.11		
Myrtenol	C10H16O		LibSearch	25.547	9.997		515-00-4	73.45		
Caryophyllene	C15H24		LibSearch	25.547	0.647		87-44-5	73.43		
(+)-3-Carene, 2-.alpha.-isopropenyl-	C13H20		LibSearch	25.547	5.964		1000151-27-1	73.38		
Amorphene<gamma->	C15H24		LibSearch	25.547	-3.083		6980-46-7	73.31		
Bicyclo[5.2.0]nonane, 2-methylene-4,8,8-trimethyl-4-vinyl-	C15H24		LibSearch	25.547	2.097		242794-76-9	73.22		
.alpha.-Farnesene	C15H24		LibSearch	25.547	1.247		502-61-4	73.21		
Aristolochene<4,5-di-epi->	C15H24		LibSearch	25.547	-2.083		54868-40-5	72.91		
Aromandendrene	C15H24		LibSearch	25.547	2.447		489-39-4	72.90		
Cyclohexane, 1,5-diethenyl-3-methyl-2-methylene-, (1.alpha.,3.alpha.,5.alpha.)-	C12H18		LibSearch	25.547	6.414		74742-35-1	72.88		
Panaxjapyne A	C17H26O		LibSearch	25.547	-6.386		1242413-82-6	72.86		
10,12-Octadecadiynoic acid	C18H28O2		LibSearch	25.547	-11.153		7333-25-7	72.83		
(6Z,9Z,12Z,15Z)-Methyl octadeca-6,9,12,15-tetraenoate	C19H30O2		LibSearch	25.547	-9.603		73097-00-4	72.60		
Bisabolene<(Z)-alpha->	C15H24		LibSearch	25.547	-3.543		70332-15-9	72.44		
Caryophyllene <(E)->	C15H24		LibSearch	25.547			13877-93-5	72.20		
Bicyclo[7.2.0]undec-4-ene, 4,11,11-trimethyl-8-methylene-,[1R-(1R*,4Z,9S*)]-	C15H24		LibSearch	25.547	0.647		118-65-0	72.17		
Aristolochene <4,5-di-epi->	C15H24		LibSearch	25.547			54868-40-5	72.06		
(1R,2S,6S,7S,8S)-8-Isopropyl-1-methyl-3-methylenetricyclo[4.4.0.02,7]decane-rel-	C15H24		LibSearch	25.547	5.281		18252-44-3	72.03		
Germacrene D	C15H24		LibSearch	25.547	-2.603		23986-74-5	72.02		
trans-3-Cyclopropyl-7-(2-methoxyethyl)norcarane	C13H22O		LibSearch	25.547	3.231		1000223-15-8	71.98		
1R,3Z,9S-4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-3-ene	C15H24		LibSearch	25.547	0.647		1000159-39-4	71.97		
(S,1Z,6Z)-8-Isopropyl-1-methyl-5-methylenecyclodeca-1,6-diene	C15H24		LibSearch	25.547	0.297		317819-80-0	71.91		
1R,3Z,9S-4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-3-ene	C15H24		LibSearch	25.547	0.647		1000159-39-4	71.89		
trans-.alpha.-Bergamotene	C15H24		LibSearch	25.547	1.714		13474-59-4	71.86		
1,8-Nonadiene, 2-methyl-5,7-dimethylene-	C12H18		LibSearch	25.547	7.114		1000152-68-8	71.83		
(+)-3-Carene, 4-isopropenyl-	C13H20		LibSearch	25.547	5.497		161395-29-5	71.76		
Tricyclo[7.2.0.0(3,8)]undec-4-ene, 4,8,11,11-tetramethyl-	C15H24		LibSearch	25.547	2.164		1000161-04-2	71.68		
11,11-Dimethyl-spiro[2,9]dodeca-3,7-dien	C14H22		LibSearch	25.547	1.347		1000062-28-4	71.62		
Bicyclo[4.3.0]nonane, 7-methylene-2,4,4-trimethyl-2-vinyl-	C15H24		LibSearch	25.547	2.097		1000156-11-9	71.58		
1,7-Octadiene, 2,7-dimethyl-3,6-bis(methylene)-	C12H18		LibSearch	25.547	7.497		16714-60-6	71.54		
3-Cyclohexene-1-methanol, 3(or 4)-(4-methyl-3-penten-1-yl)-, 1-acetate	C15H24O2		LibSearch	25.547			53889-39-7	71.54		
Bergamotene<alpha-cis->	C15H24		LibSearch	25.547	0.447		18252-46-5	71.54		
Methyl trans-2-(3-cyclopropyl-7-norcaranyl)acetate	C13H20O2		LibSearch	25.547	1.697		1000223-15-6	71.53		
Cycloheptane, 4-methylene-1-methyl-2-(2-methyl-1-propen-1-yl)-1-vinyl-	C15H24		LibSearch	25.547	0.964		1010159-38-5	71.49		
Longipinene<alpha->	C15H24		LibSearch	25.547	3.137		5989-08-2	71.46		
Methyl cis-2-(3-cyclopropyl-7-norcaranyl)acetate	C13H20O2		LibSearch	25.547	1.697		1000223-15-7	71.25		

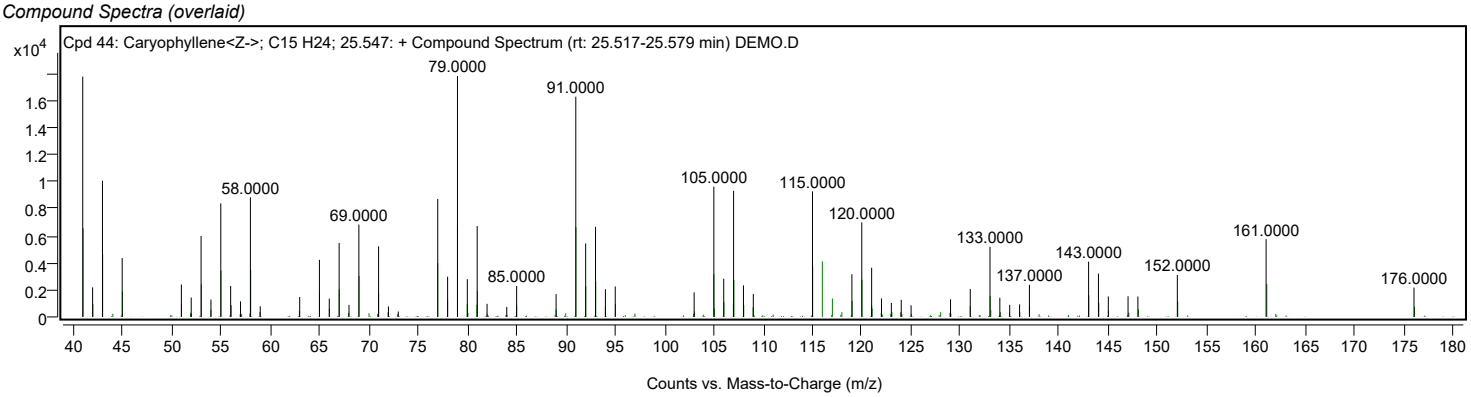
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



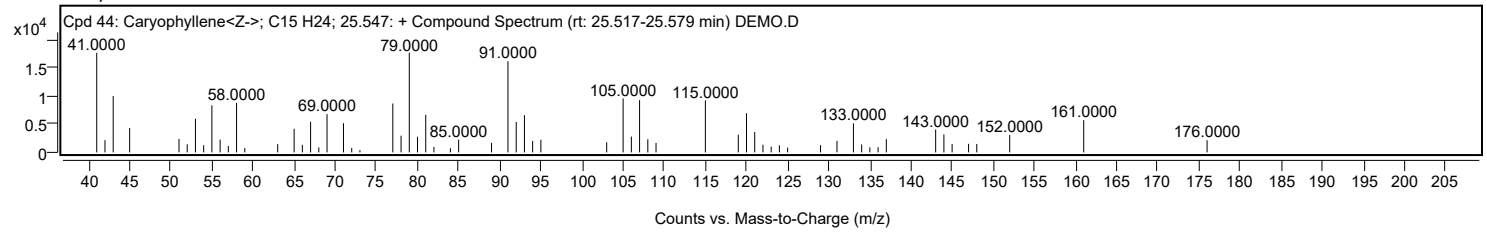
Caryophyllene<Z->

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			79.00			PWNose.xml

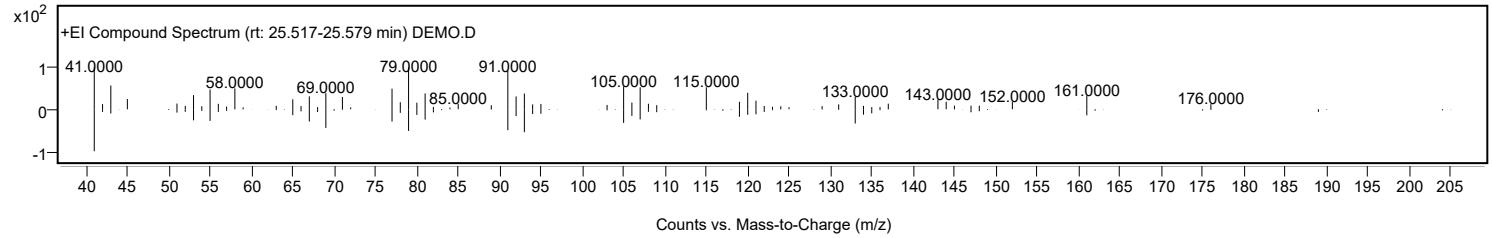
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			79.00			PWNose.xml

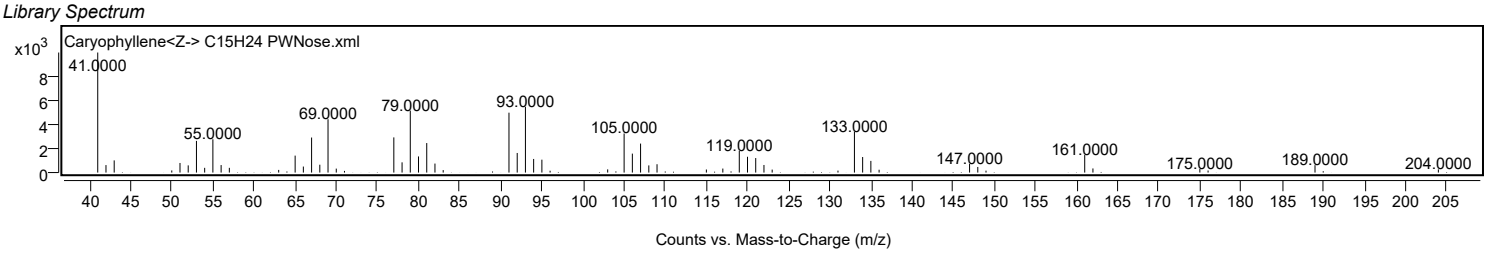
Observed Spectrum



Mirror Plot



Library Spectrum

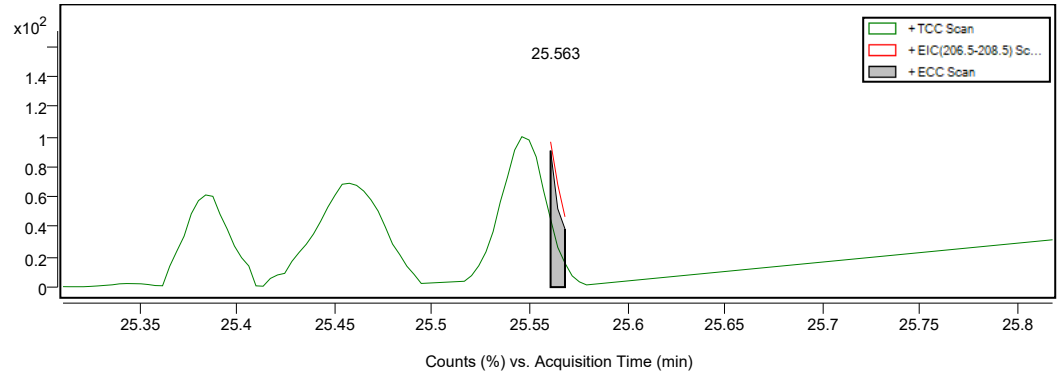


Cpd 45: 25.563

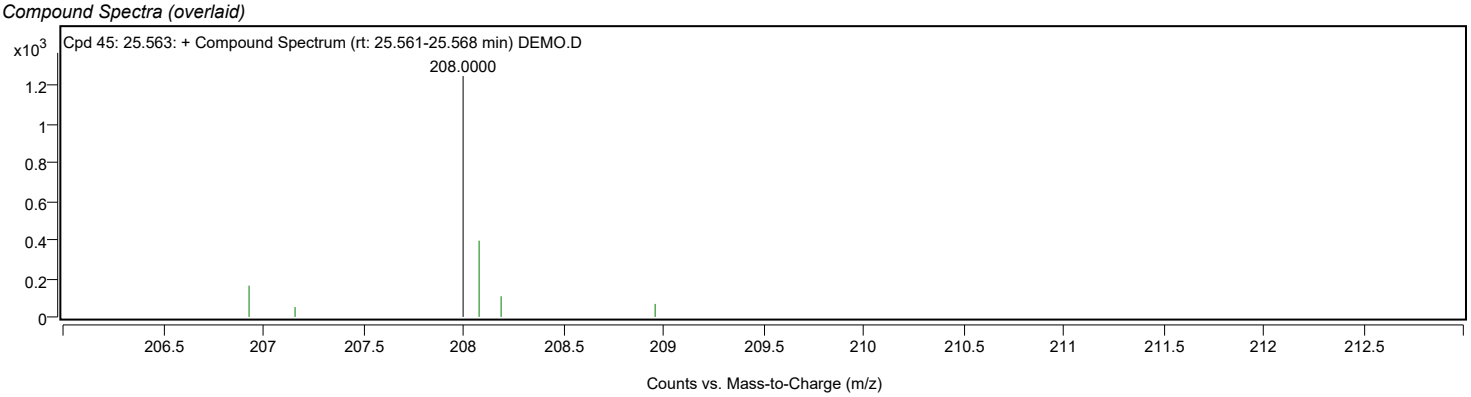
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
		25.563						Chrom Decon	

Compound Chromatograms (overlaid)

Structure



Compound Spectra (overlaid)



Cpd. 46: Magnolan, (1RS,3RS,4aSR,9aRS)

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Magnolan, (1RS,3RS,4aSR,9aRS)	C13 H16 O2	25.863			27606-09-3	LibSearch	65.73	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		65.73			50		

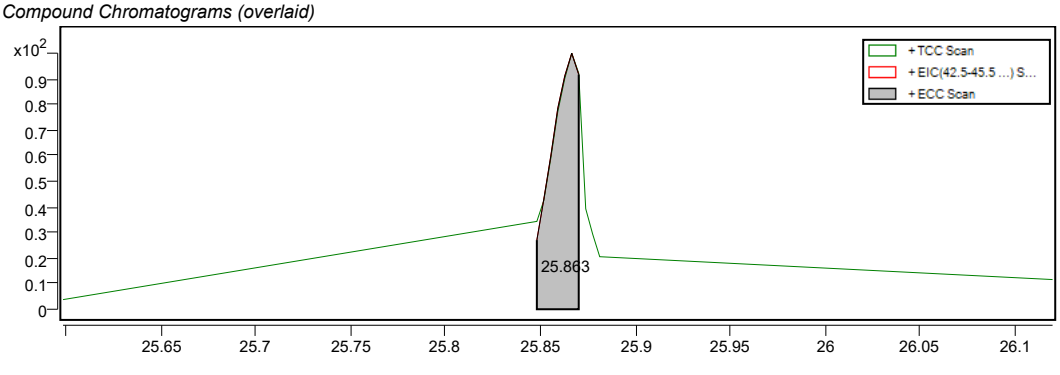
Compound Discovery Report

Agilent | Trusted Answers

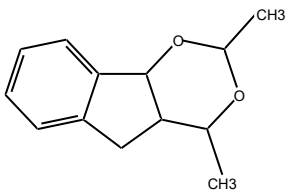
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Magnolan, (1RS,3RS,4aSR,9aRS)	C13H16O2		LibSearch	25.863			27606-09-3	65.73		
Magnolan, (1RS,3RS,4aRS,9aSR)	C13H16O2		LibSearch	25.863			27606-09-3	65.29		
Bicyclo[4.2.0]octa-1,3,5-triene, 7-(3-butenyl)-	C12H14		LibSearch	25.863	4.597		122057-61-8	59.58		
1H-Pyrrole, 1-phenyl-	C10H9N		LibSearch	25.863	5.013		635-90-5	58.70		
1-Propene, 3-cyano-1-phenyl-	C10H9N		LibSearch	25.863	3.447		1000164-96-2	57.95		
Propenoic acid, 3-(cycloheptatrien-7-yl)-, methyl ester	C11H12O2		LibSearch	25.863	3.847		1000269-64-5	57.41		
11-Azabicyclo[4.4.1]undeca-1,3,5,7,9-pentaene	C10H9N		LibSearch	25.863	3.613		4753-55-3	57.20		
1H-Pyrrole, 1-phenyl-	C10H9N		LibSearch	25.863	5.013		635-90-5	57.18		
4H-1,2,4-Triazole-3-thiol, 4-(2,3-dihydro-1H-inden-1-yl)-5-(1-methylethyl)-	C14H17N3S		LibSearch	25.863	-10.103		1000362-83-8	57.04		
1-Phenyl-1-cyclopropanecarbonitrile	C10H9N		LibSearch	25.863	3.980		935-44-4	56.63		
3-Phenyl-2-butenenitrile	C10H9N		LibSearch	25.863	3.830		14368-40-2	56.02		
1,2,4-Metheno-1H-cyclobuta[b]cyclopenta[d]furan, 2,2a,3a,4,6a,6b-hexahydro-3a-methyl-	C11H12O		LibSearch	25.863	11.713		78323-74-7	55.82		
1-Phenyl-1-cyclopropanecarbonitrile	C10H9N		LibSearch	25.863	3.980		935-44-4	55.45		
Cyclopropanecarbonitrile, 2-phenyl-, trans-	C10H9N		LibSearch	25.863	4.180		5590-14-7	55.41		
2-indanol trifluoroacetate ester	C11H9F3O2		LibSearch	25.863	5.713		1000376-43-8	55.12		
Bicyclo[4.2.1]nona-2,4,7-triene, 9-(phenylseleno)-, syn-	C15H14Se		LibSearch	25.863			72065-43-1	55.03		
Bicyclo[4.2.1]nona-2,4,7-triene, 9-(phenylseleno)-, (anti-)	C15H14Se		LibSearch	25.863			72065-50-0	54.66		
Bicyclo[4.2.1]nona-2,4,7-triene, 9-acetyl-, syn-	C11H12O		LibSearch	25.863	5.463		1000141-51-6	54.62		
1-Phenyl-1-pentyn-4-ol	C11H12O		LibSearch	25.863	3.013		16330-23-7	54.50		
Vinylphenylacetonitrile	C10H9N		LibSearch	25.863	3.513		110013-89-3	54.31		
2,3-Diazabicyclo[2.2.1]hept-2-ene, 5-phenyl-	C11H12N2		LibSearch	25.863			146562-77-8	54.25		
1-Naphthalenamine	C10H9N		LibSearch	25.863	0.147		134-32-7	54.00		
Benzene, (1-ethyl-2-propenyl)-	C11H14		LibSearch	25.863	7.247		19947-22-9	53.89		
trans-Cinnamyl bromide	C9H9Br		LibSearch	25.863	4.247		26146-77-0	53.58		
Benzenepropanenitrile, .alpha.-methylene-	C10H9N		LibSearch	25.863	4.130		28769-48-4	53.55		
Cyclopropanecarbonyl chloride, 2-phenyl-, trans-	C10H9ClO		LibSearch	25.863	3.063		939-87-7	53.44		
Acrylic acid, 3-cyano-2-hydroxy-3-phenyl-, methyl ester	C11H9NO3		LibSearch	25.863	-2.570		1000305-19-2	53.31		
2-Naphthalenamine	C10H9N		LibSearch	25.863	0.147		91-59-8	52.83		
Benzene, (1-ethyl-1-propenyl)-	C11H14		LibSearch	25.863	6.263		4701-36-4	52.70		
Benzeneethanol, .beta.-ethenyl-	C10H12O		LibSearch	25.863	4.847		6052-63-7	52.70		
(1-Phenylcyclopentyl)methanamine	C12H17N		LibSearch	25.863	0.013		17511-89-6	52.64		
Pentacyclo[8.2.1.1(4,7).0(2,9).0(3,8)]exo-trans-exo-tetradeca-5,11-diene	C14H16		LibSearch	25.863	7.047		2957-68-8	52.60		
Lepidine	C10H9N		LibSearch	25.863			491-35-0	52.60		
(2-Nitroallyl)-benzene	C9H9NO2		LibSearch	25.863	3.513		62811-39-6	52.55		
Benzene, (1-ethyl-1-propenyl)-	C11H14		LibSearch	25.863	6.263		4701-36-4	52.51		
1-Naphthalenamine	C10H9N		LibSearch	25.863	0.147		134-32-7	52.50		
1-Naphthalenamine	C10H9N		LibSearch	25.863	0.147		134-32-7	52.44		
2-Naphthalenamine	C10H9N		LibSearch	25.863	0.147		91-59-8	52.43		
1H-Pyrrole, 2-phenyl-	C10H9N		LibSearch	25.863	2.980		3042-22-6	52.35		
1-indanol trifluoroacetate ester	C11H9F3O2		LibSearch	25.863	5.713		1000376-43-6	52.29		
2-Naphthalenamine	C10H9N		LibSearch	25.863	0.147		91-59-8	52.27		
1,2,4-Metheno-1H-cyclobuta[cd]pentalene, octahydro-	C10H12		LibSearch	25.863	14.447		6707-86-4	52.22		
Benzonitrile, 4-(1,2,3,4-tetrahydro-1-isoquinolyl)-	C16H14N2		LibSearch	25.863	-11.220		199479-20-4	52.21		
1,3-Cyclopentadiene, 5-(trans-2-ethyl-3-methylcyclopropylidene)-	C11H14		LibSearch	25.863	7.763		79209-36-2	52.19		
1-Phenyl-1-nonyne	C15H20		LibSearch	25.863	-0.903		57718-18-0	52.18		
5-Norbornene-2,3-diacetonitrile	C11H12N2		LibSearch	25.863	0.280		101832-55-7	52.17		
2-Naphthalenamine	C10H9N		LibSearch	25.863	0.147		91-59-8	52.09		
Benzene, 1-cyclopenten-1-yl-	C11H12		LibSearch	25.863	5.113		825-54-7	52.07		
3-Penten-2-one, 5-phenyl-	C11H12O		LibSearch	25.863	3.613		10521-97-8	52.00		
Deltacyclene	C9H10		LibSearch	25.863	15.113		7785-10-6	51.97		

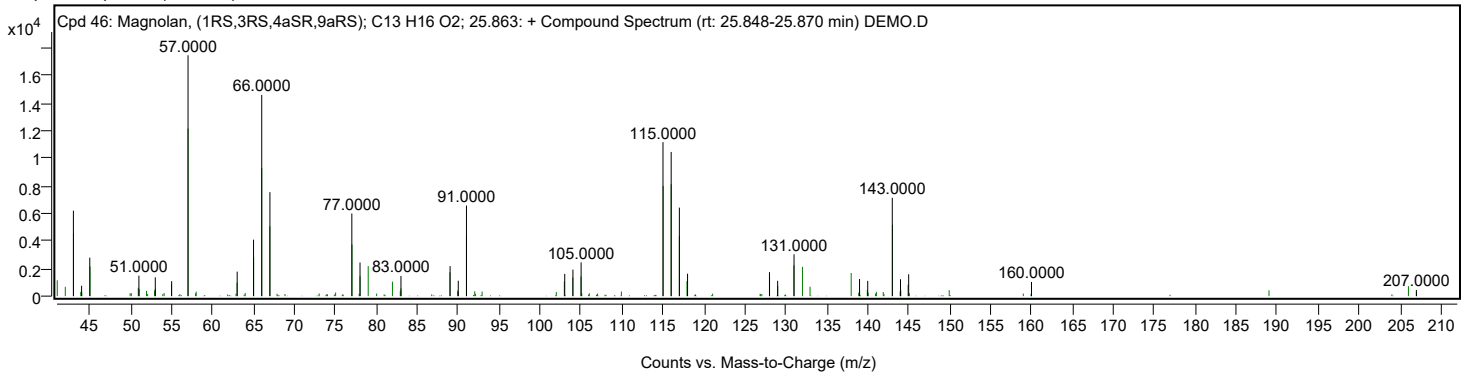
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



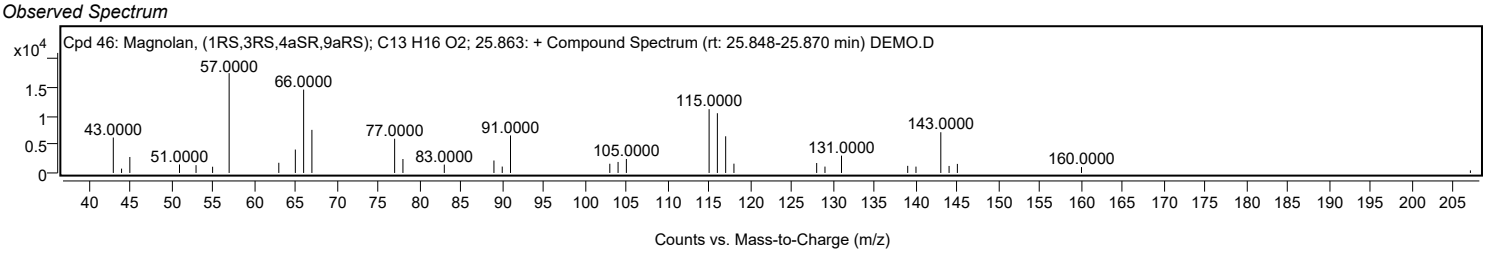
Magnolan, (1RS,3RS,4aSR,9aRS)

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			65.73			PWNose.xml

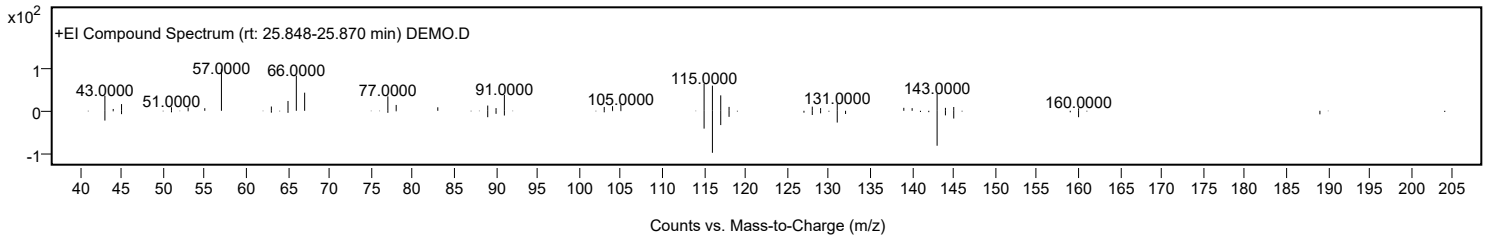
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			65.73			PWNose.xml

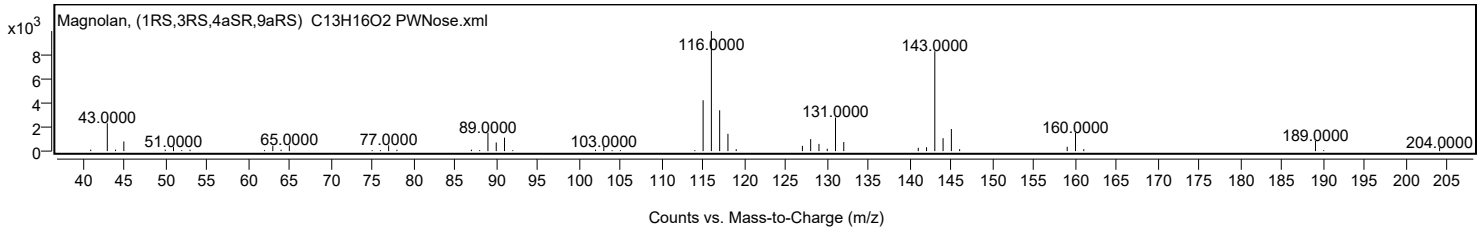
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 47: Cyclaprop

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Cyclaprop	C13 H18 O2	25.870			17511-60-3	LibSearch	63.13	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		63.13			50		

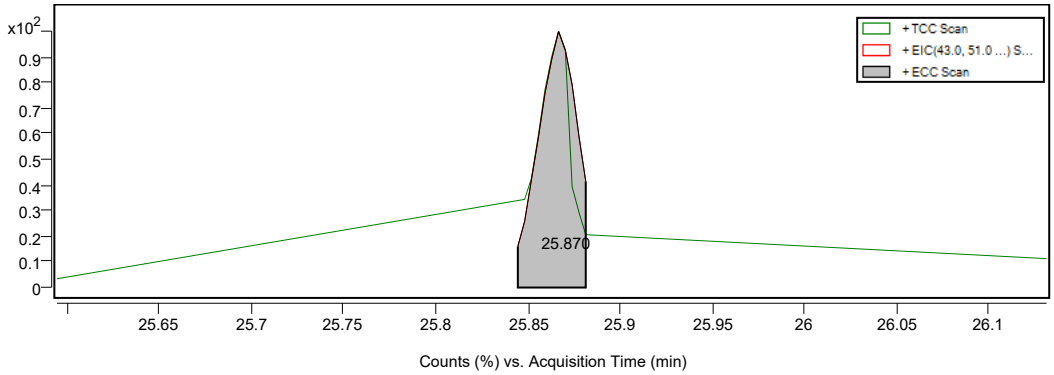
Compound Discovery Report

Agilent | Trusted Answers

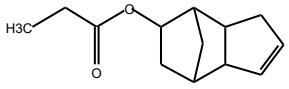
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Cyclaprop	C13H18O2		LibSearch	25.870			17511-60-3	63.13		
(3aR,4S,7S,7aS)-3a,4,5,6,7,7a-Hexahydro-1H-4,7-methanoinden-6-yl propionate	C13H18O2		LibSearch	25.870	4.370		1000498-52-8	59.45		
Propenoic acid, 3-(cycloheptatrien-7-yl)-, methyl ester	C11H12O2		LibSearch	25.870	3.854		1000269-64-5	55.30		
1,2,4-Metheno-1H-cyclobuta[cd]pentalene, octahydro-	C10H12		LibSearch	25.870	14.454		6707-86-4	53.65		
Magnolan, (1RS,3RS,4aSR,9aRS)	C13H16O2		LibSearch	25.870			27606-09-3	53.51		
Cinnamyl propionate <(E)->	C12H14O2		LibSearch	25.870			78761-38-3	53.38		
Dicyclopentadiene	C10H12		LibSearch	25.870	11.787		77-73-6	53.30		
Dicyclopentadiene	C10H12		LibSearch	25.870	11.787		77-73-6	53.11		
Benzene, 1-ethenyl-4-ethyl-	C10H12		LibSearch	25.870	7.604		3454-07-7	52.79		
1,3,4-Metheno-1H-cyclobuta[cd]pentalene, octahydro-	C10H12		LibSearch	25.870	14.454		6707-88-6	52.50		
Cyclobuta[1,2:3,4]dicyclopentene, 1,3a,3b,4,6a,6b-hexahydro-	C10H12		LibSearch	25.870	9.737		105226-58-2	52.48		
Magnolan, (1RS,3RS,4aRS,9aSR)	C13H16O2		LibSearch	25.870			27606-09-3	52.37		
Indan-1,3-diol monopropionate	C12H14O3		LibSearch	25.870	-1.830		1000132-07-5	52.34		
Bicyclo[4.2.1]nona-2,4,7-triene, 9-acetyl-, syn-	C11H12O		LibSearch	25.870	5.470		1000141-51-6	52.22		
Dicyclopentadiene	C10H12		LibSearch	25.870	11.787		77-73-6	52.18		
Bicyclo[4.2.1]nona-2,4,7-triene, 9-(phenylseleno)-, syn-	C15H14Se		LibSearch	25.870			72065-43-1	52.12		
Bicyclo[4.2.1]nona-2,4,7-triene, 9-(phenylseleno)-, (anti-)	C15H14Se		LibSearch	25.870			72065-50-0	51.99		
Benzene, (2-methyl-1-propenyl)-	C10H12		LibSearch	25.870	7.920		768-49-0	51.95		
trans-Cinnamyl bromide	C9H9Br		LibSearch	25.870	4.254		26146-77-0	51.85		
1H-Pyrrole, 1-phenyl-	C10H9N		LibSearch	25.870	5.020		635-90-5	51.82		
Benzene, 1-methyl-4-(2-propenyl)-	C10H12		LibSearch	25.870	7.604		3333-13-9	51.68		
Cyclobuta[1,2:3,4]dicyclopentene, 1,3a,3b,6,6a,6b-hexahydro-	C10H12		LibSearch	25.870	9.737		612-09-9	51.63		
Benzene, (2-methyl-1-propenyl)-	C10H12		LibSearch	25.870	7.920		768-49-0	51.62		
1-Propene, 3-cyano-1-phenyl-	C10H9N		LibSearch	25.870	3.454		1000164-96-2	51.58		
Dicyclopentadiene	C10H12		LibSearch	25.870	11.787		77-73-6	51.42		
2-Propen-1-ol, 3-phenyl-, propanoate	C12H14O2		LibSearch	25.870	1.437		103-56-0	51.42		
Benzene, 2-ethenyl-1,3-dimethyl-	C10H12		LibSearch	25.870	7.370		2039-90-9	51.39		
Benzene, 1-methyl-2-(2-propenyl)-	C10H12		LibSearch	25.870	7.604		1587-04-8	51.27		
Herbanate isomer I	C13H20O2		LibSearch	25.870			116126-82-0	51.16		
5-Norbornene-2,3-diacetonitrile	C11H12N2		LibSearch	25.870	0.287		101832-55-7	51.06		
Benzene, 2-butenyl-	C10H12		LibSearch	25.870	7.537		1560-06-1	50.97		
1H-Pyrrole, 1-phenyl-	C10H9N		LibSearch	25.870	5.020		635-90-5	50.96		
Herbanate isomer II	C13H20O2		LibSearch	25.870			116126-82-0	50.95		
Benzene, 2-ethenyl-1,4-dimethyl-	C10H12		LibSearch	25.870	7.370		2039-89-6	50.85		
2,2,2-Trifluoro-N-(2-phenylcyclopropyl)acetamide, trans-	C11H10F3NO		LibSearch	25.870	2.720		721-60-8	50.81		
(E)-1-Phenyl-1-butene	C10H12		LibSearch	25.870	7.537		1005-64-7	50.80		
4H-1,2,4-Triazole-3-thiol, 4-(2,3-dihydro-1H-inden-1-yl)-5-(1-methylethyl)-	C14H17N3S		LibSearch	25.870	-10.096		1000362-83-8	50.70		
Benzene, (2-methyl-1-propenyl)-	C10H12		LibSearch	25.870	7.920		768-49-0	50.63		
2-indanol trifluoroacetate ester	C11H9F3O2		LibSearch	25.870	5.720		1000376-43-8	50.58		
(2-Nitroallyl)-benzene	C9H9NO2		LibSearch	25.870	3.520		62811-39-6	50.51		
o-Isopropenyltoluene	C10H12		LibSearch	25.870	7.987		7399-49-7	50.37		
Benzene, 2-ethenyl-1,4-dimethyl-	C10H12		LibSearch	25.870	7.370		2039-89-6	50.17		
Dimethyl styrene<2,5->	C10H12		LibSearch	25.870	14.430		27576-03-0	49.94		
2-Propen-1-ol, 3-phenyl-, propanoate	C12H14O2		LibSearch	25.870	1.437		103-56-0	49.77		
Pentacyclo[8.2.1.1(4,7).0(2,9).0(3,8)]exo-trans-exo-tetradeca-5,11-diene	C14H16		LibSearch	25.870	7.054		2957-68-8	49.73		
Dimethyl styrene <2,5->	C10H12		LibSearch	25.870			27576-03-0	49.70		
Benzocyclobutene, 1-bromo-1-methyl-	C9H9Br		LibSearch	25.870	4.904		1000161-76-4	49.48		
Benzonitrile, 4-(1,2,3,4-tetrahydro-1-isoquinolyl)-	C16H14N2		LibSearch	25.870	-11.213		199479-20-4	49.33		
Benzene, (1-methyl-1-propenyl)-, (E)-	C10H12		LibSearch	25.870	7.920		768-00-3	49.33		
trans-2-Phenylcyclopropylamine, N-chlorodifluoroacetyl-	C11H10ClF2NO		LibSearch	25.870	-0.363		1000447-48-6	49.24		

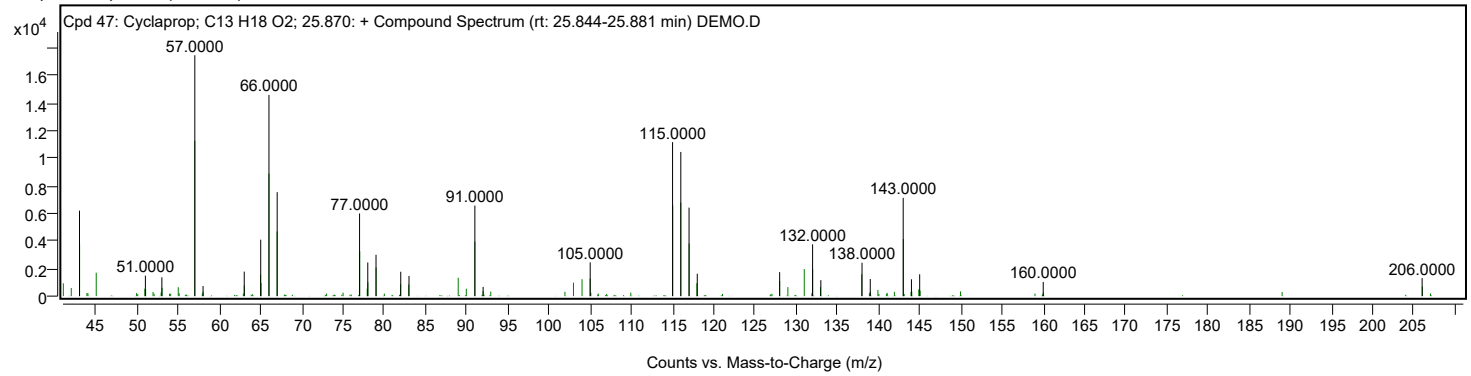
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



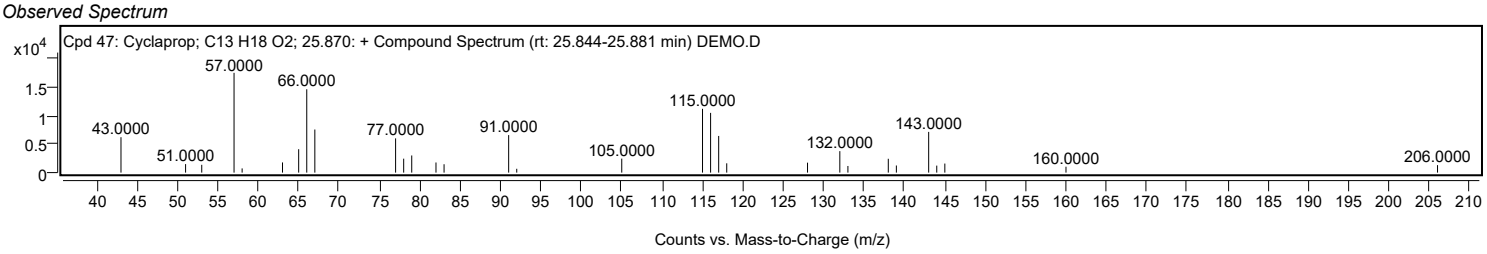
Cyclaprop

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			63.13			PWNose.xml

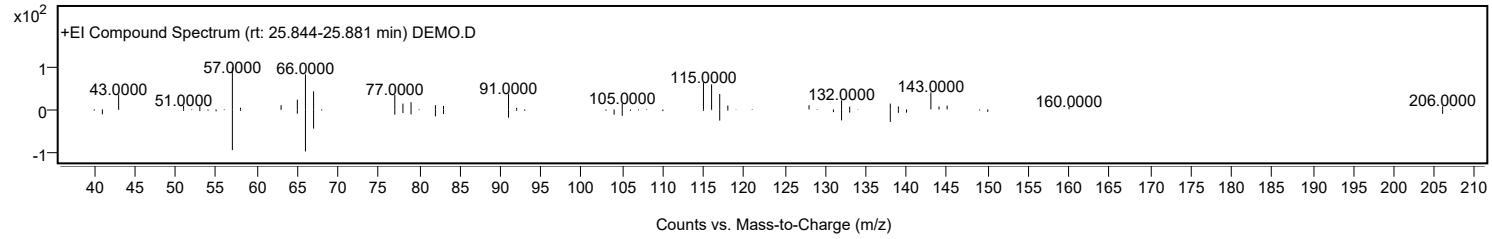
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			63.13			PWNose.xml

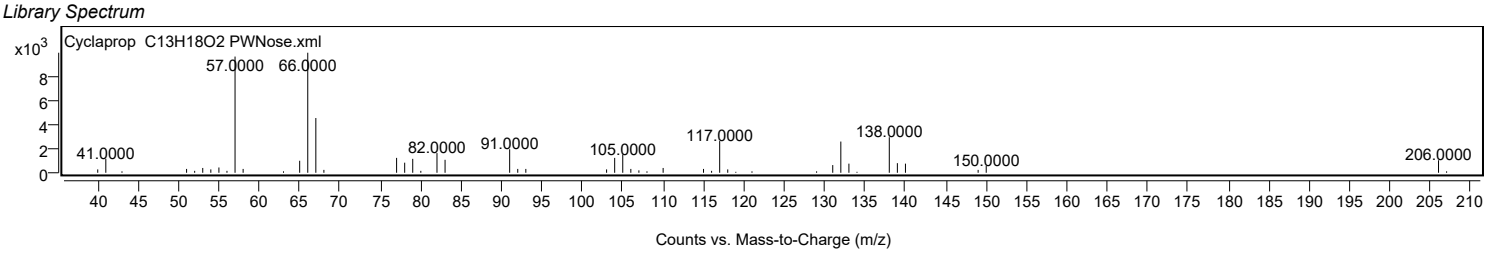
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 48: Valeric anhydride

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Valeric anhydride	C10 H18 O3	26.391			2082-59-9	LibSearch	80.71	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		80.71			50		

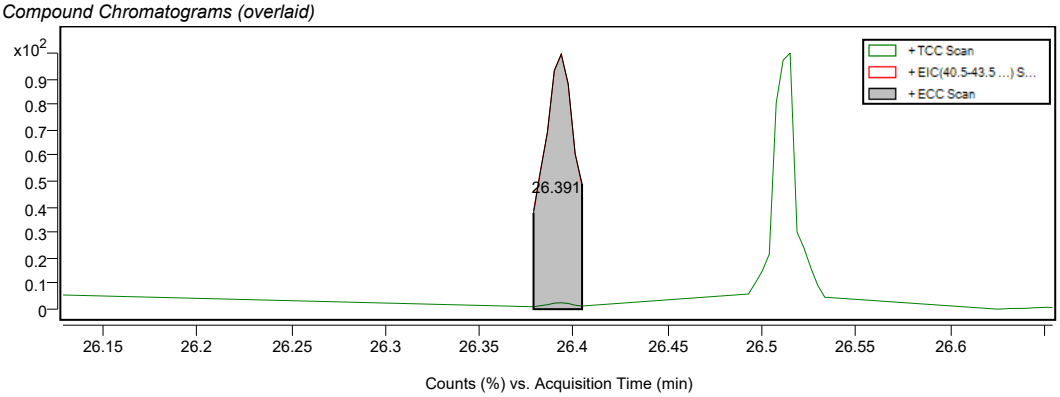
Compound Discovery Report

Agilent | Trusted Answers

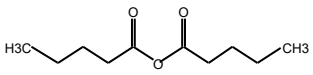
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Valeric anhydride	C10H18O3		LibSearch	26.391	4.408		2082-59-9	80.71		
Valeric anhydride	C10H18O3		LibSearch	26.391			2082-59-9	78.89		
2-Methylbutanoic anhydride	C10H18O3		LibSearch	26.391	6.558		1468-39-9	78.81		
Hexane, 2-bromo-	C6H13Br		LibSearch	26.391	12.224		3377-86-4	78.17		
2H-Pyran, 2-(bromomethyl)tetrahydro-	C6H11BrO		LibSearch	26.391	8.624		34723-82-5	77.94		
Valeric anhydride	C10H18O3		LibSearch	26.391	4.408		2082-59-9	77.35		
Hexane, 3-bromo-	C6H13Br		LibSearch	26.391	12.224		3377-87-5	76.63		
Hexane, 2-bromo-	C6H13Br		LibSearch	26.391	12.224		3377-86-4	76.55		
Furfuryl alcohol, tetrahydro-5-methyl-, cis-	C6H12O2		LibSearch	26.391	10.508		16015-08-0	76.11		
Oxetane, 2-ethyl-3-methyl-	C6H12O		LibSearch	26.391	14.891		53778-62-4	75.35		
Hexane, 3-bromo-	C6H13Br		LibSearch	26.391	12.224		3377-87-5	75.20		
2-Furanmethanol, tetrahydro-5-methyl-, trans-	C6H12O2		LibSearch	26.391	10.508		54774-28-6	74.96		
Pentane, 2,2-dimethyl-	C7H16		LibSearch	26.391	15.841		590-35-2	74.36		
2(3H)-Furanone, 5-ethyldihydro-	C6H10O2		LibSearch	26.391	9.958		695-06-7	74.05		
2(3H)-Furanone, 5-acetyldihydro-	C6H8O3		LibSearch	26.391	7.691		29393-32-6	73.84		
Furan, tetrahydro-2,4-dimethyl-, cis-	C6H12O		LibSearch	26.391	14.541		39168-01-9	73.66		
Hexane, 3-bromo-	C6H13Br		LibSearch	26.391	12.224		3377-87-5	73.49		
2-Propyltetrahydropyran	C8H16O		LibSearch	26.391	10.258		3857-17-8	73.40		
2-Methylbutanoic anhydride	C10H18O3		LibSearch	26.391	6.558		1468-39-9	73.35		
Hexane, 2-bromo-	C6H13Br		LibSearch	26.391	12.224		3377-86-4	73.34		
5H-Tetrazol-5-amine	CH3N5		LibSearch	26.391			1000273-02-0	72.93		
2(3H)-Furanone, 5-ethyldihydro-	C6H10O2		LibSearch	26.391	9.958		695-06-7	72.88		
Butane, 2,2,3-trimethyl-	C7H16		LibSearch	26.391	16.924		464-06-2	72.86		
Furan, tetrahydro-2,4-dimethyl-, trans-	C6H12O		LibSearch	26.391	14.541		39168-02-0	72.70		
2H-Pyran-2-methanol, tetrahydro-	C6H12O2		LibSearch	26.391	9.524		100-72-1	72.42		
2(3H)-Furanone, 5-acetyldihydro-	C6H8O3		LibSearch	26.391	7.691		29393-32-6	72.39		
Furan, tetrahydro-2,5-dimethyl-, cis-	C6H12O		LibSearch	26.391	14.541		2144-41-4	72.25		
5-Hydroxypentanal	C5H10O2		LibSearch	26.391	10.574		4221-03-8	72.15		
Valerolactone<gamma->	C5H8O2		LibSearch	26.391	20.291		108-29-2	72.04		
Hexane, 2-iodo-	C6H13I		LibSearch	26.391	10.258		18589-27-0	71.99		
Hexane, 2-methyl-	C7H16		LibSearch	26.391	15.508		591-76-4	71.97		
Heptalactone<gamma->	C7H12O2		LibSearch	26.391	13.011		105-21-5	71.94		
2(3H)-Furanone, 5-ethyldihydro-	C6H10O2		LibSearch	26.391	9.958		695-06-7	71.74		
2(3H)-Furanone, dihydro-5-propyl-	C7H12O2		LibSearch	26.391	8.308		105-21-5	71.49		
2H-Pyran-2-methanol, tetrahydro-	C6H12O2		LibSearch	26.391	9.524		100-72-1	71.43		
2(3H)-Furanone, dihydro-5-methyl-	C5H8O2		LibSearch	26.391	11.624		108-29-2	71.31		
5-(Bromomethyl)oxolan-2-one	C5H7BrO2		LibSearch	26.391	6.691		99393-06-3	71.17		
Acetylvaleryl	C7H12O2		LibSearch	26.391			96-04-8	71.07		
2(3H)-Furanone, dihydro-5-propyl-	C7H12O2		LibSearch	26.391	8.308		105-21-5	70.84		
Sulfurous acid, isohexyl hexyl ester	C12H26O3S		LibSearch	26.391	-3.159		1000309-12-8	70.79		
Sulfurous acid, butyl isohexyl ester	C10H22O3S		LibSearch	26.391	0.158		1000309-17-2	70.78		
Hexalactone<gamma->	C6H10O2		LibSearch	26.391	17.061		695-06-7	70.73		
5-Oxotetrahydrofuran-2-carboxylic acid, ethyl ester	C7H10O4		LibSearch	26.391	5.524		1126-51-8	70.72		
Pentane, 2,2-dimethyl-	C7H16		LibSearch	26.391	15.841		590-35-2	70.72		
2(3H)-Furanone, dihydro-5-propyl-	C7H12O2		LibSearch	26.391	8.308		105-21-5	70.71		
Pentane, 2,2-dimethyl-	C7H16		LibSearch	26.391	15.841		590-35-2	70.70		
Pentalactone <gamma->	C5H8O2		LibSearch	26.391			108-29-2	70.58		
Hexane <2-methyl->	C7H16		LibSearch	26.391			591-76-4	70.46		
Pentanoic acid, 4-methyl-2-oxo-, methyl ester	C7H12O3		LibSearch	26.391	10.458		3682-43-7	70.35		
3H-1,2,4-Triazol-3-one, 1,2-dihydro-	C2H3N3O		LibSearch	26.391	9.524		930-33-6	70.27		

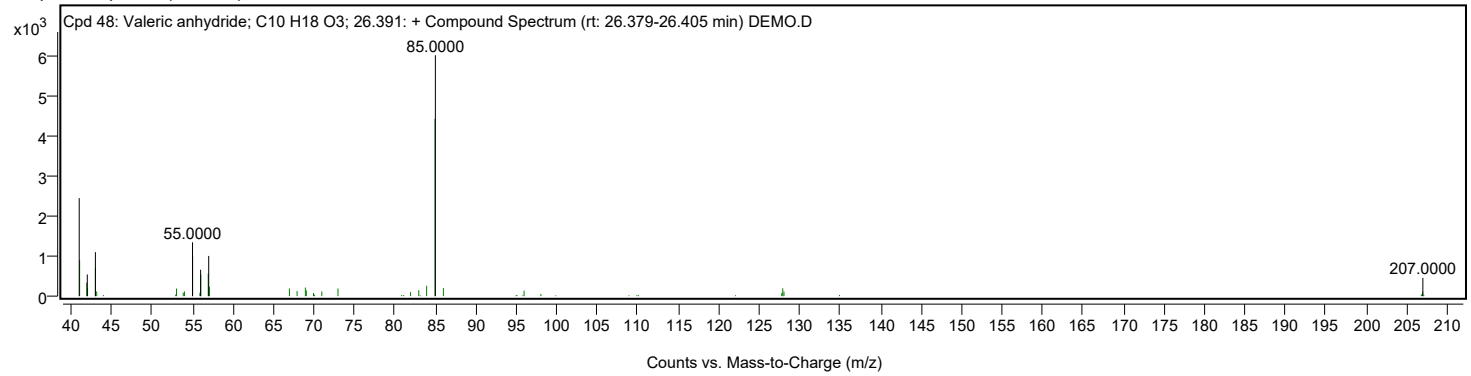
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



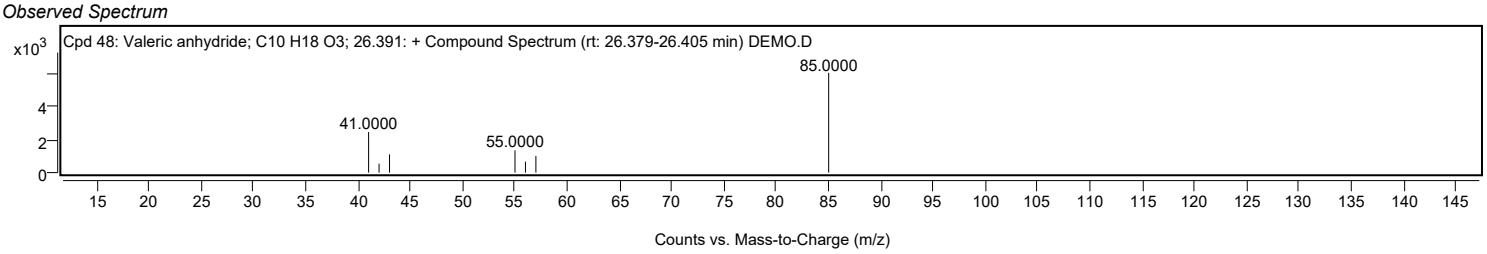
Valeric anhydride

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			80.71			NIST.L

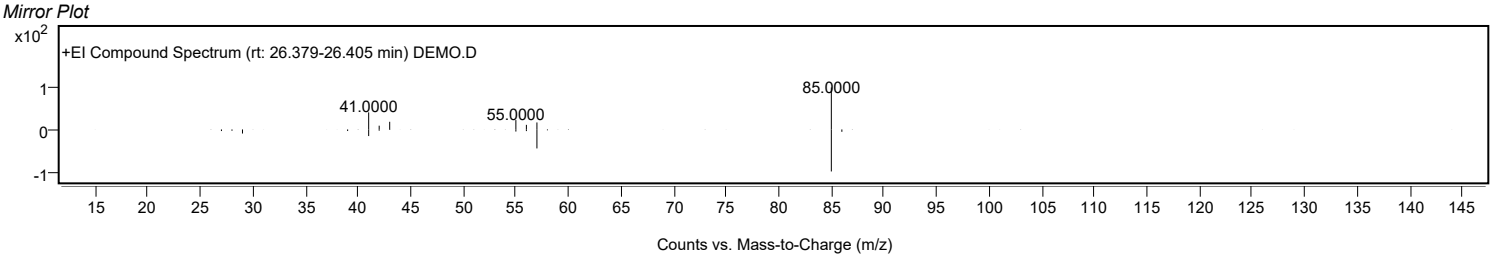
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			80.71			NIST.L

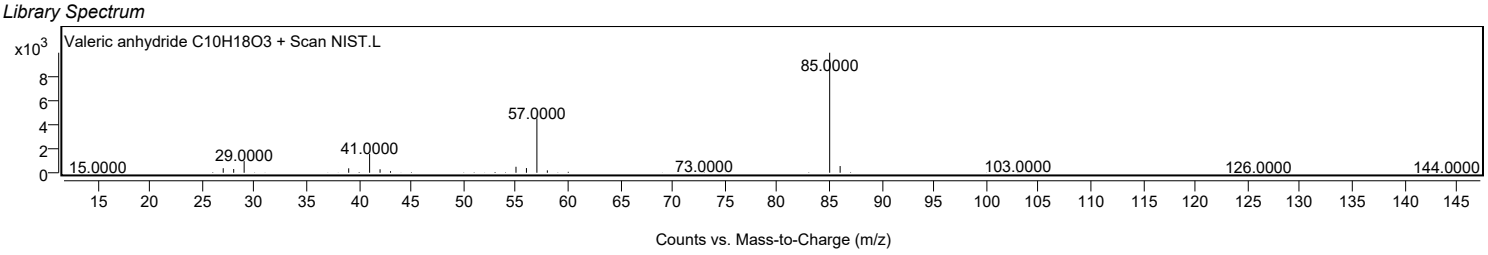
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 49: 1,2-Ethanediol, monobenzoate

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
1,2-Ethanediol, monobenzoate	C9 H10 O3	26.510			94-33-7	LibSearch	64.24	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		64.24			50		

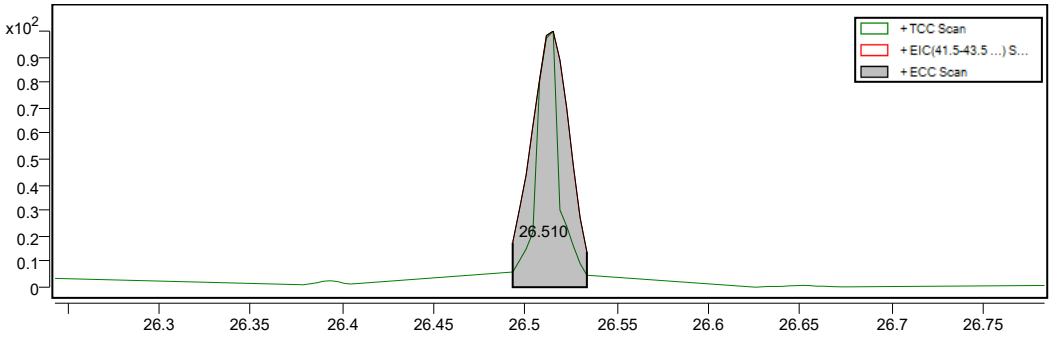
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

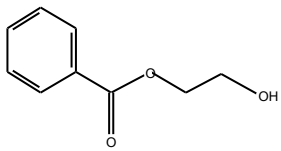
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
1,2-Ethanediol, monobenzoate	C9H10O3		LibSearch	26.510	3.143		94-33-7	64.24		
Benzhydrazide, N2-(2-methoxy-5-nitrobenzylideno)-	C15H13N3O4		LibSearch	26.510	-19.607		349572-84-5	63.92		
N'-(3-Pyridinylmethylene)benzohydrazide	C13H11N3O		LibSearch	26.510	-9.757		1215-53-8	62.63		
Benzenecarboxylic acid	C7H6O2		LibSearch	26.510			65-85-0	62.30		
Benzene, (methoxymethyl)-	C8H10O		LibSearch	26.510	10.360		538-86-3	62.23		
Benzoic acid, (4-pyridylmethylene)hydrazide	C13H11N3O		LibSearch	26.510	-9.757		1507-93-3	61.94		
Benzeneacetic acid, .alpha.-methoxy-, (S)-	C9H10O3		LibSearch	26.510	3.826		26164-26-1	61.91		
Benzoic acid	C7H6O2		LibSearch	26.510	7.343		65-85-0	61.53		
Benzene, (1-methoxyethyl)-	C9H12O		LibSearch	26.510	9.776		4013-34-7	61.18		
Methyl benzoate	C8H8O2		LibSearch	26.510	15.440		93-58-3	61.06		
Methyl Benzoate	C8H8O2		LibSearch	26.510			93-58-3	60.93		
Benzamide	C7H7NO		LibSearch	26.510	6.460		55-21-0	60.92		
Benzoic acid	C7H6O2		LibSearch	26.510	7.343		65-85-0	60.81		
Cyclobutane-1,1-dicarboxamide, N,N'-di-benzoyloxy-	C20H18N2O6		LibSearch	26.510	-28.390		1000253-25-3	60.64		
Benzoic acid	C7H6O2		LibSearch	26.510	7.343		65-85-0	60.54		
Benzenemethanol, 2-nitro-	C7H7NO3		LibSearch	26.510	2.643		612-25-9	60.50		
Benzoic acid	C7H6O2		LibSearch	26.510	7.343		65-85-0	60.41		
Benzaldehyde, dimethyl acetal	C9H12O2		LibSearch	26.510	14.610		1125-88-8	60.29		
Benzene, 2-methoxy-1,3-dimethyl-	C9H12O		LibSearch	26.510	8.243		1004-66-6	60.28		
Benzoic acid	C7H6O2		LibSearch	26.510	7.343		65-85-0	60.20		
Benzoic acid, methyl ester	C8H8O2		LibSearch	26.510	8.843		93-58-3	60.19		
Benzoic acid, methyl ester	C8H8O2		LibSearch	26.510	8.843		93-58-3	60.15		
Benzamide	C7H7NO		LibSearch	26.510	6.460		55-21-0	59.79		
(R)-(-)-.alpha.-Methoxyphenylacetic acid	C9H10O3		LibSearch	26.510	3.826		3966-32-3	59.56		
Ether, 2,4,6-cycloheptatrien-1-yl methyl	C8H10O		LibSearch	26.510	11.126		1714-38-1	59.52		
Benzene, 2-methoxy-1,3-dimethyl-	C9H12O		LibSearch	26.510	8.243		1004-66-6	59.45		
Benzamide	C7H7NO		LibSearch	26.510	6.460		55-21-0	59.45		
3-Ethylanisole	C9H12O		LibSearch	26.510	8.476		10568-38-4	59.32		
Dimethylanisole <2,4->	C9H12O		LibSearch	26.510			6738-23-4	59.29		
Benzeneacetic acid, .alpha.-methoxy-, (.+/-.)-	C9H10O3		LibSearch	26.510	3.826		7021-09-2	59.18		
Ethanone, 2-hydroxy-1-phenyl-	C8H8O2		LibSearch	26.510	5.310		582-24-1	59.16		
Benzenemethanol, 2-nitro-	C7H7NO3		LibSearch	26.510	2.643		612-25-9	59.09		
S-Benzoyl(thiohydroxylamine)	C7H7NOS		LibSearch	26.510	2.793		25740-80-1	58.96		
Anisole<para-methyl->	C8H10O		LibSearch	26.510	18.170		104-93-8	58.90		
Diazene, methylphenyl-, 1-oxide, (E)-	C7H8N2O		LibSearch	26.510			35150-75-5	58.90		
Benzoin methyl ether	C15H14O2		LibSearch	26.510	-3.707		3524-62-7	58.90		
Benzoic acid, (4-nitrophenyl)-methylenehydrozide	C14H11N3O3		LibSearch	26.510	-16.457		28123-77-5	58.78		
Cyclopropanecarboxamide, N-benzoyloxy-	C11H11NO3		LibSearch	26.510	-2.840		1000253-25-4	58.78		
Butanenitrile, 2,3-bis(benzoyloxyimino)-	C18H13N3O4		LibSearch	26.510	-22.307		1000269-66-6	58.75		
Benzoic acid, methyl ester	C8H8O2		LibSearch	26.510	8.843		93-58-3	58.68		
Benzenemethanol, 2-nitro-	C7H7NO3		LibSearch	26.510	2.643		612-25-9	58.65		
Benzene, (1-methoxyethyl)-	C9H12O		LibSearch	26.510	9.776		4013-34-7	58.53		
Benzene, 2-methoxy-1,3-dimethyl-	C9H12O		LibSearch	26.510	8.243		1004-66-6	58.43		
Methanol, oxo-, benzoate	C8H6O3		LibSearch	26.510	5.693		1000305-65-2	58.34		
Benzoic acid, methyl ester	C8H8O2		LibSearch	26.510	8.843		93-58-3	58.29		
1,2(4H)-Oxazine-3-ol, 5,6-dihydro-6-oxo-, benzoate	C11H9NO4		LibSearch	26.510	-5.074		1000253-25-6	58.21		
2-Chloroethyl benzoate	C9H9ClO2		LibSearch	26.510	3.426		939-55-9	58.15		
2-Pyridinealdoxime	C6H6N2O		LibSearch	26.510	7.460		873-69-8	58.14		
Heptanediamide, N,N'-di-benzoyloxy-	C21H22N2O6		LibSearch	26.510	-30.107		1000253-26-4	58.12		
Benzamide, N-(2-hydroxyethyl)-	C9H11NO2		LibSearch	26.510	-0.740		18838-10-3	57.98		

Compound Chromatograms (overlaid)

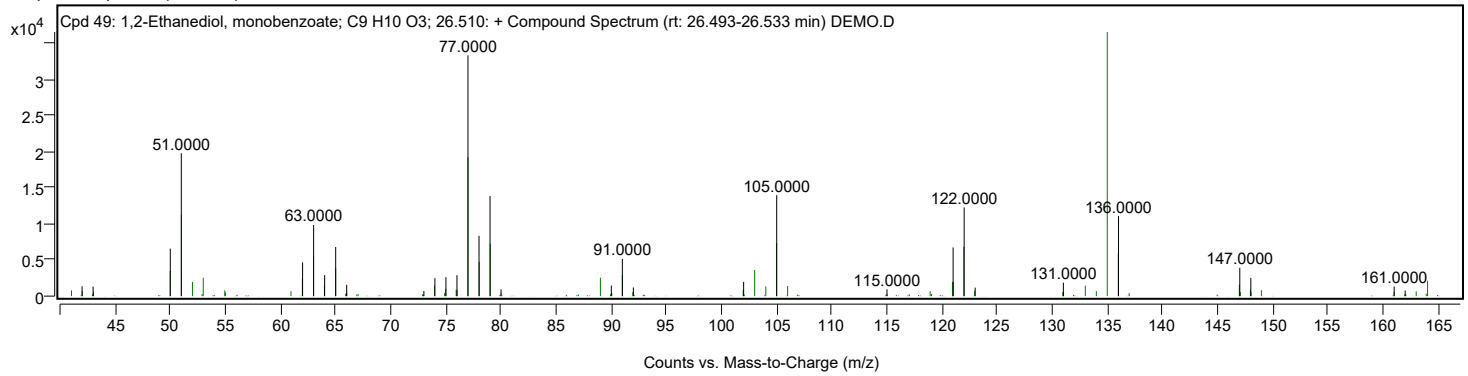


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



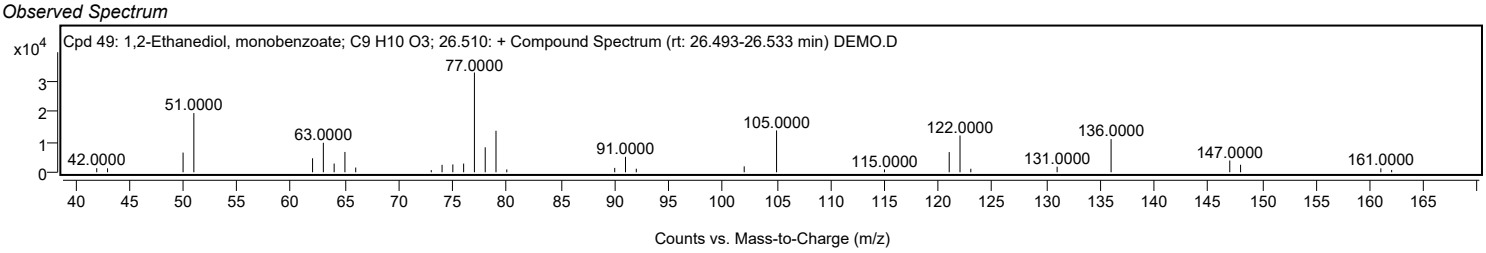
1,2-Ethanediol, monobenzoate

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			64.24			NIST.L

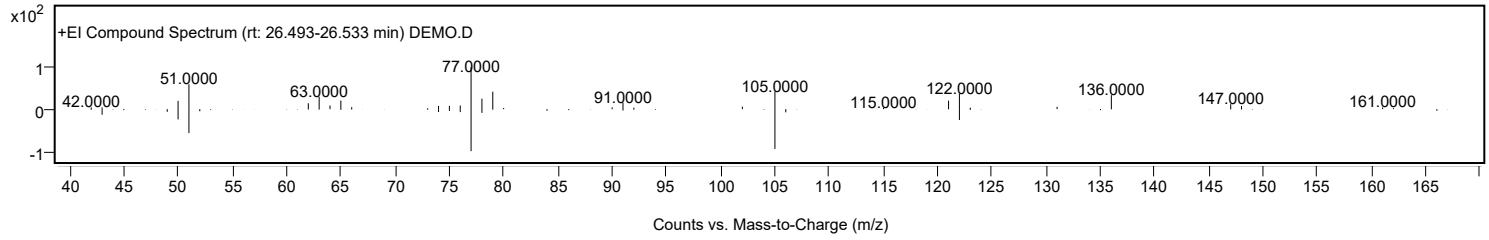
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			64.24			NIST.L

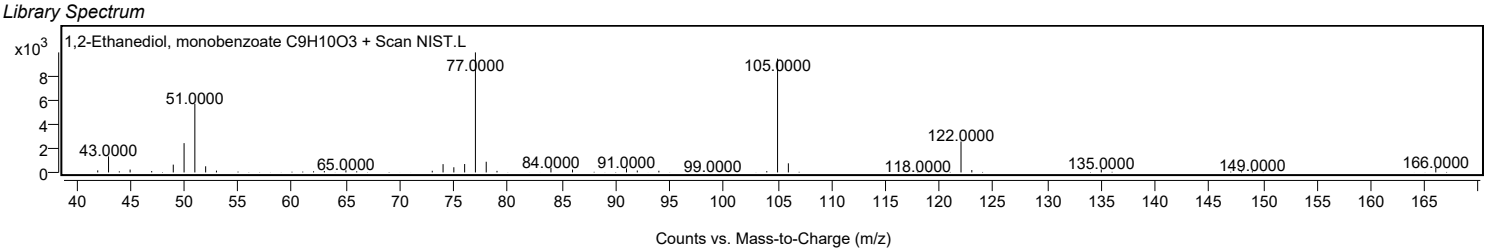
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 50: Helional (Tropional)

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Helional (Tropional)	C11 H12 O3	26.515			1205-17-0	LibSearch	97.01	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		97.01			50		

Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Helional (Tropional)	C11H12O3		LibSearch	26.515			1205-17-0	97.01		
2-Methoxy-4-methyl-1-pentylbenzene	C13H20O		LibSearch	26.515	1.615		1000408-33-6	83.23		
2-Butanone, 1-(1,3-benzodioxol-5-yl)-	C11H12O3		LibSearch	26.515	0.315		23023-13-4	82.43		
1-(1,3-benzodioxol-5-yl)-N-(1,3-benzodioxol-4-ylmethyl)-N-methylpropan-2-amine	C19H21NO4		LibSearch	26.515	-15.785		1000378-90-9	81.71		
2-Butanone, 1-(1,3-benzodioxol-5-yl)-	C11H12O3		LibSearch	26.515	0.315		23023-13-4	81.20		
1,3-Benzodioxole-5-propanal, .alpha.-methyl-	C11H12O3		LibSearch	26.515	0.515		1205-17-0	80.97		
4-(3,4-Methylenedioxyphenyl)-2-butanone	C11H12O3		LibSearch	26.515	0.315		55418-52-5	77.37		
Dulcinyl	C11H12O3		LibSearch	26.515			55418-52-5	77.36		
1,3-Benzodioxole, 5-propyl-	C10H12O2		LibSearch	26.515	4.232		94-58-6	76.08		
Benzamide, 2-methoxy-N-(2-phenylethyl)-N-ethyl-	C18H21NO2		LibSearch	26.515	-11.052		1000451-45-6	75.85		
Benzamide, 2-methoxy-N-propyl-	C11H15NO2		LibSearch	26.515	-1.502		1000420-13-0	75.81		
1,3-Benzodioxole, 5-propyl-	C10H12O2		LibSearch	26.515	4.232		94-58-6	75.65		
4-(3,4-Methylenedioxyphenyl)-2-butanone	C11H12O3		LibSearch	26.515	0.315		55418-52-5	75.04		
4-(3,4-Methylenedioxyphenyl)-2-butanone	C11H12O3		LibSearch	26.515	0.315		55418-52-5	74.84		
1,3-Benzodioxole, 5-propyl-	C10H12O2		LibSearch	26.515	4.232		94-58-6	73.90		
Benzene, 1-methoxy-4-(1-methylpropyl)-	C11H16O		LibSearch	26.515	6.232		4917-90-2	73.87		
4-(3,4-Methylenedioxyphenyl)-2-butanone	C11H12O3		LibSearch	26.515	0.315		55418-52-5	73.82		
1-(2-Methoxyphenyl)propan-1-one	C10H12O2		LibSearch	26.515	4.548		5561-92-2	73.80		
Benzamide, 4-methoxy-N-methyl-N-ethyl-	C11H15NO2		LibSearch	26.515	1.815		1000421-50-1	72.64		
m-Anisoyl amide, N-(2-phenylethyl)-N-ethyl-	C18H21NO2		LibSearch	26.515	-11.052		1000451-73-7	72.53		
Benzene, 1-methoxy-4-(1-methylpropyl)-	C11H16O		LibSearch	26.515	6.232		4917-90-2	72.46		
1-(2-Methoxyphenyl)propan-1-one	C10H12O2		LibSearch	26.515	4.548		5561-92-2	71.53		
3-Methyl-4-piperonyl-5-isoxazolone	C12H11NO4		LibSearch	26.515	-9.302		14731-85-2	70.68		
2-Methoxybenzoic acid, allyl ester	C11H12O3		LibSearch	26.515	2.548		31994-79-3	70.50		
Methyl 5-butylpyridine-2-carboxylate	C11H15NO2		LibSearch	26.515	2.082		1000408-33-1	70.05		
Benzamide, 2-methoxy-N-isobutyl-	C12H17NO2		LibSearch	26.515	-2.085		1000420-13-1	70.00		
2-Methoxy-N-methylhippuric acid, methyl ester	C12H15NO4		LibSearch	26.515	-2.635		1000250-14-9	69.62		
Benzene, 1-(1,3-dimethyl-3-butenyl)-4-methoxy-	C13H18O		LibSearch	26.515	3.465		74672-05-2	69.15		
1,3-Benzodioxole-5-propanal, .alpha.-methyl-, oxime (peak 1)	C11H13NO3		LibSearch	26.515	-2.268		1000475-84-1	68.58		
5H-Tetrazole-5-thione, 1,4-dihydro-1-methyl-4-phenyl-	C8H8N4S		LibSearch	26.515			1455-91-0	68.40		
Furazan-3-amine, 4-(3,4-methylenedioxybenzyloxy)-	C10H9N3O4		LibSearch	26.515	-7.552		1000294-23-2	68.16		
Bis-[1,3]-oxazino[5,6-f:6',5'-H]quinoline,3,10-bis(3,4-methylenedioxybenzyl)-6-trifluoromethyl-3,4,9,10(2H,11H)-tetrahydro-	C30H24F3N3O6		LibSearch	26.515	-46.535		41193-03-7	67.69		
1,3-Benzodioxole-5-propanal, .alpha.-methyl-, oxime (peak 2)	C11H13NO3		LibSearch	26.515	-2.268		1000475-84-0	67.59		
3-[3,4-Methylenedioxyphenyl]alanine	C10H11NO4		LibSearch	26.515	-4.685		33522-63-3	67.38		
3,4-Methylenedioxybenzyl isothiocyanate	C9H7NO2S		LibSearch	26.515			4430-47-1	67.26		
4-Methoxybenzoic acid, allyl ester	C11H12O3		LibSearch	26.515	2.548		6941-68-0	67.04		
Benzamide, 4-methoxy-N-methyl-N-(hept-2-yl)-	C16H25NO2		LibSearch	26.515	-5.402		1000421-50-6	66.86		
3-[2-(2-Methoxy-phenyl)-2-oxo-ethyl]-5-phenyl-3H-[1,3,4]oxadiazol-2-one	C17H14N2O4		LibSearch	26.515	-18.802		1000296-89-1	66.85		
2-Bromo-2'-methoxyacetophenone	C9H9BrO2		LibSearch	26.515	1.282		31949-21-0	66.81		
MDA 2-amido analog	C11H13NO3		LibSearch	26.515	-3.168		858215-05-1	66.64		
2-Methoxybenzoic acid, 2,5-dichlorophenyl ester	C14H10Cl2O3		LibSearch	26.515	-9.868		1000325-58-2	66.45		
Ehtyl 2-piperonyl carbazate	C11H14N2O4		LibSearch	26.515	-6.818		31203-56-2	66.43		
1H-Pyrazole-4-carboxamide, 3-[(1,3-benzodioxol-5-ylmethyl)amino]-	C12H12N4O3		LibSearch	26.515	-17.402		1000337-32-7	66.35		
5-[3,4-Methylenedioxybenzyl]hydantoin	C11H10N2O4		LibSearch	26.515	-9.452		62682-17-1	66.18		
2-Bromo-2'-methoxyacetophenone	C9H9BrO2		LibSearch	26.515	1.282		31949-21-0	66.02		
o-Methoxybenzoic acid, 2-bromo-4-fluorophenyl ester	C14H10BrFO3		LibSearch	26.515	-8.785		1000292-61-8	65.78		
Benzamide, 2-methoxy-N-methyl-	C9H11NO2		LibSearch	26.515	1.815		1000420-12-8	65.60		
5,5'-((2R,3S)-2,3-Dimethylbutane-1,4-diyl)bis(benzo[d][1,3]dioxole)	C20H22O4		LibSearch	26.515	-15.552		110269-50-6	65.58		
4-Methoxybenzoic acid, (benzo[1,2,5]oxadiazol-5-ylmethylene)hydrazide	C15H12N4O3		LibSearch	26.515	-18.468		1010316-75-5	65.53		
1-Propanone, 1-(3-methoxyphenyl)-	C10H12O2		LibSearch	26.515	4.548		37951-49-8	65.32		

Compound Discovery Report

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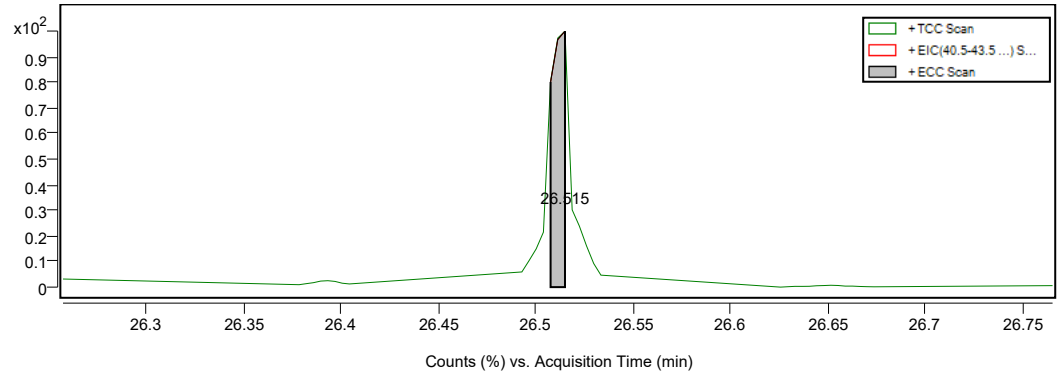
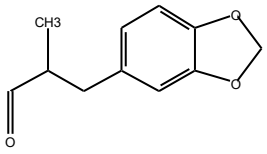
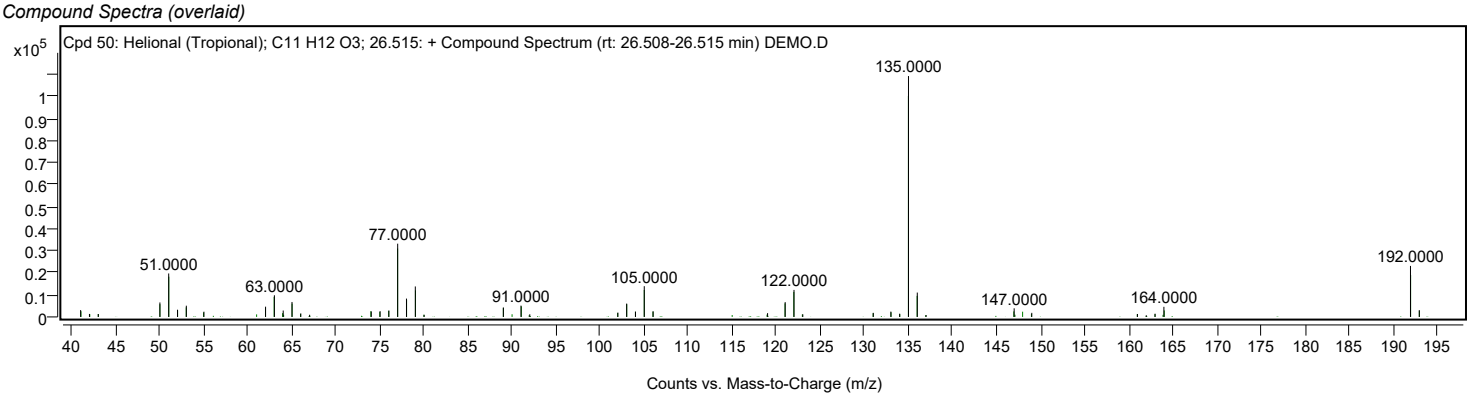
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



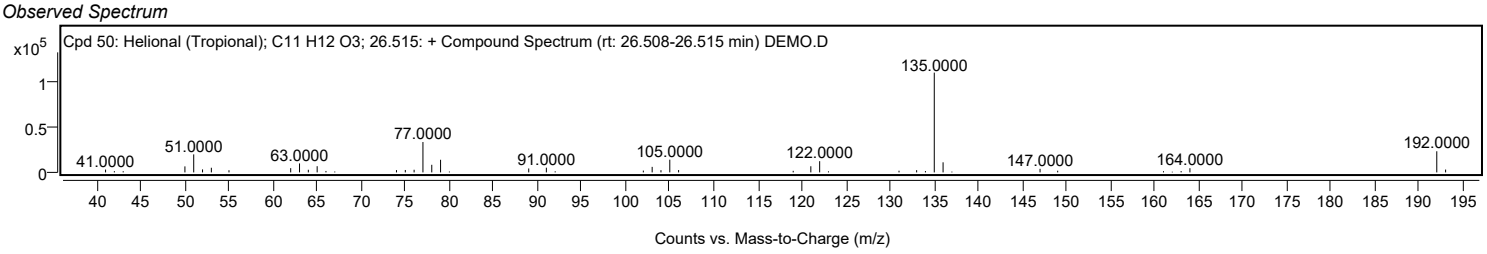
Helional (Tropional)

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			97.01			PWNose.xml

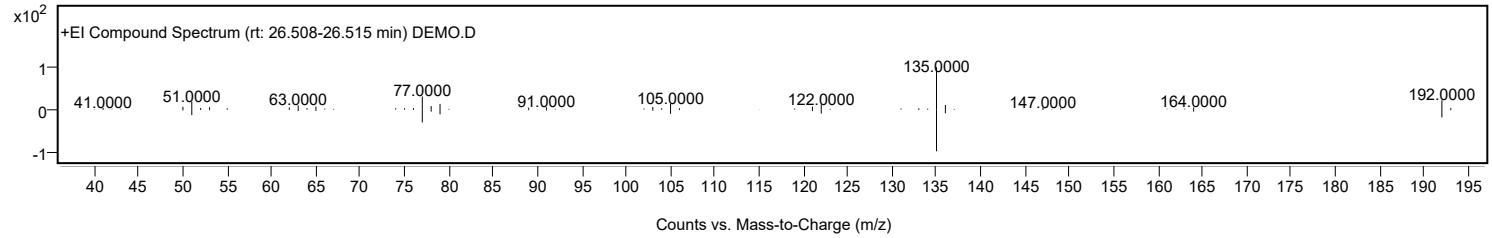
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			97.01			PWNose.xml

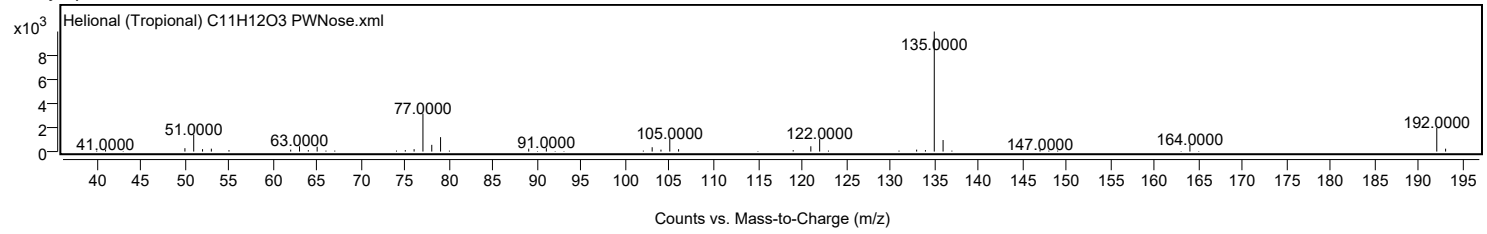
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 51: 4-tert-Octylphenol, TMS derivative

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
4-tert-Octylphenol, TMS derivative	C17 H30 O Si	26.654			78721-87-6	LibSearch	42.24	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		42.24			50		

Compound Discovery Report

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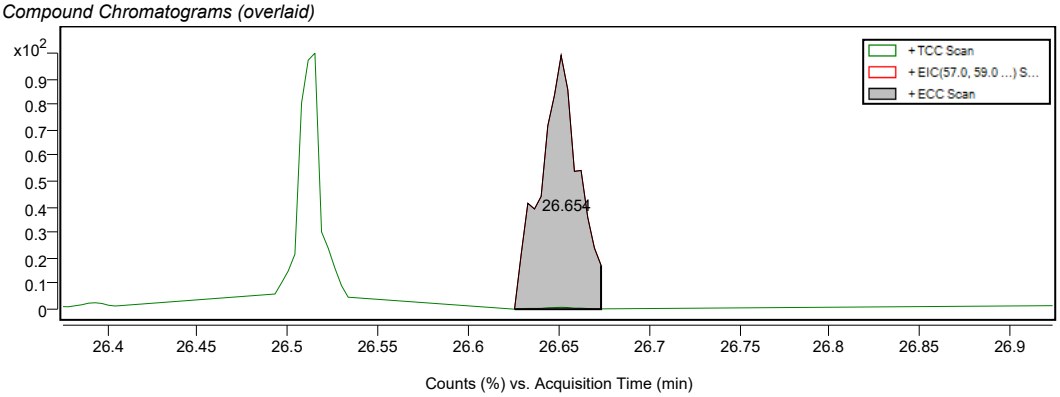
Compound ID Table

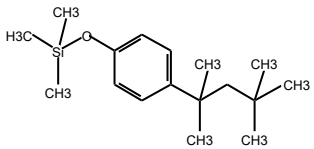
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
4-tert-Octylphenol, TMS derivative	C17H30OSi		LibSearch	26.654	-0.312		78721-87-6	42.24		
DL-Lactamide, methyl ether	C4H9NO2		LibSearch	26.654	12.654		1000452-56-7	42.22		
Silane, trimethyl-	C3H10Si		LibSearch	26.654	20.438		993-07-7	41.58		
1,1,1,3,5,5,5-Heptamethyltrisiloxane	C7H22O2Si3		LibSearch	26.654	14.271		1873-88-7	39.86		
1-(2-Methoxyethoxy)-2-methyl-2-propanol, methyl ether	C8H18O3		LibSearch	26.654	10.654		1000364-24-4	38.64		
4-tert-Octylphenol, TMS derivative	C17H30OSi		LibSearch	26.654	-0.312		78721-87-6	38.63		
Silane, trimethyl-	C3H10Si		LibSearch	26.654	20.438		993-07-7	38.11		
Methane, tert-butoxyisopropoxy-	C8H18O2		LibSearch	26.654	12.988		4346-01-4	37.95		
Butane, 2-methoxy-	C5H12O		LibSearch	26.654	17.821		6795-87-5	37.80		
Amylene hydrate	C5H12O		LibSearch	26.654	16.488		75-85-4	37.43		
1,3-Bis-t-butylperoxy-phthalan	C16H24O5		LibSearch	26.654	-4.829		97526-35-7	37.39		
2-Dodecylphenol, TMS	C21H38OSi		LibSearch	26.654	-9.762		345933-33-7	37.19		
4-tert-Octylphenol, TMS derivative	C17H30OSi		LibSearch	26.654	-0.312		78721-87-6	37.18		
3-Pentanol, 2-methyl-	C6H14O		LibSearch	26.654	14.721		565-67-3	36.77		
3-Methylene-cyclopropane-1,2-carboxylic acid peroxide t-butyl ester	C14H22O6		LibSearch	26.654	-1.029		1000143-92-5	35.79		
tert-Butyldimethylsilyl iodide	C6H15ISi		LibSearch	26.654	12.371		1000366-61-3	35.62		
p-Dioxane, 2,3-bis(tert-butyloxy)-	C12H24O4		LibSearch	26.654	3.338		1000149-87-9	35.51		
Amylene hydrate	C5H12O		LibSearch	26.654	16.488		75-85-4	35.42		
3-Pentanol, 2-methyl-	C6H14O		LibSearch	26.654	14.721		565-67-3	35.24		
Amylene hydrate	C5H12O		LibSearch	26.654	16.488		75-85-4	35.19		
3-Pentanol, 2-methyl-	C6H14O		LibSearch	26.654	14.721		565-67-3	34.97		
1,2-Propanediol, 2-methyl-, 1-methanesulfonate	C5H12O4S		LibSearch	26.654	6.771		74792-80-6	34.80		
4-tert-Butylphenol, TMS derivative	C13H22OSi		LibSearch	26.654	4.904		25237-79-0	34.71		
Propane, 2-methyl-2-(1-methylethoxy)-	C7H16O		LibSearch	26.654	15.921		17348-59-3	34.53		
tert-Butyl methyl carbonate	C6H12O3		LibSearch	26.654	13.721		32793-05-8	34.51		
2,4,6-Cycloheptatrien-1-one, 3,5-bis-trimethylsilyl-	C13H22OSi2		LibSearch	26.654	4.088		1000161-21-8	34.41		
1-Propanol, 2-(2-methoxypropoxy)-	C7H16O3		LibSearch	26.654	10.271		13588-28-8	34.40		
4-Hydroxy-3-hexanone	C6H12O2		LibSearch	26.654	11.388		4984-85-4	34.36		
Hydrazine, 2-butyl-1,1-dimethyl-	C6H16N2		LibSearch	26.654	12.238		54007-23-7	34.30		
Butane, 1-ethoxy-	C6H14O		LibSearch	26.654	15.088		628-81-9	34.28		
Butane, 1-ethoxy-	C6H14O		LibSearch	26.654	15.088		628-81-9	34.10		
2-Butanol, 3-methoxy-	C5H12O2		LibSearch	26.654	15.121		53778-72-6	33.81		
2-Propanol, 1-isopropoxy-2-methyl-	C7H16O2		LibSearch	26.654	12.971		3587-75-5	33.76		
Amylene hydrate	C5H12O		LibSearch	26.654	16.488		75-85-4	33.74		
3-Pentanol, 2-methyl-	C6H14O		LibSearch	26.654	14.721		565-67-3	33.74		
1-(1-Methoxypropan-2-yloxy)propan-2-yl 2-methylbutanoate	C12H24O4		LibSearch	26.654	4.304		1000367-11-4	33.70		
3-Hexanol	C6H14O		LibSearch	26.654	13.654		623-37-0	33.60		
2-Propanol, 1-(2-methoxypropoxy)-	C7H16O3		LibSearch	26.654	10.538		13429-07-7	33.25		
4-Hydroxy-3-hexanone	C6H12O2		LibSearch	26.654	11.388		4984-85-4	32.95		
Propane, 1-ethoxy-2-methyl-	C6H14O		LibSearch	26.654	16.171		627-02-1	32.44		
Thymol, TBDMS derivative	C16H28OSi		LibSearch	26.654	0.771		330455-64-6	32.39		
Hydrazine, 1,1-dimethyl-2-pentyl-	C7H18N2		LibSearch	26.654	10.571		67398-36-1	32.32		
Tri(1,2-propyleneglycol), monomethyl ether	C10H22O4		LibSearch	26.654	5.371		1000262-26-6	32.17		
3-Hexanol	C6H14O		LibSearch	26.654	13.654		623-37-0	31.84		
3-Hexanol	C6H14O		LibSearch	26.654	13.654		623-37-0	31.78		
Butanamide, 3,3-dimethyl-	C6H13NO		LibSearch	26.654	10.938		926-04-5	31.75		
Methyl propanoate	C4H8O2		LibSearch	26.654	24.724		554-12-1	31.71		
sec-Butyl ethyl ether	C6H14O		LibSearch	26.654			2679-87-0	31.68		
Hexan-3-ol	C6H14O		LibSearch	26.654			623-37-0	31.57		
4-Hydroxy-3-hexanone	C6H12O2		LibSearch	26.654	11.388		4984-85-4	31.48		

Compound Chromatograms (overlaid)

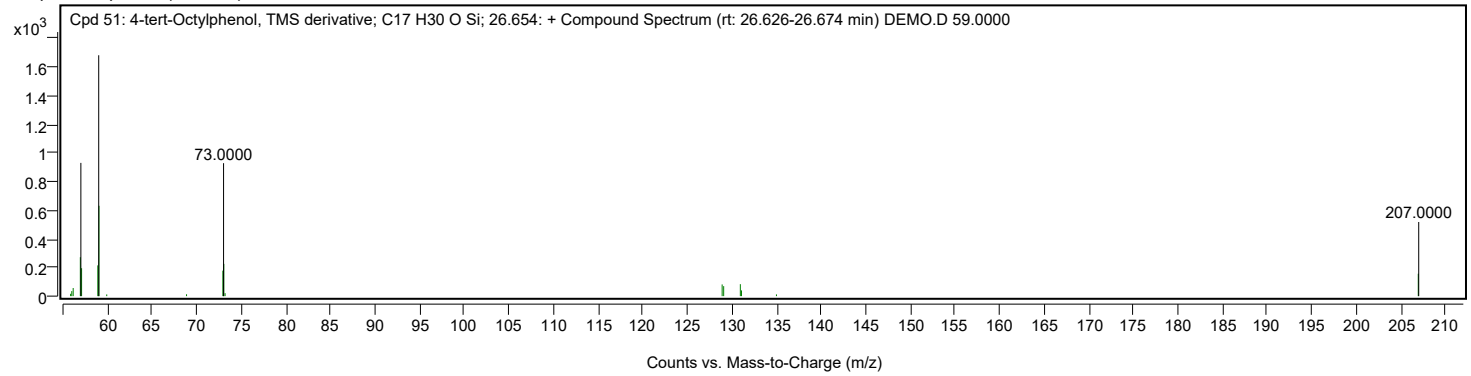


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



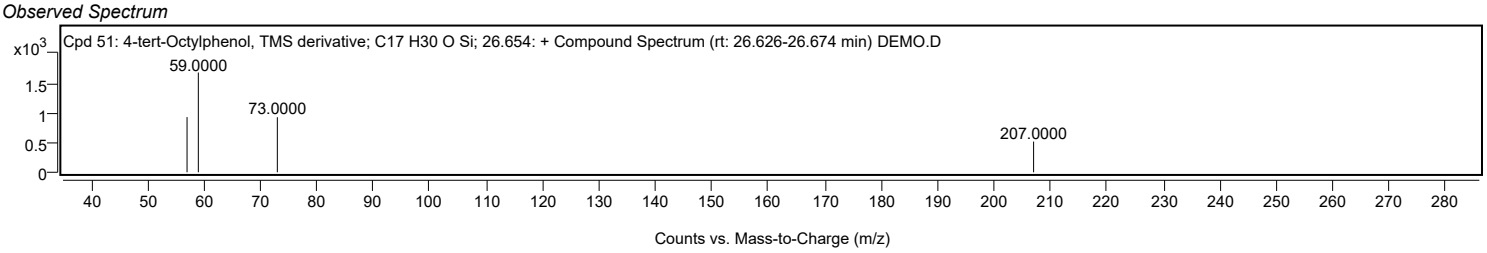
4-tert-Octylphenol, TMS derivative

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			42.24			NIST.L

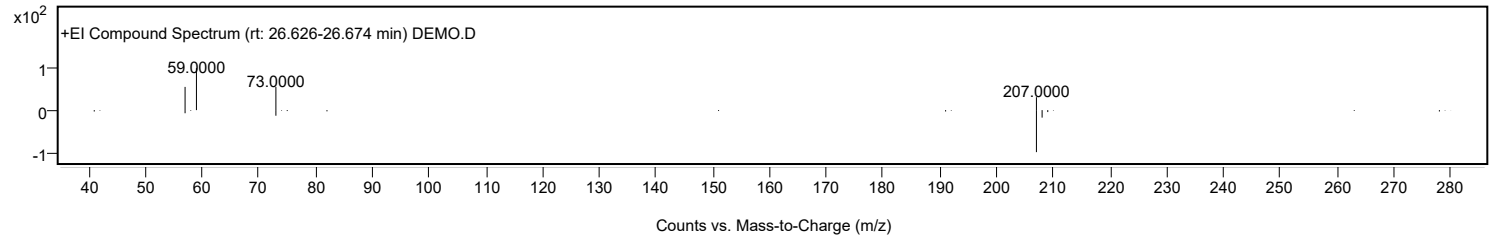
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			42.24			NIST.L

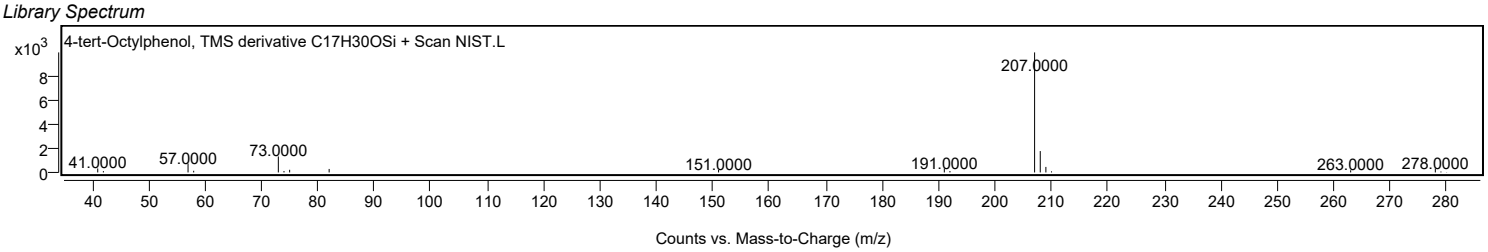
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 52: Propanedinitrile, cyclohexyl(2-methylcyclohexyl)-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Propanedinitrile, cyclohexyl(2-methylcyclohexyl)-	C16 H24 N2	27.171			74764-55-9	LibSearch	50.70	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		50.70			50		

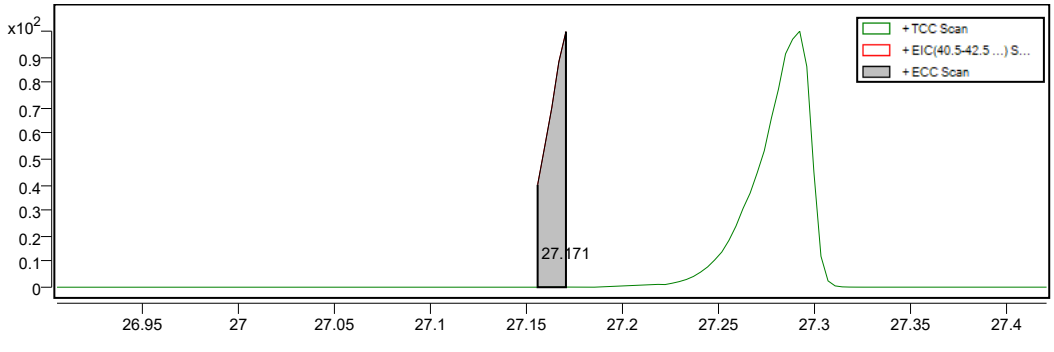
Compound Discovery Report

Agilent | Trusted Answers

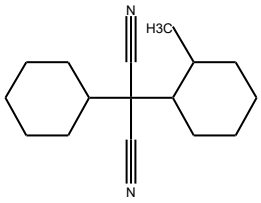
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Propanedinitrile, cyclohexyl(2-methylcyclohexyl)-	C16H24N2		LibSearch	27.171	-7.929		74764-55-9	50.70		
Cyclohexane, nitro-	C6H11NO2		LibSearch	27.171	9.454		1122-60-7	49.45		
Cyclohexane, nitro-	C6H11NO2		LibSearch	27.171	9.454		1122-60-7	49.38		
1,5-Heptadien-4-one, 3,3,6-trimethyl-	C10H16O		LibSearch	27.171	9.804		546-49-6	48.91		
Cyclopentane acetic acid hydrazide	C7H14N2O		LibSearch	27.171	3.788		20287-25-6	48.62		
Cyclohexane, (bromomethyl)-	C7H13Br		LibSearch	27.171	9.221		2550-36-9	48.59		
Hexadienyl tiglate, (2E,4E)-	C11H16O2		LibSearch	27.171			1231959-42-4	48.47		
5-Methyl-N-nitro-1H-1,2,4-triazol-3-amine	C3H5N5O2		LibSearch	27.171	2.088		42216-41-1	48.46		
(4-Bromobutan-2-yl)cyclopropane	C7H13Br		LibSearch	27.171	11.321		1000444-18-1	48.26		
1-Pentyne, 3-methoxy-3-methyl-	C7H12O		LibSearch	27.171	15.404		22802-35-3	47.93		
Dicyclohexyl methylphosphonate	C13H25O3P		LibSearch	27.171			7040-53-1	47.88		
Sulfurous acid, cyclohexylmethyl ethyl ester	C9H18O3S		LibSearch	27.171	0.454		1000309-21-2	47.60		
Cyclohexane, bromo-	C6H11Br		LibSearch	27.171	10.888		108-85-0	47.45		
Cyclohexanemethanol, chlorodifluoroacetate	C9H13ClF2O2		LibSearch	27.171	7.754		1010376-25-9	47.11		
Cyclohexane, 1-bromo-4-methyl-	C7H13Br		LibSearch	27.171	9.871		6294-40-2	46.89		
Oxalic acid, dicyclohexyl ester	C14H22O4		LibSearch	27.171	-4.062		1000309-30-9	46.82		
Cycloheptane, bromo-	C7H13Br		LibSearch	27.171	8.888		2404-35-5	46.65		
Cyclohexane, (2-nitro-2-propenyl)-	C9H15NO2		LibSearch	27.171	5.038		80255-17-0	46.52		
Cyclohexane, bromo-	C6H11Br		LibSearch	27.171	10.888		108-85-0	46.44		
Oxalic acid, cyclohexyl propyl ester	C11H18O4		LibSearch	27.171	1.954		1000309-30-3	46.34		
Cyclohexane, 1-bromo-2-methyl-	C7H13Br		LibSearch	27.171	9.871		6294-39-9	46.29		
Hexadienyl angelate, 2E, 4E-	C11H16O2		LibSearch	27.171	5.788		1000383-63-9	46.26		
Sulfurous acid, di(cyclohexylmethyl) ester	C14H26O3S		LibSearch	27.171	-8.879		1010309-22-7	46.18		
Cyclopropane, 2-bromo-1,1,3-trimethyl-	C6H11Br		LibSearch	27.171	13.621		36617-00-2	46.10		
Phosphorous acid, dicyclohexyl ester	C12H23O3P		LibSearch	27.171	-2.146		139-69-5	46.06		
Oxalic acid, cyclohexyl ethyl ester	C10H16O4		LibSearch	27.171	3.621		1000309-30-2	45.98		
Artemisia ketone	C10H16O		LibSearch	27.171	17.291		546-49-6	45.91		
Oxalic acid, cyclohexyl butyl ester	C12H20O4		LibSearch	27.171	0.304		1000309-30-5	45.91		
Pentadecafluorooctanoic acid, cyclohexylmethyl ester	C15H13F15O2		LibSearch	27.171	14.754		1000406-81-0	45.90		
Dicyclohexyl methylphosphonate	C13H25O3P		LibSearch	27.171			7040-53-1	45.66		
Cyclohexanemethanol	C7H14O		LibSearch	27.171	10.121		100-49-2	45.56		
1,5-Octadiene, 7-methyl-3-(1-methylethyl)-	C12H22		LibSearch	27.171	10.171		74630-12-9	45.55		
Cyclohexyl methylphosphonate	C7H15O3P		LibSearch	27.171			1932-60-1	45.55		
Cyclohexanemethanol	C7H14O		LibSearch	27.171	10.121		100-49-2	45.50		
2,6-Octadiene, 2,4-dimethyl-	C10H18		LibSearch	27.171	11.438		63843-03-8	45.49		
Phosphonous dibromide, cyclohexyl-	C6H11Br2P		LibSearch	27.171	3.838		86012-32-0	45.36		
Cyclopentane, 1-methyl-2-(2-propenyl)-, trans-	C9H16		LibSearch	27.171	11.988		50746-53-7	45.27		
Cyclohexane, 1-bromo-4-methyl-	C7H13Br		LibSearch	27.171	9.871		6294-40-2	45.21		
Cyclohexane, azido-	C6H11N3		LibSearch	27.171			19573-22-9	45.20		
Cycloheptane, bromo-	C7H13Br		LibSearch	27.171	8.888		2404-35-5	45.13		
Cyclohexane, 1-bromo-4-methyl-	C7H13Br		LibSearch	27.171	9.871		6294-40-2	45.12		
Cyclohexanemethanol	C7H14O		LibSearch	27.171	10.121		100-49-2	45.10		
Cyclohexanemethanol	C7H14O		LibSearch	27.171	10.121		100-49-2	45.09		
Octadienyl angelate, 2E, 4E-	C13H20O2		LibSearch	27.171	2.471		1000383-60-4	44.86		
Cyclohexylmethanol, trifluoroacetate (ester)	C9H13F3O2		LibSearch	27.171	10.821		164071-20-9	44.81		
Pentyl methanesulfonate	C6H14O3S		LibSearch	27.171			6968-20-3	44.79		
Pinocamphone<trans->	C10H16O		LibSearch	27.171	13.171		547-60-4	44.70		
Cyclobutanecarboxylic acid, 2-propenyl ester	C8H12O2		LibSearch	27.171	10.571		1000282-60-3	44.53		
Cyclohexane, bromo-	C6H11Br		LibSearch	27.171	10.888		108-85-0	44.44		
acetic acid, 2,2,2-trifluoro-, [1,1'-bicyclohexyl]-4-yl ester	C14H21F3O2		LibSearch	27.171	2.121		1000397-13-2	44.43		

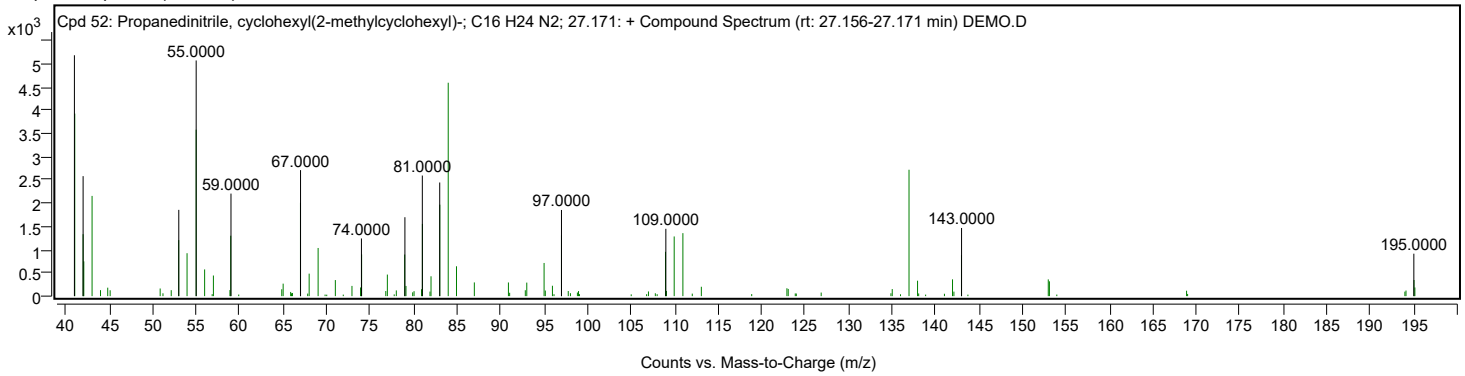
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



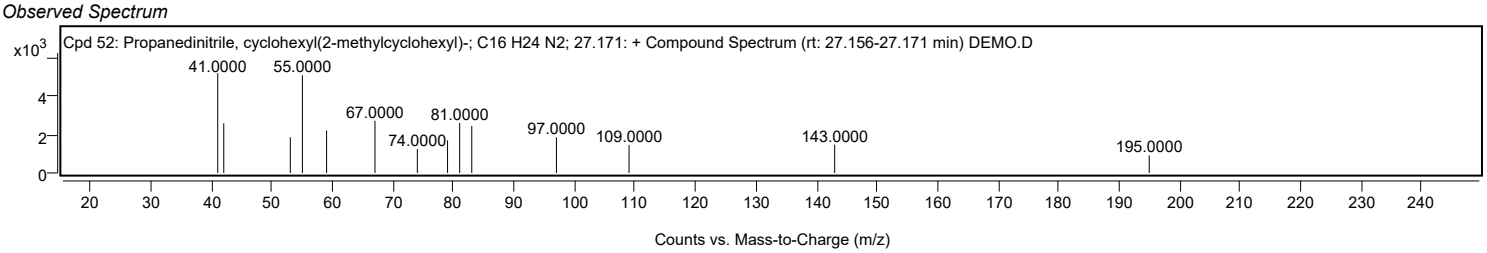
Propanedinitrile, cyclohexyl(2-methylcyclohexyl)-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			50.70			NIST.L

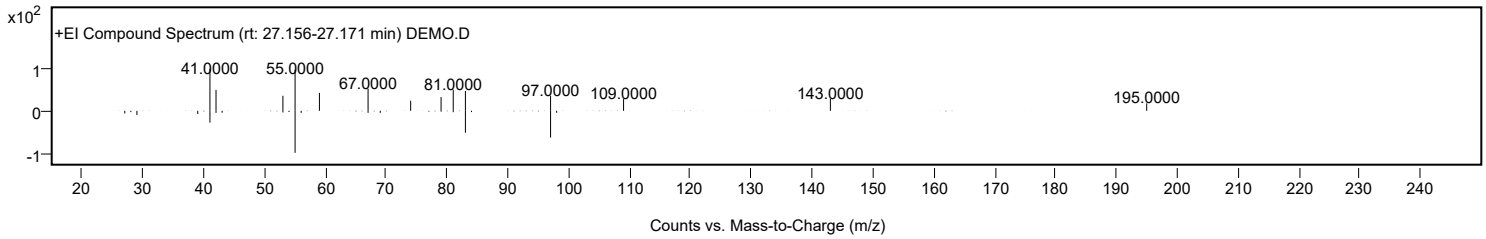
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			50.70			NIST.L

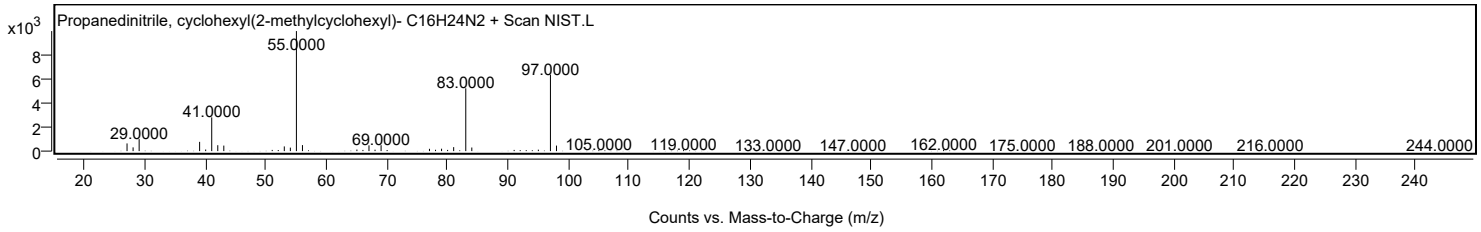
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 53: 1,4-Pentadiene, 2-methyl-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
1,4-Pentadiene, 2-methyl-	C6 H10	27.182			763-30-4	LibSearch	39.87	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		39.87			50		

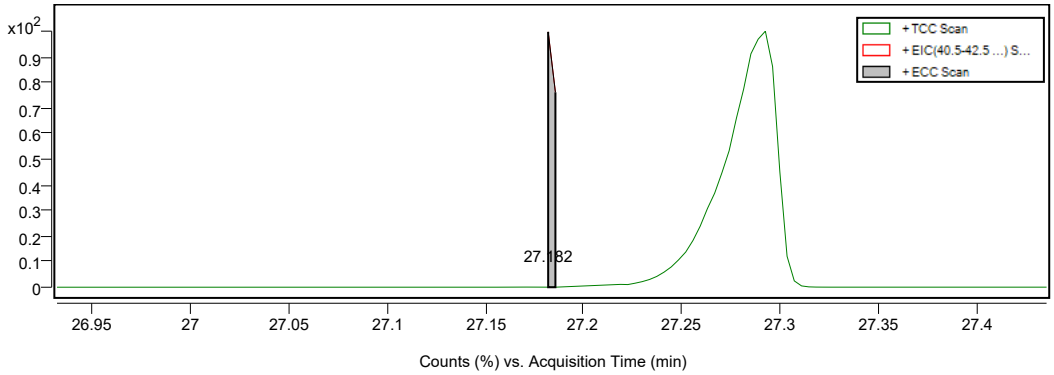
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

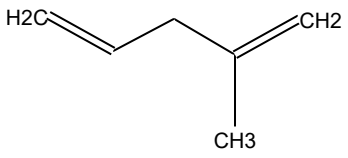
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
1,4-Pentadiene, 2-methyl-	C6H10		LibSearch	27.182	17.599		763-30-4	39.87		
4-Pyrimidinamine, 6-methyl-	C5H7N3		LibSearch	27.182	8.965		3435-28-7	39.67		
Cyclopentane, 2-ethylidene-1,1-dimethyl-	C9H16		LibSearch	27.182	11.882		56324-66-4	39.45		
3,3,5,5-Tetramethylcyclopentene	C9H16		LibSearch	27.182	12.999		38667-10-6	39.23		
Cyclooctanethiol, 2-(diethylboryloxy)-	C12H25BOS		LibSearch	27.182			1000161-69-7	38.83		
Cyclopropane, 1,2-dimethyl-3-methylene-, cis-	C6H10		LibSearch	27.182	18.032		4866-55-1	38.69		
1-Cyclooctene, 3-bromo-	C8H13Br		LibSearch	27.182	7.199		1000163-39-0	38.65		
Hexadienal<2E,4E->	C6H8O		LibSearch	27.182	22.042		142-83-6	38.38		
1-Propanone, 1-(1-cyclohexen-1-yl)-	C9H14O		LibSearch	27.182	8.415		1655-03-4	38.05		
Salvene<E->	C9H16		LibSearch	27.182	22.982		33746-69-9	38.04		
Senecionitrile	C5H7N		LibSearch	27.182			4786-24-7	37.68		
trans-8a-Methylperhydroazulen-4(1H)-one	C11H18O		LibSearch	27.182	4.749		32166-45-3	37.61		
1,4-Pentadiene, 3-methyl-	C6H10		LibSearch	27.182	18.282		1115-08-8	37.09		
Salvene<Z->	C9H16		LibSearch	27.182	23.172		33746-70-2	36.92		
Cyclopropane, 1,2-dimethyl-3-methylene-, trans-	C6H10		LibSearch	27.182	18.032		5070-00-8	36.73		
(3S,3aS,6R,7[a]R)-Perhydro-3,6-dimethyl-benzo-[b]-furan-2-one	C10H16O2		LibSearch	27.182			103666-97-3	36.53		
Cyclopentane, (2-methylbutylidene)-	C10H18		LibSearch	27.182	10.215		53366-54-4	36.44		
2,4-Hexadienal, (E,E)-	C6H8O		LibSearch	27.182	13.482		142-83-6	36.32		
Cyclopropane, 2-methylene-1-propionyl-	C7H10O		LibSearch	27.182	13.482		1000157-08-1	36.06		
1,4-Hexadiene, 3-ethyl-4,5-dimethyl-	C10H18		LibSearch	27.182	12.132		1000154-09-2	36.05		
3-Hexyne-2,5-diol, 2,5-dimethyl-	C8H14O2		LibSearch	27.182	10.232		142-30-3	35.94		
Cyclohexanone, 2-nitro-	C6H9NO3		LibSearch	27.182	6.615		4883-67-4	35.93		
(3R,3aR,6R,7[a]S)-Perhydro-3,6-dimethyl-benzo-[b]-furan-2-one	C10H16O2		LibSearch	27.182			92015-65-1	35.88		
Furane-2-carboxaldehyde, 5-(4-nitrophenoxymethyl)-	C12H9NO5		LibSearch	27.182	-7.235		1000273-82-3	35.88		
1-Allyl-cyclopropanecarboxylic acid, 2,6-di-t-butyl-4-methyl-phenyl ester	C22H32O2		LibSearch	27.182	-11.001		108546-69-6	35.87		
1,5-Hexadiene	C6H10		LibSearch	27.182	17.215		592-42-7	35.82		
2,2,6,6-Tetramethylthiabicyclohexane	C9H18S		LibSearch	27.182	8.349		78050-22-3	35.75		
3-Cyclohexene-1-acetic acid, .alpha.-oxo-, methyl ester	C9H12O3		LibSearch	27.182	6.099		77846-83-4	35.73		
Cyclohexane, butylidene-	C10H18		LibSearch	27.182	8.815		2272-03-9	35.72		
3-Heptyne, 5-ethyl-5-methyl-	C10H18		LibSearch	27.182	11.382		61228-10-2	35.70		
(3R,3aS,6R,7[a]R)-Perhydro-3,6-dimethyl-benzo-[b]-furan-2-one	C10H16O2		LibSearch	27.182			92015-65-1	35.62		
Borinic acid, diethyl-, 1-methyl-2-propynyl ester	C8H15BO		LibSearch	27.182			55848-32-3	35.58		
1,4-Pentadiene, 3-methyl-	C6H10		LibSearch	27.182	18.282		1115-08-8	35.55		
Sorbaldehyde	C6H8O		LibSearch	27.182			4488-48-6	35.48		
1-Hexyne	C6H10		LibSearch	27.182	16.932		693-02-7	35.48		
Pentane, 1-chloro-5-(methylenecyclopropyl)-	C9H15Cl		LibSearch	27.182	8.682		1000158-49-0	35.41		
Cyclooctene, 3-(2-propenyl)-	C11H18		LibSearch	27.182	7.332		61141-59-1	35.37		
3-Octyne, 7-methyl-	C9H16		LibSearch	27.182	12.699		37050-06-9	35.36		
Sorbic aldehyde	C6H8O		LibSearch	27.182			142-83-6	35.33		
Ethanone, 1-(1,3-dimethyl-3-cyclohexen-1-yl)-	C10H16O		LibSearch	27.182	7.832		51733-68-7	35.26		
2(1H)-Pyridinone, 1-methyl-	C6H7NO		LibSearch	27.182	10.432		694-85-9	35.23		
Cyclohexene,3-(1-methylpropyl)-	C10H18		LibSearch	27.182	10.565		15232-91-4	35.18		
2-Hexyne, 4-methyl-	C7H12		LibSearch	27.182	16.015		20198-49-6	35.07		
1-(1,2,3-Trimethyl-cyclopent-2-enyl)-ethanone	C10H16O		LibSearch	27.182	8.332		70987-81-4	35.05		
Heptadienal <2,4-trans,trans->	C7H10O		LibSearch	27.182			4313-03-5	35.03		
1,3-Hexadiene, 2,3,5-trimethyl-	C9H16		LibSearch	27.182	13.782		61142-34-5	34.98		
Cyclopentanepropanethiol, thiolacetate	C10H18OS		LibSearch	27.182	3.099		28796-76-1	34.94		
Cyclopropene, 3,3-diethyl-	C7H12		LibSearch	27.182	15.932		78578-86-6	34.88		
1,3,3-Trimethylcyclopropene	C6H10		LibSearch	27.182	17.749		3664-56-0	34.85		
Cyclopentene, 3-methyl-1-(1-methylethyl)-	C9H16		LibSearch	27.182	12.732		51115-02-7	34.84		

Compound Chromatograms (overlaid)

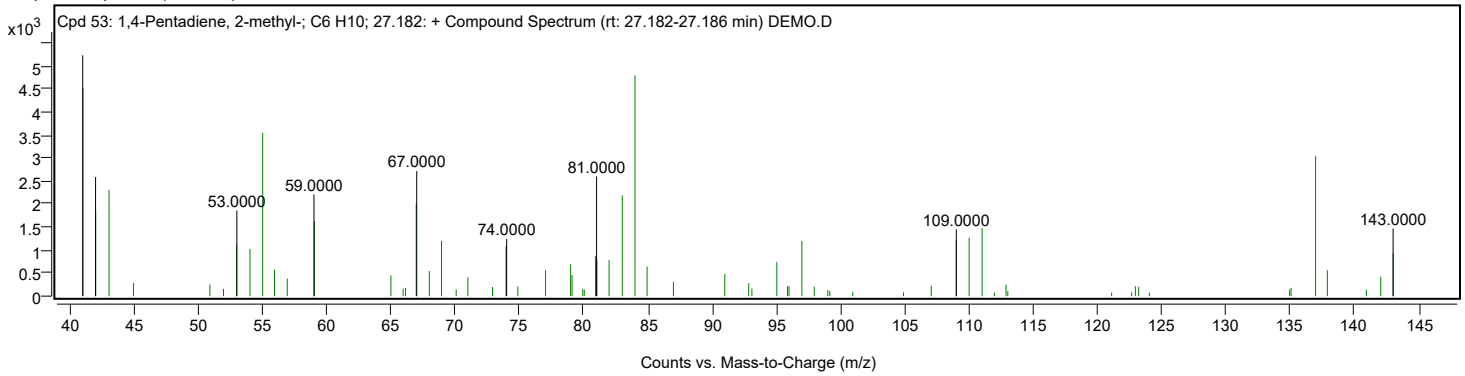


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



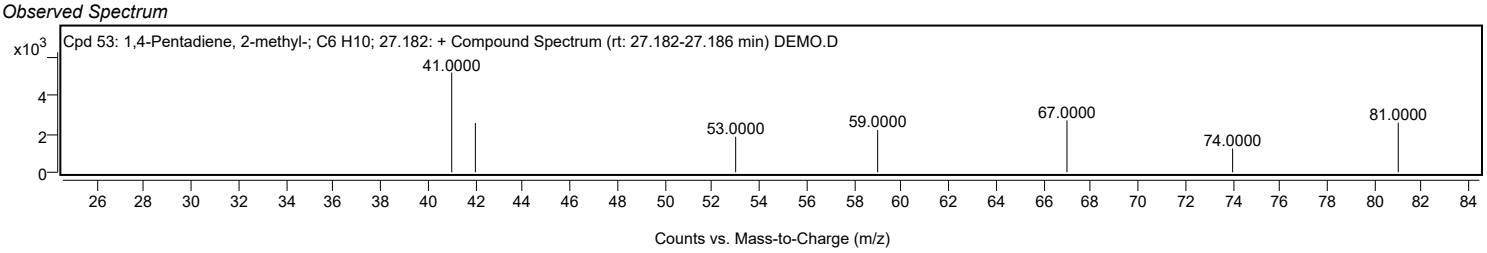
1,4-Pentadiene, 2-methyl-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			39.87			NIST.L

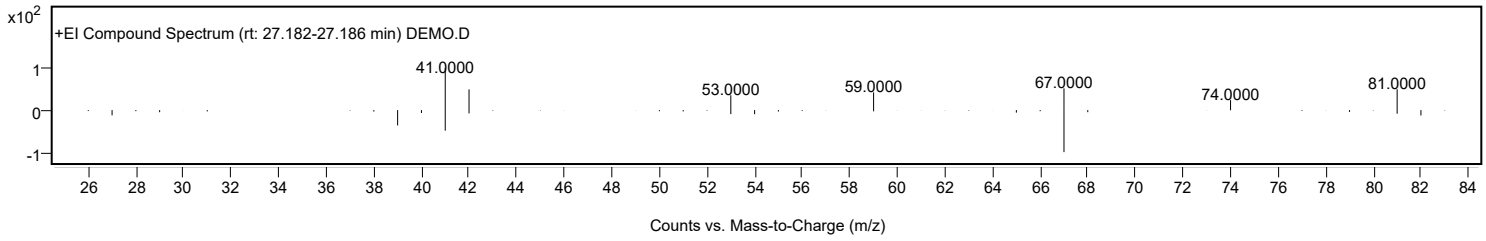
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			39.87			NIST.L

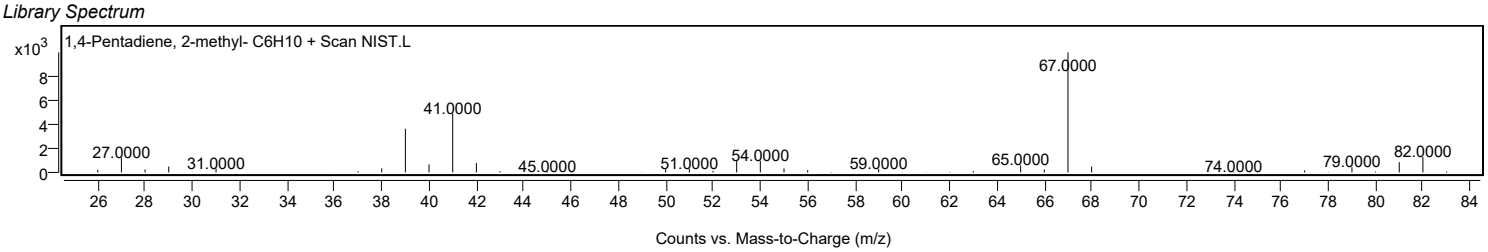
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 54: [2-(3,3a,4,5,6,10c-Hexahydro-1H-pyrrolo[3,4-c]carbazol-2-yl)-ethyl]-dimethyl-amine

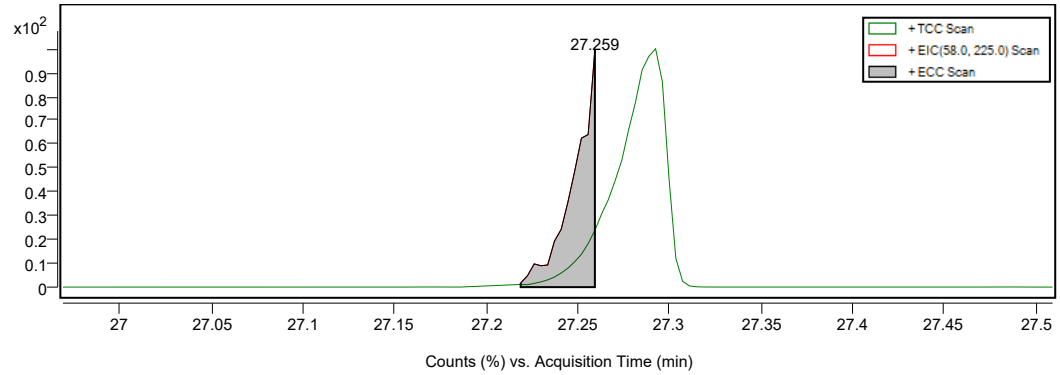
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
[2-(3,3a,4,5,6,10c-Hexahydro-1H-pyrrolo[3,4-c]carbazol-2-yl)-ethyl]-dimethyl-amine	C18 H25 N3	27.259			1000297-41-9	LibSearch	27.87	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		27.87			2		

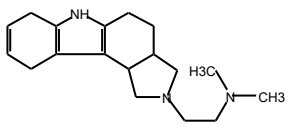
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
[2-(3,3a,4,5,6,10c-Hexahydro-1H-pyrrolo[3,4-c]carbazol-2-yl)-ethyl]-dimethyl-amine	C18H25N3		LibSearch	27.259	-9.607		1000297-41-9	27.87		
1H-Pyrrolo[2,3-f]quinoline-7-carboxylic acid, 6,9-dihydro-5-methoxy-2,3-dimethyl-9-oxo-, ethyl ester	C17H18N2O4		LibSearch	27.259	-19.124		1000350-72-1	5.95		

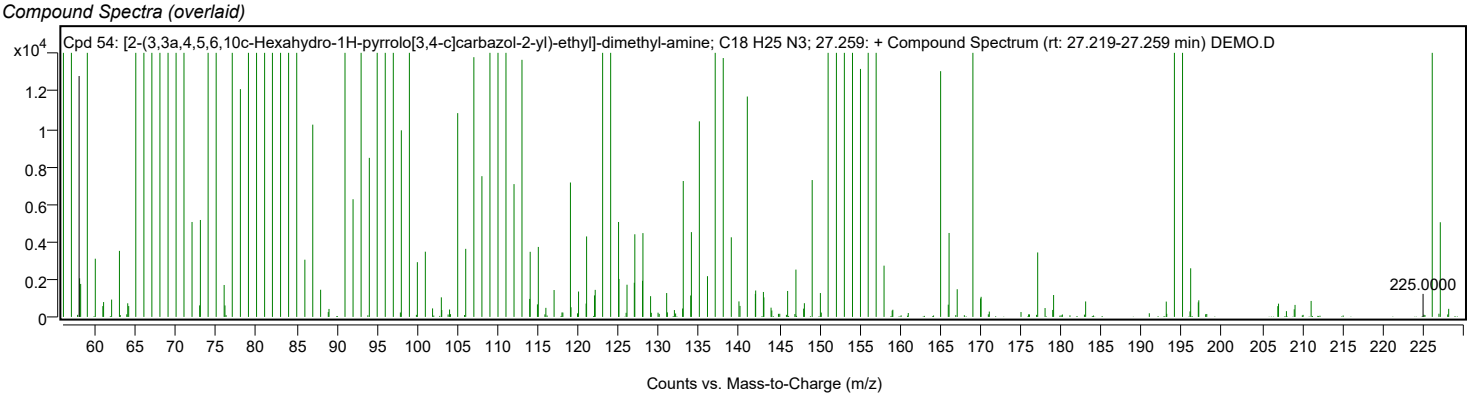
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



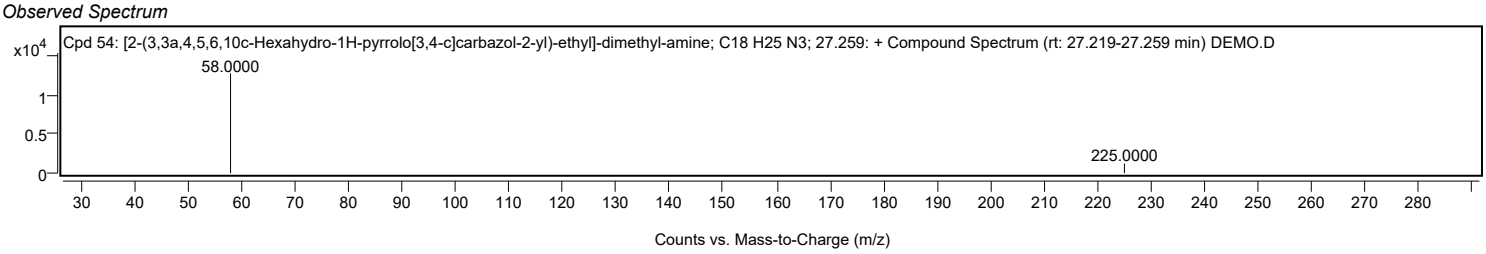
[2-(3,3a,4,5,6,10c-Hexahydro-1H-pyrrolo[3,4-c]carbazol-2-yl)-ethyl]-dimethyl-amine

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			27.87			NIST.L

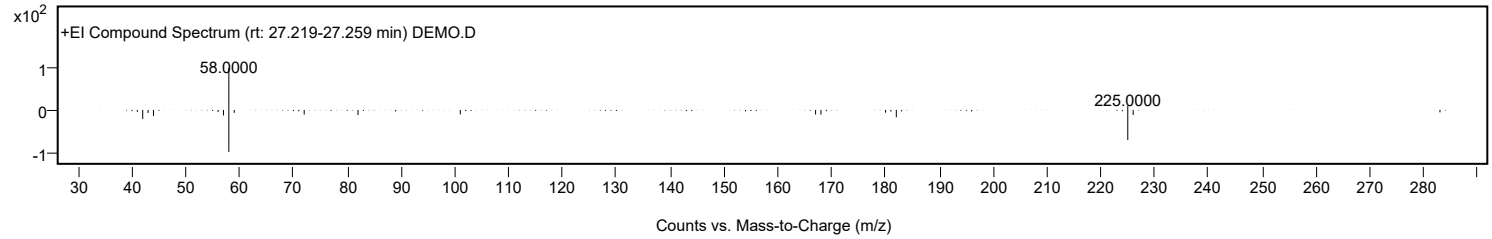
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			27.87			NIST.L

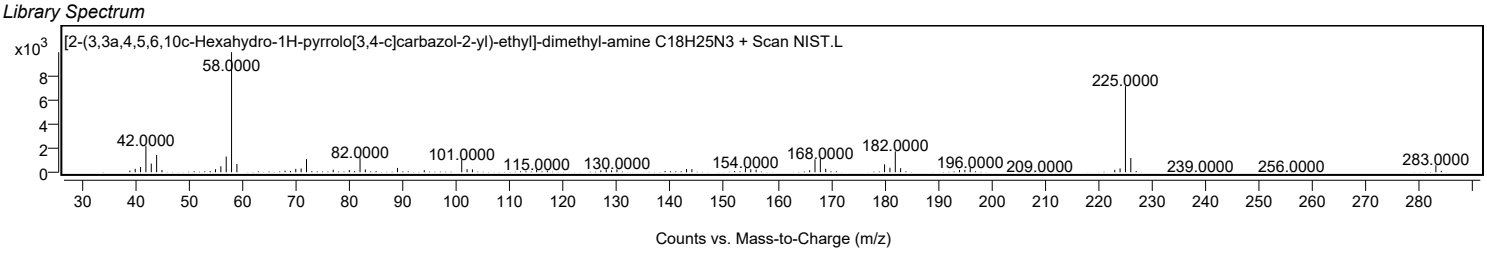
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 55: Methyl dihydrojasmonate<cis->

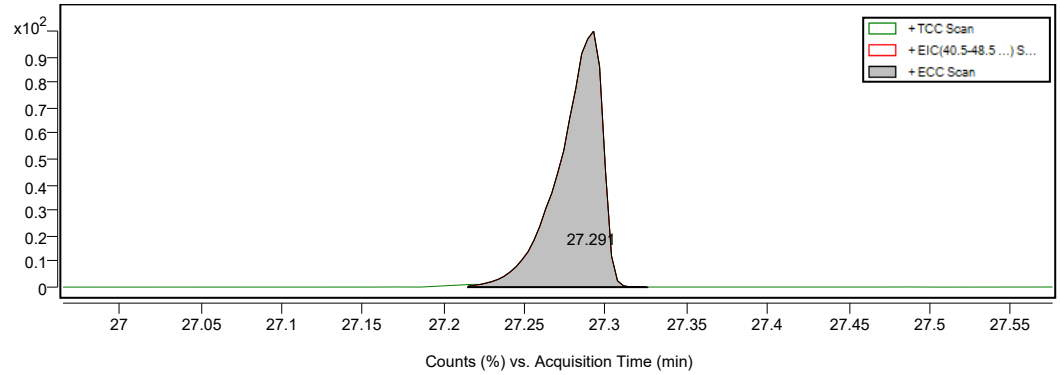
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Methyl dihydrojasmonate<cis->	C13 H22 O3	27.291			39647-11-5	LibSearch	97.09	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		97.09			50		

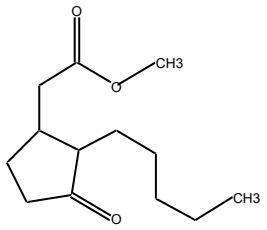
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Methyl dihydrojasmonate<cis->	C13H22O3		LibSearch	27.291	-7.699		39647-11-5	97.09		
Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester	C13H22O3		LibSearch	27.291	-0.326		24851-98-7	96.54		
Methyl dihydrojasmonate<trans->	C13H22O3		LibSearch	27.291	-8.759		2630-39-9	95.71		
Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester	C13H22O3		LibSearch	27.291	-0.326		24851-98-7	89.21		
Dihydrojasmonate <methyl-, trans->	C13H22O3		LibSearch	27.291			2630-39-9	88.35		
Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester	C13H22O3		LibSearch	27.291	-0.326		24851-98-7	88.24		
Dihydrojasmonate <methyl-, cis->	C13H22O3		LibSearch	27.291			39647-11-5	88.03		
Hedione	C13H22O3		LibSearch	27.291			24851-98-7	86.11		
S-(2-((1R,4R)-4-Methyl-2-oxocyclohexyl)propan-2-yl) ethanethioate	C12H20O2S		LibSearch	27.291	-1.259		166022-17-9	68.08		
ethyl 2-oxo-1-pentylcyclopentanecarboxylate	C13H22O3		LibSearch	27.291	-0.526		1000441-61-0	67.03		
1,1-Dicyclohexylpentane	C17H32		LibSearch	27.291	-2.276		54833-30-6	66.98		
7-Hexadecenoic acid, methyl ester, (Z)-	C17H32O2		LibSearch	27.291	-4.142		56875-67-3	66.46		
S-(2-((1R,4S)-4-methyl-2-oxocyclohexyl)propan-2-yl) ethanethioate, rel-	C12H20O2S		LibSearch	27.291	-1.259		166022-16-8	66.16		
2-Hexenoic acid, 3,4,4-trimethyl-5-oxo-, ethyl ester, (E)-	C11H18O3		LibSearch	27.291	5.308		6994-98-5	65.82		
Cyclopentanone, 2-(2-octenyl)-	C13H22O		LibSearch	27.291	1.691		1000131-94-9	65.52		
E-9-Tetradecenoic acid	C14H26O2		LibSearch	27.291	-2.326		50286-30-1	65.44		
7-Hexadecenoic acid, methyl ester, (Z)-	C17H32O2		LibSearch	27.291	-4.142		56875-67-3	65.38		
2,6-Nonadienal, 3,7-dimethyl-	C11H18O		LibSearch	27.291	6.074		41448-29-7	65.35		
1,6,10,14-Phytatetraene-3,5,9-triol	C20H34O3		LibSearch	27.291	-12.226		263873-69-4	65.22		
Methyl jasmonate<Z->	C13H20O3		LibSearch	27.291	-7.449		1211-29-6	65.10		
17-Octadecynoic acid	C18H32O2		LibSearch	27.291	-8.792		34450-18-5	64.90		
2,6,10-trimethylundecanoic Acid, 2,2,2- trifluoroethyl ester	C16H29F3O2		LibSearch	27.291	3.608		1000376-59-4	64.84		
Z-11-Tetradecenoic acid	C14H26O2		LibSearch	27.291	-2.326		1000130-83-3	64.66		
Cyclohexane, 1,1'-(1,5-pentanediyl)bis-	C17H32		LibSearch	27.291	-3.342		54833-31-7	64.60		
Z-7-Tetradecenoic acid	C14H26O2		LibSearch	27.291	-2.326		1000130-98-4	64.49		
Methyl jasmonate	C13H20O3		LibSearch	27.291	-0.459		1211-29-6	64.16		
11-Dodecen-1-ol, 2,4,6-trimethyl-, (R,R,R)-	C15H30O		LibSearch	27.291	1.408		27829-54-5	64.12		
10-Undecen-1-yl acetate	C13H24O2		LibSearch	27.291	2.774		112-19-6	64.12		
Methyl epi-jasmonate<Z->	C13H20O3		LibSearch	27.291	-8.619		42536-97-0	64.10		
Oxacyclotetradecan-2-one	C13H24O2		LibSearch	27.291	-4.442		1725-04-8	64.09		
Myristoleic acid	C14H26O2		LibSearch	27.291	-2.326		544-64-9	63.76		
Cyclopentaneacetic acid, 3-oxo-2-(2-pentenyl)-, methyl ester, [1.alpha.,2.alpha.(Z)]-	C13H20O3		LibSearch	27.291	-0.459		42536-97-0	63.71		
13-Heptadecyn-1-ol	C17H32O		LibSearch	27.291	-5.559		56554-77-9	63.70		
Z-(13,14-Epoxy)tetradec-11-en-1-ol acetate	C16H28O3		LibSearch	27.291	-3.992		1000131-33-2	63.69		
Z-8-Methyl-9-tetradecenoic acid	C15H28O2		LibSearch	27.291	-2.926		1000130-84-5	63.65		
Z-9-Pentadecenol	C15H30O		LibSearch	27.291	-2.092		1000130-76-9	63.56		
Z-2-Tetradecen-1-ol acetate	C16H30O2		LibSearch	27.291	-2.492		1000130-81-9	63.51		
Cyclopentadecanone, 2-hydroxy-	C15H28O2		LibSearch	27.291	-8.676		4727-18-8	63.50		
Z-8-Octadecen-1-ol acetate	C20H38O2		LibSearch	27.291	-9.126		1000130-92-5	63.47		
cis-7-Tetradecen-1-yl acetate	C16H30O2		LibSearch	27.291	-2.492		16974-10-0	63.47		
11-Tetradecyn-1-ol acetate	C16H28O2		LibSearch	27.291	-2.642		33925-72-3	63.45		
Isocitronellol	C10H20O		LibSearch	27.291	9.391		18479-52-2	63.41		
Benzocyclodecene, tetradecahydro-	C14H26		LibSearch	27.291	0.941		61142-06-1	63.37		
Cyclopentadecanolide	C15H28O2		LibSearch	27.291	-14.269		106-02-5	63.34		
Cyclobutanecarboxylic acid, tridec-2-ynyl ester	C18H30O2		LibSearch	27.291	-6.342		1010299-13-7	63.26		
Myristoleic acid	C14H26O2		LibSearch	27.291	-2.326		544-64-9	63.26		
Myristoleic acid	C14H26O2		LibSearch	27.291	-2.326		544-64-9	63.26		
Musk ambrette	C16H28O2		LibSearch	27.291	-17.629		123-69-3	63.19		
n-Decylsuccinic anhydride	C14H24O3		LibSearch	27.291	-5.242		18470-76-3	63.17		
Cyclopentanone <3-acetonyl-, 2-pentyl->	C13H22O2		LibSearch	27.291			40942-73-2	63.09		

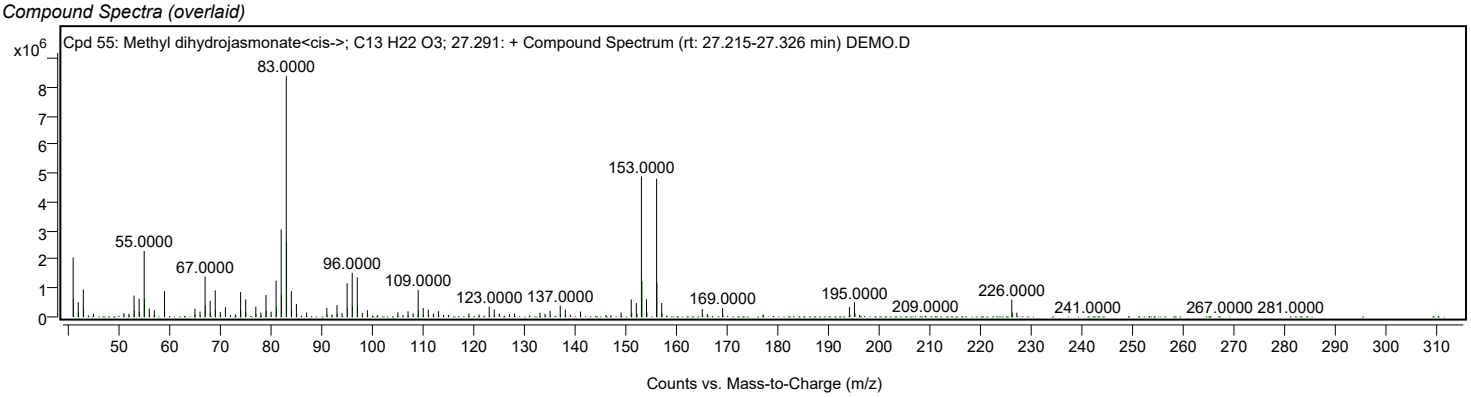
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



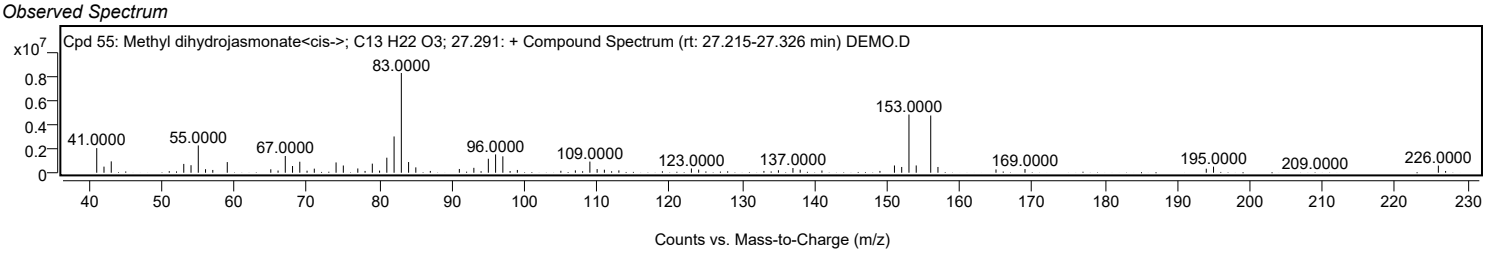
Methyl dihydrojasmonate<cis->

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			97.09			PWNose.xml

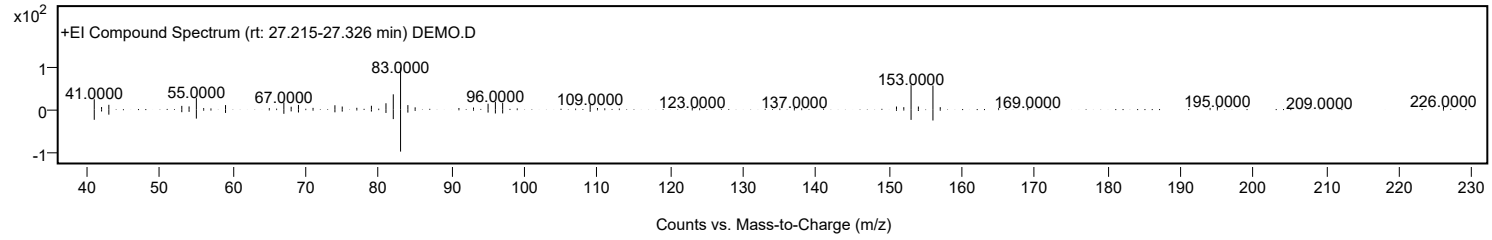
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			97.09			PWNose.xml

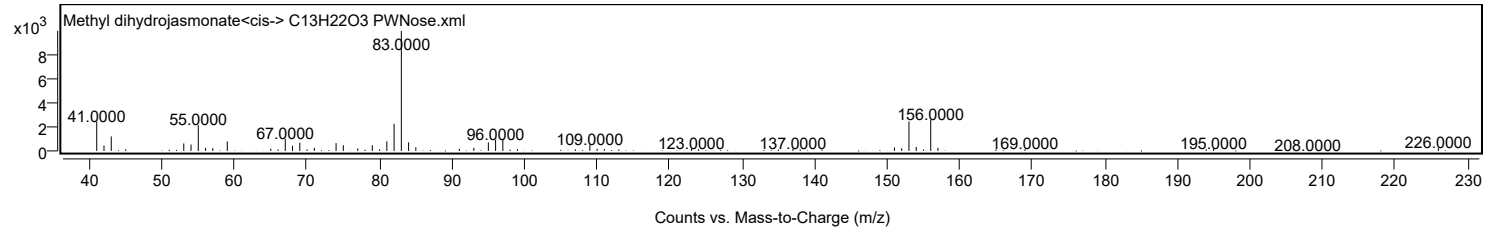
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 56: Norbornen-2-ol acetate<endo-5->

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Norbornen-2-ol acetate<endo-5->	C9 H12 O2	27.485			99295-40-6	LibSearch	53.23	Chrom Decon	PWNose.xml

Compound Discovery Report

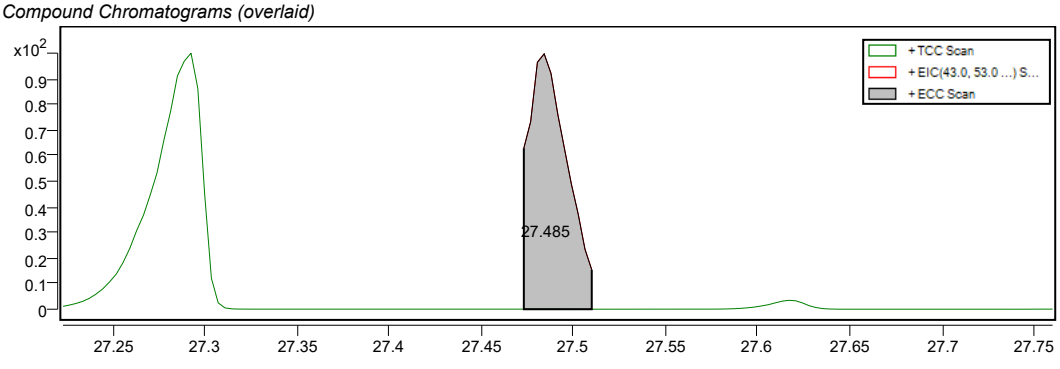
Agilent | Trusted Answers

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		53.23			50		

Compound ID Table

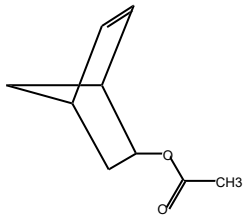
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Norbornen-2-ol acetate<endo-5->	C9H12O2		LibSearch	27.485	16.265		99295-40-6	53.23		
Myroxide <(Z)->	C10H16O		LibSearch	27.485			33281-83-3	53.07		
Norbornen-2-ol acetate<exo-5->	C9H12O2		LibSearch	27.485	16.435		5257-37-4	53.02		
Myroxide<Z->	C10H16O		LibSearch	27.485	14.665		94607-48-4	52.43		
Epoxy-ocimene<Z->	C10H16O		LibSearch	27.485	14.765		33281-83-3	51.18		
5-Norbornen-2-yl acetate	C9H12O2		LibSearch	27.485	9.952		6143-29-9	51.12		
Norbornen-2-ol acetate <endo-5->	C9H12O2		LibSearch	27.485			99295-40-6	51.12		
Norbornen-2-ol acetate <exo-5->	C9H12O2		LibSearch	27.485			5257-37-4	50.99		
Myroxide <(E)->	C10H16O		LibSearch	27.485			28977-57-3	50.62		
5-Norbornen-2-yl acetate	C9H12O2		LibSearch	27.485	9.952		6143-29-9	50.47		
Nonadien-1-yl acetate <3,6->	C11H18O2		LibSearch	27.485			76649-26-8	50.23		
1,9-Decadiyne	C10H14		LibSearch	27.485	10.635		1720-38-3	49.33		
Spiro[bicyclo[2.2.1]hept-5-ene-2,4'-[1,2]dioxolan]-3'-one, 5'-methyl-	C10H12O3		LibSearch	27.485	4.252		1000142-21-3	49.15		
Norbornene-2-methanol acetate<endo-5->	C10H14O2		LibSearch	27.485	11.365		16053-06-8	48.97		
2-Acetyl-5-norbornene	C9H12O		LibSearch	27.485	10.485		5063-03-6	48.91		
1,9-Decadiyne	C10H14		LibSearch	27.485	10.635		1720-38-3	48.70		
Cyclopropane, (R,R)-1-((Z),(Z)-hexa-1',3'-dienyl)-2-ethenyl-	C11H16		LibSearch	27.485	9.418		77210-41-4	48.62		
Norbornene-2-methanol acetate <endo-5->	C10H14O2		LibSearch	27.485			16053-06-8	48.58		
Norbornene-2-methanol acetate<exo-5->	C10H14O2		LibSearch	27.485	11.585		128435-13-2	48.36		
Nonadienol acetate<3E,6Z->	C11H18O2		LibSearch	27.485	7.435		211323-05-6	48.31		
Bicyclo[3.1.0]hexane, 6-methylene-	C7H10		LibSearch	27.485	16.018		54211-16-4	48.25		
2-Acetyl-5-norbornene	C9H12O		LibSearch	27.485	10.485		5063-03-6	48.24		
2-Acetyl-5-norbornene	C9H12O		LibSearch	27.485	10.485		5063-03-6	47.31		
2-Methyl-3-nitrophenyl .beta.-phenylpropionate	C16H15NO4		LibSearch	27.485	-11.532		40300-01-4	47.24		
5-endo-(Hydroxymethyl)-6-exo-methylbicyclo[2.2.1]hept-2-ene	C9H14O		LibSearch	27.485	9.335		18377-05-4	47.15		
1,11-Dodecadiyne	C12H18		LibSearch	27.485	7.318		20521-44-2	47.03		
6-exo-Methylbicyclo[2.2.1]hept-2-ene-5-endo-carboxylic acid	C9H12O2		LibSearch	27.485	7.452		4397-23-3	46.98		
Norbornene-2-methanol<endo-5->	C8H12O		LibSearch	27.485	17.185		67671-06-1	46.98		
Norbornene-2-methanol acetate <exo-5->	C10H14O2		LibSearch	27.485			42836-43-1	46.97		
trans, trans-Octa-2,4-dienyl acetate	C10H16O2		LibSearch	27.485	7.502		30361-34-3	46.96		
2-Acetyl-5-norbornene	C9H12O		LibSearch	27.485	10.485		5063-03-6	46.92		
Norbornene-2-methanol <endo-5->	C8H12O		LibSearch	27.485			67671-06-1	46.92		
2-Bicyclo[2.2.1]hept-5-en-2-yl-ethanol	C9H14O		LibSearch	27.485	8.702		13080-91-6	46.87		
Spiro[bicyclo[3.1.0]hexane-2,1'-cyclopropane]	C8H12		LibSearch	27.485	14.552		1000460-73-6	46.86		
Sinensal <beta->	C15H22O		LibSearch	27.485			60066-88-8	46.77		
2-Norbornen-5-ol, formate	C8H10O2		LibSearch	27.485	10.002		1000142-75-9	46.70		
Epoxy-ocimene<E->	C10H16O		LibSearch	27.485	14.385		28977-57-3	46.46		
Cyclopropane, 1-(2-methylene-3-butenyl)-1-(1-methylenepropyl)-	C12H18		LibSearch	27.485	8.902		51567-07-8	46.29		
Bicyclo[3.2.0]hept-6-ene	C7H10		LibSearch	27.485	15.418		4927-03-1	46.28		
Methyl trans-2-(3-cyclopropyl-7-norcaranyl)acetate	C13H20O2		LibSearch	27.485	3.635		1000223-15-6	46.24		
3-6-Nonadien-1-yl-acetate	C11H18O2		LibSearch	27.485	5.852		76649-26-8	45.85		
Methyl cis-2-(3-cyclopropyl-7-norcaranyl)acetate	C13H20O2		LibSearch	27.485	3.635		1000223-15-7	45.73		
9-Bromotricyclo[5.2.1.0(2,6)]dec-3-ene	C10H13Br		LibSearch	27.485	8.802		1010460-86-5	45.72		
Adamantan-2-ol, 4-bromo-, cis	C10H15BrO		LibSearch	27.485	5.385		33782-47-7	45.66		
Oct-7-yn-1-ol, acetate	C10H16O2		LibSearch	27.485	7.818		1000506-59-0	45.60		
Phenyl-4-methyl pentan-3-one <1->	C12H16O		LibSearch	27.485			40463-09-0	45.49		
Phenyl-4-methyl pentan-3-one<1->	C12H16O		LibSearch	27.485	3.715		40463-09-0	45.35		
Norbornene-2-methanol<exo-5->	C8H12O		LibSearch	27.485	17.535		67671-05-0	45.16		
1,3,6-Heptatriene, 5-methyl-	C8H12		LibSearch	27.485	15.135		925-52-0	44.96		
5-Exo-ethynyl-5-endo-norbornenol	C9H10O		LibSearch	27.485	10.285		106697-35-2	44.92		

Compound Chromatograms (overlaid)

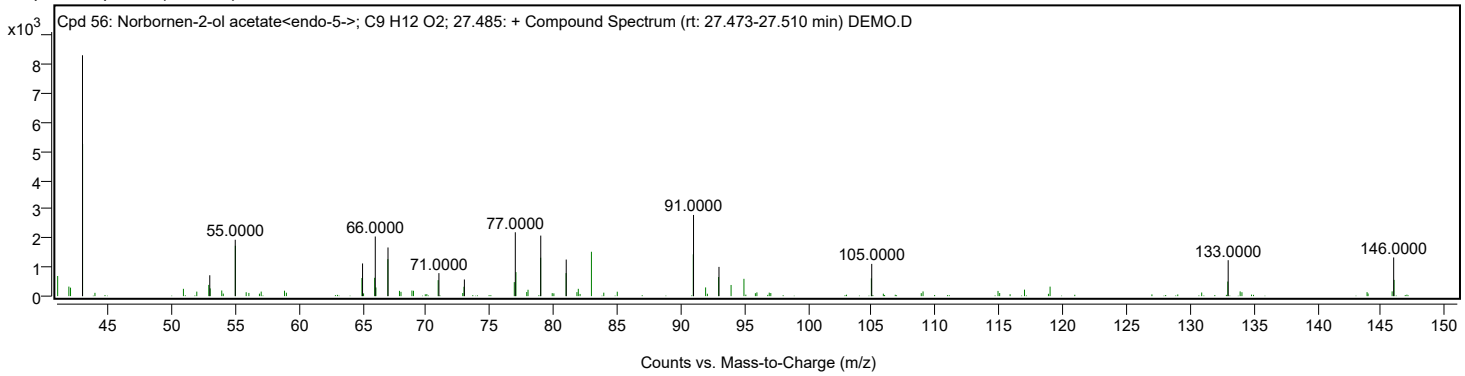


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



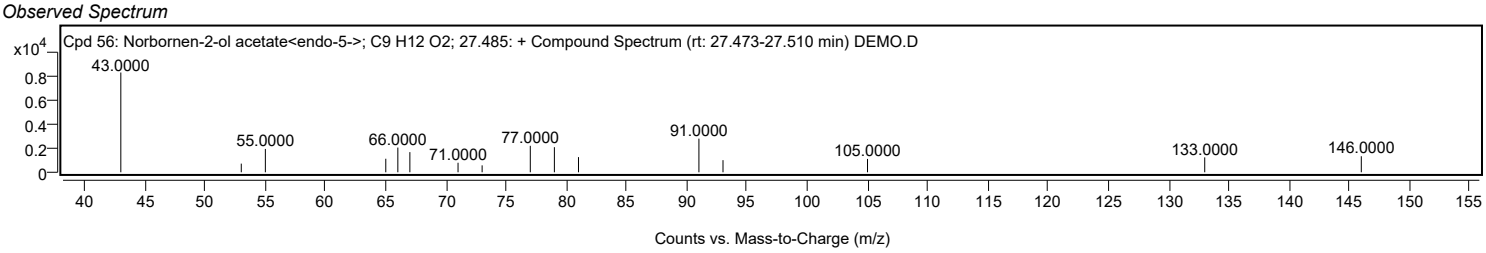
Norbornen-2-ol acetate<endo-5->

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			53.23			PWNose.xml

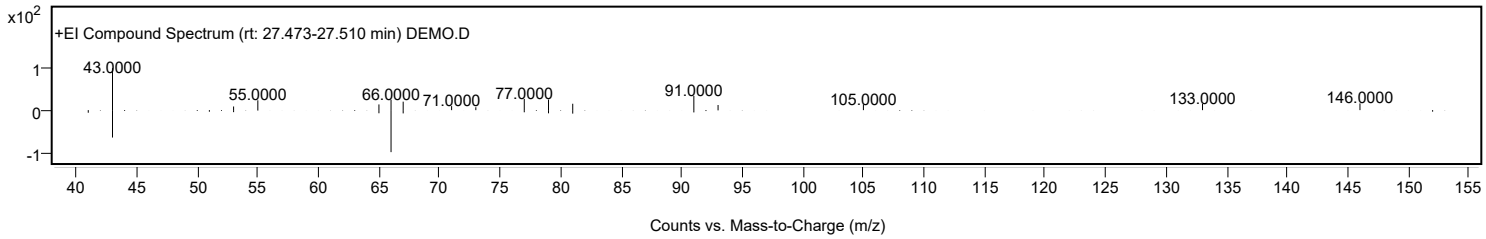
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			53.23			PWNose.xml

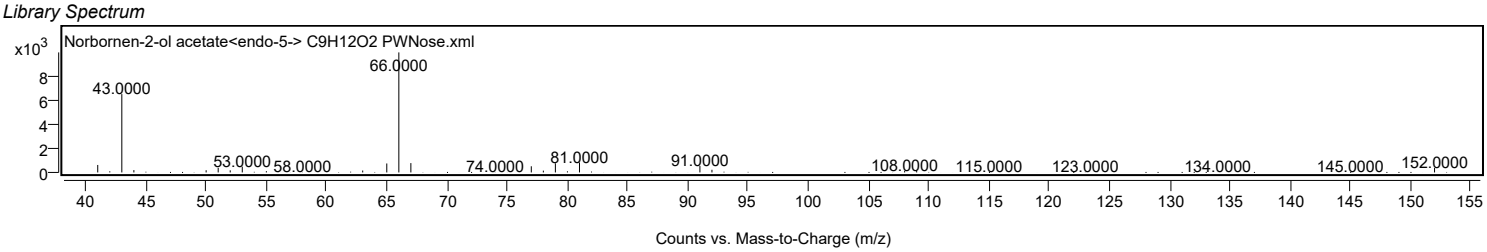
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 57: Disulfide <allyl->

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Disulfide <allyl->	C6 H10 S2	27.492			2179-57-9	LibSearch	46.24	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		46.24			50		

Compound Discovery Report

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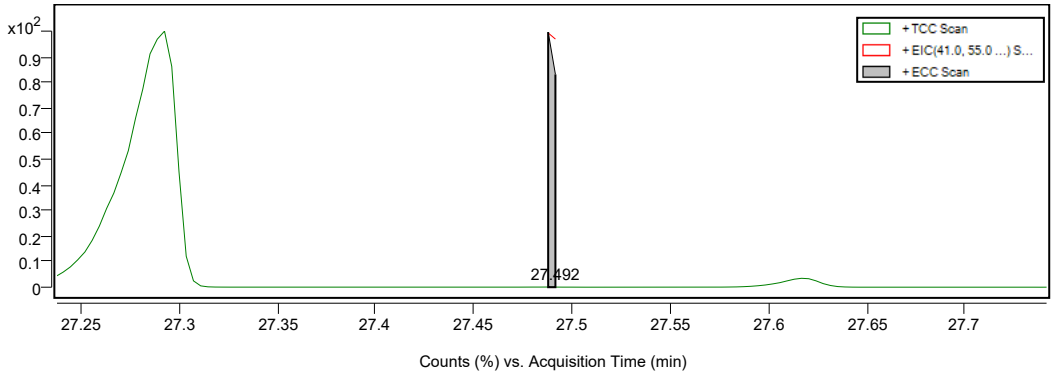
Compound ID Table

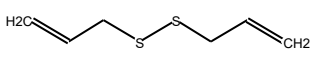
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Disulfide <allyl->	C6H10S2		LibSearch	27.492			2179-57-9	46.24		
Diallyl disulphide	C6H10S2		LibSearch	27.492	9.175		2179-57-9	44.06		
Pteridine, 4-methyl-	C7H6N4		LibSearch	27.492	5.492		2432-21-5	40.32		
Diallyl disulphide	C6H10S2		LibSearch	27.492	9.175		2179-57-9	39.44		
(1-Aminoethyl)cymantrene	C10H10MnNO3		LibSearch	27.492			12214-72-1	37.24		
(Z)-1-Allyl-2-(prop-1-en-1-yl)disulfane	C6H10S2		LibSearch	27.492	8.875		122156-03-0	36.24		
(E)-1-Allyl-2-(prop-1-en-1-yl)disulfane	C6H10S2		LibSearch	27.492	8.875		122156-02-9	33.44		
Tetrasulfide, di-2-propenyl	C6H10S4		LibSearch	27.492	0.808		2444-49-7	33.05		
Succinic acid, 2-chloro-6-fluorophenyl but-2-en-1-yl ester	C14H14ClFO4		LibSearch	27.492	-5.625		1000391-22-5	32.61		
3-Hepten-1-ol	C7H14O		LibSearch	27.492	11.358		10606-47-0	32.25		
Pteridine, 4-methyl-	C7H6N4		LibSearch	27.492	5.492		2432-21-5	31.99		
2,2'-Dithiodicyclohexanol	C12H22O2S2		LibSearch	27.492	-9.492		27040-92-2	31.77		
2-Chloro-6-fluorophenol, 2-methylpropionate	C10H10ClFO2		LibSearch	27.492	4.992		1000447-32-0	31.61		
2-Ethylbutyric acid, 2-chloro-6-fluorophenyl ester	C12H14ClFO2		LibSearch	27.492	1.675		1000369-68-9	31.25		
Tetrasulfide <diallyl->	C6H10S4		LibSearch	27.492			2444-49-7	31.21		
1,5-Hexadiene, 3-methyl-	C7H12		LibSearch	27.492	16.942		1541-33-9	31.16		
1,5-Heptadiene	C7H12		LibSearch	27.492	15.575		1541-23-7	31.05		
Bis(2-methylallyl) carbonate	C9H14O3		LibSearch	27.492	9.275		64057-79-0	30.90		
Diallyl disulphide	C6H10S2		LibSearch	27.492	9.175		2179-57-9	30.72		
Propanedinitrile, cyclohexylidene-	C9H10N2		LibSearch	27.492	2.975		4354-73-8	30.42		
Propanedinitrile, cyclohexylidene-	C9H10N2		LibSearch	27.492	2.975		4354-73-8	30.01		
Acrylamide, 3-(3-cyclohexenyl)-N-phenyl-	C15H17NO		LibSearch	27.492	-6.559		1000157-24-4	29.91		
Malonic acid, 10-chlorodecyl pentyl ester	C18H33ClO4		LibSearch	27.492	-12.009		1000349-04-2	29.84		
1,5-Heptadiene	C7H12		LibSearch	27.492	15.575		1541-23-7	29.73		
N-Propyl-N-(4-aminophenylsulfonyl)benzamide	C16H18N2O3S		LibSearch	27.492	-18.909		1000375-16-0	29.52		
1,5-Heptadiene, (Z)-	C7H12		LibSearch	27.492	15.575		7736-34-7	29.43		
2-Chloro-6-fluorophenol, 3-methylbutyl ether	C11H14ClFO		LibSearch	27.492	4.858		1000395-35-9	29.29		
Dioctyl malonate	C19H36O4		LibSearch	27.492	-9.909		16958-88-6	29.03		
Linalool	C10H18O		LibSearch	27.492			78-70-6	28.92		
Linalool <ethyl-, (Z)->	C11H20O		LibSearch	27.492			54592-32-4	28.92		
1,5-Hexadiene, 3-methyl-	C7H12		LibSearch	27.492	16.942		1541-33-9	28.85		
1,5-Heptadiene, (E)-	C7H12		LibSearch	27.492	15.575		7736-22-3	28.84		
Methyl dicyclohexylphosphinite	C13H25OP		LibSearch	27.492			42366-52-9	28.77		
1,5-Hexadiene, 2-methyl-	C7H12		LibSearch	27.492	16.258		4049-81-4	28.75		
Linalool	C10H18O		LibSearch	27.492			78-70-6	28.50		
Malonic acid, 8-chlorooctyl pentyl ester	C16H29ClO4		LibSearch	27.492	-8.692		1000349-00-6	28.50		
Carbonic acid, monoamide, N-hexyl-, 2-ethylhexyl ester	C15H31NO2		LibSearch	27.492	-2.742		1000406-84-1	28.45		
Linalool <ethyl-, (E)->	C11H20O		LibSearch	27.492			92590-71-1	28.42		
2,5-Difluorothiophenol, S-(2-methylpropionyl)-	C10H10F2OS		LibSearch	27.492	4.758		1000463-04-3	28.24		
Senecionitrile	C5H7N		LibSearch	27.492			4786-24-7	28.19		
4-Chlorobutyric acid, 3-methylbutyl-2 ester	C9H17ClO2		LibSearch	27.492	7.825		1000360-63-6	28.17		
2-Hexenamide, N-phenyl-	C12H15NO		LibSearch	27.492	-0.825		1483-36-9	28.13		
Carbonic acid, monoamide, N-hexyl-, decyl ester	C17H35NO2		LibSearch	27.492	-7.125		1000415-18-0	28.12		
Carbonic acid, monoamide, N-hexyl-, octyl ester	C15H31NO2		LibSearch	27.492	-3.809		1000406-45-7	27.91		
Linalyl benzoate	C17H22O2		LibSearch	27.492			126-64-7	27.87		
Linalool	C10H18O		LibSearch	27.492	16.172		78-70-6	27.84		
1,5-Dimethyl-1-vinyl-4-hexenyl butyrate	C14H24O2		LibSearch	27.492	2.975		78-36-4	27.48		
Ethyllinalool	C11H20O		LibSearch	27.492	7.792		1000430-72-3	27.47		
1,1,2,2-Tetrakis(allyloxy)ethane	C14H22O4		LibSearch	27.492	1.675		16646-44-9	27.46		
Tetrahydrofurfuryl bromide	C5H9BrO		LibSearch	27.492	11.725		1192-30-9	27.29		

Compound Chromatograms (overlaid)

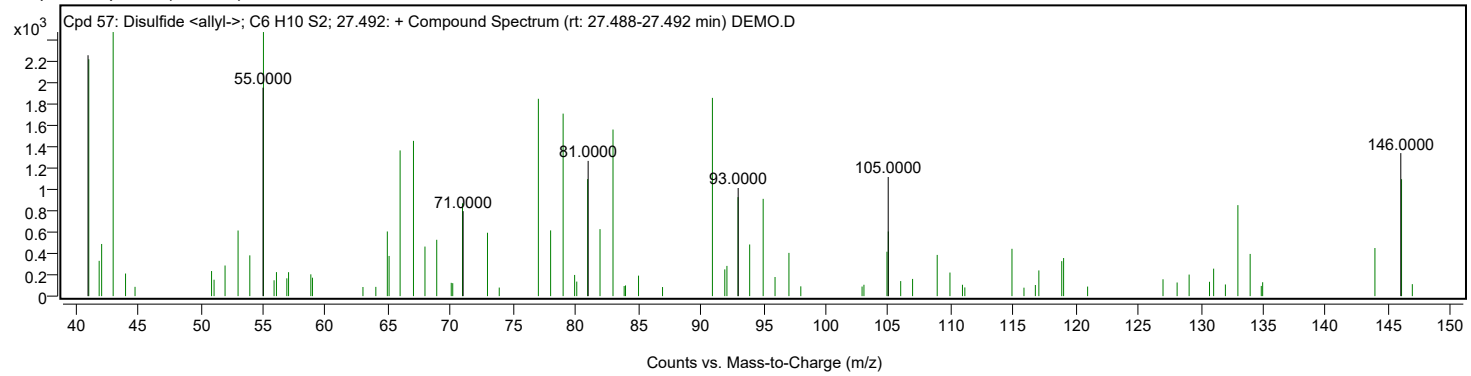


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



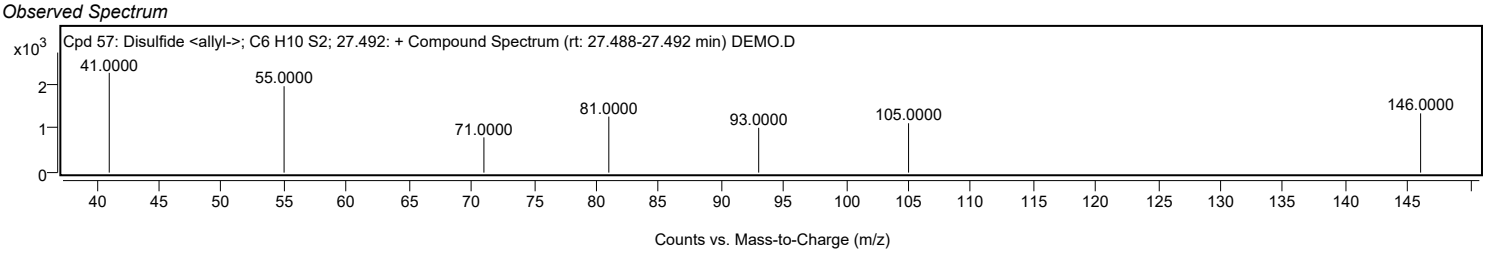
Disulfide <allyl->

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			46.24			PWNose.xml

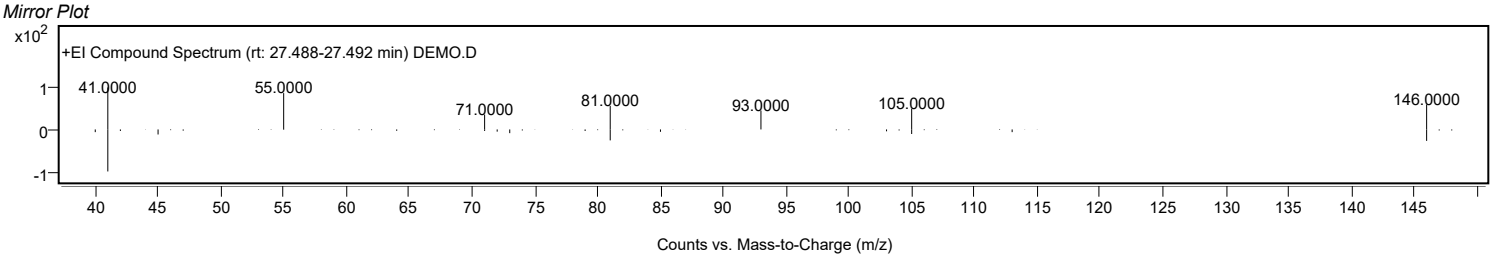
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			46.24			PWNose.xml

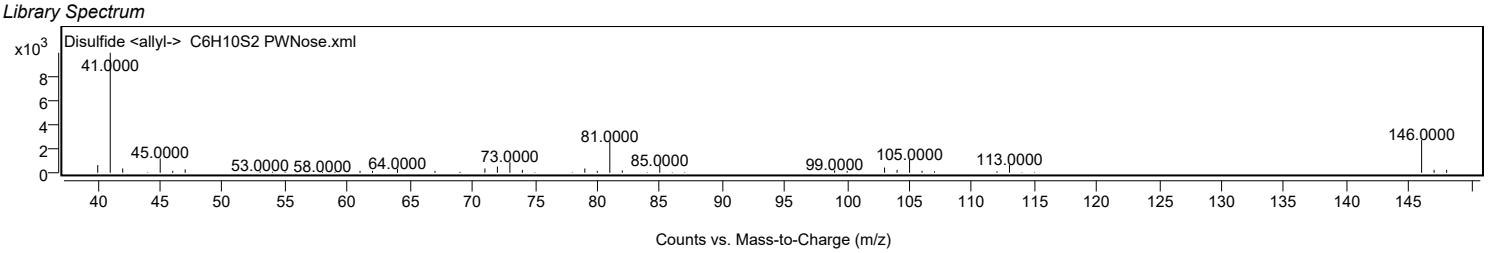
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 58: Methyl dihydrojasmonate<trans->

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Methyl dihydrojasmonate<trans->	C13 H22 O3	27.617			2630-39-9	LibSearch	98.23	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		98.23			50		

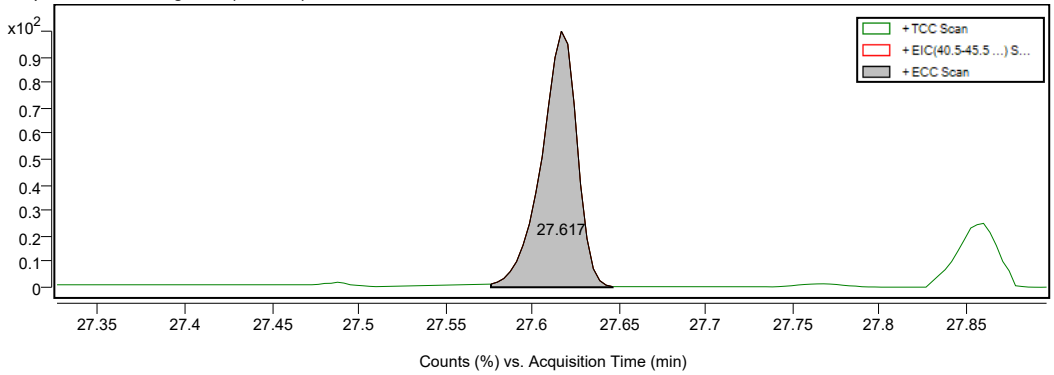
Compound Discovery Report

Agilent | Trusted Answers

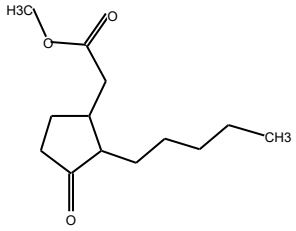
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Methyl dihydrojasmonate<trans->	C13H22O3		LibSearch	27.617	-8.433		2630-39-9	98.23		
Methyl dihydrojasmonate<cis->	C13H22O3		LibSearch	27.617	-7.373		39647-11-5	97.15		
Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester	C13H22O3		LibSearch	27.617	0.000		24851-98-7	95.24		
Dihydrojasmonate <methyl-, trans->	C13H22O3		LibSearch	27.617			2630-39-9	91.66		
Hedione	C13H22O3		LibSearch	27.617			24851-98-7	91.56		
Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester	C13H22O3		LibSearch	27.617	0.000		24851-98-7	90.25		
Dihydrojasmonate <methyl-, cis->	C13H22O3		LibSearch	27.617			39647-11-5	87.55		
Cyclopentaneacetic acid, 3-oxo-2-pentyl-, methyl ester	C13H22O3		LibSearch	27.617	0.000		24851-98-7	86.72		
2,6-Nonadienal, 3,7-dimethyl-	C11H18O		LibSearch	27.617	6.400		41448-29-7	72.93		
Isocitronellol	C10H20O		LibSearch	27.617	9.717		18479-52-2	72.41		
Cyclohexane, 1,1'-(1,5-pentanediyl)bis-	C17H32		LibSearch	27.617	-3.017		54833-31-7	71.73		
Cyclobutanecarboxylic acid, undec-2-enyl ester	C16H28O2		LibSearch	27.617	-2.533		1000299-13-6	70.77		
1,1-Dicyclohexylpentane	C17H32		LibSearch	27.617	-1.950		54833-30-6	70.63		
7-Hexadecenoic acid, methyl ester, (Z)-	C17H32O2		LibSearch	27.617	-3.817		56875-67-3	70.47		
11-Dodecen-1-ol, 2,4,6-trimethyl-, (R,R,R)-	C15H30O		LibSearch	27.617	1.733		27829-54-5	69.83		
3-Hexen-1-ol, 2,5-dimethyl-, acetate, (Z)-	C10H18O2		LibSearch	27.617	9.917		1000132-12-5	69.77		
Cyclobutanecarboxylic acid, tridec-2-ynyl ester	C18H30O2		LibSearch	27.617	-6.017		1010299-13-7	69.69		
6-Nonenal, 3,7-dimethyl-	C11H20O		LibSearch	27.617	7.217		1000132-43-9	69.67		
17-Octadecynoic acid	C18H32O2		LibSearch	27.617	-8.467		34450-18-5	69.66		
9-Eicosyne	C20H38		LibSearch	27.617	-6.167		71899-38-2	69.65		
S-(2-((1R,4R)-4-Methyl-2-oxocyclohexyl)propan-2-yl) ethanethioate	C12H20O2S		LibSearch	27.617	-0.933		166022-17-9	69.59		
Hexanol-1, 6-cyclohexyl-	C12H24O		LibSearch	27.617	2.283		4354-58-9	69.53		
10-Undecen-1-yl acetate	C13H24O2		LibSearch	27.617	3.100		112-19-6	69.41		
Cyclohexane, (2-nitro-2-propenyl)-	C9H15NO2		LibSearch	27.617	5.483		80255-17-0	69.29		
Dec-1-en-3-yl tiglate	C15H26O2		LibSearch	27.617			1231958-90-9	69.03		
Nopinone	C9H14O		LibSearch	27.617	14.597		38651-65-9	68.99		
Pentanoic acid, 10-undecenyl ester	C16H30O2		LibSearch	27.617	-1.867		1000159-93-4	68.96		
E-2-Octadecadecen-1-ol	C18H36O		LibSearch	27.617	-6.733		1000131-10-2	68.83		
Isocitronellene	C10H18		LibSearch	27.617	22.157		85006-04-8	68.70		
1-Methylbicyclo[3.3.0]octane-3,7-dione	C9H12O2		LibSearch	27.617	6.317		21170-08-1	68.67		
E-9-Tetradecenoic acid	C14H26O2		LibSearch	27.617	-2.000		50286-30-1	68.67		
Oxacyclotetradecan-2-one	C13H24O2		LibSearch	27.617	-4.117		1725-04-8	68.49		
Bicyclo[3.1.1]heptan-2-one, 3,6,6-trimethyl-	C10H16O		LibSearch	27.617	9.133		16022-08-5	68.42		
1,9-Tetradecadiene	C14H26		LibSearch	27.617	4.100		112929-06-3	68.39		
S-(2-((1R,4S)-4-methyl-2-oxocyclohexyl)propan-2-yl) ethanethioate, rel-	C12H20O2S		LibSearch	27.617	-0.933		166022-16-8	68.31		
3,7-Dimethyl-2,6-nonadien-1-ol	C11H20O		LibSearch	27.617	5.483		1000131-31-2	68.28		
2-Octen-1-ol, 3,7-dimethyl-	C10H20O		LibSearch	27.617	7.967		40607-48-5	68.25		
9-Borabicyclo[3.3.1]nonane, 9-(3-methoxycyclohexyl)oxy-	C15H27BO2		LibSearch	27.617			1000150-57-9	68.18		
E-7-Tetradecenol	C14H28O		LibSearch	27.617	-0.117		37011-95-3	68.14		
Methyl jasmonate<Z->	C13H20O3		LibSearch	27.617	-7.123		1211-29-6	68.11		
Myristoleic acid	C14H26O2		LibSearch	27.617	-2.000		544-64-9	68.00		
5-Nonadecen-1-ol	C19H38O		LibSearch	27.617	-8.400		1000131-11-9	67.98		
Nonenyl tiglate, (2Z)-	C14H24O2		LibSearch	27.617			1231959-70-8	67.98		
Pinocamphone<trans->	C10H16O		LibSearch	27.617	13.617		547-60-4	67.89		
10-Methyl-E-11-tridecen-1-ol propionate	C17H32O2		LibSearch	27.617	-2.750		1000130-97-4	67.85		
1,19-Eicosadiene	C20H38		LibSearch	27.617	-5.533		14811-95-1	67.84		
2,2-Dimethyl-4-octenal	C10H18O		LibSearch	27.617	8.833		30390-60-4	67.83		
2,7-Dioxatricyclo[4.3.1.0(3,8)]decan-4-ol	C8H12O3		LibSearch	27.617	10.167		1010191-02-5	67.82		
(E)-2-undecenyl tiglate	C16H28O2		LibSearch	27.617			1231960-09-0	67.79		
cisZ-11,12-Epoxytetradecan-1-ol	C14H28O2		LibSearch	27.617	-0.850		1000131-00-1	67.78		

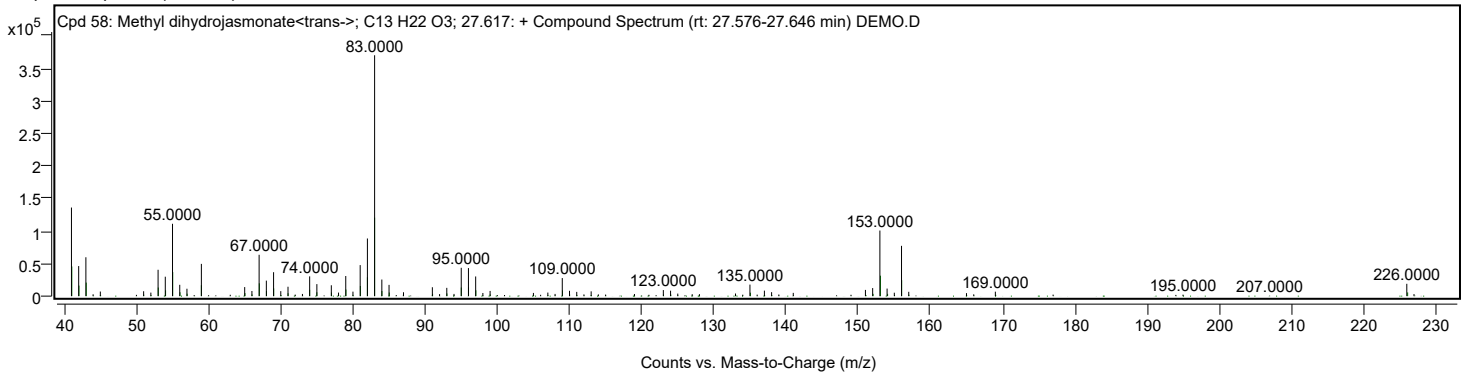
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



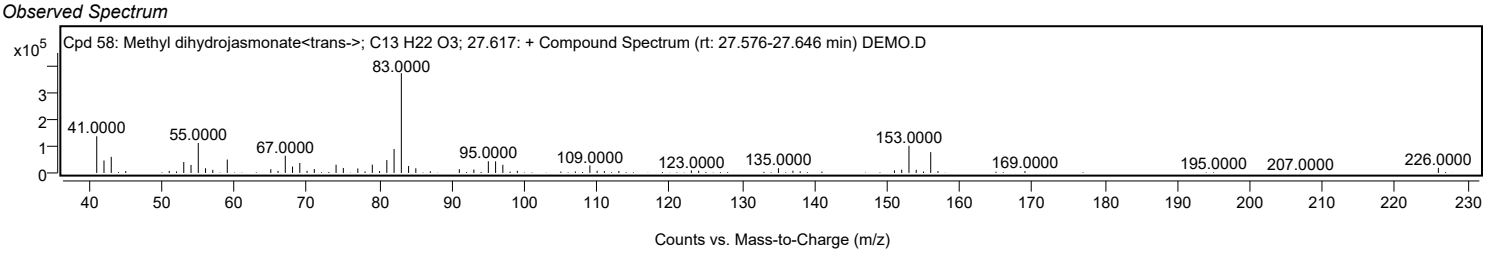
Methyl dihydrojasmonate<trans->

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			98.23			PWNose.xml

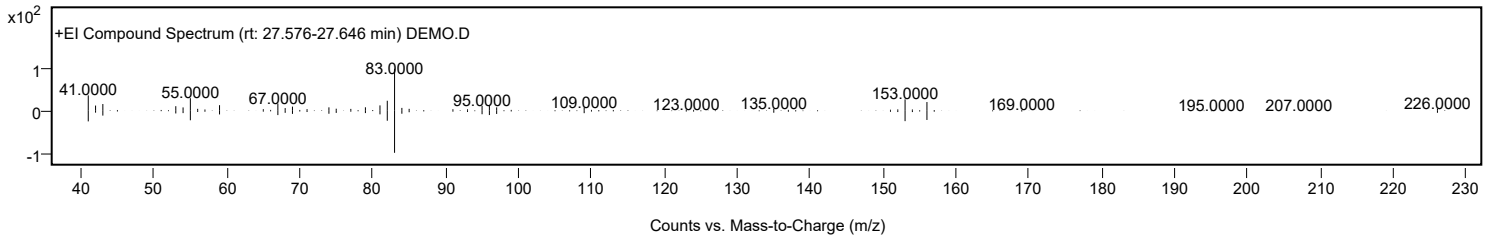
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			98.23			PWNose.xml

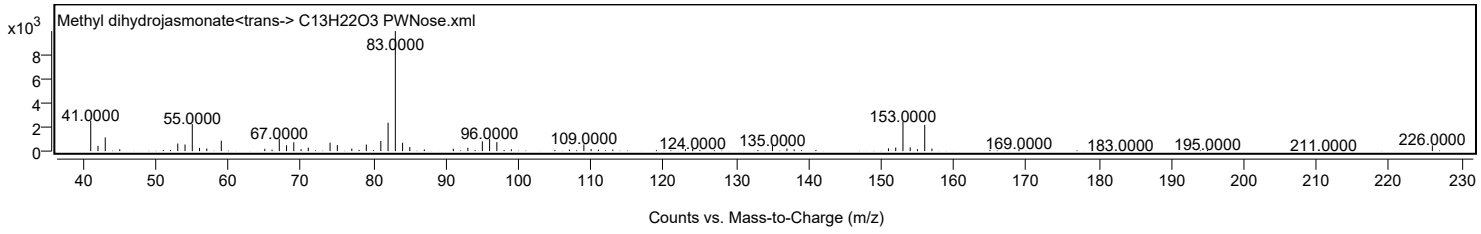
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 59: Ethyl 1-(1-adamantylcarbonyl)piperidine-4-carboxylate

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Ethyl 1-(1-adamantylcarbonyl)piperidine-4-carboxylate	C19 H29 N O3	27.757			260553-08-0	LibSearch	44.17	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		44.17			50		

Compound Discovery Report

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Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Ethyl 1-(1-adamantylcarbonyl)piperidine-4-carboxylate	C19H29NO3		LibSearch	27.757	-9.393		260553-08-0	44.17		
DL-Alanine, N-methyl-N-(byt-3-en-1-yloxycarbonyl)-, byt-3-en-1-yl ester	C13H21NO4		LibSearch	27.757	0.874		1010392-74-4	44.05		
Furan, 2-[[(1-methylethyl)thio]methyl]-	C8H12OS		LibSearch	27.757	8.974		1883-78-9	42.90		
Furan, 2-[[(1-methylethyl)thio]methyl]-	C8H12OS		LibSearch	27.757	8.974		1883-78-9	38.87		
Furan, 2-[[(1-methylethyl)thio]methyl]-	C8H12OS		LibSearch	27.757	8.974		1883-78-9	38.54		
5,10-Pentadecadien-1-ol, (Z,Z)-	C15H28O		LibSearch	27.757	-1.759		64275-51-0	38.29		
Furfuryl sulfide <isopropyl->	C8H12OS		LibSearch	27.757			1883-78-9	38.16		
N-Cyclohexyl-1-(2-methoxyethyl)-2-methyl-5-oxopyrrolidine-2-carboxamide	C15H26N2O3		LibSearch	27.757	-12.076		1000458-29-1	37.71		
N-Cyclopentyl-1-(2-methoxyethyl)-2-methyl-5-oxopyrrolidine-2-carboxamide	C14H24N2O3		LibSearch	27.757	-10.076		1000458-29-5	35.82		
N-(.beta.-Hydroxyethyl)-4-(.gamma.-hydroxypropyl)piperidine	C10H21NO2		LibSearch	27.757	-0.193		19780-85-9	35.43		
N-Butyl-1-(2-methoxyethyl)-2-methyl-5-oxopyrrolidine-2-carboxamide	C13H24N2O3		LibSearch	27.757	-7.693		1000458-30-4	35.20		
Cyclobutanecarboxamide, N-(2-phenylethyl)-N-nonyl-	C22H35NO		LibSearch	27.757	-14.043		1000451-61-1	35.10		
DL-Alanyl-DL-alanine, N,N'-dimethyl-N'-(byt-3-en-1-yloxycarbonyl)-, byt-3-en-1-yl ester	C17H28N2O5		LibSearch	27.757	-8.043		1000392-75-0	34.78		
N-(tert-Butyl)-1-(2-methoxyethyl)-2-methyl-5-oxopyrrolidine-2-carboxamide	C13H24N2O3		LibSearch	27.757	-6.293		1000458-29-4	33.99		
1,5-Heptadiene	C7H12		LibSearch	27.757	15.841		1541-23-7	33.83		
Tricyclo[3.3.1.1(3,7)]decane, 2-bromo-	C10H15Br		LibSearch	27.757	8.791		7314-85-4	33.70		
1,5-Heptadiene, (E)-	C7H12		LibSearch	27.757	15.841		7736-22-3	33.40		
9-Iodotricyclo[4.2.1.1(2,5)]decane	C10H15I		LibSearch	27.757	6.824		1000194-77-8	33.36		
1,5-Hexadiene, 3-methyl-	C7H12		LibSearch	27.757	17.207		1541-33-9	33.18		
N-(2,6-Dimethylphenyl)-1-(2-methoxyethyl)-2-methyl-5-oxopyrrolidine-2-carboxamide	C17H24N2O3		LibSearch	27.757	-16.059		1000458-28-9	33.05		
N-(.beta.-Hydroxyethyl)-4-(.gamma.-hydroxypropyl)piperidine	C10H21NO2		LibSearch	27.757	-0.193		19780-85-9	33.03		
3-Hydroxyimino-2,5,5-trimethyl-1-pyrroline, 1-oxide	C7H12N2O2		LibSearch	27.757			1000305-90-1	32.95		
1,5-Heptadiene, (Z)-	C7H12		LibSearch	27.757	15.841		7736-34-7	32.80		
4,5-Dimethoxypyrimidine N-oxide	C6H8N2O3		LibSearch	27.757			114969-59-4	32.46		
1,5-Heptadiene	C7H12		LibSearch	27.757	15.841		1541-23-7	32.36		
1-n-butyladamantane	C14H24		LibSearch	27.757	6.891		14449-41-3	31.91		
Coranol	C11H22O		LibSearch	27.757			83926-73-2	31.88		
N-(3-(p-tert-Butylphenoxy)-2-hydroxypropyl)succinimide	C17H23NO4		LibSearch	27.757	-14.376		1000240-55-2	31.85		
1,5-Hexadiene, 3-methyl-	C7H12		LibSearch	27.757	17.207		1541-33-9	31.07		
Butanedioic acid, 2-(1-oxo-2-propenylamino)-, dimethyl ester	C9H13NO5		LibSearch	27.757	1.474		1010272-38-7	31.02		
Adamantane, 2-(dicyanocyclohexylmethyl)-	C19H26N2		LibSearch	27.757	-9.009		1000164-91-8	30.91		
1,1'-Bis(2-bromocyclopentane), (E)-	C10H16Br2		LibSearch	27.757	0.807		1000162-03-0	30.69		
1-Adamantan-1-yl-6-chloro-7-fluoro-4-oxo-1,4-dihydroquinoline-3-carboxylic acid,N methyl ester	C21H21ClFNO3		LibSearch	27.757	-16.876		1000210-85-2	30.62		
2-Methyl-5-(1-adamantyl)pentan-2-ol	C16H28O		LibSearch	27.757	2.041		95477-25-1	30.61		
1,5-Heptadiene, (E)-	C7H12		LibSearch	27.757	15.841		7736-22-3	30.44		
2-Iodoadamantane	C10H15I		LibSearch	27.757	6.824		18971-91-0	30.25		
Cyclohexanemethanol, .alpha.,.alpha.,4-trimethyl-	C10H20O		LibSearch	27.757	8.891		498-81-7	29.82		
N-(2,3-Dihydrobenzo[b][1,4]dioxin-6-yl)-1-(2-methoxyethyl)-2-methyl-5-oxopyrrolidine-2-carboxamide	C17H22N2O5		LibSearch	27.757	-20.026		1010458-28-5	29.49		
o-Menthan-8-ol	C10H20O		LibSearch	27.757	8.891		343855-44-7	28.95		
1-(2-Methoxyethyl)-2-methyl-N-(naphthalen-2-yl)-5-oxopyrrolidine-2-carboxamide	C19H22N2O3		LibSearch	27.757	-21.476		1010458-32-1	28.90		
3-Hexene, 1-(1-methoxyethoxy)-, (Z)-	C9H18O2		LibSearch	27.757	10.891		54340-96-4	28.80		
Terpineol <cis- dihydro- alpha->	C10H20O		LibSearch	27.757			7322-63-6	28.39		
2,6-Dioxa-adamantan-4-ol	C8H12O3		LibSearch	27.757	10.307		1000188-72-3	28.32		
4,5-Diamino-6-methyl-2-thiopyrimidine	C5H8N4S		LibSearch	27.757	-0.976		6305-99-3	28.30		
Terpineol<cis-dihydro-alpha->	C10H20O		LibSearch	27.757	13.667		7322-63-6	28.10		
1-Butene, 4-cyclopropyl-	C7H12		LibSearch	27.757	15.941		7736-35-8	28.02		
Cyclohexanemethanol, .alpha.,.alpha.,4-trimethyl-	C10H20O		LibSearch	27.757	8.891		498-81-7	27.98		
2,6-Octadiene, (E,E)-	C8H14		LibSearch	27.757	13.891		18152-31-3	27.73		
Terpineol<trans-dihydro-alpha->	C10H20O		LibSearch	27.757	14.427		5114-00-1	27.65		
Cyclohexanemethanol, .alpha.,.alpha.,4-trimethyl-, trans-	C10H20O		LibSearch	27.757	8.891		5114-00-1	27.59		

Compound Discovery Report

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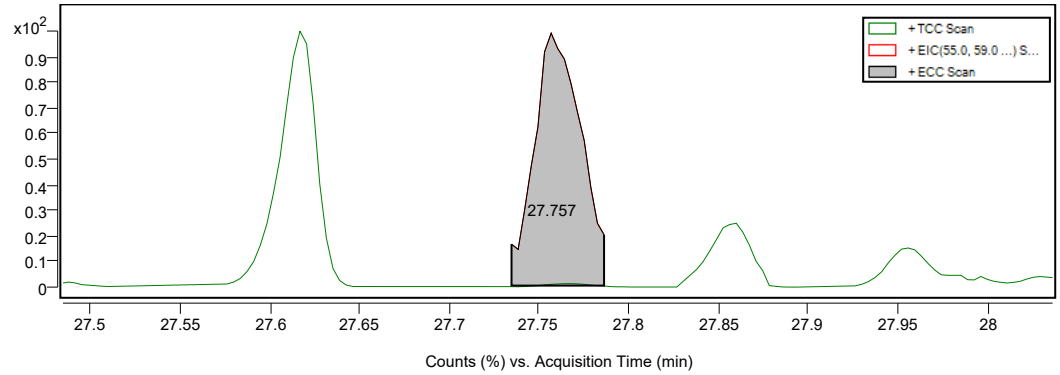
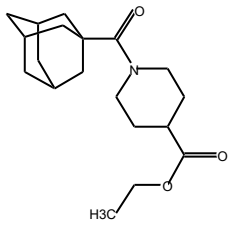
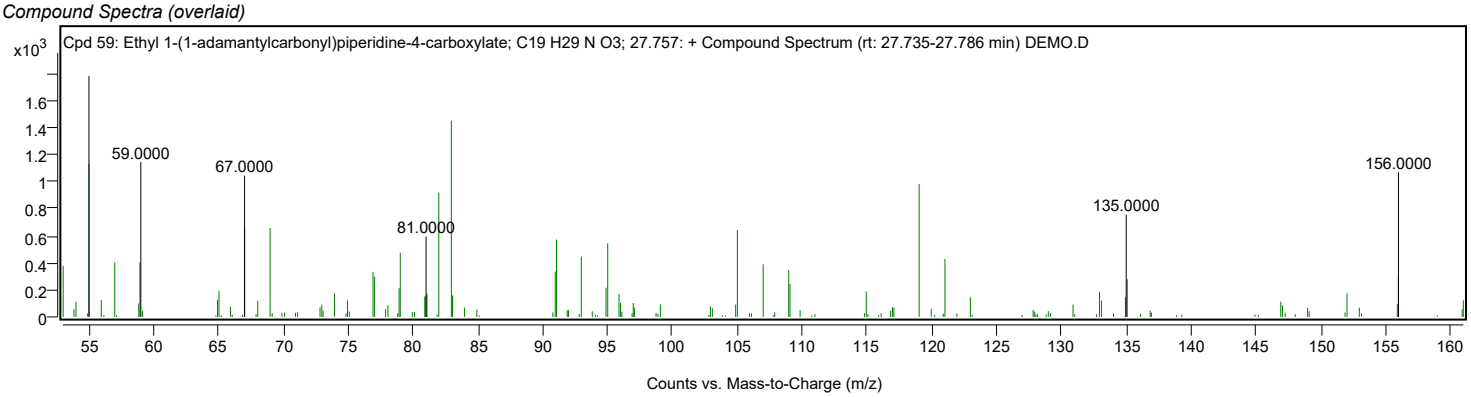
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



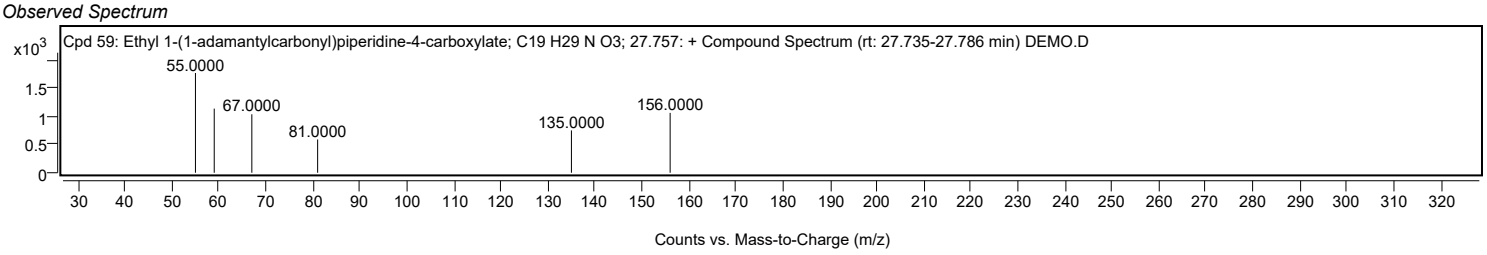
Ethyl 1-(1-adamantylcarbonyl)piperidine-4-carboxylate

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			44.17			NIST.L

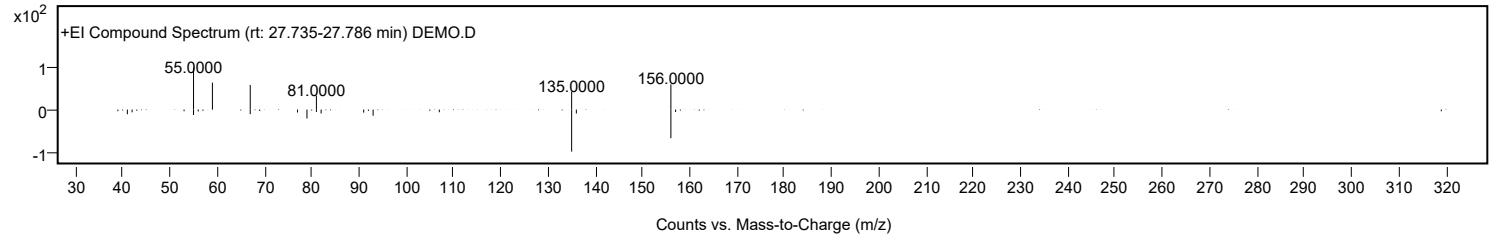
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			44.17			NIST.L

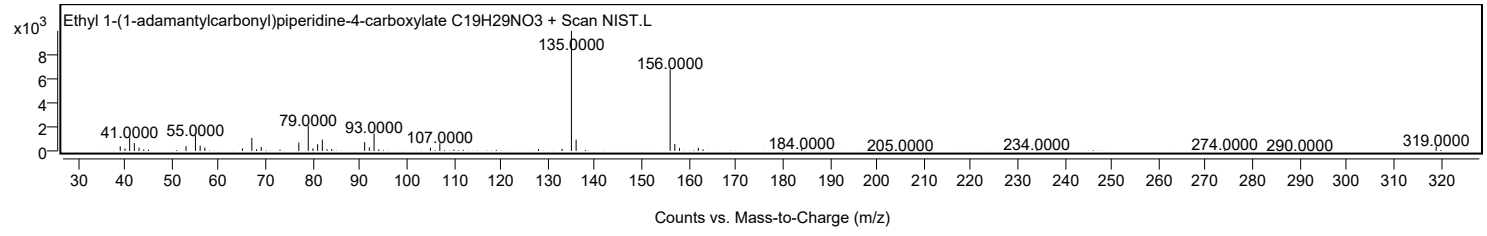
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 60: Iso E Super <gamma->

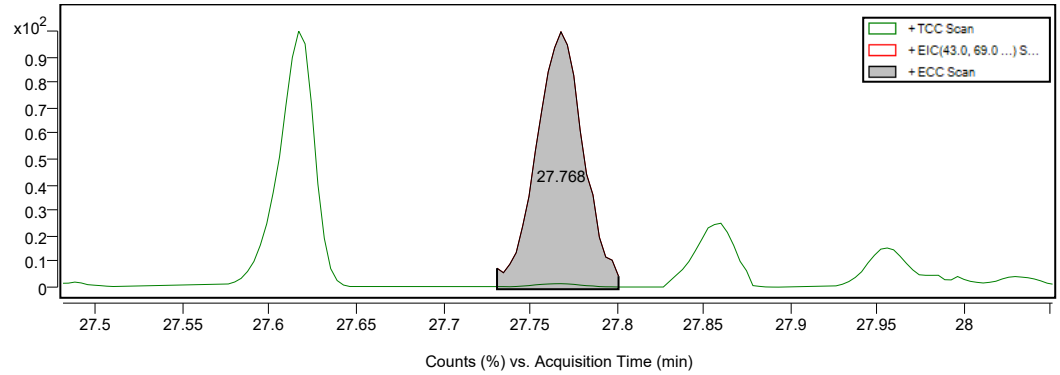
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Iso E Super <gamma->	C16 H26 O	27.768			68155-67-9	LibSearch	53.30	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		53.30			50		

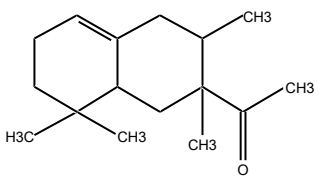
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Iso E Super <gamma->	C16H26O		LibSearch	27.768			68155-67-9	53.30		
Benzene, [1-methyl-1-(pentyloxy)ethyl]-	C14H22O		LibSearch	27.768	3.085		54932-79-5	48.64		
Amberonne (isomer 3)	C16H26O		LibSearch	27.768	-0.665		1000470-69-9	48.55		
Amberonne (isomer 2)	C16H26O		LibSearch	27.768	-0.665		1010470-69-8	45.87		
2-[2-(2,2,3,3,3-Pentafluoropropanoyl)oxyethoxy]ethyl 2,2,3,3,3-pentafluoropropanoate	C10H8F10O5		LibSearch	27.768	14.151		1010352-00-0	45.71		
4-Phenyl-morpholine-2,6-dione	C10H9NO3		LibSearch	27.768	-2.282		56956-66-2	45.35		
1-[1,6-Dimethyl-4-(4-methyl-3-pentenyl)-3-cyclohexen-1-yl]ethanone	C16H26O		LibSearch	27.768	-0.632		57499-57-7	44.06		
3-Buten-2-one, 4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)-	C14H22O		LibSearch	27.768	2.451		79-70-9	42.54		
2-(2-Hydroxyethoxy)phenol, bis(pentafluoropropionate)	C14H8F10O5		LibSearch	27.768	6.018		1000376-16-9	42.27		
1,3-Dioxolane, 2,4,5-trimethyl-2-(p-tolyl)-	C13H18O2		LibSearch	27.768	2.418		1000149-74-3	42.17		
3-Oxypentanol, 5-chloro, pentafluoropropionate	C7H8ClF5O3		LibSearch	27.768	13.085		1000374-84-0	41.98		
Amberonne (isomer 1)	C16H26O		LibSearch	27.768	-0.665		1000470-69-7	41.97		
2,4,4-Trimethyl-3-hydroxymethyl-5a-(3-methyl-but-2-enyl)-cyclohexene	C15H26O		LibSearch	27.768	-0.115		1000144-10-5	41.63		
Acetohydrazide, 2-(4-tolyloxy)-N2-benzoylmethylene-	C17H16N2O3		LibSearch	27.768	-17.332		1000258-81-8	40.87		
Iso E Super <alpha->	C16H26O		LibSearch	27.768			68155-66-8	39.90		
Dicumyl peroxide	C18H22O2		LibSearch	27.768	-4.665		80-43-3	39.42		
1,4-Benzenediol, 2-[(1,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)methyl]-, [1R-(1.alpha.,4a.beta.,8a.alpha.)]-	C21H30O2		LibSearch	27.768	-14.832		39707-55-6	38.70		
Succinic acid, monochloride, 2,4-dimethylpent-3-yl ester	C11H19ClO3		LibSearch	27.768	4.401		1000349-36-8	37.97		
Succinic acid, di(3-methylphenyl) ester	C18H18O4		LibSearch	27.768	-10.999		1000329-96-8	37.86		
Chrysanthenyl acetate <trans->	C12H18O2		LibSearch	27.768			50764-55-1	37.80		
1-Penten-3-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	C14H22O		LibSearch	27.768	1.818		127-43-5	37.64		
Verbenyl acetate <trans->	C12H18O2		LibSearch	27.768			1203-21-0	36.98		
Benzamide, N,N-diethyl-4-methyl-	C12H17NO		LibSearch	27.768	2.685		2728-05-4	36.91		
1-(4-Methylbenzoyl)-2,3-diphenyl-cyclopropane	C23H20O		LibSearch	27.768	-15.765		1000145-81-1	36.71		
Benzamide, 3-methyl-N-methyl-N-propyl-	C12H17NO		LibSearch	27.768	2.685		1000421-46-2	36.70		
Benzamide, 3-methyl-N-isobutyl-	C12H17NO		LibSearch	27.768	0.418		1000407-41-0	36.70		
.beta.-BERGAMOTENE	C15H24		LibSearch	27.768	4.018		1000425-19-8	36.64		
3-Methylbenzoic acid, 2,5-dichlorophenyl ester	C14H10Cl2O2		LibSearch	27.768	-7.349		1000325-71-3	36.60		
Labd-8-en-15-ol	C20H36O		LibSearch	27.768	-7.999		220766-83-6	36.54		
4-(Fluoromethyl)-5-methyl-2-phenyl-2H-1,2,3-triazole	C10H10FN3		LibSearch	27.768	3.135		1000098-68-5	36.47		
Benzoic acid, 4-methyl-, 2-hydroxy-2-phenylpropyl ester	C17H18O3		LibSearch	27.768	-7.849		1000160-37-2	36.46		
Dicumyl peroxide	C18H22O2		LibSearch	27.768	-4.665		80-43-3	36.45		
Chrysanthenyl acetate<cis->	C12H18O2		LibSearch	27.768	9.258		67999-48-8	36.31		
2-Phenoxyethanol, pentafluoropropionate	C11H9F5O3		LibSearch	27.768	8.935		1000365-49-7	36.18		
Chrysanthenyl acetate<trans->	C12H18O2		LibSearch	27.768	10.438		50764-55-1	36.15		
Isoxazole, 4,5-dihydro-5-[(4-methoxyphenyl)methyl]-	C11H13NO2		LibSearch	27.768	2.235		1010362-14-0	36.12		
(1R,5S,6R)-2,7,7-Trimethylbicyclo[3.1.1]hept-2-en-6-yl acetate	C12H18O2		LibSearch	27.768	6.501		67999-48-8	35.97		
1,3-Benzenediol, o-(2-furoyl)-o'-(4-methylbenzoyl)-	C19H14O5		LibSearch	27.768	-14.715		1000330-75-7	35.97		
Verbenyl acetate <cis->	C12H18O2		LibSearch	27.768			29135-27-1	35.90		
6,8-Nonadien-2-one, 6-methyl-5-(1-methylethylidene)-	C13H20O		LibSearch	27.768	4.651		60714-16-1	35.86		
Verbenyl acetate<trans->	C12H18O2		LibSearch	27.768	7.938		1203-21-0	35.83		
Benzamide, N,N-diethyl-4-methyl-	C12H17NO		LibSearch	27.768	2.685		2728-05-4	35.72		
Bicyclo[3.1.1]hept-2-en-6-ol, 2,7,7-trimethyl-, acetate, [1S-(1.alpha.,5.alpha.,6.beta.)]-	C12H18O2		LibSearch	27.768	6.501		50764-55-1	35.58		
3-Hydroxy-3-phenylbutan-2-one	C10H12O2		LibSearch	27.768	5.768		3155-01-9	35.33		
5,9-methanobenzocyclooctene-5(1H)-ol, 2,3,4,6,7,8,9,10-octahydro-2,2,8,8,9-pentamethyl-	C18H30O		LibSearch	27.768	-3.815		1000396-83-9	35.30		
benzoic acid, 2-chloro-4-[[4-(pentyloxy)benzoyl]oxy]-	C19H19ClO5		LibSearch	27.768	-20.065		1000398-52-3	35.23		
5(1-Ethoxycarbonyl-1,4-dihydropyridin-4-ylidene)-2,2-dimethyl-1,3-dioxan-4,6-dione	C14H15NO6		LibSearch	27.768	-12.382		142131-81-5	35.21		
Benzamide, 2-methyl-N-isobutyl-	C12H17NO		LibSearch	27.768	0.418		1000407-39-3	35.20		
dl-2-Phenyl-1,2-propanediol	C9H12O2		LibSearch	27.768	5.651		4217-66-7	35.15		
Bisabolol acetate <alpha->	C17H28O2		LibSearch	27.768			25428-44-8	35.09		

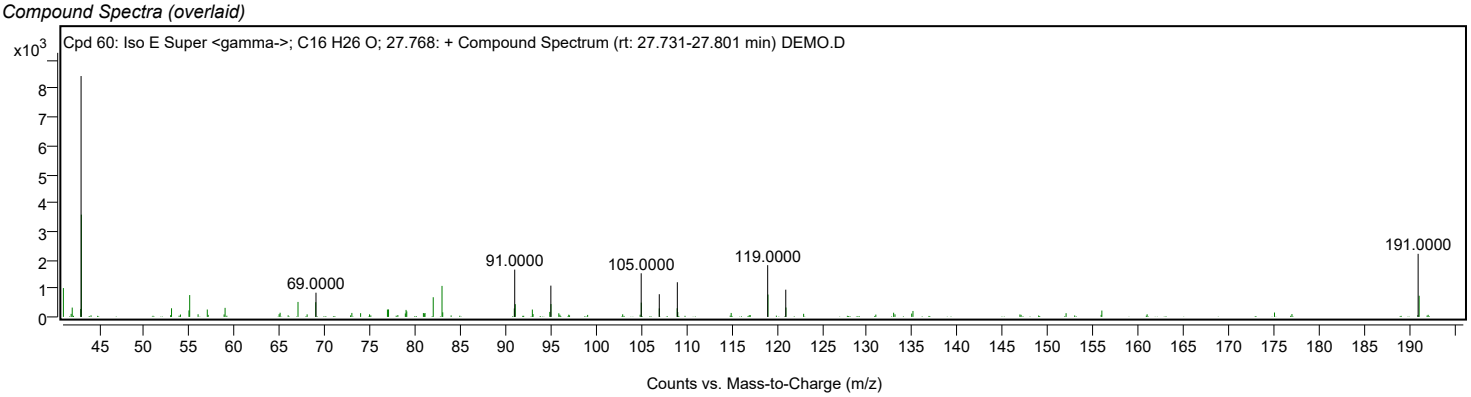
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



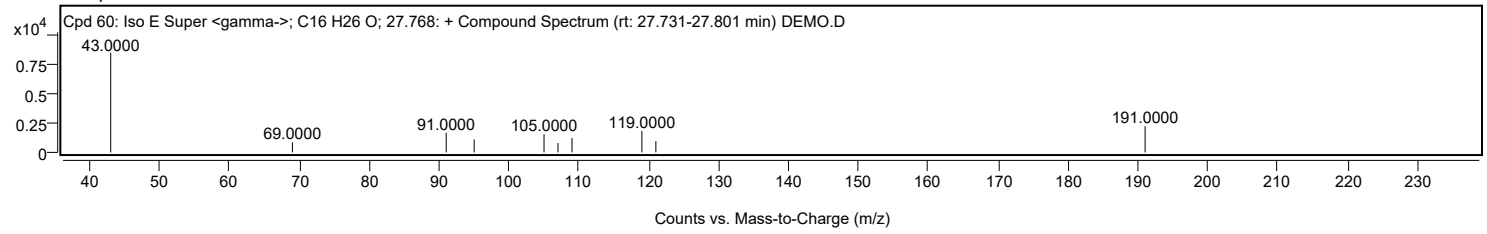
Iso E Super <gamma->

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			53.30			PWNose.xml

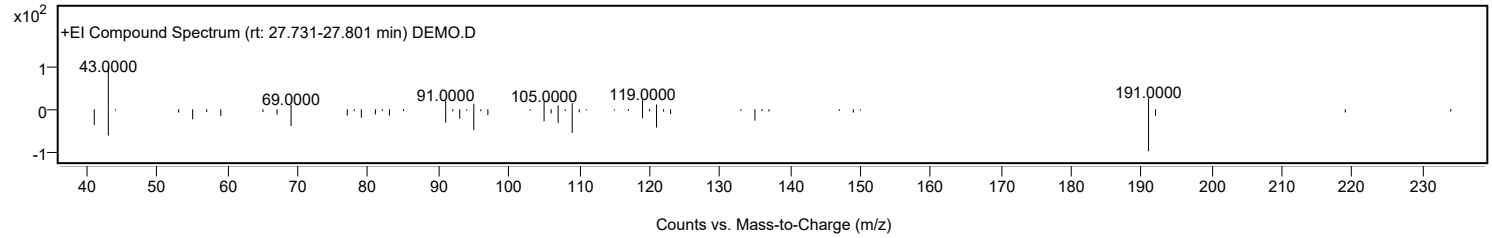
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			53.30			PWNose.xml

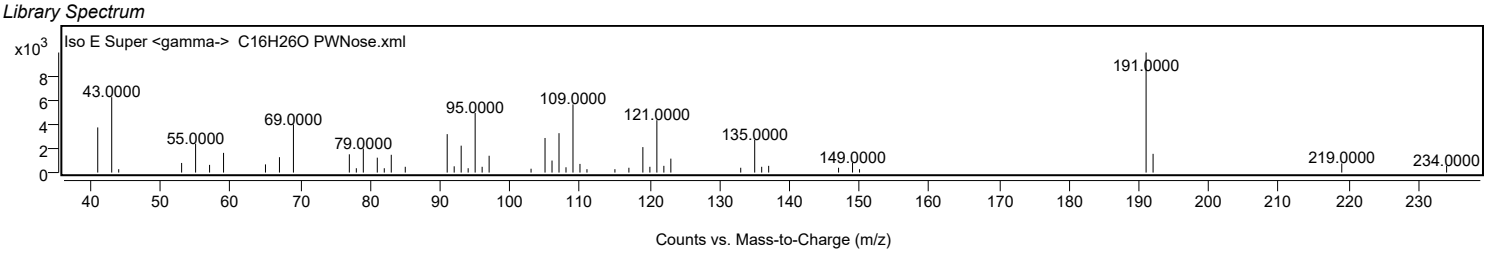
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 61: Fumaric acid, di(cis-hex-3-enyl) ester

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Fumaric acid, di(cis-hex-3-enyl) ester	C16 H24 O4	27.854			1000348-87-6	LibSearch	46.14	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		46.14			50		

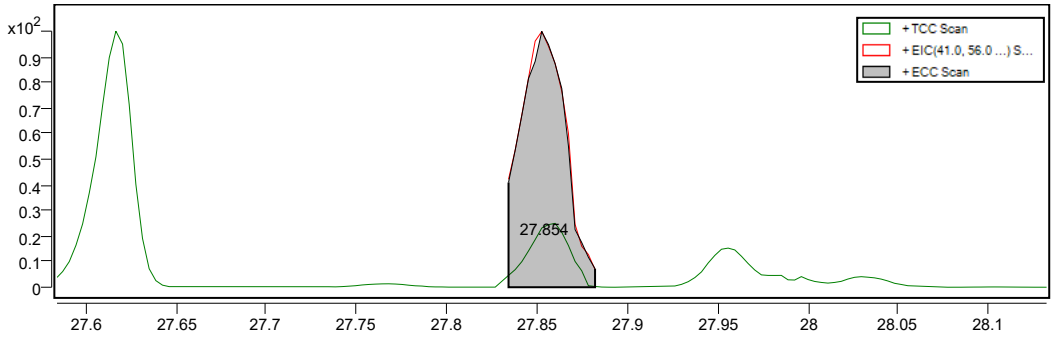
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

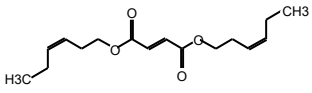
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Fumaric acid, di(cis-hex-3-enyl) ester	C16H24O4		LibSearch	27.854	-4.979		1000348-87-6	46.14		
Cyclohexanemethanol	C7H14O		LibSearch	27.854	10.804		100-49-2	44.61		
2-Butyl-.delta.1-pyrroline	C8H15N		LibSearch	27.854	11.071		64319-86-4	44.37		
Fumaric acid, di(trans-hex-3-enyl) ester	C16H24O4		LibSearch	27.854	-4.979		1000348-90-0	44.33		
Hex-(3Z)-enyl formate	C7H12O2		LibSearch	27.854			33467-73-1	44.27		
Tropinone	C8H13NO		LibSearch	27.854	8.754		532-24-1	44.23		
Tropinone	C8H13NO		LibSearch	27.854	8.754		532-24-1	44.18		
Histidine	C6H9N3O2		LibSearch	27.854	1.671		71-00-1	44.14		
Cyclohexanemethanol	C7H14O		LibSearch	27.854	10.804		100-49-2	44.08		
1H-Pyrrole, 2,3-dihydro-1-methyl-	C5H9N		LibSearch	27.854	16.271		33838-11-8	44.07		
Ethyl (E)-hex-3-enyl carbonate	C9H16O3		LibSearch	27.854	8.404		1000373-83-8	43.83		
Octenyl tiglate, (5Z)-	C13H22O2		LibSearch	27.854			1231959-79-7	43.82		
Adipic acid, di(trans-hex-3-enyl) ester	C18H30O4		LibSearch	27.854	-8.163		1000354-02-3	43.74		
Pentalene, octahydro-, cis-	C8H14		LibSearch	27.854	13.504		1755-05-1	43.65		
Ethyl (Z)-hex-3-enyl carbonate	C9H16O3		LibSearch	27.854	8.404		1000373-83-6	43.56		
(E)-Hex-3-enyl isobutyl carbonate	C11H20O3		LibSearch	27.854	6.154		1000372-74-9	43.43		
(E)-Hex-3-en-1-yl propyl carbonate	C10H18O3		LibSearch	27.854	6.754		1000372-83-0	43.42		
(Z)-Hex-3-en-1-yl propyl carbonate	C10H18O3		LibSearch	27.854	6.754		1000372-80-5	43.28		
Hexenyl hexenoate<3Z->	C12H22O2		LibSearch	27.854	4.204		31501-11-8	43.10		
Adipic acid, di(cis-hex-3-enyl) ester	C18H30O4		LibSearch	27.854	-8.163		1000353-98-7	43.04		
Cyclohexanemethanol	C7H14O		LibSearch	27.854	10.804		100-49-2	43.02		
3-Aminocrotononitrile	C4H6N2		LibSearch	27.854	12.987		1118-61-2	42.94		
Pentalene, octahydro-	C8H14		LibSearch	27.854	13.504		694-72-4	42.93		
(Z)-Hex-3-enyl isobutyl carbonate	C11H20O3		LibSearch	27.854	6.154		1000372-75-0	42.81		
Tiglate <(3Z)-hexenyl->	C11H18O2		LibSearch	27.854			67883-79-8	42.78		
Methylphosphonic acid, fluoroanhydride, 2-cyclohexylethyl ester	C9H18FO2P		LibSearch	27.854			1000273-29-4	42.73		
Cyclopentane, 1,3-dimethyl-2-(1-methylethenyl)-, (1.alpha.,2.alpha.,3.beta.)-	C10H18		LibSearch	27.854	12.037		61142-31-2	42.62		
Hexanal ethyl trans-2-hexenyl acetal	C14H28O2		LibSearch	27.854	2.704		1000431-42-6	42.59		
Cyclohexaneethanol <2->	C8H16O		LibSearch	27.854			4442-79-9	42.53		
Cyclopentane, 1-methyl-2-(2-propenyl)-, trans-	C9H16		LibSearch	27.854	12.671		50746-53-7	42.52		
Hexanoic acid, 3-hexenyl ester	C12H22O2		LibSearch	27.854	4.704		84434-19-5	42.45		
Pentalene, octahydro-, cis-	C8H14		LibSearch	27.854	13.504		1755-05-1	42.45		
Cyclohexane, chloro-	C6H11Cl		LibSearch	27.854	13.087		542-18-7	42.35		
Cyclohexane, chloro-	C6H11Cl		LibSearch	27.854	13.087		542-18-7	42.24		
DL-Histidine	C6H9N3O2		LibSearch	27.854	1.671		4998-57-6	42.19		
Oxalic acid, dicyclohexyl ester	C14H22O4		LibSearch	27.854	-3.379		1000309-30-9	42.14		
Hexanoate <(3Z)-hexenyl->	C12H22O2		LibSearch	27.854			31501-11-8	42.13		
Cyclohexaneethanol	C8H16O		LibSearch	27.854	9.137		4442-79-9	42.12		
1H-Imidazole-2-sulfonamide, N,N,N'-tris-methyl	C6H11N3O2S		LibSearch	27.854	3.521		1862493-58-0	42.08		
Isocitronellol	C10H20O		LibSearch	27.854	9.954		18479-52-2	42.03		
Octenyl angelate, 5Z-	C13H22O2		LibSearch	27.854	3.287		1000383-60-2	41.99		
Cyclohexanepropanol-	C9H18O		LibSearch	27.854	7.487		1124-63-6	41.96		
(E)-Hex-3-enyl (E)-2-methylbut-2-enoate	C11H18O2		LibSearch	27.854	6.604		120603-00-1	41.78		
Octenyl tiglate, 5Z-	C13H22O2		LibSearch	27.854	3.287		1000383-60-1	41.77		
Hexenyl tiglate<3Z->	C11H18O2		LibSearch	27.854	6.784		67883-79-8	41.76		
Hexenyl tiglate<3E->	C11H18O2		LibSearch	27.854	6.974		120603-00-1	41.76		
Histidine	C6H9N3O2		LibSearch	27.854	1.671		71-00-1	41.75		
Tropinone	C8H13NO		LibSearch	27.854	8.754		532-24-1	41.72		
(Z)-Hex-3-enyl (E)-2-methylbut-2-enoate	C11H18O2		LibSearch	27.854	6.604		67883-79-8	41.71		
Cyclohexylmethyl formate	C8H14O2		LibSearch	27.854	8.787		2888-49-5	41.65		

Compound Chromatograms (overlaid)

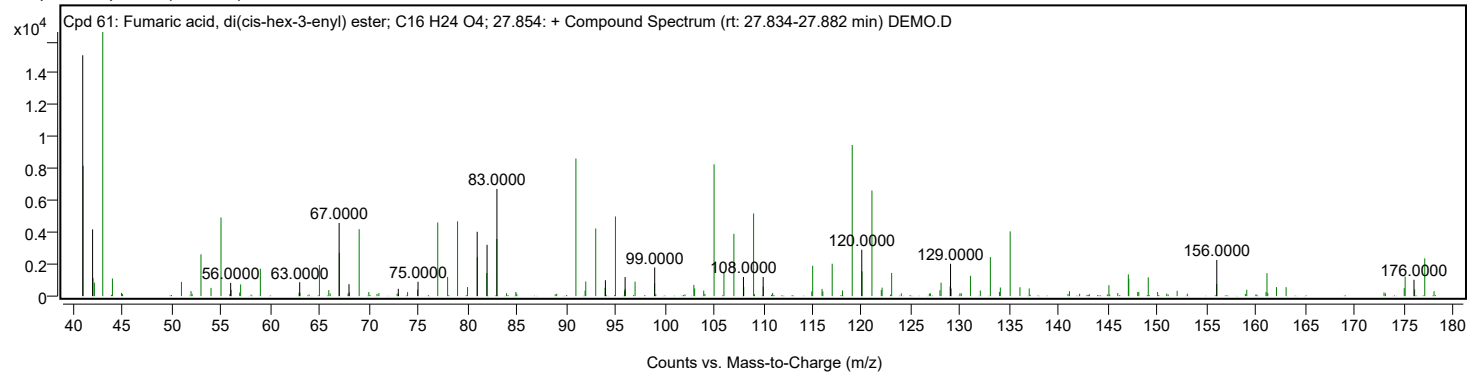


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



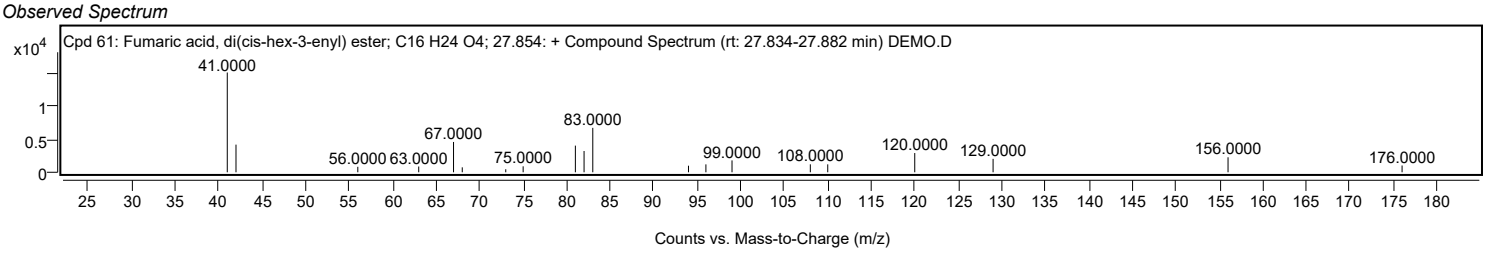
Fumaric acid, di(cis-hex-3-enyl) ester

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			46.14			NIST.L

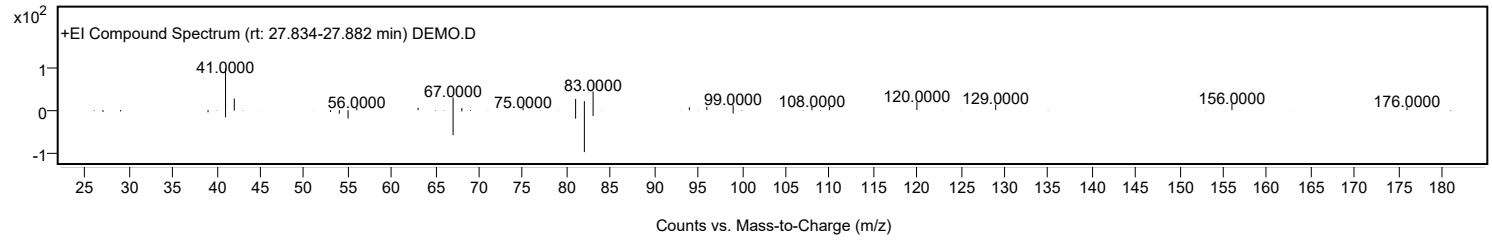
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			46.14			NIST.L

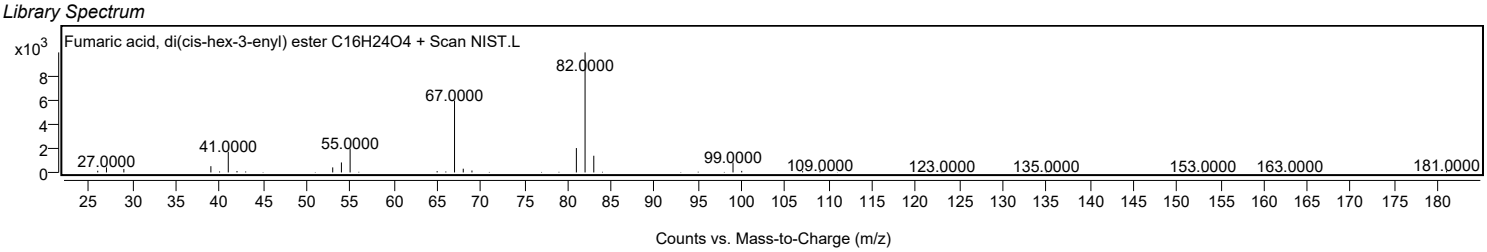
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 62: Amberonne (isomer 2)

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Amberonne (isomer 2)	C16 H26 O	27.855			1010470-69-8	LibSearch	91.02	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		91.02			50		

Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Amberonne (isomer 2)	C16H26O		LibSearch	27.855	-0.578		1010470-69-8	91.02		
Amberonne (isomer 1)	C16H26O		LibSearch	27.855	-0.578		1000470-69-7	89.89		
Amberonne (isomer 3)	C16H26O		LibSearch	27.855	-0.578		1000470-69-9	86.54		
Iso E Super <gamma->	C16H26O		LibSearch	27.855			68155-67-9	79.07		
1-[1,6-Dimethyl-4-(4-methyl-3-pentenyl)-3-cyclohexen-1-yl]ethanone	C16H26O		LibSearch	27.855	-0.545		57499-57-7	77.05		
3-Buten-2-one, 4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)-	C14H22O		LibSearch	27.855	2.538		79-70-9	75.81		
1-Penten-3-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	C14H22O		LibSearch	27.855	1.905		127-43-5	75.50		
Iso E Super <alpha->	C16H26O		LibSearch	27.855			68155-66-8	72.42		
(7a-Isopropenyl-4,5-dimethyloctahydroinden-4-yl)methanol	C15H26O		LibSearch	27.855	0.205		1010187-02-9	71.69		
[5-(Hydroxymethyl)-2,5,8a-trimethyl-1,4,4a,6,7,8-hexahydronaphthalen-1-yl]methanol	C15H26O2		LibSearch	27.855	-4.278		1796930-60-3	70.98		
Bicyclo[4.3.0]nonan-1-ol, 7,9-bis(methylene)-2,2,6-trimethyl-	C14H22O		LibSearch	27.855	3.305		125257-63-8	70.49		
2-(4a,8-Dimethyl-6-oxo-1,2,3,4,4a,5,6,8a-octahydronaphthalen-2-yl)-propionaldehyde	C15H22O2		LibSearch	27.855	-2.178		1000190-21-8	70.26		
Curcumenol	C15H22O2		LibSearch	27.855	0.055		19431-84-6	69.21		
(7S,7aR,13aS)-9-Methoxy-4,4,7,7a-tetramethyl-1,2,3,4,4a,5,6,7,7a,8-decahydrobenzo[d]xanthen-12-ol	C22H32O3		LibSearch	27.855	-13.595		1000482-45-3	69.02		
[3,3-Dimethyl-2-(3-methylbuta-1,3-dienyl)cyclohex-1-enyl]methanol	C14H22O		LibSearch	27.855	0.672		1000195-13-8	68.80		
1,4,5,6-Tetrahydrocyclopentapyrazole-3-carboxylic acid, (1-adamantan-1-ylethylidene)hydrazide	C19H26N4O		LibSearch	27.855	-19.878		1000265-46-6	68.10		
7-(1,3-Dimethylbuta-1,3-dienyl)-1,6,6-trimethyl-3,8-dioxatricyclo[5.1.0.0(2,4)]octane	C15H22O2		LibSearch	27.855	3.305		1000190-22-7	68.03		
1,5,9,9-Tetramethyl-2-methylene-spiro[3.5]non-5-ene	C14H22		LibSearch	27.855	5.722		1000186-71-7	67.88		
Acetic acid, (1,2,3,4,5,6,7,8-octahydro-3,8,8-trimethylnaphth-2-yl)methyl ester	C16H26O2		LibSearch	27.855	-1.528		314773-27-8	67.57		
1,3-Cyclopentadiene, 2,3,4,5-tetramethyl-1-(4-pentenyl)-	C14H22		LibSearch	27.855	5.005		1000161-28-7	67.50		
2,4a,5,8a-Tetramethyl-1,2,3,4,4a,7,8,8a-octahydronaphthalen-1-yl formate (isomer 3)	C15H24O2		LibSearch	27.855	-0.578		1000497-98-5	67.29		
3-Epi-cedrenol, methyl ether	C16H26O		LibSearch	27.855	1.555		1000465-29-7	67.13		
Alloaromadendrene oxide-(1)	C15H24O		LibSearch	27.855	3.488		1000156-12-8	67.03		
1,3,6,10-Cyclotetradecatetraene, 3,7,11-trimethyl-14-(1-methylethyl)-, [S-(E,Z,E,E)]-	C20H32		LibSearch	27.855	-6.678		1898-13-1	67.03		
4,8a-Dimethyl-6-(2-methyl-oxiran-2-yl)-4a,5,6,7,8,8a-hexahydro-1H-naphthalen-2-one	C15H22O2		LibSearch	27.855	-1.178		1000189-11-4	66.93		
Elemol acetate	C17H28O2		LibSearch	27.855	-8.115		60031-93-8	66.85		
5-(7a-Isopropenyl-4,5-dimethyl-octahydroinden-4-yl)-3-methyl-pent-2-en-1-ol	C20H34O		LibSearch	27.855	-7.828		1000193-54-0	66.70		
Tetracyclo[6.1.0.0(2,4).0(5,7)]nonane, 3,3,6,6,9,9-hexamethyl-, cis,cis,trans--	C15H24		LibSearch	27.855	10.072		1000151-74-7	66.10		
2-Methyl-4-(2,6,6-trimethylcyclohex-1-enyl)but-2-en-1-ol	C14H24O		LibSearch	27.855	0.505		62924-17-8	66.03		
1R,3Z,9S-4,11,11-Trimethyl-8-methylenebicyclo[7.2.0]undec-3-ene	C15H24		LibSearch	27.855	2.955		1000159-39-4	65.98		
9-Isopropyl-1-methyl-2-methylene-5-oxatricyclo[5.4.0.0(3,8)]undecane	C15H24O		LibSearch	27.855	5.772		1000185-86-6	65.95		
Longipinene<alpha->	C15H24		LibSearch	27.855	5.445		5989-08-2	65.93		
Viridiflorene	C15H24		LibSearch	27.855	-0.825		21747-46-6	65.70		
Spiro[2.7]dec-4-ene, 1,1,5,6,6,9,9-heptamethyl-10-methylene-	C18H30		LibSearch	27.855	0.255		1000150-39-7	65.70		
Elemene<gamma->	C15H24		LibSearch	27.855	1.775		29873-99-2	65.57		
Longifolol acetate<iso->	C17H28O2		LibSearch	27.855	-13.235		205697-15-0	65.55		
5,9-methanobenzocyclooctene-5(1H)-ol, 2,3,4,6,7,8,9,10-octahydro-2,2,8,8,9-pentamethyl-	C18H30O		LibSearch	27.855	-3.728		1000396-83-9	65.49		
Khusimone	C14H20O		LibSearch	27.855	-5.195		30557-76-7	65.46		
Cyclopenta[1,3]cyclopropa[1,2]cycloheptene-3(3aH)-one, 1,2,3b,6,7,8-hexahydro-6,6-dimethyl-	C13H18O		LibSearch	27.855	4.122		91531-58-7	65.40		
1-Hydroxy-6-(3-isopropenyl-cycloprop-1-enyl)-6-methyl-heptan-2-one	C14H22O2		LibSearch	27.855	0.372		1010189-14-9	65.12		
2-Octenoic acid, 4-isopropylidene-7-methyl-6-methylene-, methyl ester	C14H22O2		LibSearch	27.855	3.638		1000151-99-2	64.89		
(-)-Aristolene	C15H24		LibSearch	27.855	4.472		6831-16-9	64.79		
Duprezianene<beta->	C15H24		LibSearch	27.855	2.345		178443-10-2	64.63		
Longicyclene	C15H24		LibSearch	27.855	4.485		1137-12-8	64.60		
4,6,6-Trimethyl-2-(3-methylbuta-1,3-dienyl)-3-oxatricyclo[5.1.0.0(2,4)]octane	C15H22O		LibSearch	27.855	4.405		1000190-22-2	64.54		
Funebrene<alpha->	C15H24		LibSearch	27.855	3.145		50894-66-1	64.47		
Tricyclo[5.4.0.0(2,8)]undec-9-ene, 2,6,6,9-tetramethyl-, (1R,2S,7R,8R)-	C15H24		LibSearch	27.855	4.472		5989-08-2	64.45		
Amber formate	C15H24O2		LibSearch	27.855			65405-72-3	64.28		
Eremoligenol	C15H26O		LibSearch	27.855	-6.185		10219-71-3	64.27		

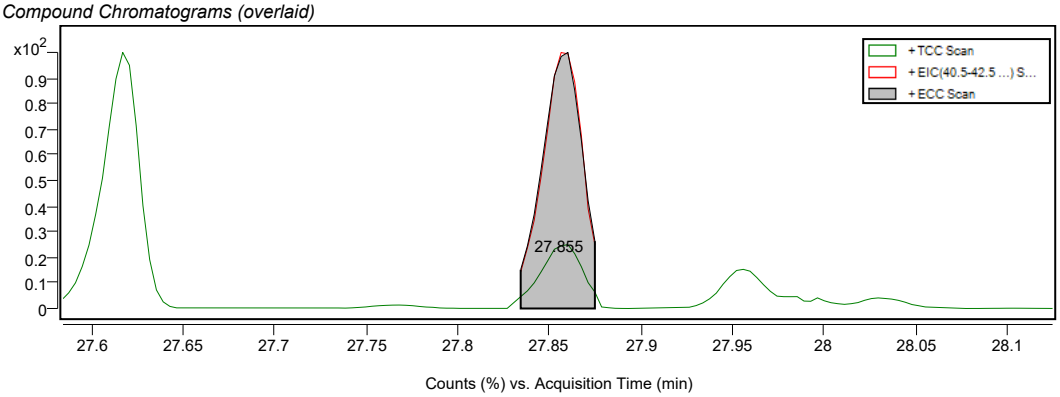
Compound Discovery Report

Agilent | Trusted Answers

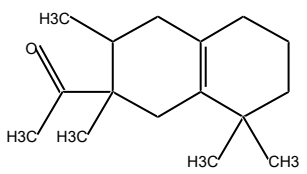
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Alloaromadendrene oxide-(2)	C15H24O		LibSearch	27.855	3.488		1000156-12-7	64.25		

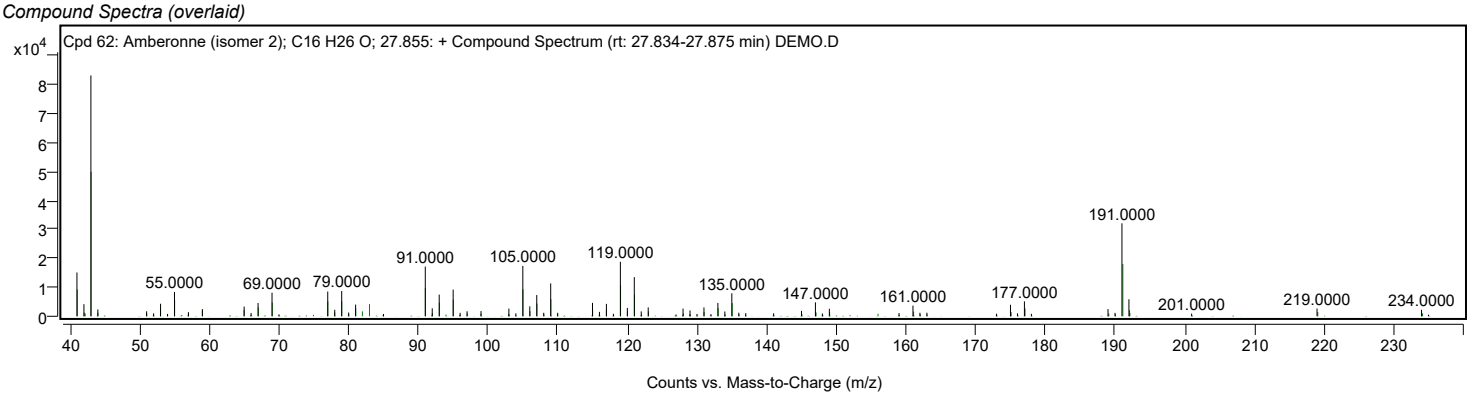
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



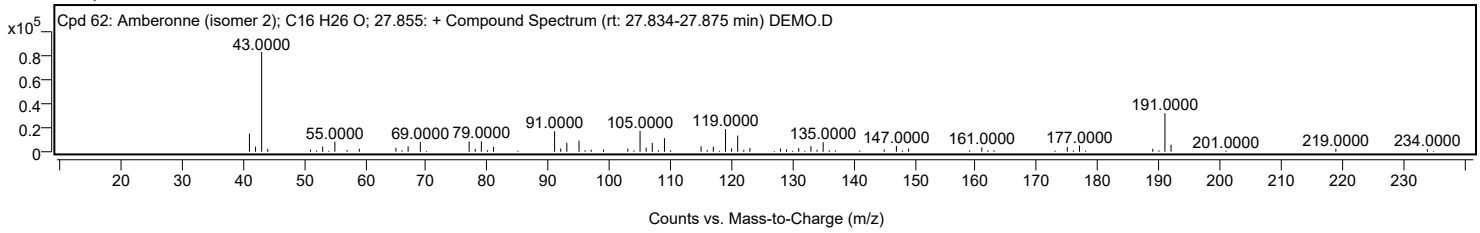
Amberonne (isomer 2)

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			91.02			NIST.L

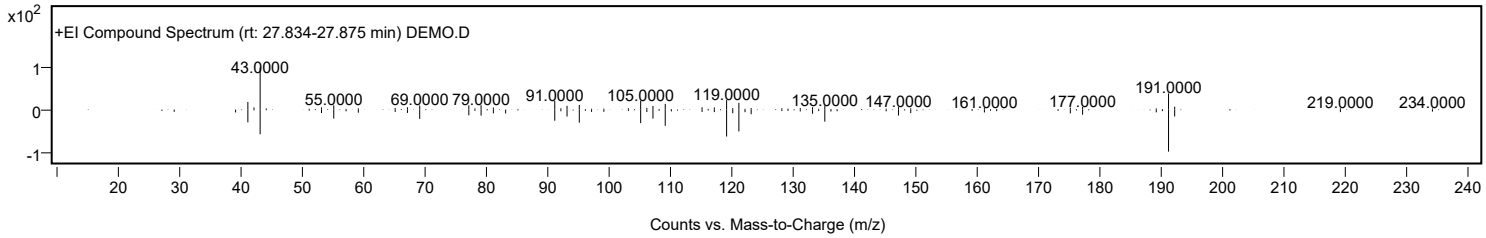
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			91.02			NIST.L

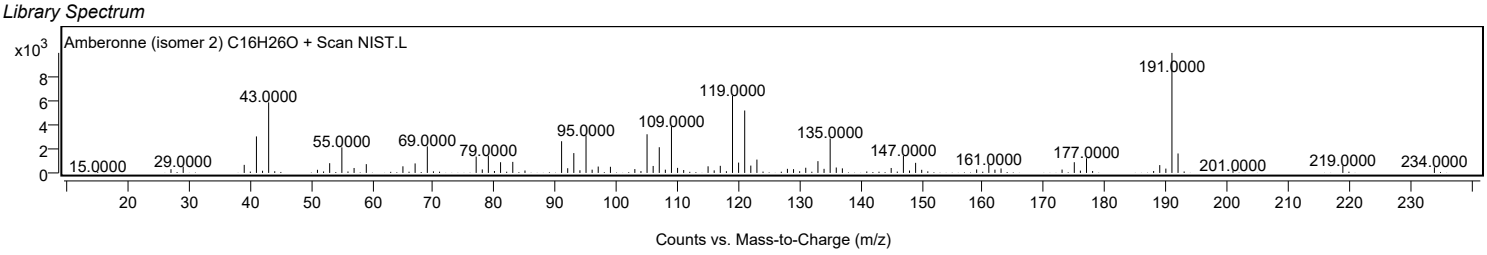
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 63: [2,2'-Bifuran]-3-carboxylic acid, methyl ester

Compound Discovery Report

Agilent | Trusted Answers

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
[2,2'-Bifuran]-3-carboxylic acid, methyl ester	C10 H8 O4	27.867			5905-07-7	LibSearch	42.63	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		42.63			50		

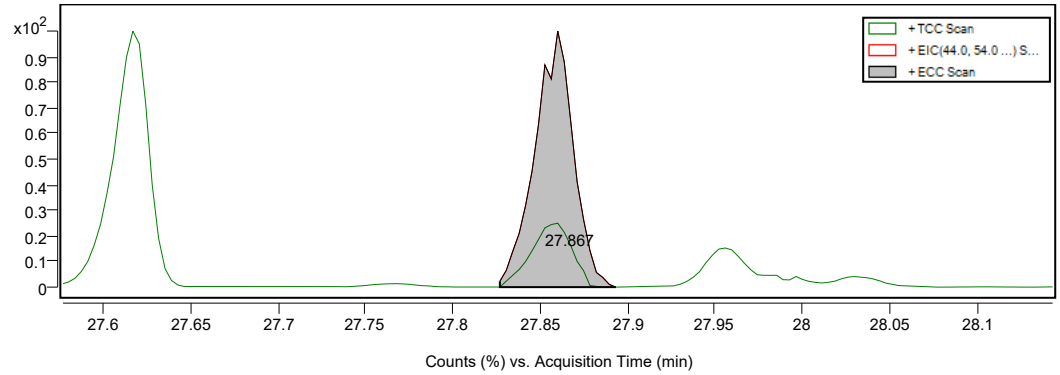
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
[2,2'-Bifuran]-3-carboxylic acid, methyl ester	C10H8O4		LibSearch	27.867	4.183		5905-07-7	42.63		
2-Propenoic acid, 3-(4-methoxyphenyl)-, methyl ester	C11H12O3		LibSearch	27.867	3.600		832-01-9	41.92		
(2S,3S)-3-Benzyloxy-4-(tert-butyldimethylsilyloxy)butan-1,2-diol isopropylidene acetal	C20H34O4Si		LibSearch	27.867	-8.050		1000429-64-1	39.69		
Dimethyl 2,4-bis(4-hydroxyphenyl)cyclobutane-1,3-dicarboxylate, dimethyl ether (isomer 2)	C22H24O6		LibSearch	27.867	-18.517		1000513-15-6	38.84		
Methyl 4-hydroxy-1-benzofuran-6-carboxylate	C10H8O4		LibSearch	27.867	0.900		1279218-51-7	38.07		
Retrofractamide-A	C20H25NO3		LibSearch	27.867	-16.983		94079-67-1	37.50		
Benzoic acid, 4-butyl-, methyl ester	C12H16O2		LibSearch	27.867	3.333		20651-69-8	37.45		
trans-2-Hydroxycinnamic acid, methyl ether, methyl ester	C11H12O3		LibSearch	27.867	3.600		98288-15-4	37.41		
2-Propenoic acid, 3-(4-methoxyphenyl)-, methyl ester	C11H12O3		LibSearch	27.867	3.600		832-01-9	37.25		
3-(2-Methoxy-5-methylphenyl)acrylic acid	C11H12O3		LibSearch	27.867	0.217		103986-76-1	37.05		
2-Propenoic acid, 3-(2-methoxyphenyl)-, methyl ester	C11H12O3		LibSearch	27.867	3.600		15854-58-7	37.01		
2-Propenoic acid, 3-(4-methoxyphenyl)-, methyl ester, (E)-	C11H12O3		LibSearch	27.867	3.600		3901-07-3	36.93		
2-Propenoic acid, 3-(4-methoxyphenyl)-, methyl ester	C11H12O3		LibSearch	27.867	3.600		832-01-9	36.57		
(2E,4E,8E)-9-(Benzo[d][1,3]dioxol-5-yl)-1-(piperidin-1-yl)nona-2,4,8-trien-1-one	C21H25NO3		LibSearch	27.867	-18.883		107584-38-3	36.35		
2-Propenoic acid, 3-(4-methoxyphenyl)-, methyl ester, (E)-	C11H12O3		LibSearch	27.867	3.600		3901-07-3	35.95		
(2E,4E,8E)-9-(Benzo[d][1,3]dioxol-5-yl)-1-(piperidin-1-yl)nona-2,4,8-trien-1-one	C21H25NO3		LibSearch	27.867	-18.883		107584-38-3	35.83		
2-Propenoic acid, 3-(4-methoxyphenyl)-, methyl ester	C11H12O3		LibSearch	27.867	3.600		832-01-9	35.65		
2-Propenoic acid, 3-phenyl-, methyl ester, (E)-	C10H10O2		LibSearch	27.867	6.750		1754-62-7	35.50		
(2,5-Dimethylbenzo(b)thien-3-yl)acetamide	C12H13NOS		LibSearch	27.867	-4.983		1000244-56-6	34.98		
1H-Isoindole-1,3(2H)-dione, 5-nitro-	C8H4N2O4		LibSearch	27.867	-1.750		89-40-7	34.96		
Methyl 3-(3-methoxyphenyl)prop-2-enoate	C11H12O3		LibSearch	27.867	3.600		79432-91-0	34.88		
2-Pyrrolidinone, 4-phenyl-	C10H11NO		LibSearch	27.867	4.567		1198-97-6	34.78		
(2E,4E,8E)-9-(Benzo[d][1,3]dioxol-5-yl)-1-(pyrrolidin-1-yl)nona-2,4,8-trien-1-one	C20H23NO3		LibSearch	27.867	-16.883		117137-68-5	34.72		
Methyl p-methoxycinnamate, cis	C11H12O3		LibSearch	27.867	3.600		19310-29-3	34.33		
Benzo[1,3]dioxole-5-carboxylic acid, [2-(4-cyclohexylphenoxy)ethyl]amide	C22H25NO4		LibSearch	27.867	-24.783		1000302-47-4	34.23		
2-Propenoic acid, 3-phenyl-, methyl ester	C10H10O2		LibSearch	27.867	6.750		103-26-4	34.16		
N-(p-Vinylbenzoyl)-l-alanine	C12H13NO3		LibSearch	27.867	-5.250		139184-60-4	34.09		
3-(4-Methoxyphenyl)-4H-1,2,4-oxadiazol-5-one	C9H8N2O3		LibSearch	27.867	-3.833		59812-04-3	34.02		
3-Benzyl-1,4,7,10,13-pentaoxacyclopentadecane-2,5,9-trione	C17H20O8		LibSearch	27.867	-25.250		79687-34-6	33.99		
2-Propenal, 3-(3,4-dimethoxyphenyl)-	C11H12O3		LibSearch	27.867	1.750		4497-40-9	33.72		
Dimethyl 2,4-bis(4-hydroxyphenyl)cyclobutane-1,3-dicarboxylate, dimethyl ether (isomer 1)	C22H24O6		LibSearch	27.867	-18.517		1000513-20-6	33.39		
Methyl cinnamate<E->	C10H10O2		LibSearch	27.867	4.287		1754-62-7	33.16		
2-Propenoic acid, 3-phenyl-, methyl ester, (E)-	C10H10O2		LibSearch	27.867	6.750		1754-62-7	33.09		
1,3-Cyclobutanedicarboxylic acid, 2,4-bis(4-hydroxyphenyl)-, 1,3-dimethyl ester, dimethyl ether	C22H24O6		LibSearch	27.867	-18.517		867017-01-4	33.03		
3-Allyl-4-hydroxy-5-methoxybenzaldehyde	C11H12O3		LibSearch	27.867	-0.367		20240-58-8	32.96		
Methyl cinnamate<Z->	C10H10O2		LibSearch	27.867	7.687		19713-73-6	32.85		
Methyl cis-cinnamate	C10H10O2		LibSearch	27.867	6.750		19713-73-6	32.70		
Phthalic acid, propyl 4-trifluoromethoxybenzyl ester	C19H17F3O5		LibSearch	27.867	-11.050		1000377-68-4	32.65		
(E)-2-[1-(3-Acetoxy-2-furanyl)ethylidene]-2H-furan-3-one	C12H10O5		LibSearch	27.867	-1.817		105399-04-0	32.64		
2-Propenoic acid, 3-phenyl-, methyl ester	C10H10O2		LibSearch	27.867	6.750		103-26-4	32.48		
m-Trifluoromethoxybenzyl alcohol	C8H7F3O2		LibSearch	27.867	10.200		50823-90-0	32.12		
(2E,6E)-7-(Benzo[d][1,3]dioxol-5-yl)-1-(piperidin-1-yl)hepta-2,6-dien-1-one	C19H23NO3		LibSearch	27.867	-15.433		147030-09-9	31.97		
2-Propenal, 3-(3,4-dimethoxyphenyl)-	C11H12O3		LibSearch	27.867	1.750		4497-40-9	31.94		
4-Hydroxycoumarin, TBDMS derivative	C15H20O3Si		LibSearch	27.867	-3.167		1000333-10-3	31.84		
2-Oxazoline, 4,5-diethyl-2-(p-nitrophenyl)-, trans-	C13H16N2O3		LibSearch	27.867	-5.267		25943-15-1	31.84		
1,3-Benzodioxole, 4-methoxy-6-(2-propenyl)-	C11H12O3		LibSearch	27.867	2.600		607-91-0	31.60		
3-(Allyloxy)-N-(1,3-thiazol-2-yl)benzamide	C13H12N2O2S		LibSearch	27.867	-10.200		499989-63-8	31.52		
Cinnamate <(E)-, methyl->	C10H10O2		LibSearch	27.867			1754-62-7	31.34		
1,3-Cyclobutanedicarboxylic acid, 2,4-bis(4-hydroxyphenyl)-, 1,3-dimethyl ester, dimethyl ether	C22H24O6		LibSearch	27.867	-18.517		867017-01-4	31.31		
2-Methoxycinnamic acid, TMS derivative	C13H18O3Si		LibSearch	27.867	1.783		1000352-48-2	31.16		

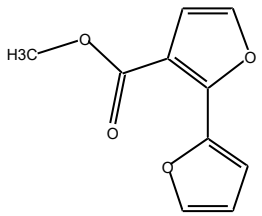
Compound Discovery Report

Agilent | Trusted Answers

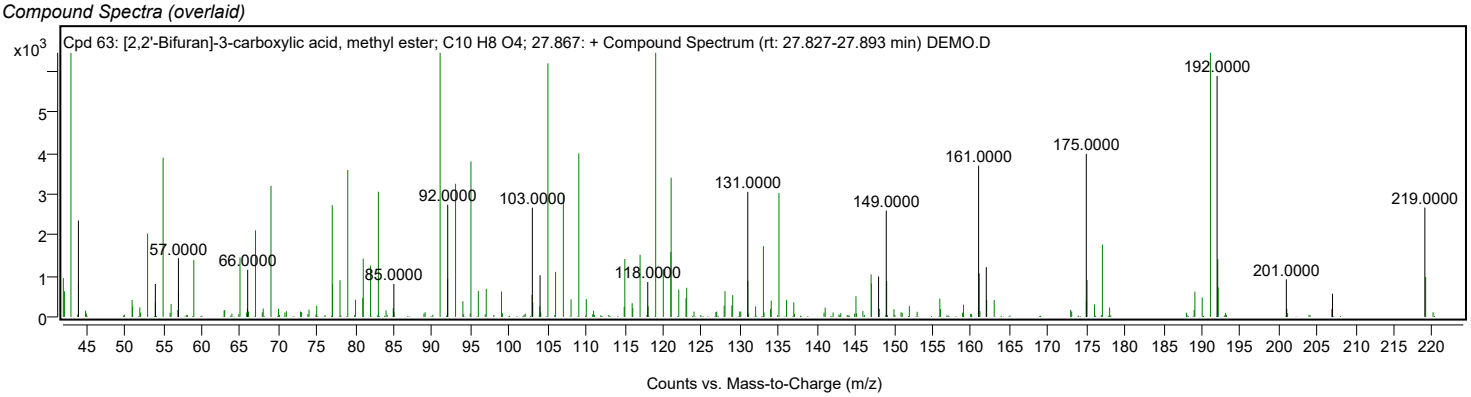
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



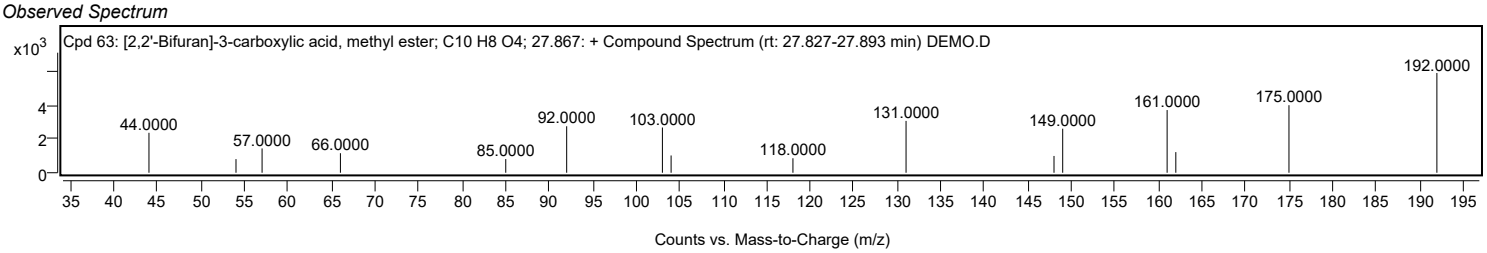
[2,2'-Bifuran]-3-carboxylic acid, methyl ester

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			42.63			NIST.L

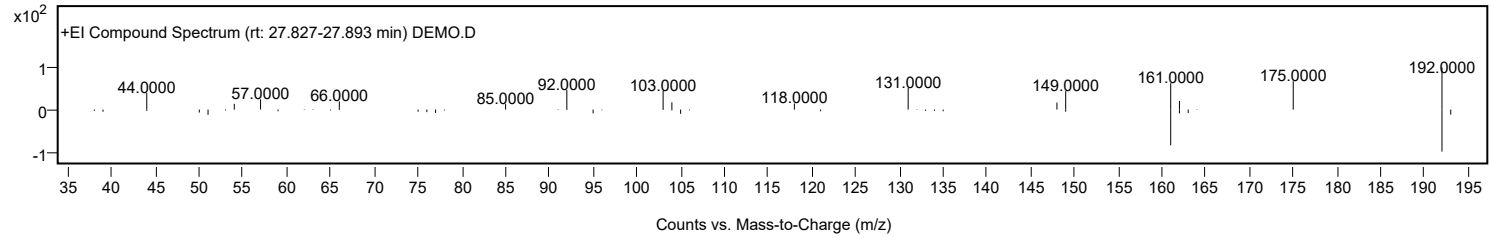
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			42.63			NIST.L

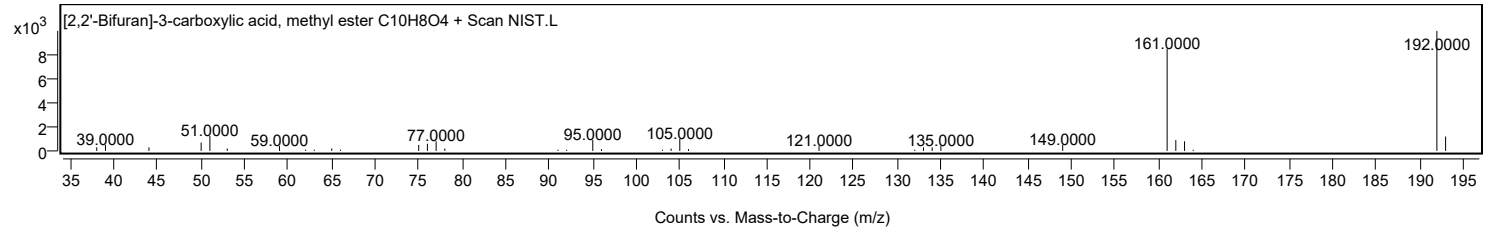
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 64: Helvetolide

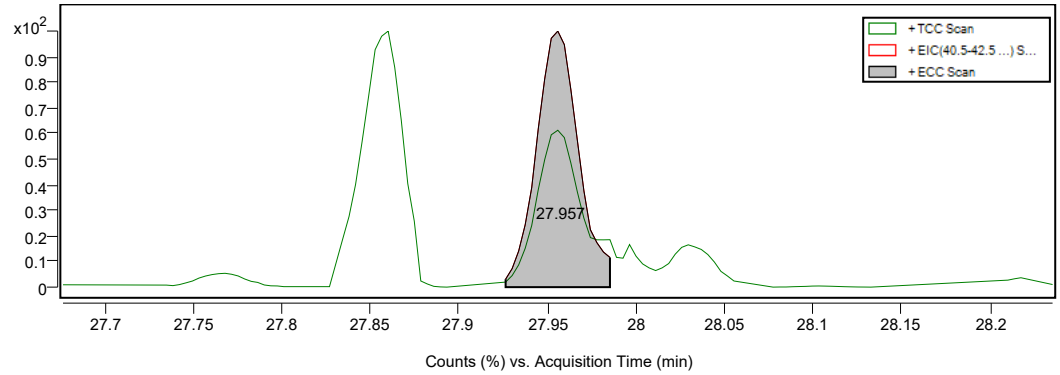
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Helvetolide	C17 H32 O3	27.957			141773-73-1	LibSearch	93.34	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		93.34			50		

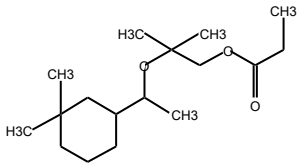
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Helvetolide	C17H32O3		LibSearch	27.957			141773-73-1	93.34		
t-butylsulfinate,-O-menthyl-	C14H28O2S		LibSearch	27.957	-2.009		1000151-39-9	66.14		
Oxalic acid, butyl 1-menthyl ester	C16H28O4		LibSearch	27.957	-3.193		1000314-97-2	62.44		
1,1,3,3,5-Pentamethylcyclohexane	C11H22		LibSearch	27.957	10.457		70810-19-4	62.28		
Hexanal ethyl cis-3-hexenyl acetal	C14H28O2		LibSearch	27.957	2.807		1000431-42-9	62.17		
Cyclohexane, 2-iodo-4-methyl-1-(1-methylethyl)-	C10H19I		LibSearch	27.957	5.424		64240-81-9	61.79		
Oxalic acid, heptyl 1-menthyl ester	C19H34O4		LibSearch	27.957	-8.159		1010314-97-5	61.08		
2-Heptenoic acid, tetradecyl ester	C21H40O2		LibSearch	27.957	-10.109		1000406-09-9	61.03		
Oxalic acid, 1-menthyl octyl ester	C20H36O4		LibSearch	27.957	-9.826		1000314-97-6	60.61		
2-Heptenoic acid, tridecyl ester	C20H38O2		LibSearch	27.957	-8.459		1000406-09-8	59.95		
Cyclohexane, 1,5-diethyl-2,3-dimethyl-	C12H24		LibSearch	27.957	8.574		74663-66-4	59.94		
Menthyl lactate	C13H24O3		LibSearch	27.957	-0.093		59259-38-0	59.60		
Oxalic acid, isohexyl 1-menthyl ester	C18H32O4		LibSearch	27.957	-5.443		1000314-98-7	59.56		
Oxalic acid, 1-menthyl pentyl ester	C17H30O4		LibSearch	27.957	-4.843		1000314-97-3	59.54		
Decanol<3->	C10H22O		LibSearch	27.957	12.357		1565-81-7	59.47		
Oxalic acid, hexyl 1-menthyl ester	C18H32O4		LibSearch	27.957	-6.509		1000314-97-4	59.39		
Menthyl lactate<iso->	C13H24O3		LibSearch	27.957	-0.533		0-00-0	59.23		
Menthyl lactate	C13H24O3		LibSearch	27.957			17162-29-7	59.23		
Oxalic acid, 1-menthyl nonyl ester	C21H38O4		LibSearch	27.957	-11.476		1000314-97-7	59.12		
2-Heptenoic acid, dodecyl ester	C19H36O2		LibSearch	27.957	-6.793		1000406-09-7	59.11		
2-Heptenoic acid, pentadecyl ester	C22H42O2		LibSearch	27.957	-11.759		1000406-10-0	59.00		
Cyclohexanecarboxylic acid, butyl ester	C11H20O2		LibSearch	27.957	5.541		6553-81-7	58.94		
Pyrrolidin-5-one, 2,3-dedihydro-3-nitro-	C4H3NO4		LibSearch	27.957	8.307		1000124-44-1	58.92		
Decanol <3->	C10H22O		LibSearch	27.957			1565-81-7	58.87		
L-Menthyl lactate	C13H24O3		LibSearch	27.957	1.857		185915-25-7	58.85		
Phosphine, dichloro-D-menthyl-	C10H19Cl2P		LibSearch	27.957	4.341		83021-21-0	58.84		
Oxalic acid, di(1-menthyl) ester	C22H38O4		LibSearch	27.957	-11.843		1010314-98-6	58.72		
3-Heptene, 2,2,3,5,5,6,6-heptamethyl-	C14H28		LibSearch	27.957	8.891		54845-26-0	58.59		
Oxalic acid, 1-menthyl undecyl ester	C23H42O4		LibSearch	27.957	-14.793		1000314-97-9	58.58		
Oxalic acid, 1-menthyl tetradecyl ester	C26H48O4		LibSearch	27.957	-19.759		1000314-98-1	58.45		
2-Heptenoic acid, undecyl ester	C18H34O2		LibSearch	27.957	-5.143		1010406-09-6	58.45		
5,6-Dihydropenicillic acid	C8H12O4		LibSearch	27.957	5.974		35973-53-6	58.34		
Oxalic acid, dodecyl 1-menthyl ester	C24H44O4		LibSearch	27.957	-16.443		1000314-98-0	58.17		
3-Decanol	C10H22O		LibSearch	27.957	8.324		1565-81-7	57.86		
Nonylol	C9H20O		LibSearch	27.957			3452-97-9	57.64		
Oxalic acid, decyl 1-menthyl ester	C22H40O4		LibSearch	27.957	-13.126		1000314-97-8	57.57		
Cyclohexanol, 5-methyl-2-(1-methylethyl)-, sulfite (2:1), [1R-[1.alpha.(1R*,2S*,5R*),2.beta.,5.alpha.]]-	C20H38O3S		LibSearch	27.957	-13.343		26510-92-9	57.39		
2-Heptenoic acid, nonyl ester	C16H30O2		LibSearch	27.957	-1.826		1000406-09-5	57.38		
Cyclohexanecarboxylic acid, decyl ester	C17H32O2		LibSearch	27.957	-4.409		93479-48-2	57.26		
2-Heptenoic acid, hexadecyl ester	C23H44O2		LibSearch	27.957	-13.426		1000406-10-1	57.18		
5,6-Dihydropenicillic acid	C8H12O4		LibSearch	27.957	5.974		35973-53-6	57.08		
Hexanal ethyl trans-2-hexenyl acetal	C14H28O2		LibSearch	27.957	2.807		1000431-42-6	57.05		
Cyclohexanecarboxylic acid, 2-methylpropyl ester	C11H20O2		LibSearch	27.957	6.607		37139-85-8	57.00		
1-Hexanol, 3,5,5-trimethyl-	C9H20O		LibSearch	27.957	11.124		3452-97-9	56.97		
1-Hexanol, 3,5,5-trimethyl-	C9H20O		LibSearch	27.957	11.124		3452-97-9	56.95		
4-Propionyloxytridecane	C16H32O2		LibSearch	27.957	-0.626		1000245-62-6	56.93		
Ambercore isomer IV	C14H28O2		LibSearch	27.957			139504-68-0	56.87		
3-Decanol	C10H22O		LibSearch	27.957	8.324		1565-81-7	56.86		
4-tert-Butylcyclohexanecarboxylic acid	C11H20O2		LibSearch	27.957	4.424		5451-55-8	56.79		
Cyclohexanecarboxylic acid, 3-(1,1-dimethylethyl)-, cis-	C11H20O2		LibSearch	27.957	4.424		27392-17-2	56.76		

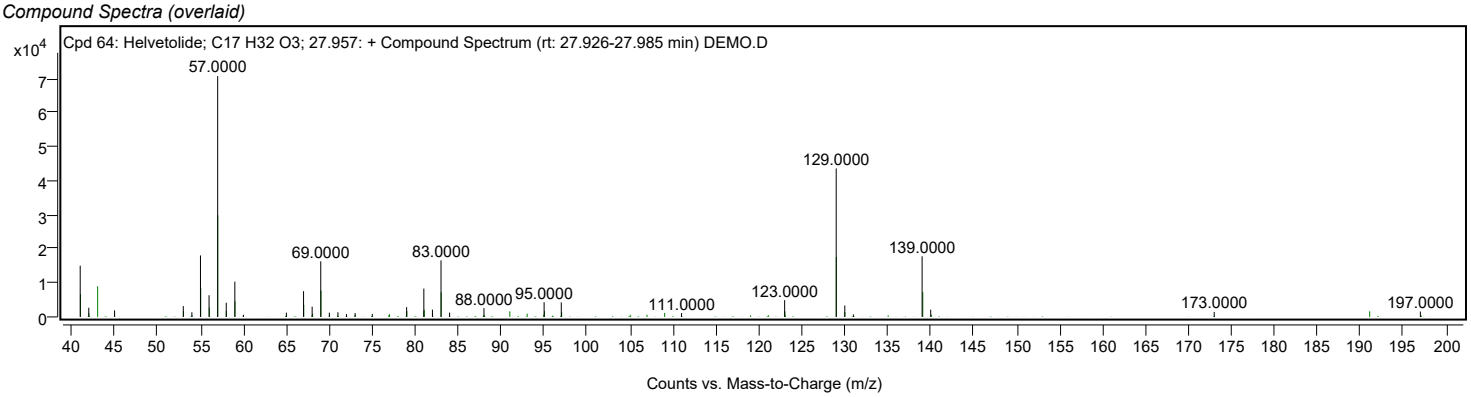
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



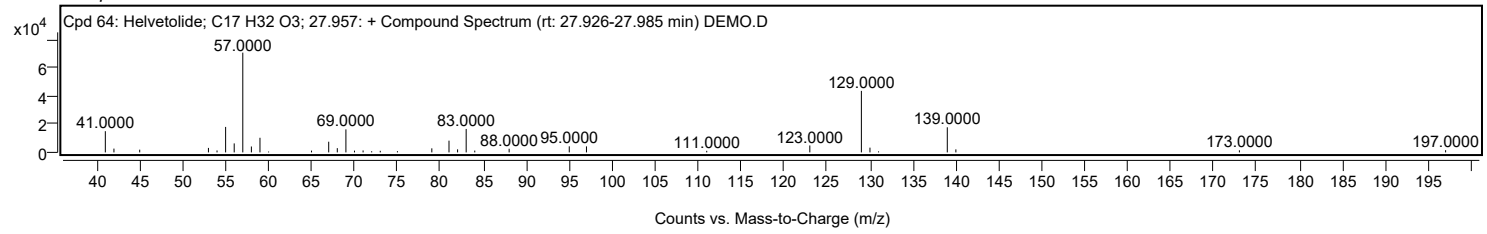
Helvetolide

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			93.34			PWNose.xml

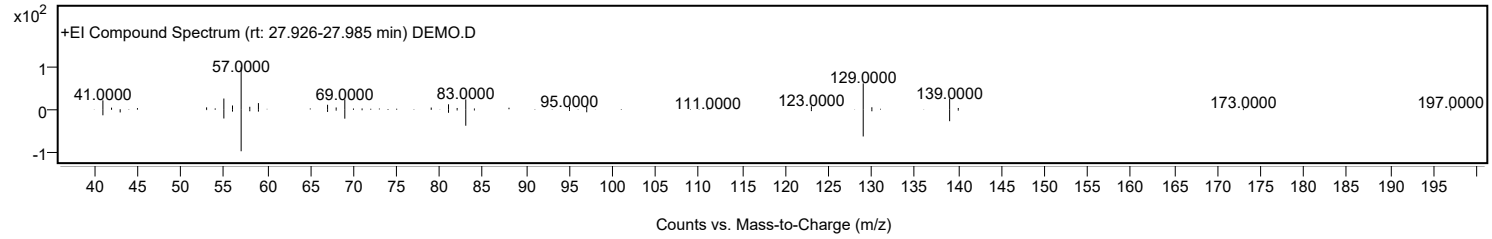
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			93.34			PWNose.xml

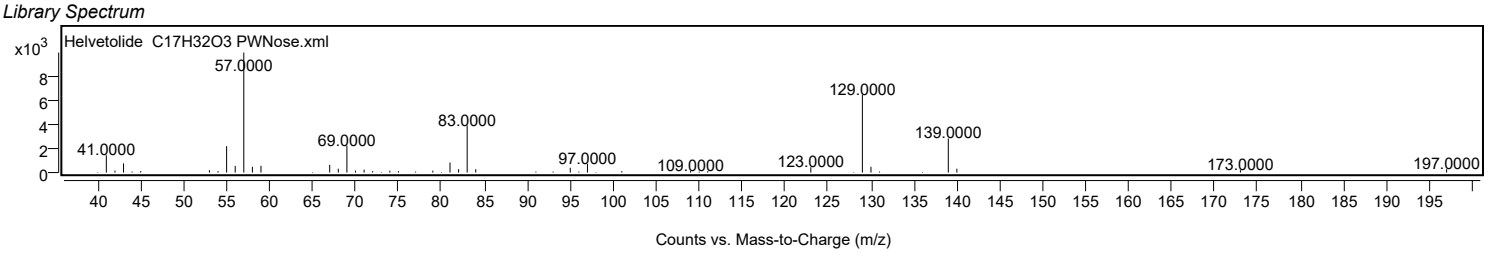
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 65: Iso E Super <gamma->

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Iso E Super <gamma->	C16 H26 O	27.987			68155-67-9	LibSearch	61.90	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		61.90			50		

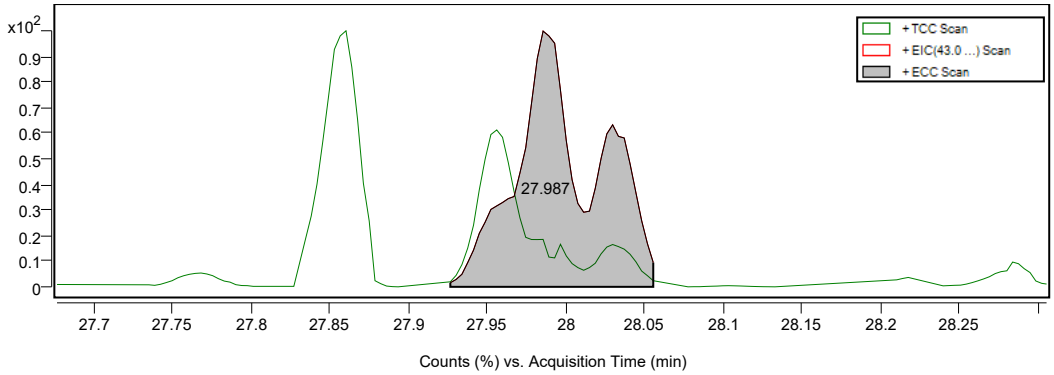
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Iso E Super <gamma->	C16H26O		LibSearch	27.987			68155-67-9	61.90		
Amberonne (isomer 3)	C16H26O		LibSearch	27.987	-0.446		1000470-69-9	57.75		
Benzene, [1-methyl-1-(pentyloxy)ethyl]-	C14H22O		LibSearch	27.987	3.304		54932-79-5	56.82		
3-Buten-2-one, 4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)-	C14H22O		LibSearch	27.987	2.670		79-70-9	55.46		
1,4,5,6-Tetrahydrocyclopentapyrazole-3-carboxylic acid, (1-adamantan-1-ylethylidene)hydrazide	C19H26N4O		LibSearch	27.987	-19.746		1000265-46-6	55.23		
4-Phenyl-morpholine-2,6-dione	C10H9NO3		LibSearch	27.987	-2.063		56956-66-2	54.32		
Amberonne (isomer 2)	C16H26O		LibSearch	27.987	-0.446		1010470-69-8	52.81		
Oxirane, [[4-(1,1-dimethylethyl)phenoxy]methyl]-	C13H18O2		LibSearch	27.987	3.220		3101-60-8	52.76		
Oxirane, [[4-(1,1-dimethylethyl)phenoxy]methyl]-	C13H18O2		LibSearch	27.987	3.220		3101-60-8	51.99		
Acetamide, N-benzyl-2-[2,3-dihydro-2-methyl-5-(4-methylphenyl)-1,3,4-thiadiazol-2-yl]-	C19H21N3OS		LibSearch	27.987	-24.896		1000272-50-7	50.90		
benzoic acid, 2-chloro-4-[[4-(pentyloxy)benzoyl]oxy]-	C19H19ClO5		LibSearch	27.987	-19.846		1000398-52-3	50.66		
Oxirane, [[4-(1,1-dimethylethyl)phenoxy]methyl]-	C13H18O2		LibSearch	27.987	3.220		3101-60-8	50.61		
Acetohydrazide, 2-(4-tolyloxy)-N2-benzoylmethylene-	C17H16N2O3		LibSearch	27.987	-17.113		1000258-81-8	50.26		
1,3-Dioxolane, 2,4,5-trimethyl-2-(p-tolyl)-	C13H18O2		LibSearch	27.987	2.637		1000149-74-3	49.97		
3-Buten-2-one, 4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)-	C14H22O		LibSearch	27.987	2.670		79-70-9	49.95		
Succinic acid, di(3-methylphenyl) ester	C18H18O4		LibSearch	27.987	-10.780		1000329-96-8	49.79		
Oxalic acid, diamide, N,N'-bis(4-methylbenzyl)-	C18H20N2O2		LibSearch	27.987	-18.546		1000309-62-7	49.77		
1-[1,6-Dimethyl-4-(4-methyl-3-pentenyl)-3-cyclohexen-1-yl]ethanone	C16H26O		LibSearch	27.987	-0.413		57499-57-7	49.29		
Isoxazole, 4,5-dihydro-5-[(4-methoxyphenyl)methyl]-	C11H13NO2		LibSearch	27.987	2.454		1010362-14-0	49.21		
Amberonne (isomer 1)	C16H26O		LibSearch	27.987	-0.446		1000470-69-7	48.15		
1-Penten-3-one, 1-(2,6,6-trimethyl-1-cyclohexen-1-yl)-	C14H22O		LibSearch	27.987	2.037		127-43-5	48.13		
Succinic acid, di(2-methylphenyl) ester	C18H18O4		LibSearch	27.987	-10.780		1000325-06-7	47.63		
Acetamide, N-acetyl-N-(phenylmethyl)-	C11H13NO2		LibSearch	27.987	2.520		3027-02-9	47.62		
4-(Fluoromethyl)-5-methyl-2-phenyl-2H-1,2,3-triazole	C10H10FN3		LibSearch	27.987	3.354		1000098-68-5	47.60		
Isophthalic acid, propyl tridec-2-ynyl ester	C24H34O4		LibSearch	27.987	-19.496		1000343-91-3	47.02		
.beta.-iso-Methyl ionone	C14H22O		LibSearch	27.987	2.420		1000285-40-2	46.42		
3,4-Dimethyl-2-(3-methyl-butyryl)-benzoic acid, methyl ester	C15H20O3		LibSearch	27.987	-3.163		71940-29-9	46.21		
Acetamide, N-[3-[[(2,5-dioxo-1-pyrrolidinyl)ethyl]ethylamino]phenyl]-	C16H21N3O3		LibSearch	27.987	-17.430		27550-64-7	46.02		
Iron, acetyldicarbonyl[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadienyl]-	C14H18FeO3		LibSearch	27.987			1000146-24-2	45.90		
3,3-Dimethyl-4-phenylamino-butan-2-one	C12H17NO		LibSearch	27.987	2.304		115437-14-4	45.81		
1,3-Dioxane-4,6-dione, 2-methyl-2-phenyl-	C11H10O4		LibSearch	27.987	-3.330		58413-46-0	45.54		
2-[2-[2-(2,2,3,3,3-Pentafluoropropanoyl)oxyethoxy]ethoxy]ethyl 2,2,3,3,3-pentafluoropropanoate	C12H12F10O6		LibSearch	27.987	9.804		1000351-99-9	45.13		
2-[2-[2-[2-(2,2,3,3,3-Pentafluoropropanoyl)oxyethoxy]ethoxy]ethoxy]ethyl 2,2,3,3,3-pentafluoropropanoate	C14H16F10O7		LibSearch	27.987	5.220		1000351-99-8	44.63		
Terephthalic acid, propyl tridec-2-yn-1-yl ester	C24H34O4		LibSearch	27.987	-19.496		1000323-92-3	44.19		
2,4-Oxazolidinedione, 3-methyl-5-phenyl-	C10H9NO3		LibSearch	27.987	-1.680		5841-66-7	44.18		
2-Ethyl-2-phenyl-1,3-dioxan-4,6-dion	C12H12O4		LibSearch	27.987	-4.980		142131-90-6	43.92		
Acetamide, 2-[2,3-dihydro-2-methyl-5-(4-methylphenyl)-1,3,4-thiadiazol-2-yl]-N-phenyl-	C18H19N3OS		LibSearch	27.987	-23.230		1010276-37-8	43.87		
Propanamide, 3-phenyl-N-propyl-	C12H17NO		LibSearch	27.987	-0.196		1000407-14-8	43.86		
3-Oxypentanol, 5-chloro, pentafluoropropionate	C7H8ClF5O3		LibSearch	27.987	13.304		1000374-84-0	43.64		
(4-Methylphenyl) methanol, n-pentyl ether	C13H20O		LibSearch	27.987	3.320		1000374-65-8	43.60		
3-[(4-Methoxy-benzoyl)-hydrazono]-N-(1-phenyl-ethyl)-butyramide	C20H23N3O3		LibSearch	27.987	-25.030		1000295-96-5	43.59		
p-Heptylaniline	C13H21N		LibSearch	27.987	-0.380		37529-27-4	43.50		
2-[2-[2-[2-[2-(2,2,3,3,3-Pentafluoropropanoyl)oxyethoxy]ethoxy]ethoxy]ethyl 2,2,3,3,3-pentafluoropropanoate	C16H20F10O8		LibSearch	27.987	0.637		1000351-99-7	43.46		
N-Phenyliminodiacetic acid	C10H11NO4		LibSearch	27.987	-2.913		1137-73-1	43.39		
(4-Methylphenyl) methanol, 3-methylbutyl ether	C13H20O		LibSearch	27.987	4.387		1000374-65-7	43.34		
2-[1-(1,3-Benzodioxol-5-yl)propan-2-yl]-6-methoxy-4-prop-2-enylphenol	C20H22O4		LibSearch	27.987	-16.296		1235092-34-8	43.25		
[1,2,4]Triazole-3-thione, 5-amino-2-phenyl-2,4-dihydro-	C8H8N4S		LibSearch	27.987	-6.230		1010303-72-9	43.17		
Ethanediamide, N,N'-bis(1-phenylethyl)-	C18H20N2O2		LibSearch	27.987	-15.946		70864-05-0	42.95		

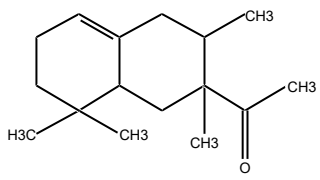
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
4-(4-Methyl-1-piperazinyl)aniline	C11H17N3		LibSearch	27.987	-2.530		16153-81-4	42.91		
Dithiocarbaminic acid, N-cyano-, S-[3-(4-ethylphenyl)-3-oxo-1-propenyl]-S'-methyl diester	C14H14N2OS2		LibSearch	27.987	-15.130		274691-67-7	42.82		

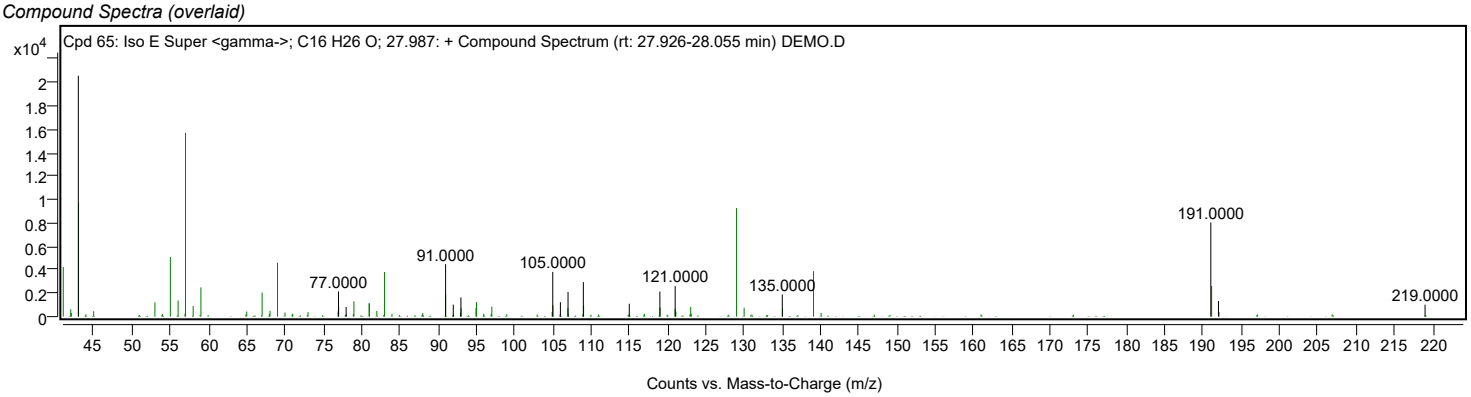
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



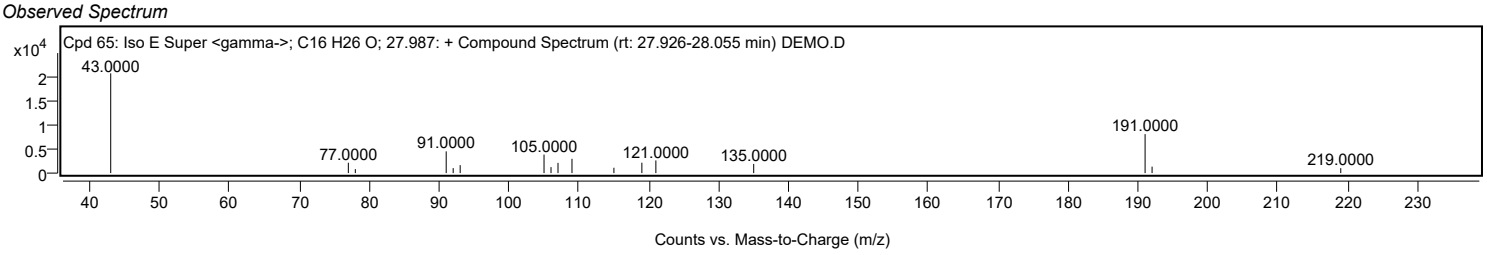
Iso E Super <gamma->

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			61.90			PWNose.xml

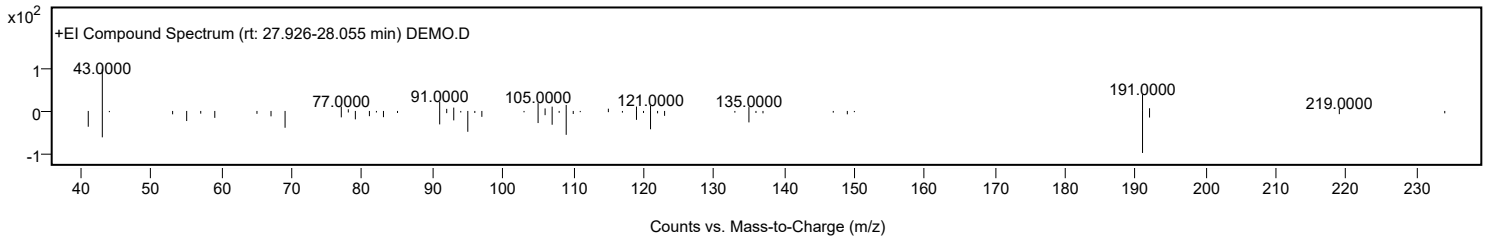
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			61.90			PWNose.xml

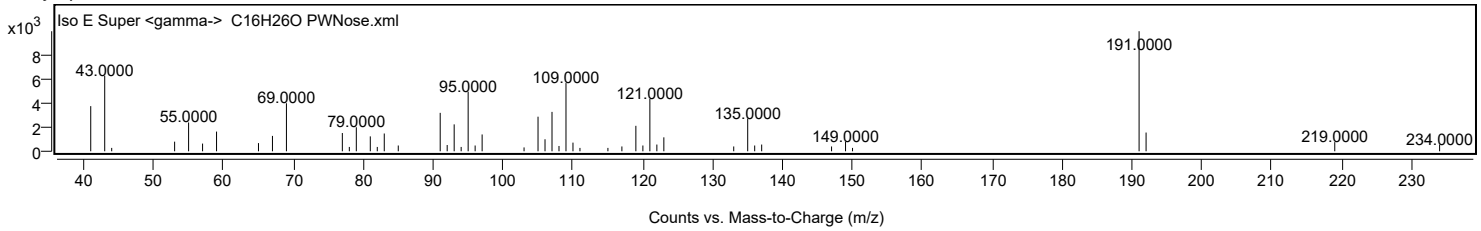
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 66: 1-Octen-4-ol acetate

Compound Discovery Report

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Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
1-Octen-4-ol acetate	C10 H18 O2	28.032			150666-71-0	LibSearch	43.32	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		43.32			50		

Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
1-Octen-4-ol acetate	C10H18O2		LibSearch	28.032	9.549		150666-71-0	43.32		
2-(1-Phenylethyl)-6-isopropyl-1,3-dioxane	C15H22O2		LibSearch	28.032	0.316		1000431-40-0	39.83		
Benzene, [1-methyl-1-(pentyloxy)ethyl]-	C14H22O		LibSearch	28.032	3.349		54932-79-5	39.51		
2-Isopropyl-5-methylcyclohexyl 3-(1-(4-chlorophenyl)-3-oxobutyl)-coumarin-4-yl carbonate	C30H33ClO6		LibSearch	28.032	-37.568		1000143-59-5	39.46		
3-Isopropyl-4-methyl-dec-1-en-4-ol	C14H28O		LibSearch	28.032	5.266		1000194-91-8	38.80		
4-Hepten-2-one, (E)-	C7H12O		LibSearch	28.032	13.682		36678-43-0	38.64		
4-Heptanol, 2,6-dimethyl-, acetate	C11H22O2		LibSearch	28.032	9.866		10250-45-0	38.60		
Propanedioic acid, dipropyl ester	C9H16O4		LibSearch	28.032	7.199		1117-19-7	38.45		
Benzoyl chloride, 4-(pentyloxy)-	C12H15ClO2		LibSearch	28.032	-0.184		36823-84-4	37.91		
Cyclohexanecarboxylic acid, 8-chlorooctyl ester	C15H27ClO2		LibSearch	28.032	-4.768		1000354-65-2	37.73		
2-Hydroxyisocaproic acid, acetate	C8H14O4		LibSearch	28.032	7.832		1000374-89-3	37.62		
Iso E Super <gamma->	C16H26O		LibSearch	28.032			68155-67-9	37.51		
4,8-Dimethyl-4-hydroxy-1-nonene	C11H22O		LibSearch	28.032	9.166		1000432-13-0	37.40		
Paramethadione	C7H11NO3		LibSearch	28.032	5.032		115-67-3	37.34		
Alicate	C11H22O2		LibSearch	28.032			10250-45-0	37.20		
1,3-Dioxane, 5-ethyl-2,2-dimethyl-	C8H16O2		LibSearch	28.032	11.482		25796-26-3	37.20		
5-Nonanol, acetate	C11H22O2		LibSearch	28.032	7.732		3857-24-7	37.16		
Paramethadione	C7H11NO3		LibSearch	28.032	5.032		115-67-3	37.04		
Anthracene, 9-dodecyltetradecahydro-	C26H48		LibSearch	28.032	-15.934		55401-75-7	36.92		
5,5-Dimethyltetrahydrofuran-3-carboxylic acid	C7H12O3		LibSearch	28.032	9.016		1000461-01-8	36.75		
2,5-Dimethyl-3-hexanol acetate	C10H20O2		LibSearch	28.032	11.532		91008-85-4	36.69		
Benzenemethanol, .alpha.-methyl-.alpha.-(1-methyl-2-propenyl)-	C12H16O		LibSearch	28.032	6.232		61967-11-1	36.61		
Pinocamphone<cis->	C10H16O		LibSearch	28.032	13.462		15358-88-0	36.02		
Amberonne (isomer 3)	C16H26O		LibSearch	28.032	-0.401		1000470-69-9	36.02		
Propyl pyruvate	C6H10O3		LibSearch	28.032	12.682		1000431-41-8	35.97		
1-(1-Hydroxy-1-phenyl-ethyl)-cyclopropanecarboxylic acid, t-butyl ester	C16H22O3		LibSearch	28.032	-2.618		108547-01-9	35.90		
Pyrrolidin-5-one, 2,3-dedihydro-3-nitro-	C4H3NO4		LibSearch	28.032	8.382		1000124-44-1	35.82		
Isonitrosoacetylacetone	C5H7NO3		LibSearch	28.032	9.316		29917-12-2	35.64		
1-Undecyn-4-ol	C11H20O		LibSearch	28.032	6.782		22127-86-2	35.54		
Propane, 1-acetoxy-2-isocyano-	C6H9NO2		LibSearch	28.032			109862-24-0	35.19		
2-Methyl-3-decanol	C11H24O		LibSearch	28.032	7.816		83909-79-9	35.11		
1H-Indene, 2,3,3a,4,7,7a-hexahydro-2,2,4,4,7,7-hexamethyl-, trans-	C15H26		LibSearch	28.032	5.249		54832-81-4	35.04		
2-Methyl-2-heptanol acetate	C10H20O2		LibSearch	28.032	9.732		45021-46-3	35.00		
Allylacetone	C6H10O		LibSearch	28.032			109-49-9	34.84		
2-Heptenoic acid, hexyl ester	C13H24O2		LibSearch	28.032	3.216		1000406-09-2	34.70		
3,7-Dimethyl-1,2,3-octanetriol	C10H22O3		LibSearch	28.032	3.899		1000432-16-7	34.66		
2-Hexanone, 5-methyl-5-nitro-	C7H13NO3		LibSearch	28.032	8.866		4604-49-3	34.62		
4-Penten-2-one, 4-methyl-	C6H10O		LibSearch	28.032	16.016		3744-02-3	34.60		
2-Hexanone, 3-methyl-4-methylene-	C8H14O		LibSearch	28.032	13.766		20690-71-5	34.49		
Hexanenitrile, 5-methyl-	C7H13N		LibSearch	28.032	13.066		19424-34-1	34.44		
Benzenemethanol, .alpha.-methyl-.alpha.-(1-methyl-2-propenyl)-	C12H16O		LibSearch	28.032	6.232		61967-11-1	34.38		
5-Fluoro-2-trifluoromethylbenzoic acid, 5-tridecyl ester	C21H30F4O2		LibSearch	28.032	-7.151		1000338-55-1	34.38		
1-Propanesulfonyl chloride	C3H7ClO2S		LibSearch	28.032	11.332		10147-36-1	34.21		
Linalool<tetrahydro->	C10H22O		LibSearch	28.032	16.602		78-69-3	34.20		
5-Fluoro-2-trifluoromethylbenzoic acid, 5-tetradecyl ester	C22H32F4O2		LibSearch	28.032	-8.818		1000338-55-7	34.19		
Undecan-4-ol	C11H24O		LibSearch	28.032			4272-06-4	34.11		
1,4-Benzenediol, 2-[(1,4,4a,5,6,7,8,8a-octahydro-2,5,5,8a-tetramethyl-1-naphthalenyl)methyl]-, [1R-(1.alpha.,4a.beta.,8a.alpha.)]-	C21H30O2		LibSearch	28.032	-14.568		39707-55-6	34.08		
3-Amino-1-pyridin-3-yl-pyrrolidine-2,5-dione	C9H9N3O2		LibSearch	28.032	-3.034		1000285-96-4	34.00		
5,9-methanobenzocyclooctene-5(1H)-ol, 2,3,4,6,7,8,9,10-octahydro-2,2,8,8,9-pentamethyl-	C18H30O		LibSearch	28.032	-3.551		1000396-83-9	33.99		
Undecan-4-ol	C11H24O		LibSearch	28.032	8.432		4272-06-4	33.97		

Compound Discovery Report

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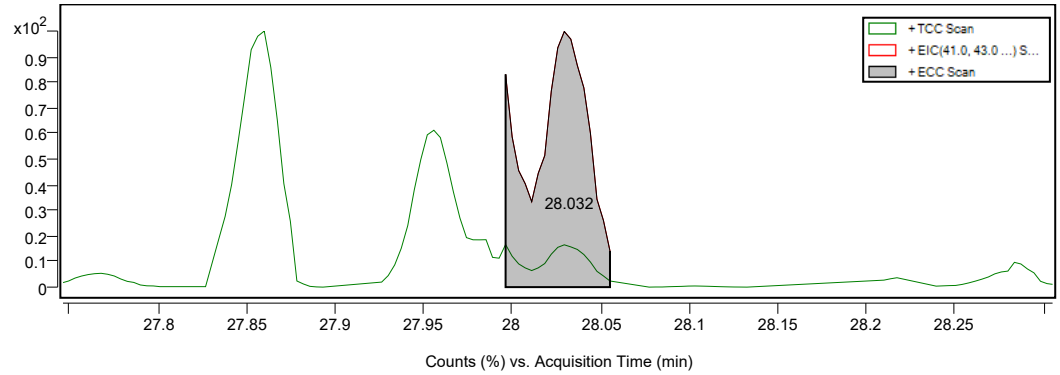
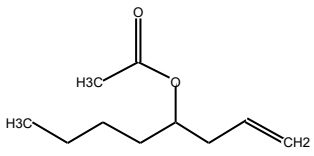
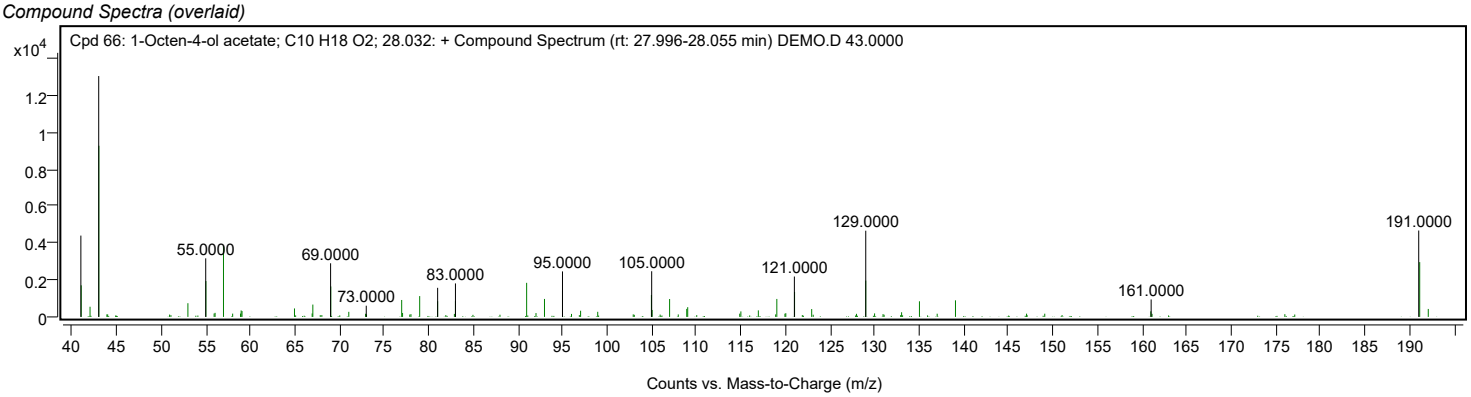
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



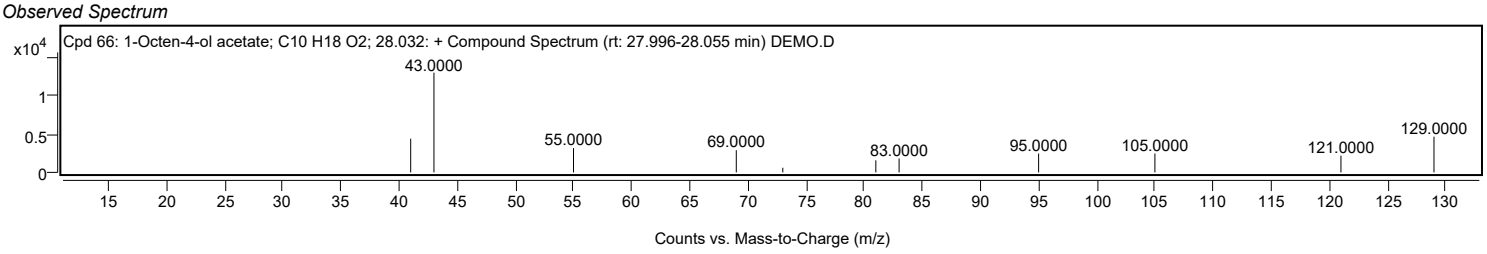
1-Octen-4-ol acetate

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			43.32			NIST.L

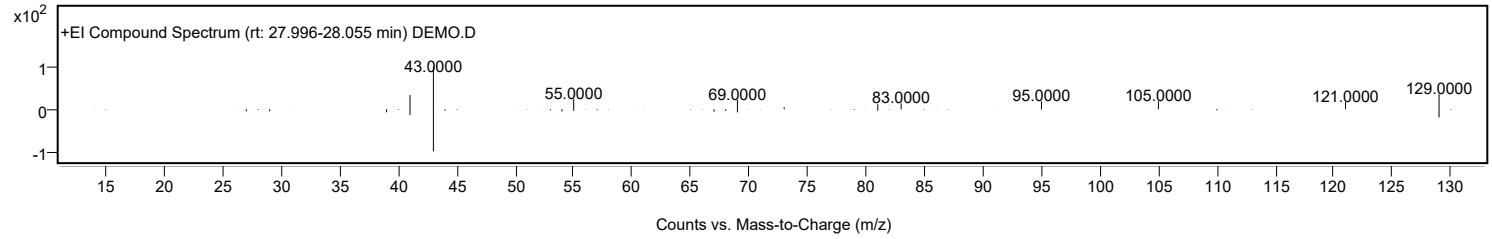
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			43.32			NIST.L

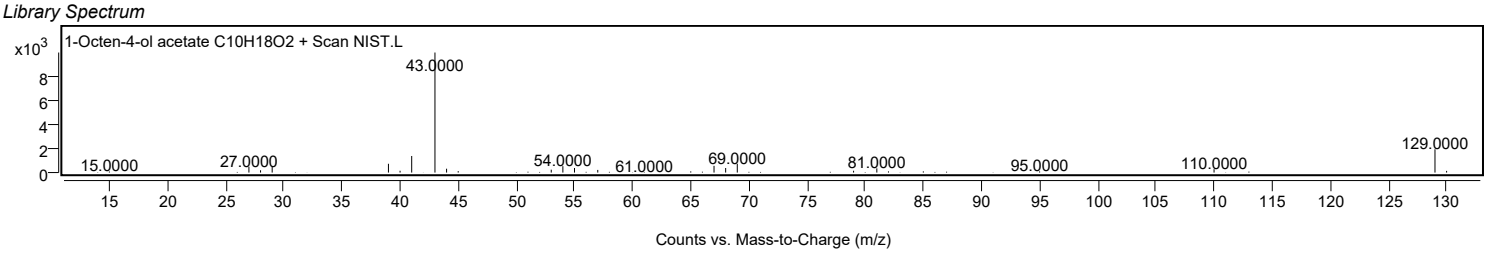
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 67: Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	C16 H24 O3	28.103			2511-22-0	LibSearch	47.18	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		47.18			11		

Compound Discovery Report

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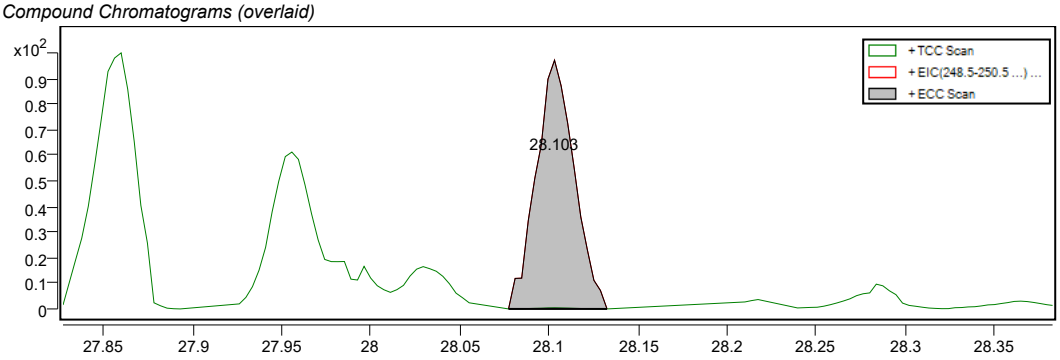
Compound ID Table

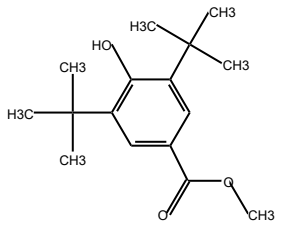
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	C16H24O3		LibSearch	28.103	-4.147		2511-22-0	47.18		
5'-Fluoro-2'-iodoacetophenone	C8H6FIO		LibSearch	28.103	4.636		914225-70-0	45.79		
4-{1-[4-(Cyanooxy)phenyl]ethyl}phenyl cyanate	C16H12N2O2		LibSearch	28.103	-11.414		47073-92-7	40.12		
2-(4-Isopropylphenyl)-4H-chromen-4-one	C18H16O2		LibSearch	28.103	-8.897		92831-11-3	39.99		
2,7-Diacetyl-9-fluorenone	C17H12O3		LibSearch	28.103	-11.264		39665-89-9	38.56		
3-Methoxy-4-pyrrolidinoaniline, TMS	C14H24N2OSi		LibSearch	28.103	-3.497		1000499-47-5	34.55		
Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester	C16H24O3		LibSearch	28.103	-4.147		2511-22-0	34.41		
2,7-Diacetyl-9-fluorenone	C17H12O3		LibSearch	28.103	-11.264		39665-89-9	32.82		
9,10-Anthracenedione, 2-(1,1-dimethylethyl)-	C18H16O2		LibSearch	28.103	-9.947		84-47-9	32.10		
4-Amino-8-chloro-2-methylquinoline, TMS derivative	C13H17ClN2Si		LibSearch	28.103	-4.214		1000484-37-9	30.64		
2(1H)-Pyrazinone, 3,5,6-tris(1,1-dimethylethyl)-	C16H28N2O		LibSearch	28.103	-1.814		39950-99-7	28.13		

Compound Chromatograms (overlaid)

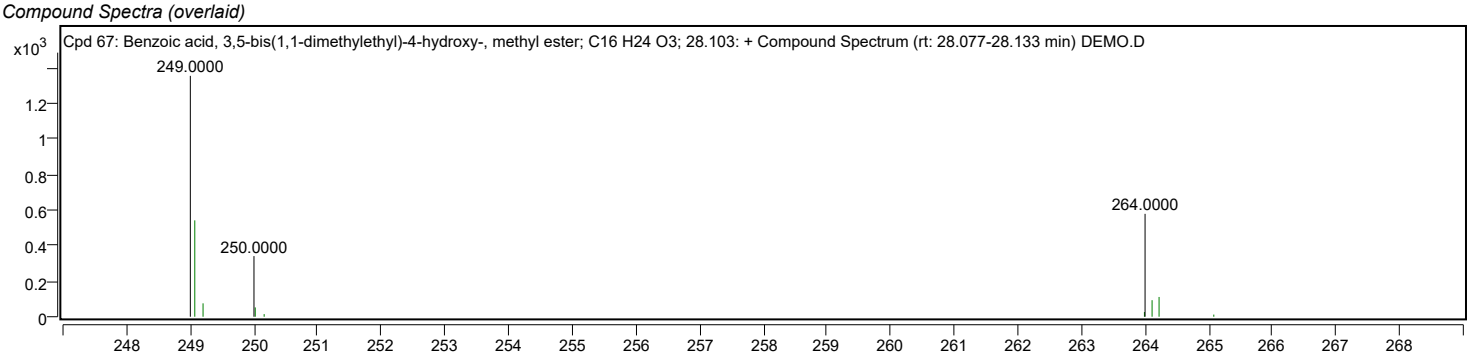


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



Counts vs. Mass-to-Charge (m/z)

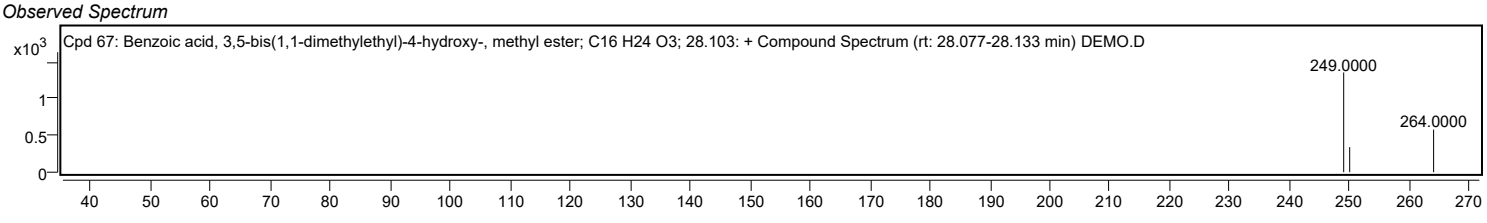
Benzoic acid, 3,5-bis(1,1-dimethylethyl)-4-hydroxy-, methyl ester

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			47.18			NIST.L

Library Match Details

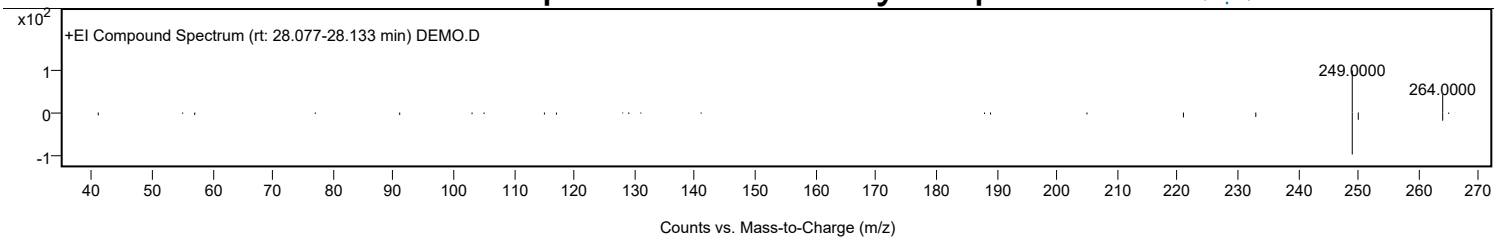
m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			47.18			NIST.L

Observed Spectrum

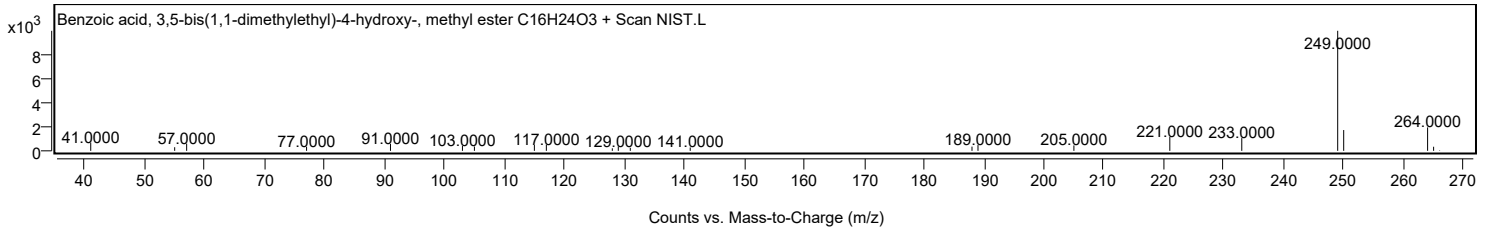


Counts vs. Mass-to-Charge (m/z)

Mirror Plot



Library Spectrum



Cpd. 68: Tiglate <(3Z)-hexenyl->

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Tiglate <(3Z)-hexenyl->	C11 H18 O2	28.217			67883-79-8	LibSearch	54.59	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		54.59			50		

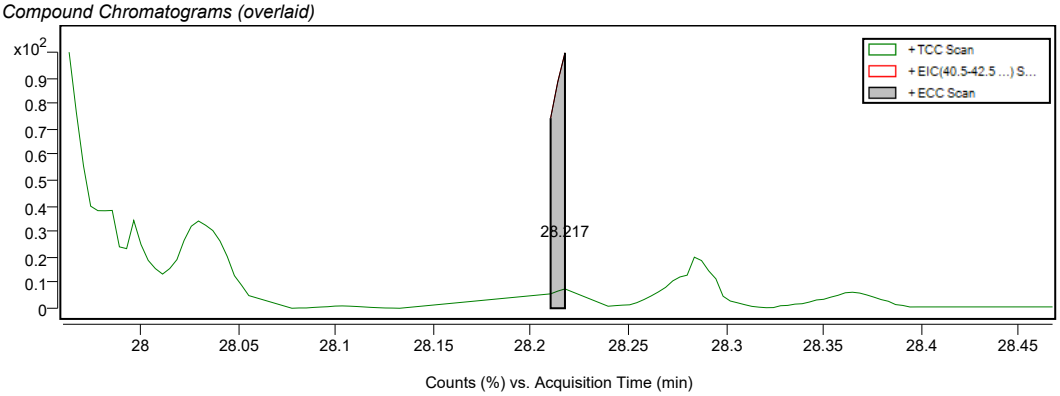
Compound Discovery Report

Agilent | Trusted Answers

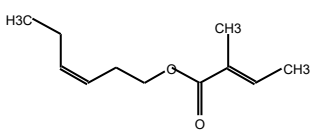
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Tiglate <(3Z)-hexenyl->	C11H18O2		LibSearch	28.217			67883-79-8	54.59		
(Z)-(Z)-Hex-3-en-1-yl 2-methylbut-2-enoate	C11H18O2		LibSearch	28.217	6.967		84060-80-0	53.89		
1(2H)-Pyrazineacetonitrile, 5-amino-3,6-dihydro-3-imino-	C6H9N5		LibSearch	28.217	5.051		35975-34-9	53.86		
Hexenyl angelate<3Z->	C11H18O2		LibSearch	28.217	9.117		84060-80-0	53.77		
Oxalic acid, dicyclohexyl ester	C14H22O4		LibSearch	28.217	-3.016		1000309-30-9	53.71		
Hexenyl tiglate<3E->	C11H18O2		LibSearch	28.217	7.337		120603-00-1	53.48		
Hexenyl tiglate<3Z->	C11H18O2		LibSearch	28.217	7.147		67883-79-8	53.48		
Hexenyl tiglate <(3E)->	C11H18O2		LibSearch	28.217			120603-00-1	53.31		
Oxalic acid, cyclohexyl butyl ester	C12H20O4		LibSearch	28.217	1.351		1000309-30-5	53.08		
(E)-Hex-3-enyl (E)-2-methylbut-2-enoate	C11H18O2		LibSearch	28.217	6.967		120603-00-1	52.82		
(Z)-Hex-3-enyl (E)-2-methylbut-2-enoate	C11H18O2		LibSearch	28.217	6.967		67883-79-8	52.81		
Oxalic acid, cyclohexyl propyl ester	C11H18O4		LibSearch	28.217	3.001		1000309-30-3	52.69		
Hexenyl angelate <(3Z)->	C11H18O2		LibSearch	28.217			84060-80-0	52.65		
Oxalic acid, cyclohexyl ethyl ester	C10H16O4		LibSearch	28.217	4.667		1000309-30-2	52.60		
2-Butyl-1,2-azaborolidine	C7H16BN		LibSearch	28.217			5357-10-8	52.36		
Hexenyl tiglate, (4Z)-	C11H18O2		LibSearch	28.217			999003-42-2	52.28		
(Z)-Hex-3-enyl (E)-2-methylbut-2-enoate	C11H18O2		LibSearch	28.217	6.967		67883-79-8	52.19		
Hexenyl tiglate, 4Z-	C11H18O2		LibSearch	28.217	6.967		1000383-63-6	51.60		
Oxalic acid, cyclohexyl pentyl ester	C13H22O4		LibSearch	28.217	-0.316		1000309-30-6	51.16		
Hexenyl angelate, 4z-	C11H18O2		LibSearch	28.217	6.967		1000383-63-7	50.61		
3-Methyl-2-butenoic acid, tridec-2-ynyl ester	C18H30O2		LibSearch	28.217	-4.783		1000299-31-7	50.10		
Carbonic acid, 3-hexenyl methyl ester, (Z)-	C8H14O3		LibSearch	28.217	10.417		67633-96-9	50.08		
Cyclohexane, 2-propenyl-	C9H16		LibSearch	28.217	12.067		2114-42-3	50.06		
Cyclohexane, (1-methylethyl)-	C9H18		LibSearch	28.217	12.967		696-29-7	49.81		
Cyclohexane, bromo-	C6H11Br		LibSearch	28.217	11.934		108-85-0	49.80		
Hexanal 2E-hexenyl 3Z-hexenyl acetal	C18H34O2		LibSearch	28.217	-3.683		1000431-43-4	49.67		
Cyclohexane, bromo-	C6H11Br		LibSearch	28.217	11.934		108-85-0	49.62		
Oxalic acid, cyclohexyl isobutyl ester	C12H20O4		LibSearch	28.217	2.417		1000309-30-4	49.57		
Isocitronellol	C10H20O		LibSearch	28.217	10.317		18479-52-2	49.53		
Hexenyl methyl carbonate<3Z->	C8H14O3		LibSearch	28.217	17.107		67633-96-9	49.52		
Vinylcyclohexyl ether	C8H14O		LibSearch	28.217	12.451		2182-55-0	49.15		
Cyclohexane, bromo-	C6H11Br		LibSearch	28.217	11.934		108-85-0	48.98		
Carbonic acid <3-hexenyl-, methyl-> ester	C8H14O3		LibSearch	28.217			67633-96-9	48.88		
Cyclopentane, 1-methyl-2-(2-propenyl)-, trans-	C9H16		LibSearch	28.217	13.034		50746-53-7	48.84		
Cyclohexane, 2-propenyl-	C9H16		LibSearch	28.217	12.067		2114-42-3	48.75		
Acetaldehyde 2E-hexenyl 3Z-hexenyl acetal	C14H26O2		LibSearch	28.217	2.934		1000431-45-5	48.70		
Cyclohexane, (1-methylethyl)-	C9H18		LibSearch	28.217	12.967		696-29-7	48.66		
Cyclohexane, octyl-	C14H28		LibSearch	28.217	3.617		1795-15-9	48.52		
Succinic acid, di(trans-hex-3-enyl) ester	C16H26O4		LibSearch	28.217	-4.483		1000353-43-7	48.51		
Oxalic acid, cyclohexyl hexyl ester	C14H24O4		LibSearch	28.217	-1.966		1000309-30-8	48.48		
Oxalic acid, cyclohexyl octyl ester	C16H28O4		LibSearch	28.217	-5.283		1000309-31-0	48.48		
1,5-Heptadien-4-one, 3,3,6-trimethyl-	C10H16O		LibSearch	28.217	10.851		546-49-6	48.39		
Cyclohexane, (1-methylethyl)-	C9H18		LibSearch	28.217	12.967		696-29-7	48.19		
Oxalic acid, cyclohexyl isohexyl ester	C14H24O4		LibSearch	28.217	-0.899		1010309-30-7	48.11		
Methoxyacetic acid, cyclohexyl ester	C9H16O3		LibSearch	28.217	7.834		1000282-69-4	47.84		
1,5-Heptadien-4-one, 3,3,6-trimethyl-	C10H16O		LibSearch	28.217	10.851		546-49-6	47.80		
(E)-Hex-3-enyl isobutyl carbonate	C11H20O3		LibSearch	28.217	6.517		1000372-74-9	47.80		
2-Hexene, 4,4,5-trimethyl-	C9H18		LibSearch	28.217	15.301		55702-61-9	47.66		
Cyclopropane, 2-bromo-1,1,3-trimethyl-	C6H11Br		LibSearch	28.217	14.667		36617-00-2	47.62		
2-Heptene, 5-ethyl-2,4-dimethyl-	C11H22		LibSearch	28.217	12.017		74421-06-0	47.59		

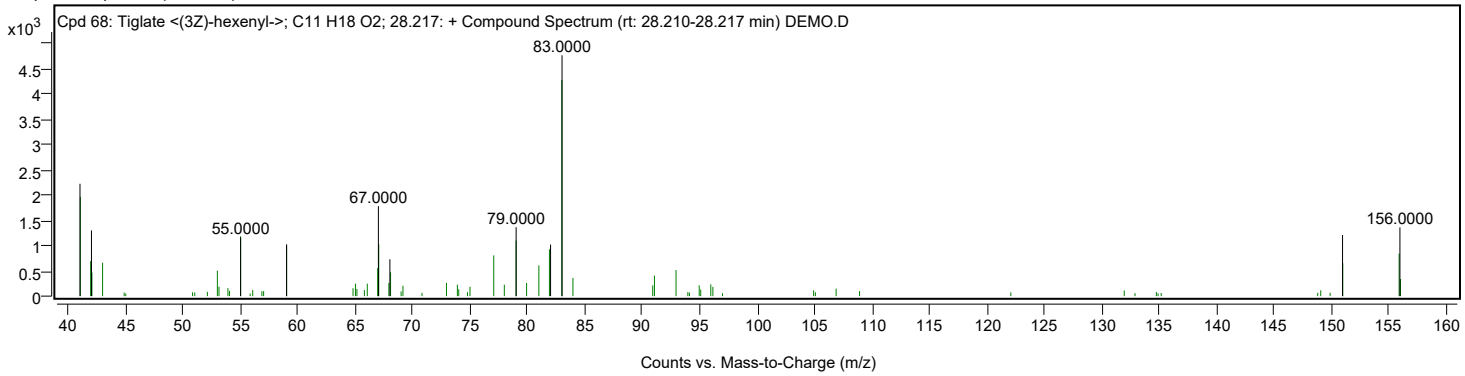
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



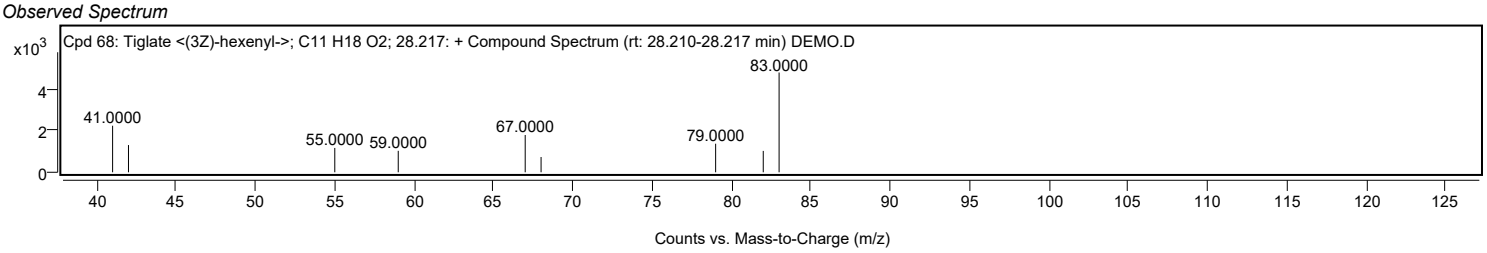
Tiglate <(3Z)-hexenyl->

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			54.59			PWNose.xml

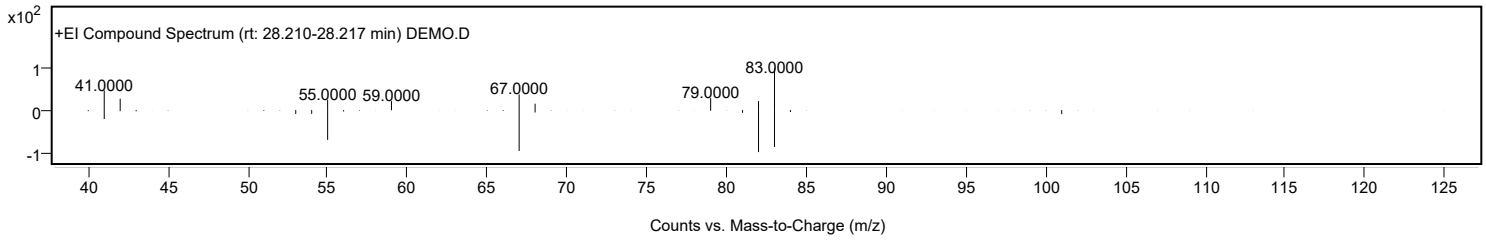
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			54.59			PWNose.xml

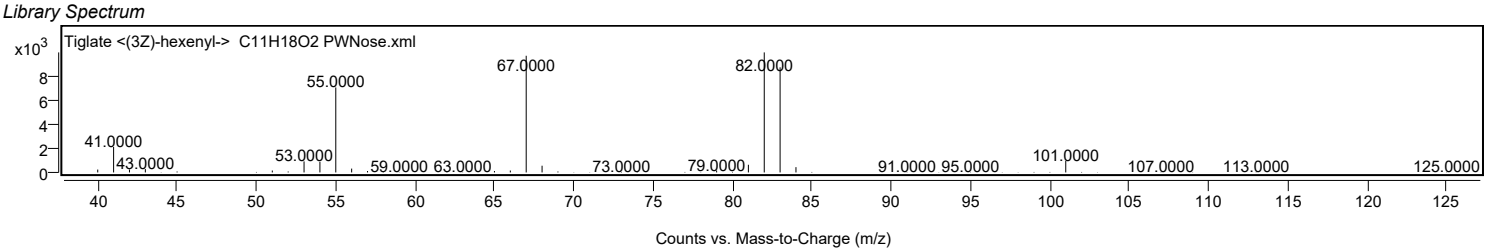
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 69: 1-Oxaspiro[2.5]oct-5-ene, 8,8-dimethyl-4-methylene-

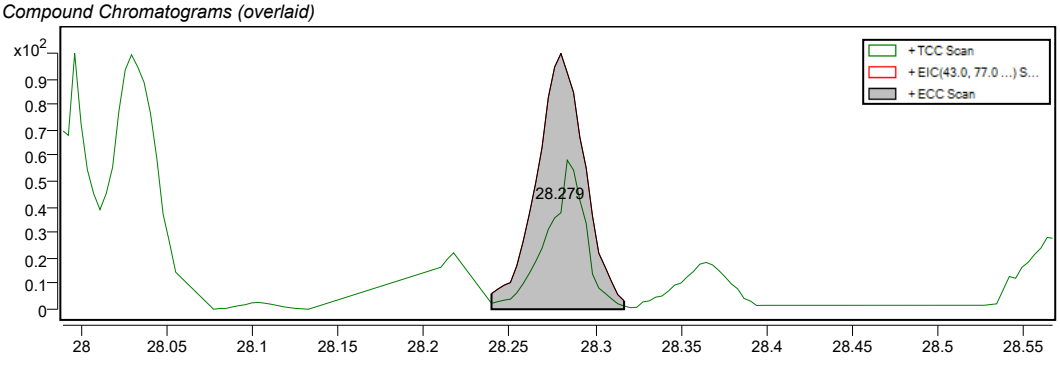
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
1-Oxaspiro[2.5]oct-5-ene, 8,8-dimethyl-4-methylene-	C10 H14 O	28.279			54345-60-7	LibSearch	69.34	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		69.34			50		

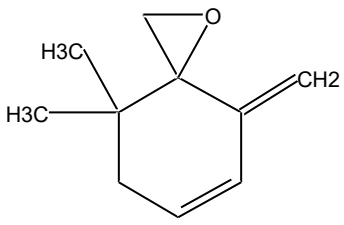
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
1-Oxaspiro[2.5]oct-5-ene, 8,8-dimethyl-4-methylene-	C10H14O		LibSearch	28.279	10.846		54345-60-7	69.34		
1,3-Cyclopentadiene, 1,3-bis(1-methylethyl)-	C11H18		LibSearch	28.279	11.413		123278-27-3	61.38		
1,3-Cyclohexadiene-1-carboxaldehyde, 2,6,6-trimethyl-	C10H14O		LibSearch	28.279	8.513		116-26-7	60.29		
Terpinen-7-al <alpha->	C10H14O		LibSearch	28.279			1197-15-5	59.33		
Ethanone,1-(2-furanylcyclopropyl)-	C9H10O2		LibSearch	28.279	9.279		1000139-62-1	57.90		
Terpinen-7-al<alpha->	C10H14O		LibSearch	28.279	8.819		1197-15-5	57.75		
Cyclohexene, 2-ethenyl-1,3,3-trimethyl-	C11H18		LibSearch	28.279	9.863		5293-90-3	57.59		
4-Hydroxy-2-methylacetophenone	C9H10O2		LibSearch	28.279	5.563		875-59-2	56.20		
3-Nonen-5-yne, 4-ethyl-	C11H18		LibSearch	28.279	9.663		74685-67-9	56.02		
Benzenemethanol, .alpha.,.alpha.,4-trimethyl-	C10H14O		LibSearch	28.279	8.329		1197-01-9	56.02		
3-Nonen-5-yne, 4-ethyl-, (Z)-	C11H18		LibSearch	28.279	9.663		74744-26-6	56.00		
Ethanone, 1-(6,6-dimethylbicyclo[3.1.0]hex-2-en-2-yl)-	C10H14O		LibSearch	28.279	10.563		24555-40-6	55.86		
4-Hydroxy-2-methylacetophenone	C9H10O2		LibSearch	28.279	5.563		875-59-2	55.73		
3-Penten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	C14H22O		LibSearch	28.279	3.179		114933-28-7	55.60		
2-tert-Butylphenol, O-isopropyloxycarbonyl-	C14H20O3		LibSearch	28.279	1.646		1000487-38-4	55.52		
4-Isopropylcyclohexa-1,3-dienecarbaldehyde	C10H14O		LibSearch	28.279	8.513		1197-15-5	55.50		
3-Nonen-5-yne, 4-ethyl-, (E)-	C11H18		LibSearch	28.279	9.663		74744-60-8	55.43		
4-Hydroxy-3-methylacetophenone	C9H10O2		LibSearch	28.279	5.563		876-02-8	55.35		
Carvacrol	C10H14O		LibSearch	28.279			499-75-2	55.00		
1-(4-Hydroxymethylphenyl)ethanone	C9H10O2		LibSearch	28.279	5.196		75633-63-5	54.88		
4-Hydroxy-2-methylacetophenone	C9H10O2		LibSearch	28.279	5.563		875-59-2	54.86		
Cyclopent-2-enone <5-methylene-2,3,4,4-tetramethyl->	C10H14O		LibSearch	28.279			864685-64-3	54.84		
3-tert-Butylphenol, acetate	C12H16O2		LibSearch	28.279	5.163		13189-51-0	54.61		
1,3-Cyclohexadiene-1-carboxaldehyde, 2,6,6-trimethyl-	C10H14O		LibSearch	28.279	8.513		116-26-7	54.57		
4-Acetoxy-3-methoxystyrene	C11H12O3		LibSearch	28.279	4.079		46316-15-8	54.52		
4-Hydroxy-3-methylacetophenone	C9H10O2		LibSearch	28.279	5.563		876-02-8	54.48		
Phenol, 2-methyl-5-(1-methylethyl)-, acetate	C12H16O2		LibSearch	28.279	4.596		6380-28-5	54.41		
Safranal	C10H14O		LibSearch	28.279			116-26-7	54.33		
3-tert-Butylphenol, O-isopropyloxycarbonyl-	C14H20O3		LibSearch	28.279	1.646		1000487-38-3	53.80		
2-tert-Butylphenol, acetate	C12H16O2		LibSearch	28.279	5.163		3245-25-8	53.70		
4-tert-Butylphenyl acetate	C12H16O2		LibSearch	28.279	5.163		3056-64-2	53.70		
Phenol, 3,5-diethyl-	C10H14O		LibSearch	28.279	6.179		1197-34-8	53.69		
4-tert-Butylphenyl acetate	C12H16O2		LibSearch	28.279	5.163		3056-64-2	53.55		
Cyclopent-2-enone<5-methylene-2,3,4,4-tetrame	C10H14O		LibSearch	28.279	13.209		0-00-0	53.39		
Phenol, m-tert-butyl-	C10H14O		LibSearch	28.279	7.813		585-34-2	53.36		
4-tert-Butylphenol, O-isopropyloxycarbonyl-	C14H20O3		LibSearch	28.279	1.646		1201410-82-3	53.35		
Phenol <4-tert-butyl->	C10H14O		LibSearch	28.279			98-54-4	53.29		
2-Caren-10-al	C10H14O		LibSearch	28.279	9.346		1000151-85-9	53.27		
Carvacrol acetate	C12H16O2		LibSearch	28.279	4.959		6380-28-5	53.15		
2,5-Cyclohexadiene, 1,4-diethyl-1,4-dimethyl-	C12H20		LibSearch	28.279	9.079		1000150-21-6	53.06		
Benzene, (1-ethoxyethyl)-	C10H14O		LibSearch	28.279	9.879		3299-05-6	53.00		
Ethanone, 1-(2-hydroxy-5-methylphenyl)-	C9H10O2		LibSearch	28.279	5.563		1450-72-2	52.96		
3-Methyl-2-(2-methyl-2-butenyl)-furan	C10H14O		LibSearch	28.279	9.696		15186-51-3	52.91		
Phenol, m-tert-butyl-	C10H14O		LibSearch	28.279	7.813		585-34-2	52.77		
Ethyltetramethylcyclopentadiene	C11H18		LibSearch	28.279	10.246		57693-77-3	52.74		
Phenol, 5-methyl-2-(1-methylethyl)-, acetate	C12H16O2		LibSearch	28.279	4.596		528-79-0	52.70		
Phenol, 5-methyl-2-(1-methylethyl)-, acetate	C12H16O2		LibSearch	28.279	4.596		528-79-0	52.67		
2-tert-Butylphenol, O-(n-propyloxycarbonyl)-	C14H20O3		LibSearch	28.279	0.579		1000487-37-9	52.61		
Cymen-7-ol <ortho->	C10H14O		LibSearch	28.279			21190-34-1	52.59		
4-t-Butylphenyl-.beta.-phenylpropionate	C19H22O2		LibSearch	28.279	-7.721		23522-70-5	52.46		

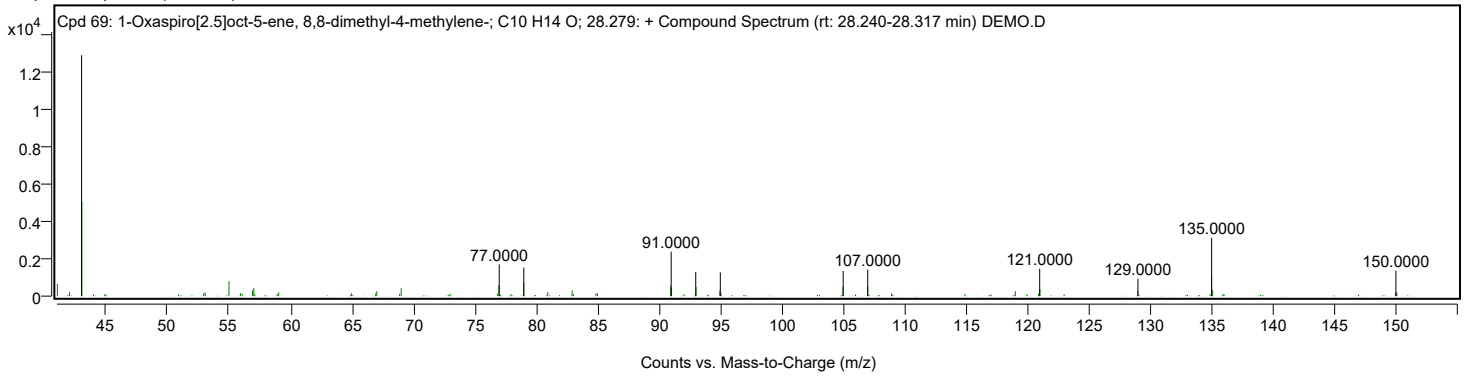
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



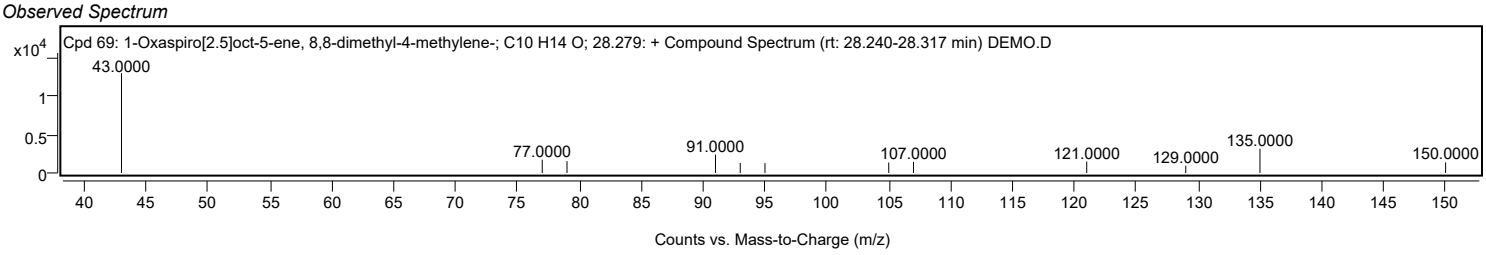
1-Oxaspiro[2.5]oct-5-ene, 8,8-dimethyl-4-methylene-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			69.34			NIST.L

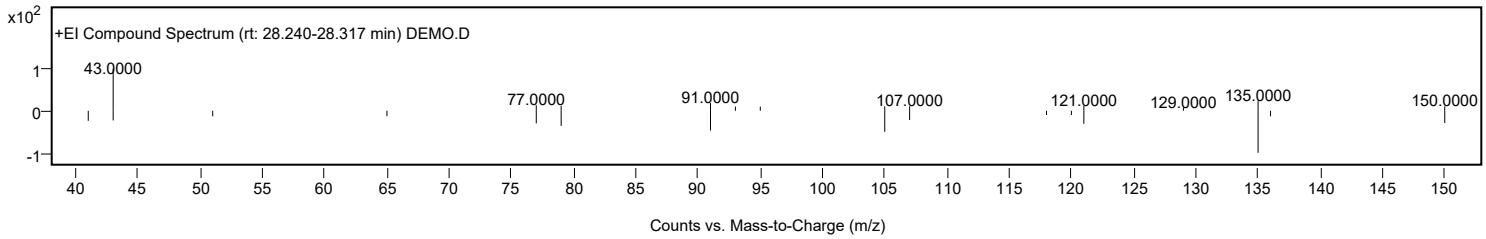
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			69.34			NIST.L

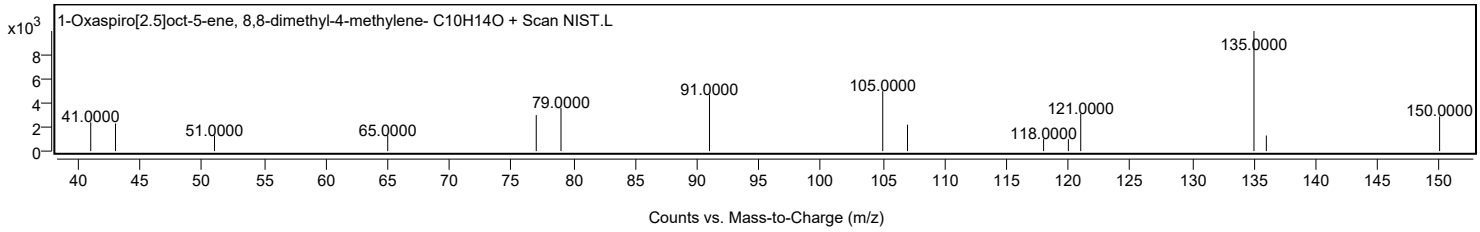
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 70: Iron, acetyldicarbonyl[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadienyl]-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Iron, acetyldicarbonyl[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadienyl]-	C14 H18 Fe O3	28.286			1000146-24-2	LibSearch	59.62	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		59.62			50		

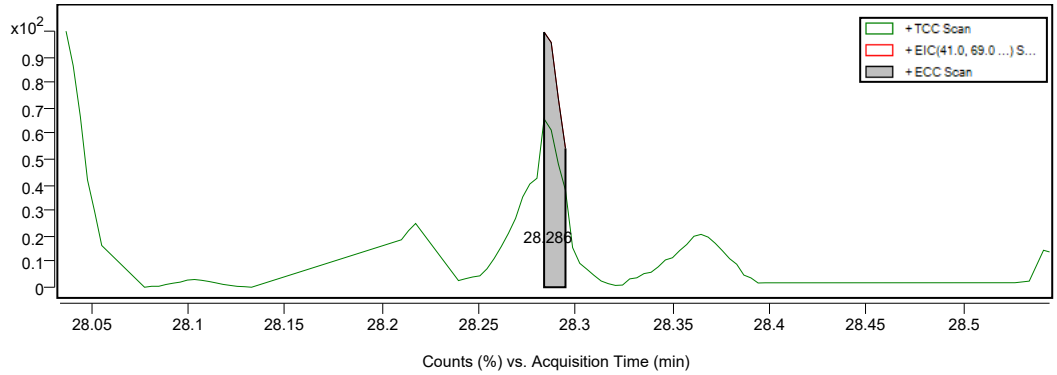
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

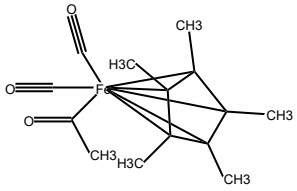
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Iron, acetyldicarbonyl[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadienyl]-	C14H18FeO3		LibSearch	28.286			1000146-24-2	59.62		
Benzamide, 2-methoxy-N-allyl-	C11H13NO2		LibSearch	28.286	0.436		1010339-10-5	52.96		
4-n-Butoxyphenyl isocyanate	C11H13NOS		LibSearch	28.286			1000342-44-4	51.51		
Iso E Super <alpha->	C16H26O		LibSearch	28.286			68155-66-8	51.38		
1,4,5,6-Tetrahydrocyclopentapyrazole-3-carboxylic acid, (1-adamantan-1-ylethylidene)hydrazide	C19H26N4O		LibSearch	28.286	-19.448		1000265-46-6	50.97		
4'-Butoxy-2'-methylacetophenone	C13H18O2		LibSearch	28.286	1.119		1000195-98-2	50.51		
4-Hydroxy-2-methylacetophenone	C9H10O2		LibSearch	28.286	5.569		875-59-2	49.61		
3-Penten-2-one, 4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-	C14H22O		LibSearch	28.286	3.186		114933-28-7	49.52		
4-Hydroxy-2-methylacetophenone	C9H10O2		LibSearch	28.286	5.569		875-59-2	49.32		
4-Hydroxy-2-methylacetophenone	C9H10O2		LibSearch	28.286	5.569		875-59-2	49.30		
4-Hydroxy-3-methylacetophenone	C9H10O2		LibSearch	28.286	5.569		876-02-8	49.17		
4-Hydroxy-3-methylacetophenone	C9H10O2		LibSearch	28.286	5.569		876-02-8	49.15		
Ethanone,1-(2-furanylcyclopropyl)-	C9H10O2		LibSearch	28.286	9.286		1000139-62-1	48.98		
Oxirane, [[4-(1,1-dimethylethyl)phenoxy]methyl]-	C13H18O2		LibSearch	28.286	3.519		3101-60-8	48.72		
Ethanone, 1-(2-hydroxy-5-methylphenyl)-	C9H10O2		LibSearch	28.286	5.569		1450-72-2	48.29		
Benzoic acid, 4-methoxy-, diethylboryl ester	C12H17BO3		LibSearch	28.286			146681-61-0	48.24		
Guaiacol <4-vinyl->	C9H10O2		LibSearch	28.286			7786-61-0	47.92		
Phenol, 5-ethenyl-2-methoxy-	C9H10O2		LibSearch	28.286	6.736		621-58-9	47.81		
4-Hydroxy-3-methylacetophenone	C9H10O2		LibSearch	28.286	5.569		876-02-8	47.75		
p-Methoxyheptanophenone	C14H20O2		LibSearch	28.286	-0.298		69287-13-4	47.20		
4'-Methoxyvalerophenone	C12H16O2		LibSearch	28.286	3.019		1671-76-7	47.11		
p-Methoxyheptanophenone	C14H20O2		LibSearch	28.286	-0.298		69287-13-4	47.08		
Pentanoic acid, 5-hydroxy-, p-t-butylphenyl ester	C15H22O3		LibSearch	28.286	-3.848		166273-37-6	46.97		
Phenol, m-tert-butyl-	C10H14O		LibSearch	28.286	7.819		585-34-2	46.86		
Phenol, m-tert-butyl-	C10H14O		LibSearch	28.286	7.819		585-34-2	46.81		
4'-Methoxyvalerophenone	C12H16O2		LibSearch	28.286	3.019		1671-76-7	46.71		
Ethanone, 1-(2-hydroxy-5-methylphenyl)-	C9H10O2		LibSearch	28.286	5.569		1450-72-2	46.53		
4-Acetoxy-3-methoxystyrene	C11H12O3		LibSearch	28.286	4.086		46316-15-8	46.51		
Phenol, p-tert-butyl-	C10H14O		LibSearch	28.286	7.819		98-54-4	46.50		
4-(7-Methyloctyl)phenol	C15H24O		LibSearch	28.286	-0.798		24518-48-7	46.49		
Phenol, 3,5-diethyl-	C10H14O		LibSearch	28.286	6.186		1197-34-8	46.48		
Cyclopent-2-enone <5-methylene-2,3,4,4-tetramethyl->	C10H14O		LibSearch	28.286			864685-64-3	46.46		
Phenol, p-tert-butyl-	C10H14O		LibSearch	28.286	7.819		98-54-4	46.41		
Benzamide, 3-methoxy-N-allyl-	C11H13NO2		LibSearch	28.286	0.436		331989-39-0	46.27		
1-Pentanone, 1-(p-anisyl)-3-methyl-	C13H18O2		LibSearch	28.286	2.419		66333-82-2	46.22		
Phenol, m-tert-butyl-	C10H14O		LibSearch	28.286	7.819		585-34-2	46.21		
1-(4-Hydroxymethylphenyl)ethanone	C9H10O2		LibSearch	28.286	5.202		75633-63-5	46.17		
Ethyl 3-(4-methoxybenzoyl)propionate	C13H16O4		LibSearch	28.286	-1.431		15118-67-9	46.00		
Phenol <4-tert-butyl->	C10H14O		LibSearch	28.286			98-54-4	45.94		
3-Methoxyacetophenone	C9H10O2		LibSearch	28.286	7.986		586-37-8	45.92		
Oxirane, [[4-(1,1-dimethylethyl)phenoxy]methyl]-	C13H18O2		LibSearch	28.286	3.519		3101-60-8	45.91		
1-Oxaspiro[2.5]oct-5-ene, 8,8-dimethyl-4-methylene-	C10H14O		LibSearch	28.286	10.852		54345-60-7	45.82		
4-tert-Butylphenyl acetate	C12H16O2		LibSearch	28.286	5.169		3056-64-2	45.78		
Pentandioic acid, (p-t-butylphenyl) ester	C15H20O4		LibSearch	28.286	-5.748		212762-88-4	45.78		
Ethyl 3-(4-methoxybenzoyl)propionate	C13H16O4		LibSearch	28.286	-1.431		15118-67-9	45.66		
4-Acetylanisole	C9H10O2		LibSearch	28.286	7.986		100-06-1	45.64		
.alpha. Isomethyl ionone	C14H22O		LibSearch	28.286	3.186		127-51-5	45.64		
Ionone <alpha-, isomethyl->	C14H22O		LibSearch	28.286			127-51-5	45.63		
Benzene, 1-ethoxy-4-ethyl-	C10H14O		LibSearch	28.286	8.586		1585-06-4	45.48		
p-Anisic acid, 3-chloroprop-2-enyl ester	C11H11ClO3		LibSearch	28.286	1.086		1000299-20-1	45.41		

Compound Chromatograms (overlaid)

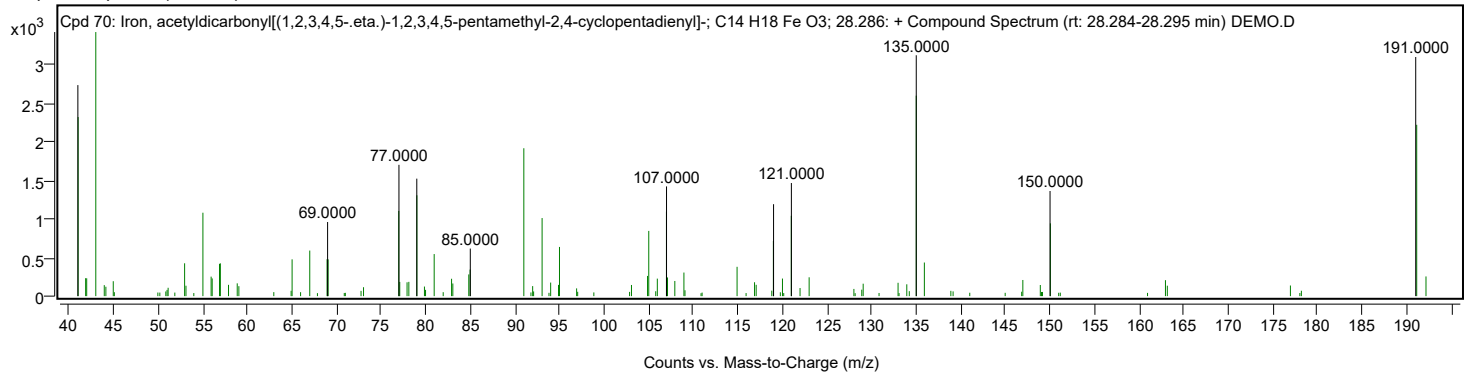


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



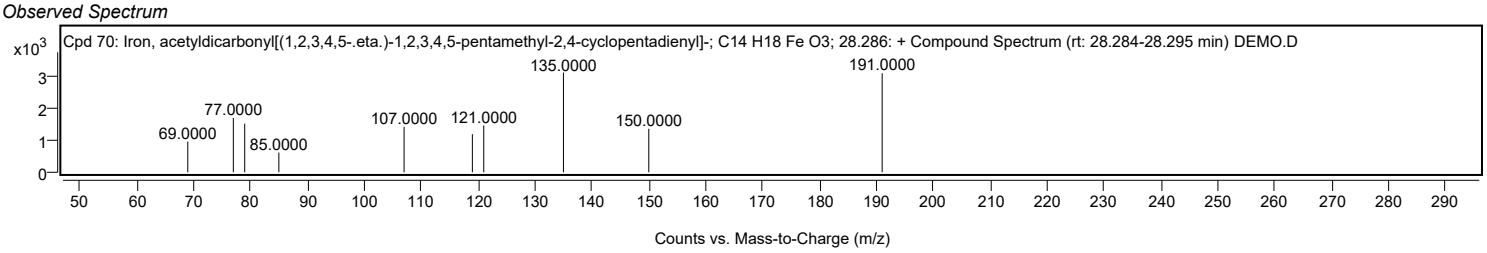
Iron, acetyldicarbonyl[(1,2,3,4,5-.eta.)-1,2,3,4,5-pentamethyl-2,4-cyclopentadienyl]-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			59.62			NIST.L

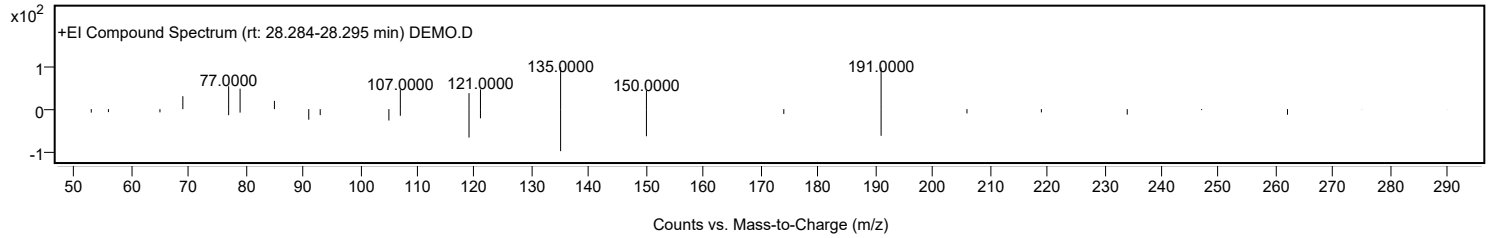
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			59.62			NIST.L

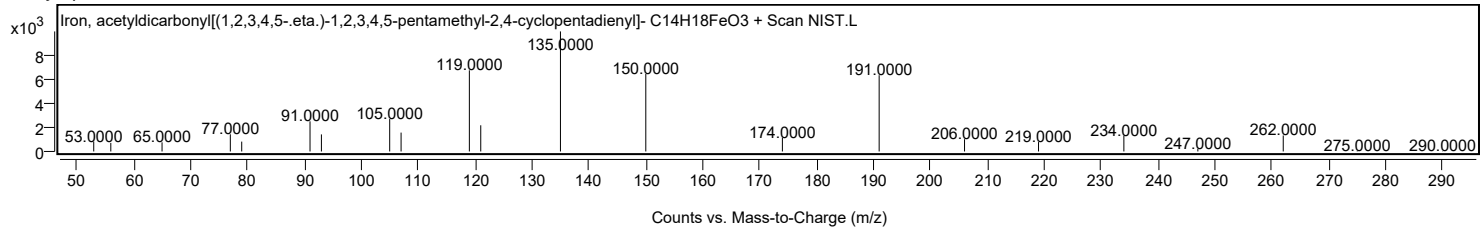
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 71: Diethylene glycol, O,O-di(pivaloyl)-

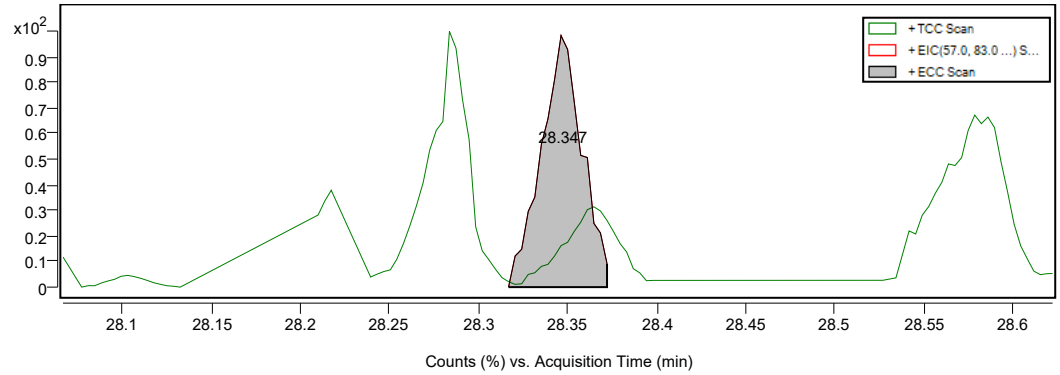
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Diethylene glycol, O,O-di(pivaloyl)-	C14 H26 O5	28.347			1000308-76-7	LibSearch	57.16	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		57.16			50		

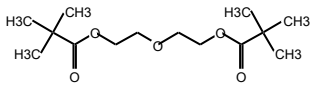
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Diethylene glycol, O,O-di(pivaloyl)-	C14H26O5		LibSearch	28.347	0.781		1000308-76-7	57.16		
Helvetolide	C17H32O3		LibSearch	28.347			141773-73-1	45.20		
Hexanal ethyl cis-3-hexenyl acetal	C14H28O2		LibSearch	28.347	3.197		1000431-42-9	44.59		
Thiophene, 2-nitro-	C4H3NO2S		LibSearch	28.347	10.397		609-40-5	43.50		
Hydrazinecarboxylic acid, (2-ethoxy-1-methyl-2-oxoethylidene)-, ethyl ester	C8H14N2O4		LibSearch	28.347	2.647		91616-14-7	43.09		
1,3-Dioxan-4-one, 2-(1,1-dimethylethyl)-6-ethyl-	C10H18O3		LibSearch	28.347	5.531		113505-80-9	42.89		
2,2'-Bi-1,3-dioxolane, 4,4,4',4',5,5,5',5'-octamethyl-	C14H26O4		LibSearch	28.347	1.747		35528-76-8	41.08		
Thiophene, 2-nitro-	C4H3NO2S		LibSearch	28.347	10.397		609-40-5	40.75		
Butanedioic acid, 2-methyl-3-oxo-, diethyl ester	C9H14O5		LibSearch	28.347	6.314		759-65-9	39.89		
2-Ethoxyheptylphthalimide	C17H23NO3		LibSearch	28.347	-10.753		1000227-41-4	39.87		
2-Butenoic acid, 3-amino-, ethyl ester	C6H11NO2		LibSearch	28.347	11.464		7318-00-5	39.39		
Malonic acid, 2,4-dimethylpent-3-yl propyl ester	C13H24O4		LibSearch	28.347	4.081		1000349-00-9	38.88		
Thiophene, 2-nitro-	C4H3NO2S		LibSearch	28.347	10.397		609-40-5	38.64		
Herboxane	C11H22O2		LibSearch	28.347			54546-26-8	38.14		
Neopentyl isothiocyanate	C6H11NS		LibSearch	28.347			597-97-7	37.66		
DL-Lactamide, N,O-dibutyl-	C11H23NO2		LibSearch	28.347	2.897		1000452-56-2	37.42		
tert-Butyl 3-(aminomethyl)piperazine-1-carboxylate	C10H21N3O2		LibSearch	28.347	-1.036		1376099-80-7	37.26		
4,4-Dimethyl-2-pentanol, chlorodifluoroacetate	C9H15ClF2O2		LibSearch	28.347	12.464		1000376-27-0	36.17		
Carbamimidothioic acid, N-cyano-N'-methyl-, methyl ester	C4H7N3S		LibSearch	28.347	6.581		5848-24-8	35.54		
Pyrazol-5-amine, 4-tert-butylsulfonyl-	C7H13N3O2S		LibSearch	28.347	-2.886		1000269-56-2	35.26		
Cyclohexanecarboxylic acid, 2-methylpropyl ester	C11H20O2		LibSearch	28.347	6.997		37139-85-8	35.16		
Cyclohexanecarboxylic acid, butyl ester	C11H20O2		LibSearch	28.347	5.931		6553-81-7	34.92		
2-Butenoic acid, 3-amino-, ethyl ester	C6H11NO2		LibSearch	28.347	11.464		7318-00-5	34.48		
Succinic acid, 4,4-dimethylpent-2-yl ethyl ester	C13H24O4		LibSearch	28.347	3.364		1000381-71-3	34.35		
4-Hydroxy-2-hexenoic acid, ethyl ester	C8H14O3		LibSearch	28.347	9.114		61454-95-3	34.27		
Cyclohexanecarboxylic acid, undecyl ester	C18H34O2		LibSearch	28.347	-5.669		94107-44-5	33.66		
1,3-Dioxan-4-one, 2-(1,1-dimethylethyl)-5,6-dimethyl-, [2R-(2.alpha.,5.alpha.,6.alpha.)]-	C10H18O3		LibSearch	28.347	6.164		107289-14-5	33.45		
2-Heptenoic acid, tridecyl ester	C20H38O2		LibSearch	28.347	-8.069		1000406-09-8	33.37		
Adipic acid, di(oct-4-yl ester)	C22H42O4		LibSearch	28.347	-11.886		1000160-80-1	32.98		
N-(3,4-Difluorophenyl)-2,2-dimethylpropanamide	C11H13F2NO		LibSearch	28.347	4.064		1000486-60-2	32.19		
2-Heptenoic acid, pentadecyl ester	C22H42O2		LibSearch	28.347	-11.369		1000406-10-0	32.17		
Butane, 1,1-dibutoxy-	C12H26O2		LibSearch	28.347	6.647		5921-80-2	32.03		
2-Heptenoic acid, tetradecyl ester	C21H40O2		LibSearch	28.347	-9.719		1000406-09-9	31.91		
Cyclohexanecarboxylic acid, heptyl ester	C14H26O2		LibSearch	28.347	0.947		92319-47-6	31.80		
Cyclohexanecarboxylic acid, heptadecyl ester	C24H46O2		LibSearch	28.347	-15.619		1010282-80-3	31.59		
1,3-Dioxolane, 2-ethyl-2-isopropyl-4,5-dimethyl-	C10H20O2		LibSearch	28.347	10.547		1010149-95-0	31.13		
Adipic acid, isobutyl trans-hex-3-enyl ester	C16H28O4		LibSearch	28.347	-3.153		1000354-00-7	30.62		
2,2-Dimethyl-3-pentanol, chlorodifluoroacetate	C9H15ClF2O2		LibSearch	28.347	12.464		1000376-26-4	30.01		
Oxirane, (bromomethyl)-	C3H5BrO		LibSearch	28.347	16.581		3132-64-7	29.51		
1,1-Hexylenedioxybutane	C10H20O2		LibSearch	28.347	6.397		1000249-77-4	29.39		
Cyclohexanecarboxylic acid, hexadecyl ester	C23H44O2		LibSearch	28.347	-13.953		1000279-54-4	29.18		
Cyclohexanecarboxylic acid, 4-(1,1-dimethylethyl)-, trans-	C11H20O2		LibSearch	28.347	4.814		943-29-3	29.14		
4-tert-Butylcyclohexanecarboxylic acid	C11H20O2		LibSearch	28.347	4.814		5451-55-8	29.07		
Cyclohexanecarboxylic acid, decyl ester	C17H32O2		LibSearch	28.347	-4.019		93479-48-2	29.03		
Cyclohexanecarboxylic acid, pentadecyl ester	C22H42O2		LibSearch	28.347	-12.303		1000279-54-3	28.74		
tert-C4H9C(O)OCH(CH3)2	C8H16O2		LibSearch	28.347	14.431		5129-36-2	28.58		
Adipic acid, cyclopentylmethyl isobutyl ester	C16H28O4		LibSearch	28.347	-3.736		1000324-77-3	28.54		
Cyclohexanecarboxylic acid, tridecyl ester	C20H38O2		LibSearch	28.347	-8.986		1000279-54-1	28.37		
Cyclohexanecarboxylic acid, octyl ester	C15H28O2		LibSearch	28.347	-0.703		89611-20-1	28.29		
2-Butenoic acid, 3-amino-, ethyl ester	C6H11NO2		LibSearch	28.347	11.464		7318-00-5	27.53		

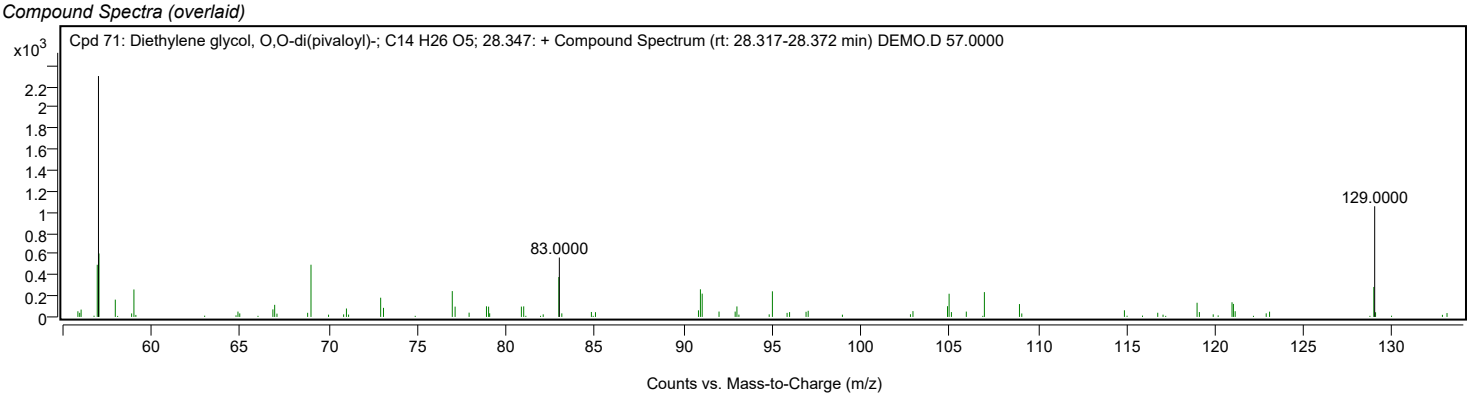
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



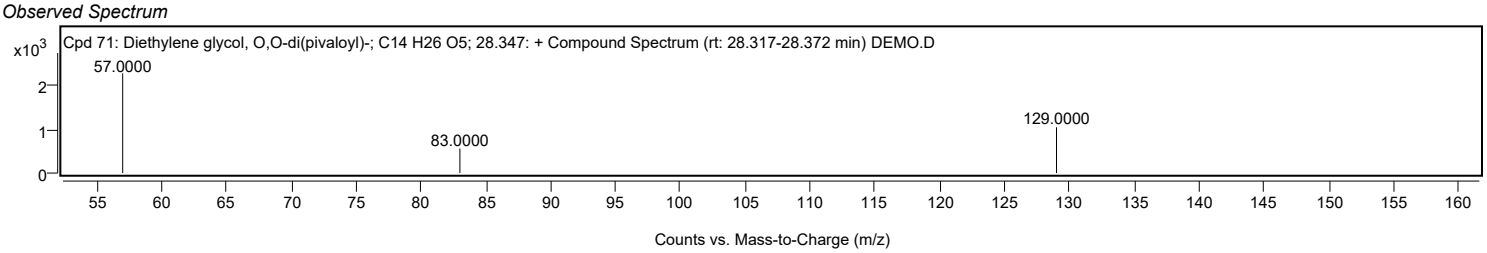
Diethylene glycol, O,O-di(pivaloyl)-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			57.16			NIST.L

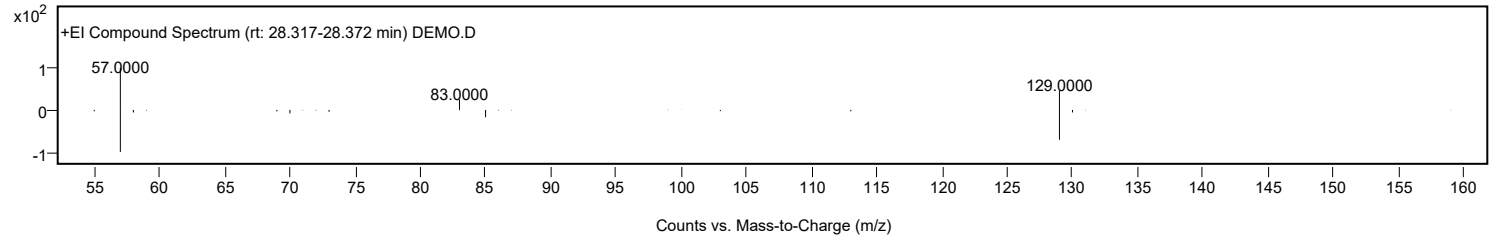
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			57.16			NIST.L

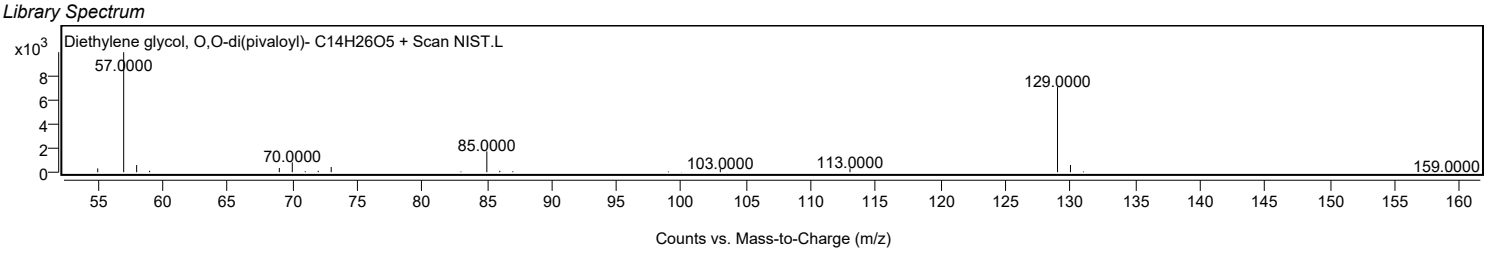
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 72: Benzene, [1-methyl-1-(pentyloxy)ethyl]-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Benzene, [1-methyl-1-(pentyloxy)ethyl]-	C14 H22 O	28.366			54932-79-5	LibSearch	50.47	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		50.47			50		

Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Benzene, [1-methyl-1-(pentyloxy)ethyl]-	C14H22O		LibSearch	28.366	3.682		54932-79-5	50.47		
3-Hydroxy-3-phenylbutan-2-one	C10H12O2		LibSearch	28.366	6.366		3155-01-9	46.30		
Iso E Super <gamma->	C16H26O		LibSearch	28.366			68155-67-9	45.39		
Atrolactic acid	C9H10O3		LibSearch	28.366	4.349		515-30-0	45.00		
p-Cyanophenyl p-(2-methylbutoxy)benzoate	C19H19NO3		LibSearch	28.366	-12.201		67951-45-5	44.19		
dl-2-Phenyl-1,2-propanediol	C9H12O2		LibSearch	28.366	6.249		4217-66-7	43.80		
Isoxazole, 4,5-dihydro-5-[(4-methoxyphenyl)methyl]-	C11H13NO2		LibSearch	28.366	2.832		1010362-14-0	43.21		
Atrolactic acid	C9H10O3		LibSearch	28.366	4.349		515-30-0	42.87		
Benzeneacetic acid, .alpha.-methoxy-, methyl ester, (.+/-.)-	C10H12O3		LibSearch	28.366	7.182		56143-21-6	42.66		
Acetohydrazide, 2-(4-tolyloxy)-N2-benzoylmethylene-	C17H16N2O3		LibSearch	28.366	-16.734		1000258-81-8	42.54		
7-Oxatetracyclo[4.2.0.0(2,4).0(3,5)]octane, 8-acetyl-8-methyl-	C10H12O2		LibSearch	28.366	13.332		120229-54-1	42.15		
4-Oxatricyclo[3.3.0.0(2,8)]oct-6-ene, 3-acetyl-3-methyl-	C10H12O2		LibSearch	28.366	11.999		1000142-20-3	42.10		
1-[1,6-Dimethyl-4-(4-methyl-3-pentenyl)-3-cyclohexen-1-yl]ethanone	C16H26O		LibSearch	28.366	-0.034		57499-57-7	41.87		
Benzeneacetic acid, .alpha.-methoxy-, (.+/-.)-	C9H10O3		LibSearch	28.366	5.682		7021-09-2	41.85		
(l-Erythro-2,3-diphenyl)-2-butanol	C16H18O		LibSearch	28.366	-1.501		4613-10-9	41.54		
4-(Fluoromethyl)-5-methyl-2-phenyl-2H-1,2,3-triazole	C10H10FN3		LibSearch	28.366	3.732		1000098-68-5	41.46		
(d-Threo-2,3-diphenyl)-2-butanol	C16H18O		LibSearch	28.366	-1.501		4539-33-7	41.44		
Amberonne (isomer 3)	C16H26O		LibSearch	28.366	-0.068		1000470-69-9	41.21		
.alpha.-Ethyl-.alpha.-methylbenzyl alcohol	C10H14O		LibSearch	28.366	8.632		1565-75-9	41.04		
Butanoic acid, 3-(1-phenylethoxy)-	C12H16O3		LibSearch	28.366	1.782		1000195-54-3	40.74		
dl-2-Phenyl-1,2-propanediol	C9H12O2		LibSearch	28.366	6.249		4217-66-7	40.73		
Silane, trimethoxymethyl-	C4H12O3Si		LibSearch	28.366	19.082		1185-55-3	40.51		
dl-2-Phenyl-1,2-propanediol	C9H12O2		LibSearch	28.366	6.249		4217-66-7	40.44		
1-Methylene-2b-hydroxymethyl-3,3-dimethyl-4b-(3-methylbut-2-enyl)-cyclohexane	C15H26O		LibSearch	28.366	0.566		1000144-10-6	40.30		
Benzene, 1,1'-(oxydiethylidene)bis-	C16H18O		LibSearch	28.366	-0.184		93-96-9	40.15		
3-Buten-2-one, 4-(2,5,6,6-tetramethyl-1-cyclohexen-1-yl)-	C14H22O		LibSearch	28.366	3.049		79-70-9	40.14		
Benzeneacetic acid, .alpha.-methoxy-, (.+/-.)-	C9H10O3		LibSearch	28.366	5.682		7021-09-2	39.75		
1-Formyl-2,2,6-trimethyl-3-cis-(3-methylbut-2-enyl)-5-cyclohexene	C15H24O		LibSearch	28.366	1.382		1000144-10-1	39.24		
Benzamide	C7H7NO		LibSearch	28.366	8.316		55-21-0	39.14		
Vertacetal <anti->	C13H18O2		LibSearch	28.366			5182-36-5	39.07		
4-Phenyl-morpholine-2,6-dione	C10H9NO3		LibSearch	28.366	-1.684		56956-66-2	38.86		
Isobutyramide, N-benzyl-N-methyl-	C12H17NO		LibSearch	28.366	4.582		1000446-60-6	38.43		
Benzeneacetic acid, .alpha.-methoxy-, (.+/-.)-	C9H10O3		LibSearch	28.366	5.682		7021-09-2	38.42		
5,9-methanobenzocycloocten-5(1H)-ol, 2,3,4,6,7,8,9,10-octahydro-2,2,8,8,9-pentamethyl-	C18H30O		LibSearch	28.366	-3.218		1000396-83-9	38.40		
2,4,4-Trimethyl-3-hydroxymethyl-5a-(3-methyl-but-2-enyl)-cyclohexene	C15H26O		LibSearch	28.366	0.482		1000144-10-5	38.33		
Benzeneacetic acid, .alpha.-methoxy-, (S)-	C9H10O3		LibSearch	28.366	5.682		26164-26-1	38.32		
Benzene, 1,1'-(oxydiethylidene)bis-	C16H18O		LibSearch	28.366	-0.184		93-96-9	38.17		
Benzamide	C7H7NO		LibSearch	28.366	8.316		55-21-0	38.10		
Benzene, (1-methoxyethyl)-	C9H12O		LibSearch	28.366	11.632		4013-34-7	37.97		
Benzaldehyde dimethyl acetal	C9H12O2		LibSearch	28.366	10.366		1125-88-8	37.88		
Benzaldehyde dimethyl acetal	C9H12O2		LibSearch	28.366	10.366		1125-88-8	37.66		
Benzeneacetic acid, .alpha.-methoxy-, methyl ester, (.+/-.)-	C10H12O3		LibSearch	28.366	7.182		56143-21-6	37.64		
Benzeneacetic acid, .alpha.-methoxy-, methyl ester, (.+/-.)-	C10H12O3		LibSearch	28.366	7.182		56143-21-6	37.59		
Benzoin methyl ether	C15H14O2		LibSearch	28.366	-1.851		3524-62-7	37.58		
Aminorex, N,N-dimethyl	C11H14N2O		LibSearch	28.366	3.682		1000447-11-0	37.54		
Safranal	C10H14O		LibSearch	28.366			116-26-7	37.53		
Cyanogen bromide	CBrN		LibSearch	28.366			506-68-3	37.49		
4-Butyl-5-(3-methylbutyl)-6-(1-methylethenyl)-2H-pyran-2-one	C17H26O2		LibSearch	28.366	-4.568		1000306-51-4	37.46		
Benzene, (1-methoxy-4-methyl-3-pentenyl)-	C13H18O		LibSearch	28.366	5.249		68705-86-2	37.43		
1-Methylene-2-benzyloxy-cyclopropane	C11H12O		LibSearch	28.366	7.766		119819-29-3	37.36		

Compound Discovery Report

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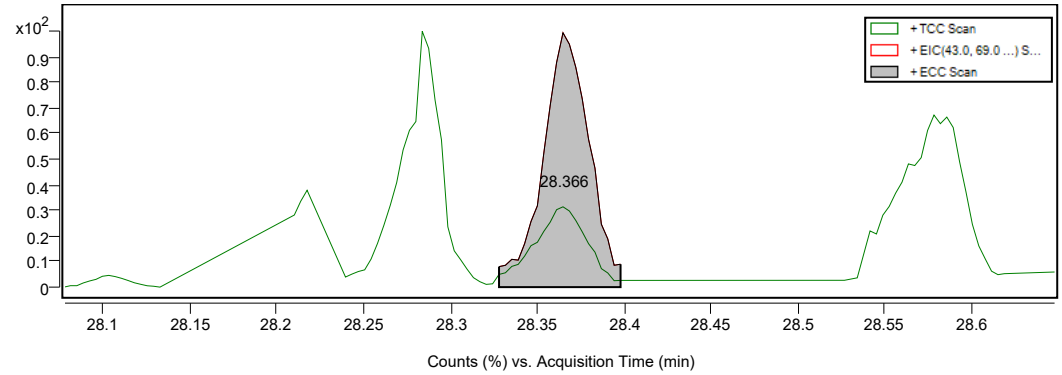
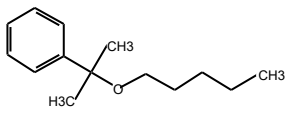
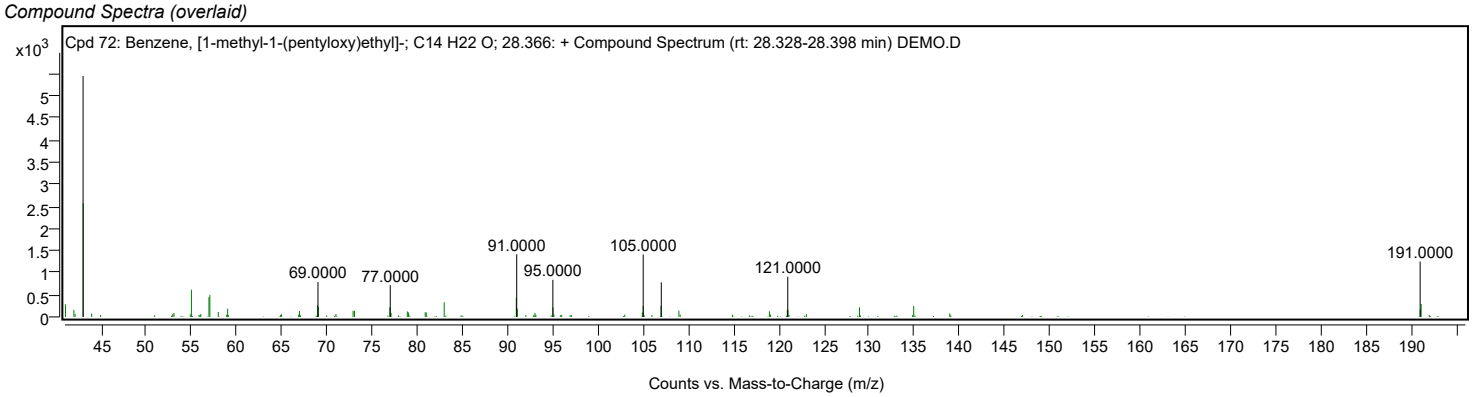
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



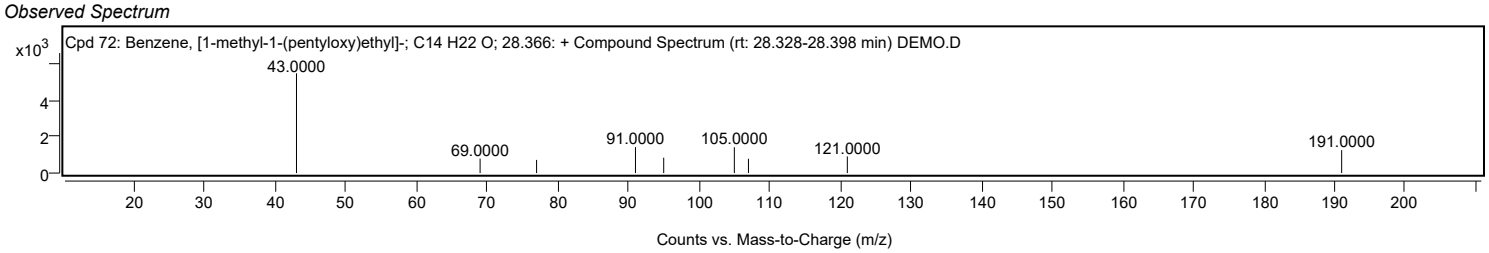
Benzene, [1-methyl-1-(pentyloxy)ethyl]-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			50.47			NIST.L

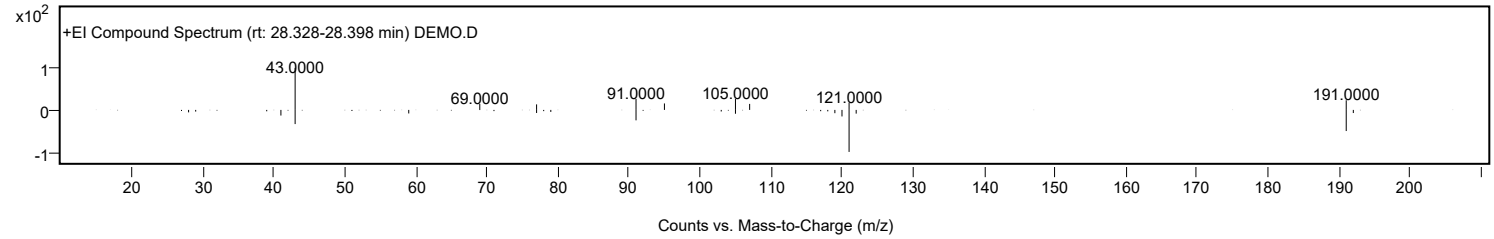
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			50.47			NIST.L

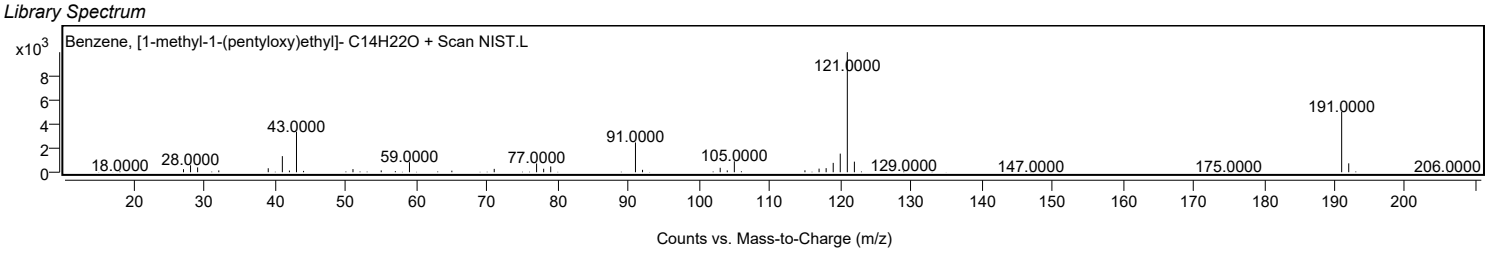
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 73: 4-(N-Methyl-N-methoxy)indancarboxamide

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
4-(N-Methyl-N-methoxy)indancarboxamide	C12 H15 N O2	28.564			1000284-45-9	LibSearch	51.74	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		51.74			50		

Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
4-(N-Methyl-N-methoxy)indancarboxamide	C12H15NO2		LibSearch	28.564	1.314		1000284-45-9	51.74		
Benzene, 1,1'-(1,5-hexadiene-1,6-diyl)bis-	C18H18		LibSearch	28.564	-4.436		4439-45-6	50.98		
Propenoic acid, 3-(cycloheptatrien-7-yl)-, methyl ester	C11H12O2		LibSearch	28.564	6.547		1000269-64-5	49.85		
1H-Indene-4-carboxaldehyde, 2,3-dihydro-	C10H10O		LibSearch	28.564	6.097		51932-70-8	49.73		
Benzene, (1-ethyl-2-propenyl)-	C11H14		LibSearch	28.564	9.947		19947-22-9	49.65		
1H-Indene-4-carboxaldehyde, 2,3-dihydro-	C10H10O		LibSearch	28.564	6.097		51932-70-8	49.15		
Benzene, 1-ethynyl-4-methyl-	C9H8		LibSearch	28.564	11.830		766-97-2	49.09		
trans-Cinnamyl bromide	C9H9Br		LibSearch	28.564	6.947		26146-77-0	48.18		
Bicyclo[4.2.1]nona-2,4,7-triene, 9-(phenylseleno)-, (anti-)	C15H14Se		LibSearch	28.564			72065-50-0	47.63		
Cyclopropanecarboxylic acid, trans-2-phenyl-, 2-chloro-6-fluorophenyl ester	C16H12ClFO2		LibSearch	28.564	-5.620		1000406-84-3	47.59		
Tricyclo[3.2.1.0(2,,4)]oct-6-ene, 8-methylene-, (1.alpha.,2.alpha.,4.alpha.,5.alpha.)-	C9H10		LibSearch	28.564	17.064		66929-90-6	47.28		
Succinic acid, 3-chlorophenyl 3-phenylprop-2-en-1-yl ester	C19H17ClO4		LibSearch	28.564	-14.536		1010391-04-7	47.26		
Benzenesulfonic acid, 4-methyl-, (2,3-dihydro-1H-inden-1-ylidene)hydrazide	C16H16N2O2S		LibSearch	28.564	-16.953		73424-46-1	47.05		
Benzocyclobutene, 1-bromo-1-methyl-	C9H9Br		LibSearch	28.564	7.597		1000161-76-4	47.04		
2-Acetoxyindane	C11H12O2		LibSearch	28.564	5.664		4254-31-3	46.92		
Benzene, 1-propynyl-	C9H8		LibSearch	28.564	11.730		673-32-5	46.72		
Benzaldehyde, 4-(1-phenyl-2-propenyloxy)-	C16H14O2		LibSearch	28.564	-4.253		1000277-56-1	46.66		
1H-Indene, 1-chloro-2,3-dihydro-	C9H9Cl		LibSearch	28.564	8.347		35275-62-8	46.60		
(2-Nitroallyl)-benzene	C9H9NO2		LibSearch	28.564	6.214		62811-39-6	46.58		
2-Methyl-3-phenyl-N-(5-trifluoromethyl-[1,3,4]thiadiazol-2-yl)acrylamide	C13H10F3N3OS		LibSearch	28.564	-7.286		1000322-25-1	46.54		
Ethanone, 1-(2,3-dihydro-1H-inden-5-yl)-	C11H12O		LibSearch	28.564	6.180		4228-10-8	46.49		
Indene	C9H8		LibSearch	28.564	11.414		95-13-6	46.40		
Cyclopropanecarboxylic acid, trans-2-phenyl-, 4-nitrophenyl ester	C16H13NO4		LibSearch	28.564	-9.620		1000406-88-4	46.30		
(+-)-2-Phenylbutyronitrile	C10H11N		LibSearch	28.564	7.347		69350-73-8	46.28		
4H-1,2,4-Triazole-3-thiol, 4-(2,3-dihydro-1H-inden-1-yl)-5-(1-methylethyl)-	C14H17N3S		LibSearch	28.564	-7.403		1000362-83-8	46.20		
1-Phenylcyclopentanecarboxylic acid	C12H14O2		LibSearch	28.564	0.830		77-55-4	46.09		
Benzene, (2-bromocyclopropyl)-	C9H9Br		LibSearch	28.564	7.697		36617-02-4	46.04		
Crotonaldehyde <2-phenyl->	C10H10O		LibSearch	28.564			4411-89-6	46.01		
Cyclopropanecarboxylic acid, trans-2-phenyl-, 3-chlorophenyl ester	C16H13ClO2		LibSearch	28.564	-6.036		1000406-84-4	45.99		
Cyclopropanecarboxylic acid, trans-2-phenyl-, 2,3-dichlorophenyl ester	C16H12Cl2O2		LibSearch	28.564	-9.036		1000406-84-6	45.96		
Benzene, (3-chloro-1-propenyl)-	C9H9Cl		LibSearch	28.564	8.130		2687-12-9	45.93		
Bicyclo[4.2.1]nona-2,4,7-triene, 9-(phenylseleno)-, syn-	C15H14Se		LibSearch	28.564			72065-43-1	45.91		
Cyclopropanecarboxylic acid, 2-phenyl-, methyl ester	C11H12O2		LibSearch	28.564	6.530		20030-70-0	45.90		
Benzene, 1,1'-(1-butene-1,4-diyl)bis-, (Z)-	C16H16		LibSearch	28.564	-0.986		70388-65-7	45.84		
Cyclopropanecarbonyl chloride, 2-phenyl-, trans-	C10H9ClO		LibSearch	28.564	5.764		939-87-7	45.64		
cis-1-Phenyl-3-methoxycarbonylcyclopropane	C11H12O2		LibSearch	28.564	6.530		1000311-93-4	45.61		
Methyl 3-(2-methylphenyl)prop-2-enoate	C11H12O2		LibSearch	28.564	5.564		75950-75-3	45.60		
.alpha.-Methyl cinnamic acid, ethyl ester	C12H14O2		LibSearch	28.564	4.514		1000454-64-3	45.57		
1H-Indene, 1-ethyl-2,3-dihydro-	C11H14		LibSearch	28.564	8.447		4830-99-3	45.56		
Benzene, 1-propynyl-	C9H8		LibSearch	28.564	11.730		673-32-5	45.55		
Phenyl trans-2-phenyl-1-cyclopropane sulfonate	C15H14O3S		LibSearch	28.564	-8.303		17299-18-2	45.50		
Indane, 1-nonyl-	C18H28		LibSearch	28.564	-3.153		29138-83-8	45.43		
Cyclopropanecarboxylic acid, trans-2-phenyl-, 4-chlorophenyl ester	C16H13ClO2		LibSearch	28.564	-6.036		1000406-88-3	45.22		
Benzeneacetaldehyde, .alpha.-ethylidene-	C10H10O		LibSearch	28.564	7.480		4411-89-6	45.01		
Methyl trans-2-phenyl-1-cyclopropanecarboxylate	C11H12O2		LibSearch	28.564	6.530		5861-31-4	44.89		
3-Ethyl-3-phenyl-1-pentene	C13H18		LibSearch	28.564	6.964		19781-34-1	44.77		
Benzeneethanol, .beta.-ethenyl-	C10H12O		LibSearch	28.564	7.547		6052-63-7	44.75		
Benzene, (3-chloro-1-propenyl)-	C9H9Cl		LibSearch	28.564	8.130		2687-12-9	44.73		
Bicyclo[2.2.2]oct-2-ene, 1,4,5,5,6,6-hexafluoro-	C8H6F6		LibSearch	28.564	20.214		31463-41-9	44.61		
2-Phenyl-1,2,3,4-tetrahydro-1,4-methanonaphthalen-2-ol	C17H16O		LibSearch	28.564	-4.336		93318-84-4	44.59		

Compound Discovery Report

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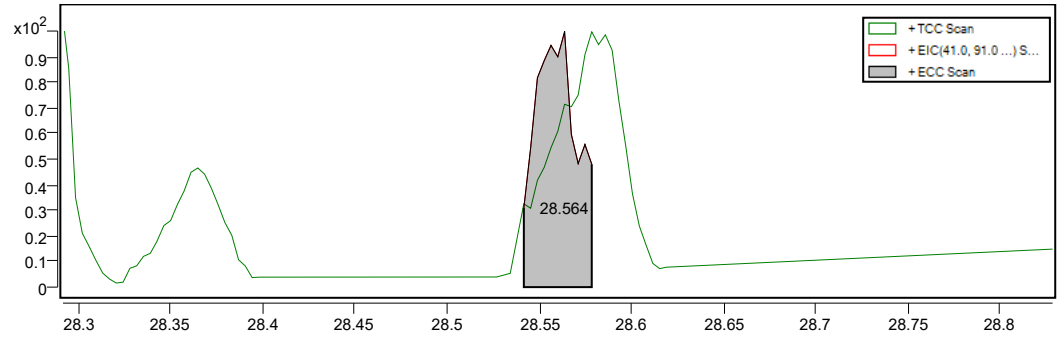
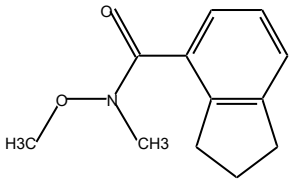
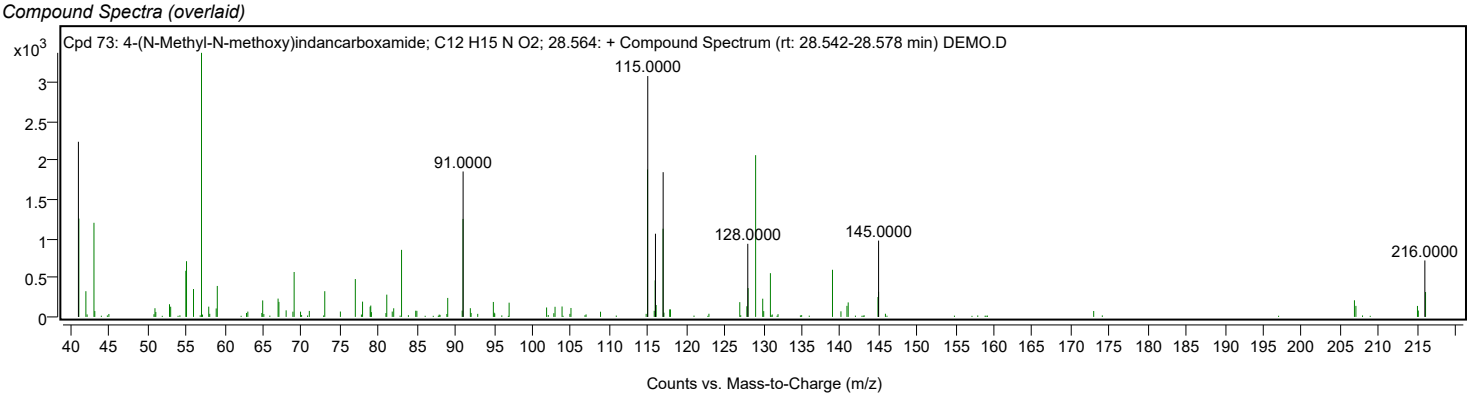
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



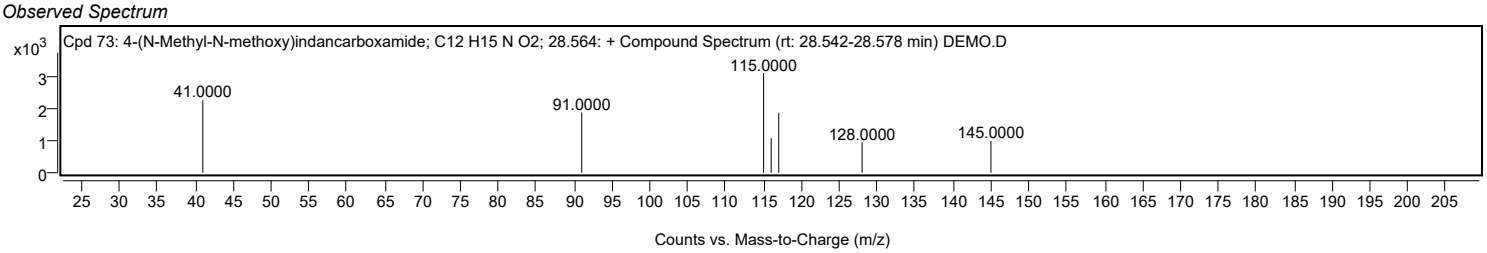
4-(N-Methyl-N-methoxy)indancarboxamide

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			51.74			NIST.L

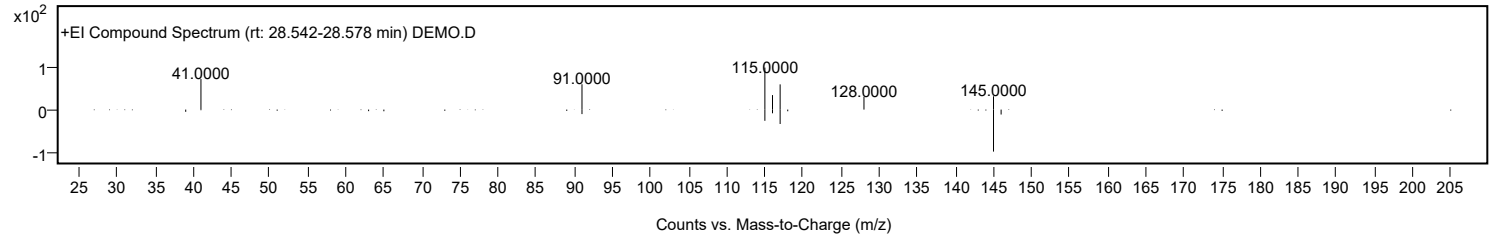
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			51.74			NIST.L

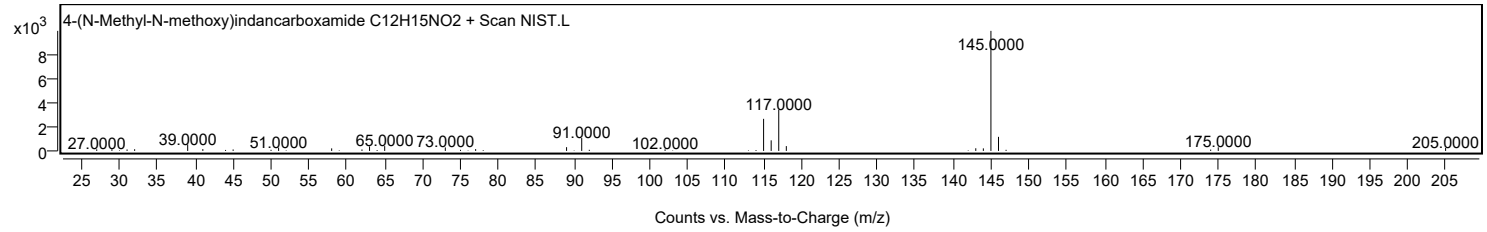
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 74: Helvetolide

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Helvetolide	C17 H32 O3	28.586			141773-73-1	LibSearch	73.00	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		73.00			50		

Compound Discovery Report

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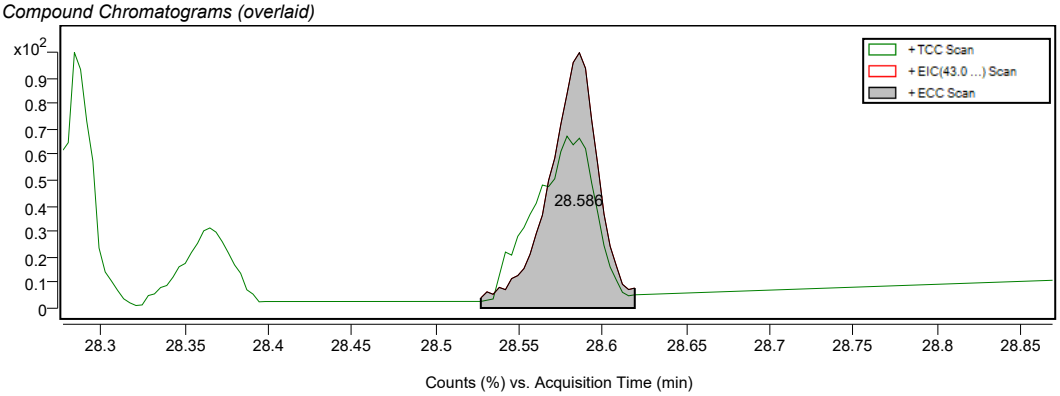
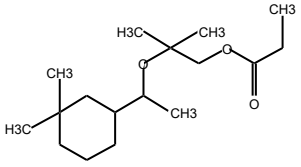
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Helvetolide	C17H32O3		LibSearch	28.586			141773-73-1	73.00		
t-butylsulfinate,-O-menthyl-	C14H28O2S		LibSearch	28.586	-1.381		1000151-39-9	58.37		
1,1,3,3,5-Pentamethylcyclohexane	C11H22		LibSearch	28.586	11.086		70810-19-4	56.56		
N,N'-di-tert-Butylcarbodiimide	C9H18N2		LibSearch	28.586			691-24-7	55.78		
Menthyl lactate<neo->	C13H24O3		LibSearch	28.586	1.146		0-00-0	55.57		
N,N'-di-tert-Butylcarbodiimide	C9H18N2		LibSearch	28.586			691-24-7	54.77		
Hexanal ethyl cis-3-hexenyl acetal	C14H28O2		LibSearch	28.586	3.436		1000431-42-9	53.92		
Phosphine, dichloro-D-menthyl-	C10H19Cl2P		LibSearch	28.586	4.969		83021-21-0	52.93		
Cyclohexane, 1,5-diethyl-2,3-dimethyl-	C12H24		LibSearch	28.586	9.202		74663-66-4	51.99		
Oxalic acid, butyl 1-menthyl ester	C16H28O4		LibSearch	28.586	-2.564		1000314-97-2	51.76		
Oxalic acid, heptyl 1-menthyl ester	C19H34O4		LibSearch	28.586	-7.531		1010314-97-5	51.73		
trans-1,4-Di-tert-butyl-cyclohexane	C14H28		LibSearch	28.586	7.436		4789-35-9	51.48		
Oxalic acid, 1-menthyl octyl ester	C20H36O4		LibSearch	28.586	-9.198		1000314-97-6	50.80		
Oxalic acid, isohexyl 1-menthyl ester	C18H32O4		LibSearch	28.586	-4.814		1000314-98-7	50.50		
Oxalic acid, hexyl 1-menthyl ester	C18H32O4		LibSearch	28.586	-5.881		1000314-97-4	50.31		
1-Hexanol, 3,5,5-trimethyl-	C9H20O		LibSearch	28.586	11.752		3452-97-9	50.25		
Herboxane	C11H22O2		LibSearch	28.586			54546-26-8	50.18		
Cyclohexane, 2-iodo-4-methyl-1-(1-methylethyl)-	C10H19I		LibSearch	28.586	6.052		64240-81-9	50.18		
1-Hexanol, 3,5,5-trimethyl-	C9H20O		LibSearch	28.586	11.752		3452-97-9	49.98		
Formic acid, 4,4-dimethylpent-2-yl ester	C8H16O2		LibSearch	28.586	13.052		1000368-69-9	49.93		
Phosphine, dibromo-L-menthyl-	C10H19Br2P		LibSearch	28.586	0.969		119512-37-7	49.88		
Hexanal ethyl trans-2-hexenyl acetal	C14H28O2		LibSearch	28.586	3.436		1000431-42-6	49.56		
Cyclodecyl formate	C11H20O2		LibSearch	28.586	3.186		1000430-79-0	49.26		
Oxalic acid, 1-menthyl nonyl ester	C21H38O4		LibSearch	28.586	-10.848		1000314-97-7	49.24		
1-Hexanol, 3,5,5-trimethyl-	C9H20O		LibSearch	28.586	11.752		3452-97-9	49.11		
4,4-Dimethyl-2-pentanol, chlorodifluoroacetate	C9H15ClF2O2		LibSearch	28.586	12.702		1000376-27-0	49.10		
Oxalic acid, 1-menthyl undecyl ester	C23H42O4		LibSearch	28.586	-14.164		1000314-97-9	49.07		
Oxalic acid, 1-menthyl pentyl ester	C17H30O4		LibSearch	28.586	-4.214		1000314-97-3	49.04		
3-Heptene, 2,2,3,5,5,6,6-heptamethyl-	C14H28		LibSearch	28.586	9.519		54845-26-0	48.80		
Oxalic acid, dodecyl 1-menthyl ester	C24H44O4		LibSearch	28.586	-15.814		1000314-98-0	48.79		
p-Tert-butylcyclohexyl formate	C11H20O2		LibSearch	28.586	6.586		1010429-39-9	48.70		
Nonylol	C9H20O		LibSearch	28.586			3452-97-9	48.63		
1-Hexanol, 3,5,5-trimethyl-	C9H20O		LibSearch	28.586	11.752		3452-97-9	48.58		
Oxalic acid, decyl 1-menthyl ester	C22H40O4		LibSearch	28.586	-12.498		1000314-97-8	48.37		
Oxalic acid, 1-menthyl tetradecyl ester	C26H48O4		LibSearch	28.586	-19.131		1000314-98-1	48.24		
Cyclohexane, (3-methylpentyl)-	C12H24		LibSearch	28.586	8.369		61142-38-9	48.24		
Oxalic acid, di(1-menthyl) ester	C22H38O4		LibSearch	28.586	-11.214		1010314-98-6	48.20		
Oxalic acid, cyclohexyl hexyl ester	C14H24O4		LibSearch	28.586	-1.598		1000309-30-8	47.93		
1-Pentene, 4,4-dimethyl-	C7H14		LibSearch	28.586	18.202		762-62-9	47.67		
Oxalic acid, cyclohexyl octyl ester	C16H28O4		LibSearch	28.586	-4.914		1000309-31-0	47.65		
Menthyl lactate<iso->	C13H24O3		LibSearch	28.586	0.096		0-00-0	47.44		
1,3-Dioxan-4-one, 2-(1,1-dimethylethyl)-6-ethyl-	C10H18O3		LibSearch	28.586	5.769		113505-80-9	47.24		
2,2-Dimethyl-3-pentanol, chlorodifluoroacetate	C9H15ClF2O2		LibSearch	28.586	12.702		1000376-26-4	47.15		
Oxalic acid, cyclohexyl butyl ester	C12H20O4		LibSearch	28.586	1.719		1000309-30-5	46.97		
1,1-Diisobutoxy-butane	C12H26O2		LibSearch	28.586	9.019		13002-16-9	46.88		
Oxalic acid, cyclohexyl isobutyl ester	C12H20O4		LibSearch	28.586	2.786		1000309-30-4	46.81		
2-Ethylthiolane, S,S-dioxide	C6H12O2S		LibSearch	28.586			10178-59-3	46.78		
Methane, isocyanato-	C2H3NO		LibSearch	28.586			624-83-9	46.64		
Paramethadione	C7H11NO3		LibSearch	28.586	5.586		115-67-3	46.54		
Methane, isocyanato-	C2H3NO		LibSearch	28.586			624-83-9	46.52		

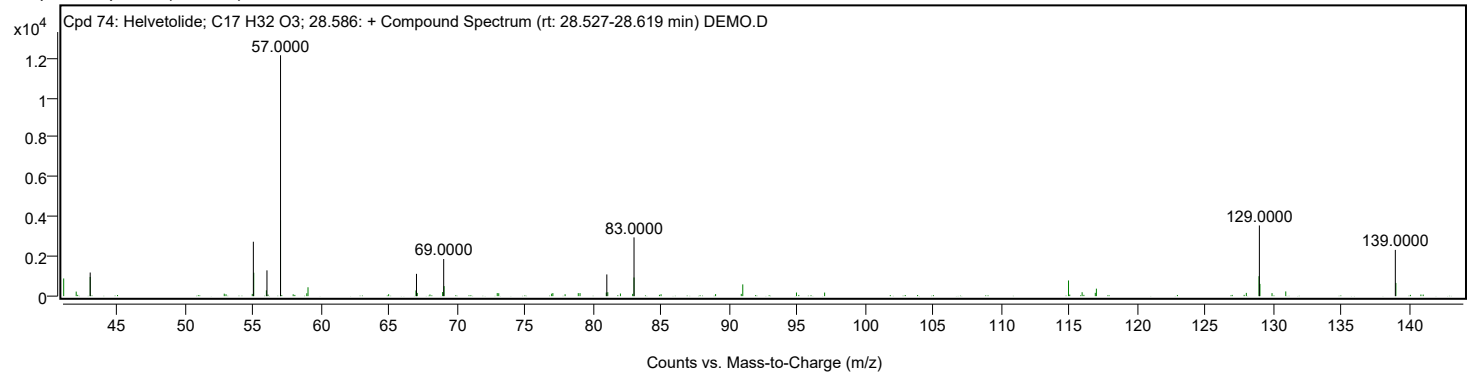
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



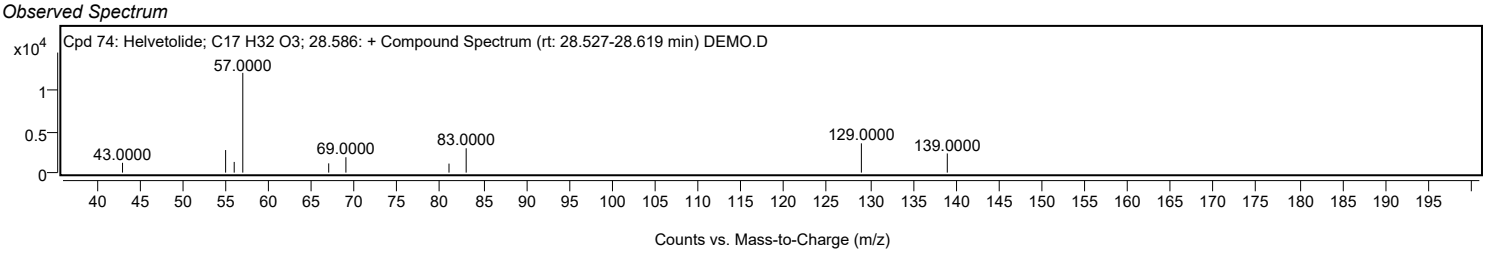
Helvetolide

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			73.00			PWNose.xml

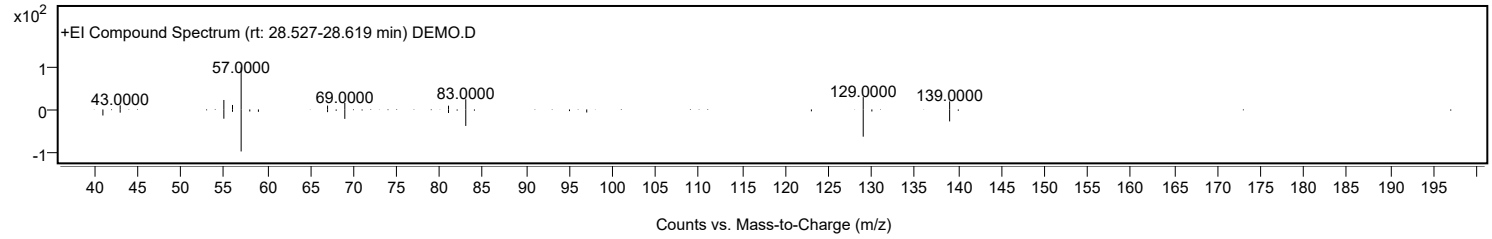
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			73.00			PWNose.xml

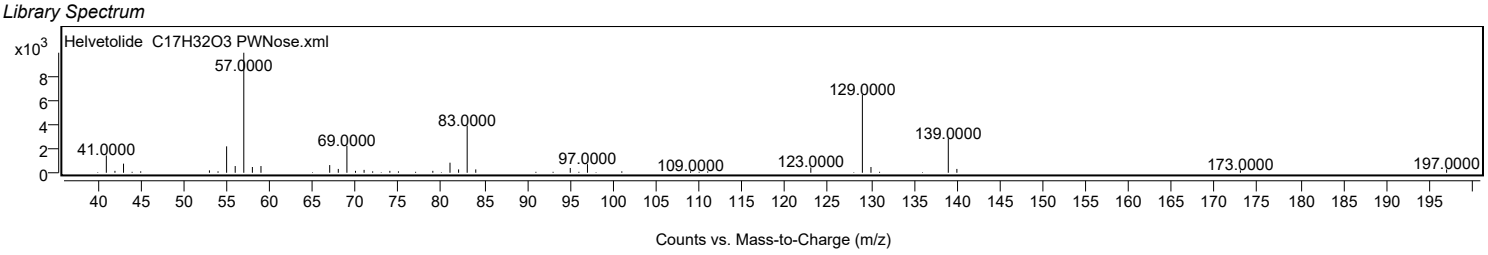
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 75: Diethylene glycol, O,O-di(pivaloyl)-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Diethylene glycol, O,O-di(pivaloyl)-	C14 H26 O5	28.950			1000308-76-7	LibSearch	51.42	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		51.42			50		

Compound Discovery Report

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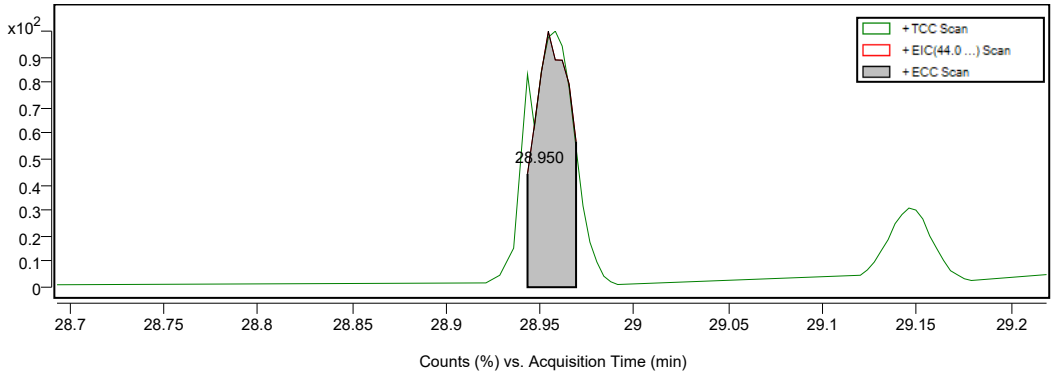
Compound ID Table

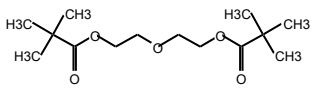
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Diethylene glycol, O,O-di(pivaloyl)-	C14H26O5		LibSearch	28.950	1.383		1000308-76-7	51.42		
Butanoic acid, 2-oxo-, ethyl ester	C6H10O3		LibSearch	28.950	13.600		15933-07-0	44.97		
Propanoic acid, anhydride	C6H10O3		LibSearch	28.950	13.600		123-62-6	44.92		
Propanoic acid, anhydride	C6H10O3		LibSearch	28.950	13.600		123-62-6	42.26		
Propanoic acid, anhydride	C6H10O3		LibSearch	28.950	13.600		123-62-6	40.82		
Paramethadione	C7H11NO3		LibSearch	28.950	5.950		115-67-3	40.03		
Paramethadione	C7H11NO3		LibSearch	28.950	5.950		115-67-3	40.02		
Paramethadione	C7H11NO3		LibSearch	28.950	5.950		115-67-3	39.37		
Butanoic acid, 2-oxo-, methyl ester	C5H8O3		LibSearch	28.950	15.250		3952-66-7	38.60		
N,N-Diethylpropionamide	C7H15NO		LibSearch	28.950	13.650		1114-51-8	38.55		
Tripropionin	C12H20O6		LibSearch	28.950			139-45-7	37.83		
1,2,3-Propanetriol, tripropanoate	C12H20O6		LibSearch	28.950	1.416		139-45-7	37.25		
1,2,3-Propanetriol, tripropanoate	C12H20O6		LibSearch	28.950	1.416		139-45-7	36.44		
2-Hydroxybutanenitrile	C4H7NO		LibSearch	28.950	15.183		1000486-93-5	36.27		
Neopentyl isothiocyanate	C6H11NS		LibSearch	28.950			597-97-7	36.04		
Paramethadione	C7H11NO3		LibSearch	28.950	5.950		115-67-3	35.63		
Allyl alcohol	C3H6O		LibSearch	28.950			107-18-6	35.61		
1,2,4-Triazin-3(2H)-one, 4,5-dihydro-5-thioxo-	C3H3N3OS		LibSearch	28.950	4.950		1627-37-8	34.99		
Allyl thiopropionate	C6H10OS		LibSearch	28.950	12.366		41820-22-8	34.20		
N,N-Diethylpropionamide	C7H15NO		LibSearch	28.950	13.650		1114-51-8	34.15		
Butyl isobutyl isobutal	C12H26O2		LibSearch	28.950	9.383		1000357-15-7	33.59		
Helvetolide	C17H32O3		LibSearch	28.950			141773-73-1	32.75		
Tripropionin	C12H20O6		LibSearch	28.950	-4.050		139-45-7	32.70		
Allyl formate	C4H6O2		LibSearch	28.950			1838-59-1	32.69		
2-(2-(2-Methoxyethoxy)ethoxy)ethyl 2-methylbutanoate	C12H24O5		LibSearch	28.950	3.200		1000366-97-4	32.63		
Oxirane, (bromomethyl)-	C3H5BrO		LibSearch	28.950	17.183		3132-64-7	32.63		
2-Hydroxy-gamma-butyrolactone	C4H6O3		LibSearch	28.950	12.066		19444-84-9	32.36		
Oxirane, (bromomethyl)-	C3H5BrO		LibSearch	28.950	17.183		3132-64-7	32.23		
3-Oxobutan-2-yl 2-methylbutanoate	C9H16O3		LibSearch	28.950	10.766		1000372-70-6	32.17		
Thiopropionate <S-allyl->	C6H10OS		LibSearch	28.950			41820-22-8	32.04		
1-Penten-3-ol	C5H10O		LibSearch	28.950	17.766		616-25-1	31.81		
Neopentane	C5H12		LibSearch	28.950	21.716		463-82-1	31.76		
DL-Lactamide, N,O-dibutyl-	C11H23NO2		LibSearch	28.950	3.500		1000452-56-2	31.55		
Adipic acid, 4-cyanophenyl isobutyl ester	C17H21NO4		LibSearch	28.950	-8.334		1000324-36-3	31.45		
Propanoate <allyl->	C6H10O2		LibSearch	28.950			2408-20-0	31.44		
2,5,8,11-Tetraoxatridecan-13-yl 2-methylbutanoate	C14H28O6		LibSearch	28.950	-1.384		1000366-96-8	30.74		
N-(3,4-Difluorophenyl)-2,2-dimethylpropanamide	C11H13F2NO		LibSearch	28.950	4.666		1000486-60-2	30.71		
3-(5-Methylpyrazol-1-yl)propanoic acid, trimethylsilyl ester	C10H18N2O2Si		LibSearch	28.950	5.966		1000472-54-9	30.68		
2-(2-Methoxyethoxy)ethyl 2-methylbutanoate	C10H20O4		LibSearch	28.950	7.783		1000366-96-5	30.38		
2-(2-(2-Methoxyethoxy)ethoxy)ethyl pentanoate	C12H24O5		LibSearch	28.950	2.133		1000367-01-3	30.24		
Butane, 1,1-dibutoxy-	C12H26O2		LibSearch	28.950	7.250		5921-80-2	29.62		
1-tert-Butyl-3-methyl-2,4,5-trioxoimidazolidine	C8H12N2O3		LibSearch	28.950	1.850		67867-39-4	29.54		
Thiolane-3,4-dicarbonitrile, 2,5-di-tert-butyl-3,4-bis(trifluoromethyl)-	C16H20F6N2S		LibSearch	28.950	0.316		1000260-74-6	29.18		
Pentene <3-hydroxy->	C5H10O		LibSearch	28.950			616-25-1	29.18		
2-Propen-1-ol	C3H6O		LibSearch	28.950	19.750		107-18-6	29.07		
5-Thiazolecarboxylic acid	C4H3NO2S		LibSearch	28.950	9.133		14527-41-4	29.06		
3-Butene-1,2-diol	C4H8O2		LibSearch	28.950	15.383		497-06-3	29.05		
tert-C4H9C(O)OCH(CH3)2	C8H16O2		LibSearch	28.950	15.033		5129-36-2	29.02		
1-Penten-3-ol	C5H10O		LibSearch	28.950	17.766		616-25-1	28.94		
Propanoic acid, 2-propenyl ester	C6H10O2		LibSearch	28.950	16.033		2408-20-0	28.89		

Compound Chromatograms (overlaid)

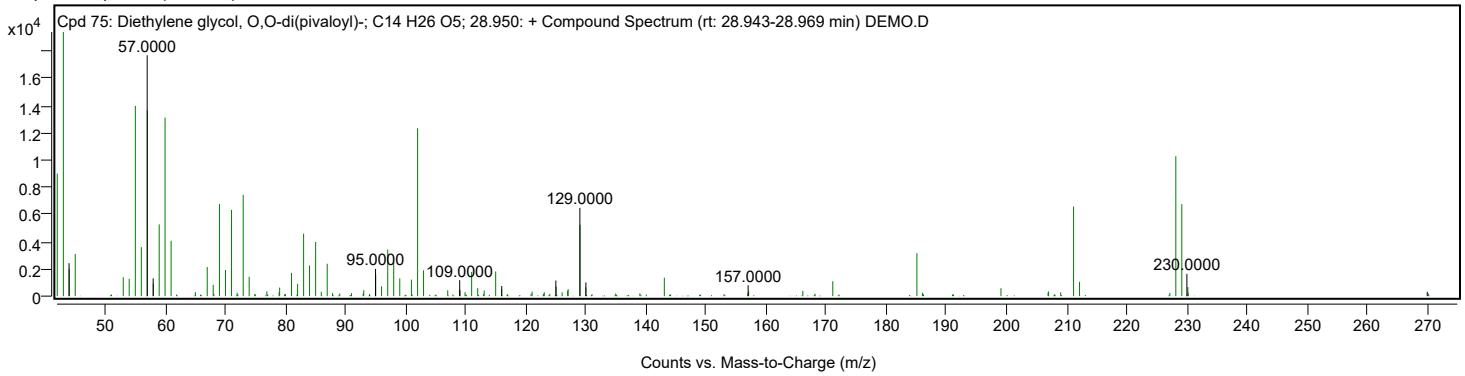


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



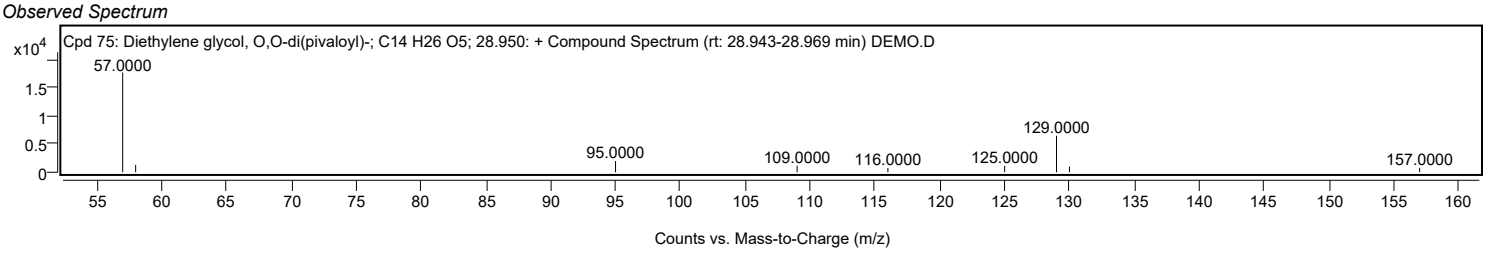
Diethylene glycol, O,O-di(pivaloyl)-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			51.42			NIST.L

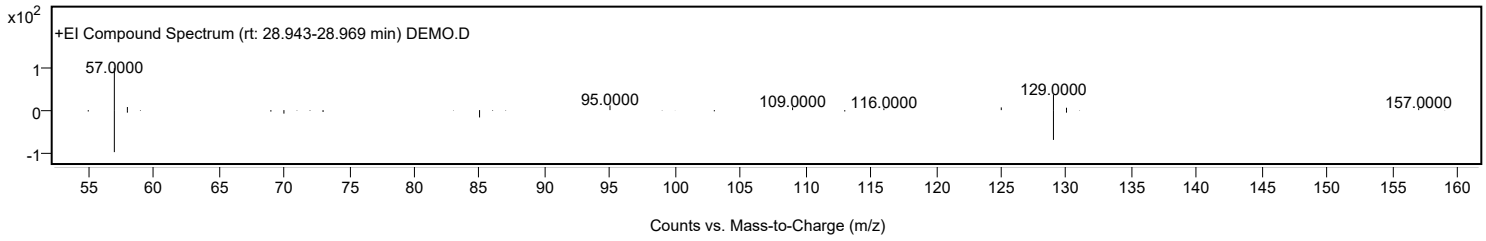
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			51.42			NIST.L

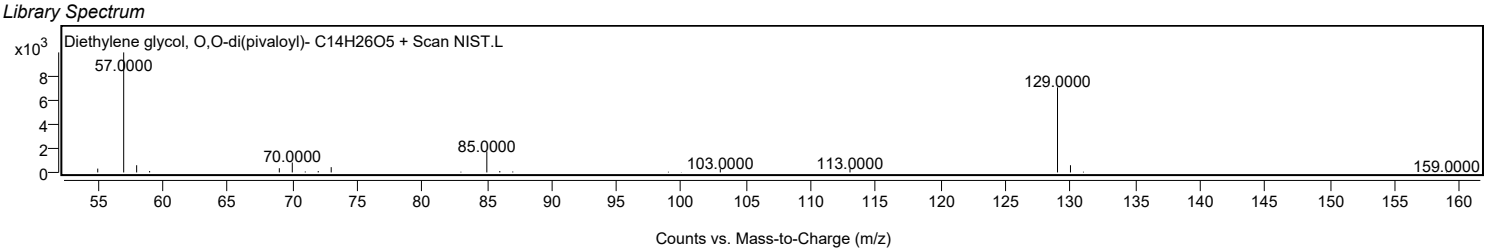
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 76: Tetradecanoate <isopropyl->

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Tetradecanoate <isopropyl->	C17 H34 O2	28.960			110-27-0	LibSearch	85.97	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		85.97			50		

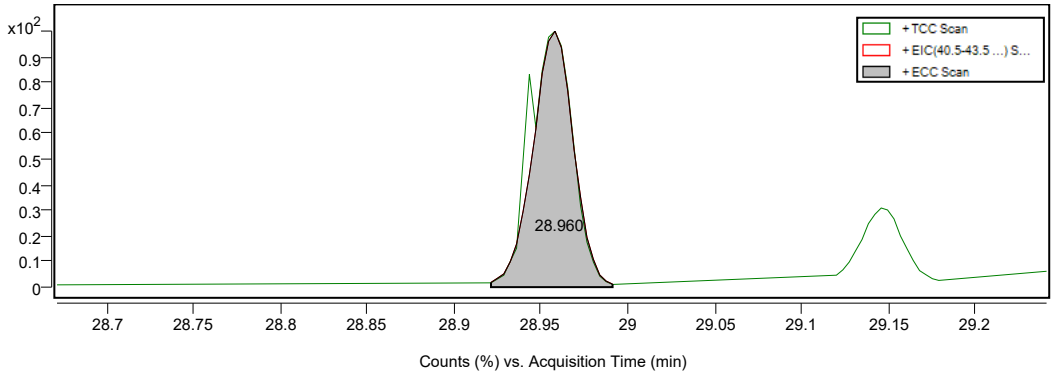
Compound Discovery Report

Agilent | Trusted Answers

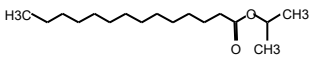
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Tetradecanoate <isopropyl->	C17H34O2		LibSearch	28.960			110-27-0	85.97		
Isopropyl tetradecanoate	C17H34O2		LibSearch	28.960	-12.460		110-27-0	81.08		
Isopropyl myristate	C17H34O2		LibSearch	28.960	-1.273		110-27-0	80.05		
Isopropyl myristate	C17H34O2		LibSearch	28.960	-1.273		110-27-0	79.44		
Isopropyl myristate	C17H34O2		LibSearch	28.960	-1.273		110-27-0	77.63		
Isopropyl myristate	C17H34O2		LibSearch	28.960	-1.273		110-27-0	76.60		
Isopropyl myristate	C17H34O2		LibSearch	28.960	-1.273		110-27-0	76.60		
Tetradecanoic acid, propyl ester	C17H34O2		LibSearch	28.960	-2.340		14303-70-9	72.62		
Tetradecanoic acid, propyl ester	C17H34O2		LibSearch	28.960	-2.340		14303-70-9	69.50		
Tetradecanoic acid	C14H28O2		LibSearch	28.960	-0.523		544-63-8	65.25		
Butyl myristate	C18H36O2		LibSearch	28.960	-4.006		110-36-1	64.65		
Butyl myristate	C18H36O2		LibSearch	28.960	-4.006		110-36-1	63.69		
i-Propyl 12-methyl-tridecanoate	C17H34O2		LibSearch	28.960	-0.206		1000336-60-4	63.67		
Myristic acid isobutyl ester	C18H36O2		LibSearch	28.960	-2.940		25263-97-2	63.64		
Myristic acid isobutyl ester	C18H36O2		LibSearch	28.960	-2.940		25263-97-2	63.52		
Tetradecanoic acid, pentyl ester	C19H38O2		LibSearch	28.960	-5.656		1000405-18-7	63.41		
Tetradecanoic acid	C14H28O2		LibSearch	28.960	-0.523		544-63-8	63.23		
2-Undecanol myristate	C25H50O2		LibSearch	28.960	-14.523		55194-47-3	62.90		
Tetradecanoic acid	C14H28O2		LibSearch	28.960	-0.523		544-63-8	61.87		
Tetradecanoic acid	C14H28O2		LibSearch	28.960	-0.523		544-63-8	61.13		
Tetradecanoic acid	C14H28O2		LibSearch	28.960	-0.523		544-63-8	61.13		
Tetradecanoic acid <n->	C14H28O2		LibSearch	28.960			544-63-8	60.37		
Butyl myristate	C18H36O2		LibSearch	28.960	-4.006		110-36-1	59.69		
Myristic anhydride	C28H54O3		LibSearch	28.960	-22.840		626-29-9	59.33		
Tetradecanoic acid	C14H28O2		LibSearch	28.960	-0.523		544-63-8	57.78		
Tetradecanoic acid, dodecyl ester	C26H52O2		LibSearch	28.960	-17.256		2040-64-4	55.89		
Octanoic acid <n->	C8H16O2		LibSearch	28.960			124-07-2	55.43		
Heptanoic acid <n->	C7H14O2		LibSearch	28.960			111-14-8	54.92		
Octanoic acid	C8H16O2		LibSearch	28.960	14.590		124-07-2	54.77		
Undecanoic acid, 2-ethyl-, methyl ester	C14H28O2		LibSearch	28.960	3.694		74810-60-9	54.57		
Octanoic acid	C8H16O2		LibSearch	28.960	9.410		124-07-2	54.53		
Pentadecylic acid	C15H30O2		LibSearch	28.960			1002-84-2	54.32		
Tetradecanoic acid, propyl ester	C17H34O2		LibSearch	28.960	-2.340		14303-70-9	54.15		
Octanoic acid	C8H16O2		LibSearch	28.960	9.410		124-07-2	53.88		
Decyl acetate	C12H24O2		LibSearch	28.960	4.020		112-17-4	53.64		
Octanol acetate	C10H20O2		LibSearch	28.960	12.660		112-14-1	53.64		
1,15-Pentadecanedioic acid	C15H28O4		LibSearch	28.960	-8.123		1460-18-0	53.57		
Heptanoic acid	C7H14O2		LibSearch	28.960	11.077		111-14-8	53.48		
Heptanoic acid	C7H14O2		LibSearch	28.960	11.077		111-14-8	53.26		
Acetic acid, hexyl ester	C8H16O2		LibSearch	28.960	12.560		142-92-7	53.15		
Hexyl acetate	C8H16O2		LibSearch	28.960	20.910		142-92-7	53.11		
Heptanoic acid	C7H14O2		LibSearch	28.960	11.077		111-14-8	53.10		
Octanoic acid	C8H16O2		LibSearch	28.960	9.410		124-07-2	52.95		
n-Capric acid isopropyl ester	C13H26O2		LibSearch	28.960	5.344		2311-59-3	52.88		
Heptanoic acid	C7H14O2		LibSearch	28.960	11.077		111-14-8	52.76		
Myristyl myristate	C28H56O2		LibSearch	28.960	-20.573		3234-85-3	52.23		
Octanoic acid	C8H16O2		LibSearch	28.960	9.410		124-07-2	51.71		
Hexanoic acid <delta-methyl->	C7H14O2		LibSearch	28.960			628-46-6	51.69		
Hexyl acetate	C8H16O2		LibSearch	28.960			142-92-7	51.44		
Acetic acid, decyl ester	C12H24O2		LibSearch	28.960	5.944		112-17-4	51.19		

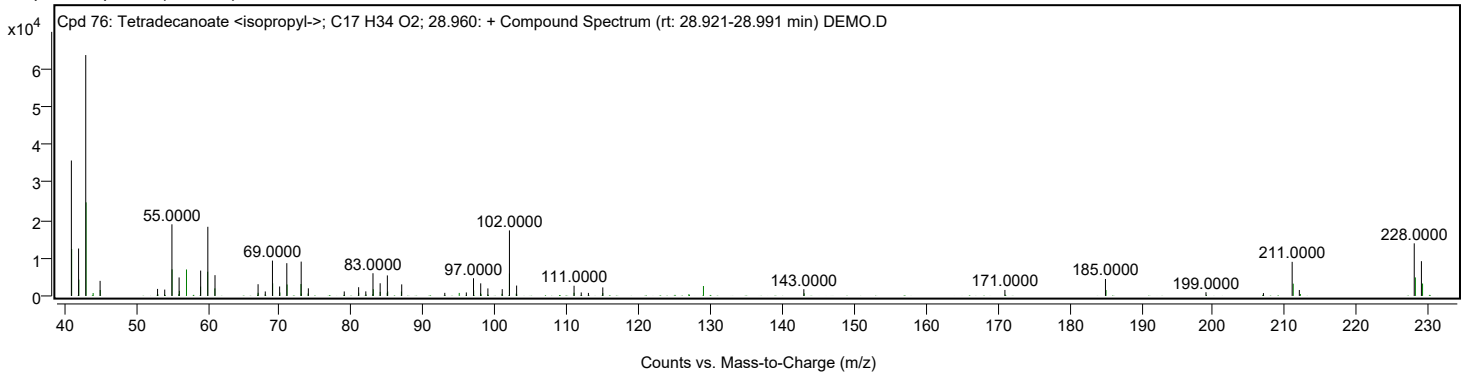
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



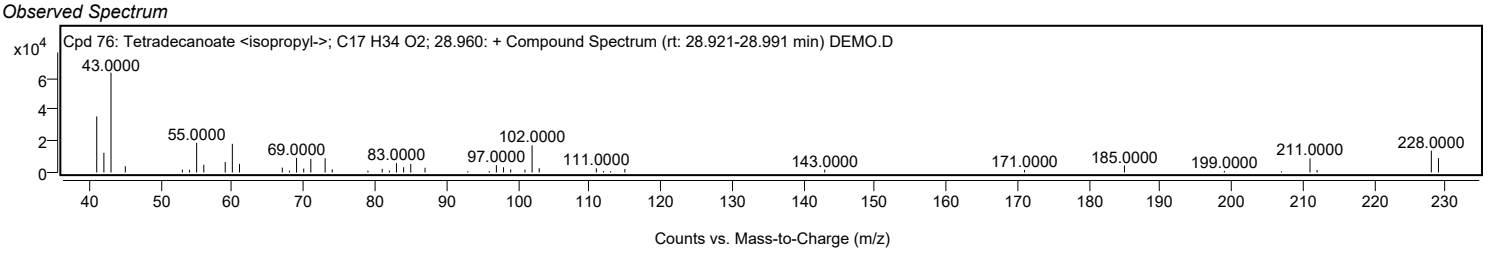
Tetradecanoate <isopropyl->

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			85.97			PWNose.xml

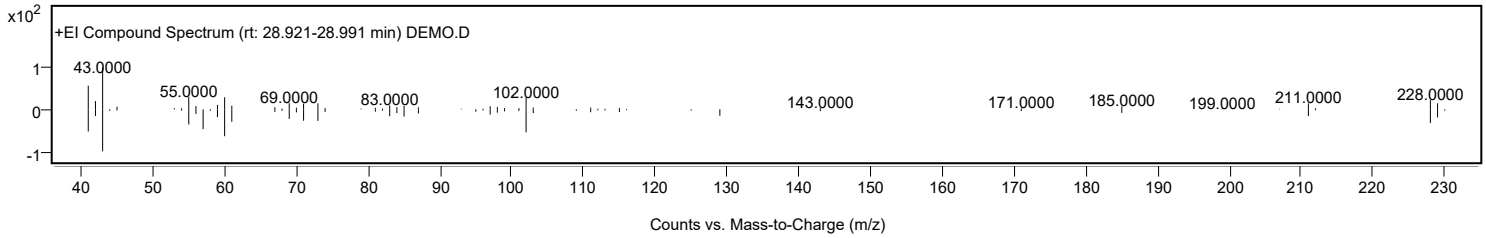
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			85.97			PWNose.xml

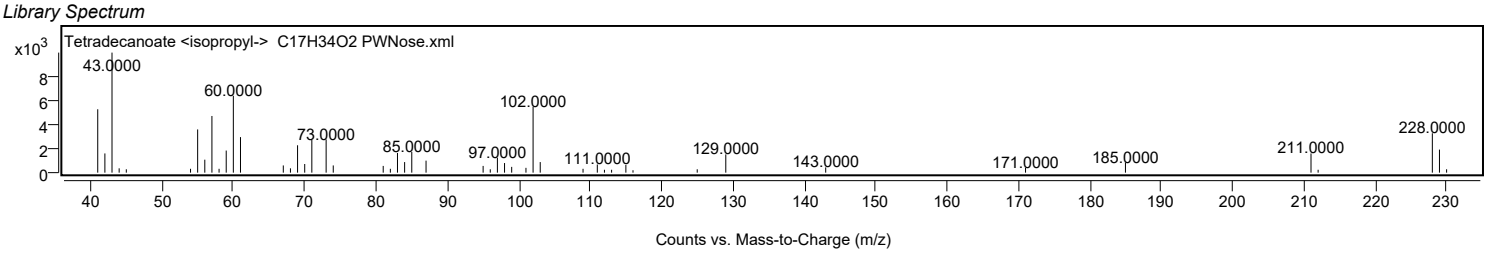
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 77: 2,2-Diethoxyacetophenone

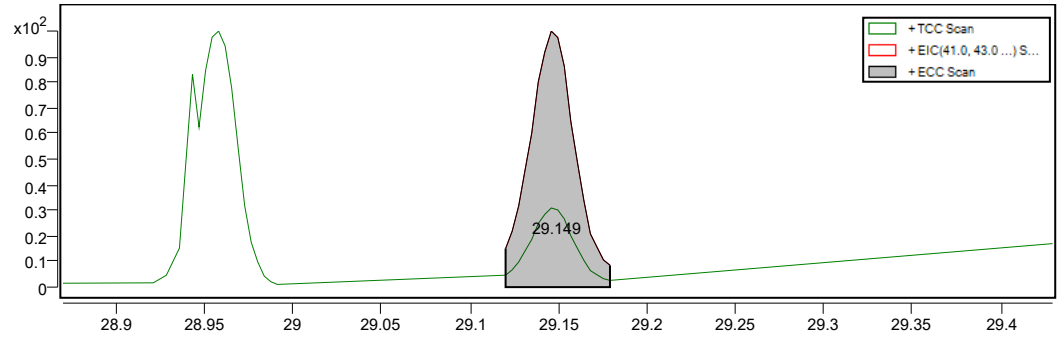
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
2,2-Diethoxyacetophenone	C12 H16 O3	29.149			6175-45-7	LibSearch	59.63	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		59.63			50		

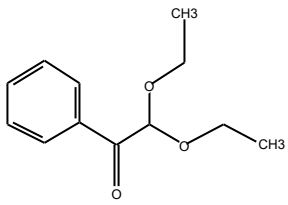
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
2,2-Diethoxyacetophenone	C12H16O3		LibSearch	29.149	3.916		6175-45-7	59.63		
2,2-Diethoxyacetophenone	C12H16O3		LibSearch	29.149	3.916		6175-45-7	58.81		
2,2-Diethoxyacetophenone	C12H16O3		LibSearch	29.149	3.916		6175-45-7	57.75		
Benzene, (3-iodo-1-methoxy-1-methylpropyl)-	C11H15IO		LibSearch	29.149	2.532		1010327-38-7	56.81		
Benzene, 1-(1,3-dimethyl-3-butenyl)-4-methoxy-	C13H18O		LibSearch	29.149	6.099		74672-05-2	56.15		
Benzamide, 4-methoxy-N-(2-phenylethyl)-N-butyl-	C20H25NO2		LibSearch	29.149	-11.734		1000451-45-2	55.78		
Benzamide, 2-methoxy-N-(2-phenylethyl)-N-butyl-	C20H25NO2		LibSearch	29.149	-11.734		1000451-45-9	55.55		
1,3-Benzodioxole-5-propanal, .alpha.-methyl-, oxime (peak 1)	C11H13NO3		LibSearch	29.149	0.366		1000475-84-1	55.05		
Benzamide, 2-methoxy-N-(2-phenylethyl)-N-isobutyl-	C20H25NO2		LibSearch	29.149	-10.668		1000451-45-8	54.41		
5,5'-((2R,3S)-2,3-Dimethylbutane-1,4-diyl)bis(benzo[d][1,3]dioxole)	C20H22O4		LibSearch	29.149	-12.918		110269-50-6	54.24		
Benzene, (2,2-dimethoxyethyl)-	C10H14O2		LibSearch	29.149	9.482		101-48-4	54.06		
di[1-(3,4-methylenedioxyphenyl)-2-propyl]methylamine	C21H25NO4		LibSearch	29.149	-15.384		1000378-88-6	54.02		
3-Phenyl-3-pentanol	C11H16O		LibSearch	29.149	7.766		1565-71-5	53.89		
1-Hexen-4-ol, 3-methyl-4-phenyl-	C13H18O		LibSearch	29.149	5.682		344308-86-7	53.81		
1-Adamantanecarboxylic acid, 2-propenyl ester	C14H20O2		LibSearch	29.149	5.649		107144-95-6	53.53		
1,3-Benzodioxole-5-propanal, .alpha.-methyl-, oxime (peak 2)	C11H13NO3		LibSearch	29.149	0.366		1000475-84-0	53.45		
m-Anisoyl amide, N-(2-phenylethyl)-N-butyl-	C20H25NO2		LibSearch	29.149	-11.734		1010451-74-0	53.18		
Benzene, (2,2-dimethoxyethyl)-	C10H14O2		LibSearch	29.149	9.482		101-48-4	53.14		
Benzene, 1-(1,3-dimethyl-3-butenyl)-3-methoxy-	C13H18O		LibSearch	29.149	6.099		74672-09-6	52.83		
o-Anisic acid, morpholide	C12H15NO3		LibSearch	29.149	-1.184		1000307-05-5	52.58		
m-Anisoyl amide, N-(2-phenylethyl)-N-isobutyl-	C20H25NO2		LibSearch	29.149	-10.668		1010451-73-9	52.52		
2-Hydroxy-2-phenylbutyramide	C10H13NO2		LibSearch	29.149	2.599		52839-87-9	52.49		
3-[2-(4-Methoxy-phenyl)-2-oxo-ethyl]-5-phenyl-3H-[1,3,4]oxadiazol-2-one	C17H14N2O4		LibSearch	29.149	-16.168		1000296-88-4	51.98		
Benzene, (2,2-dimethoxyethyl)-	C10H14O2		LibSearch	29.149	9.482		101-48-4	51.92		
Benzene, (2,2-dimethoxyethyl)-	C10H14O2		LibSearch	29.149	9.482		101-48-4	51.50		
p-Anisic acid, morpholide	C12H15NO3		LibSearch	29.149	-1.184		1010307-49-2	51.12		
Phenylacetaldehyde dimethyl acetal	C10H14O2		LibSearch	29.149			101-48-4	51.08		
MDA 2-amido analog	C11H13NO3		LibSearch	29.149	-0.534		858215-05-1	50.98		
Helional (Tropional)	C11H12O3		LibSearch	29.149			1205-17-0	50.83		
2-Methoxy-4-methyl-1-pentylbenzene	C13H20O		LibSearch	29.149	4.249		1000408-33-6	50.82		
Furazan-3-amine, 4-(3,4-methylenedioxybenzyloxy)-	C10H9N3O4		LibSearch	29.149	-4.918		1000294-23-2	50.80		
1,3-Benzodioxole-5-propanal, .alpha.-methyl-, oxime, trimethylsilyl ether (isomer 2)	C14H21NO3Si		LibSearch	29.149	-2.051		1000475-93-6	50.59		
Benzene, 1-methoxy-4-(1-methylpropyl)-	C11H16O		LibSearch	29.149	8.866		4917-90-2	49.87		
1,4-Benzenediamine, N-(1-methylheptyl)-	C14H24N2		LibSearch	29.149	-3.118		39563-50-3	49.68		
Hexahydro-1,5-dimethyl-3-phenyl-1,3,5-triazine-2-thione	C11H15N3S		LibSearch	29.149	-3.201		27023-54-7	49.59		
5-[3,4-Methylenedioxybenzyl]hydantoin	C11H10N2O4		LibSearch	29.149	-6.818		62682-17-1	49.58		
MDA 2-amido analog	C11H13NO3		LibSearch	29.149	-0.534		858215-05-1	49.42		
o-Anisic acid, 3,4-dichlorophenyl ester	C14H10Cl2O3		LibSearch	29.149	-7.234		1000307-79-4	49.42		
3-[2-(2-Methoxy-phenyl)-2-oxo-ethyl]-5-phenyl-3H-[1,3,4]oxadiazol-2-one	C17H14N2O4		LibSearch	29.149	-16.168		1000296-89-1	49.41		
Alpha-aminomethyl-alpha-ethylbenzyl alcohol	C10H15NO		LibSearch	29.149	5.366		770-65-0	49.27		
3,4-Bis(1,3-benzodioxol-5-ylmethyl)-4-hydroxyoxolan-2-one, TMS	C23H26O7Si		LibSearch	29.149	-24.851		1000503-27-9	49.26		
Piperonyl piperazine	C12H16N2O2		LibSearch	29.149	-4.101		32231-06-4	49.08		
Ethyl 5-(2H-1,3-benzodioxol-5-ylmethyl)-4,5-dihydro-1,2-oxazole-3-carboxylate	C14H15NO5		LibSearch	29.149	-6.551		1000436-98-9	49.07		
Piperonyl piperazine	C12H16N2O2		LibSearch	29.149	-4.101		32231-06-4	48.89		
Benzamide, 2-methoxy-N-methallyl-	C12H15NO2		LibSearch	29.149	0.016		1000339-10-6	48.79		
1,3-Benzenediol, O,O'-di(2-methoxybenzoyl)-	C22H18O6		LibSearch	29.149	-20.284		1000330-77-9	48.77		
1,2-Benzenediol, O-(2-methoxybenzoyl)-O'-(propargyloxycarbonyl)-	C18H14O6		LibSearch	29.149	-12.101		1000329-71-2	48.70		
o-Anisic acid, 4-chlorophenyl ester	C14H11ClO3		LibSearch	29.149	-4.234		1000307-79-0	48.69		
Benzamide, 2-methoxy-N-(2-butyl)-N-methyl-	C13H19NO2		LibSearch	29.149	2.199		1000464-25-0	48.66		
Atropic acid, TMS derivative	C12H16O2Si		LibSearch	29.149	6.899		1000484-83-7	48.55		

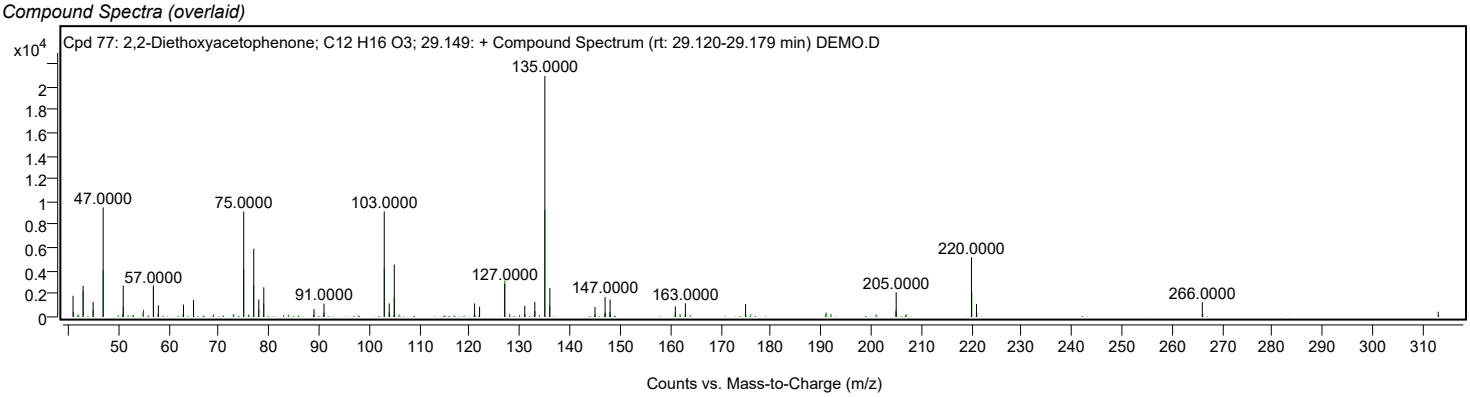
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



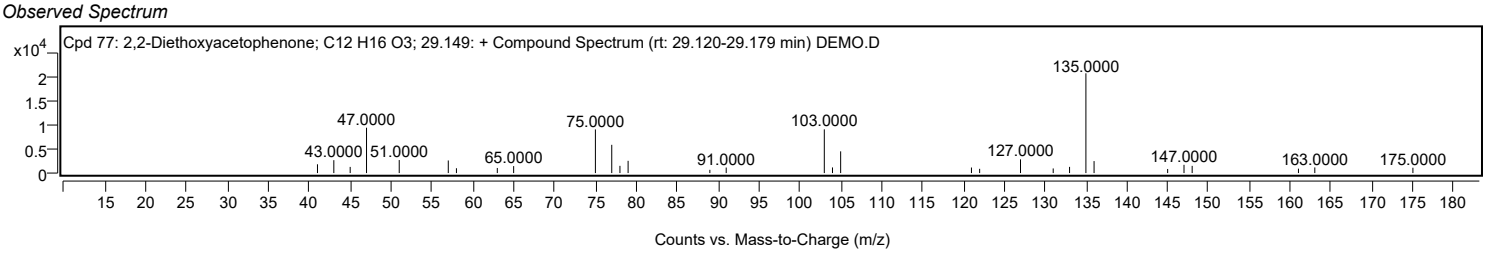
2,2-Diethoxyacetophenone

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			59.63			NIST.L

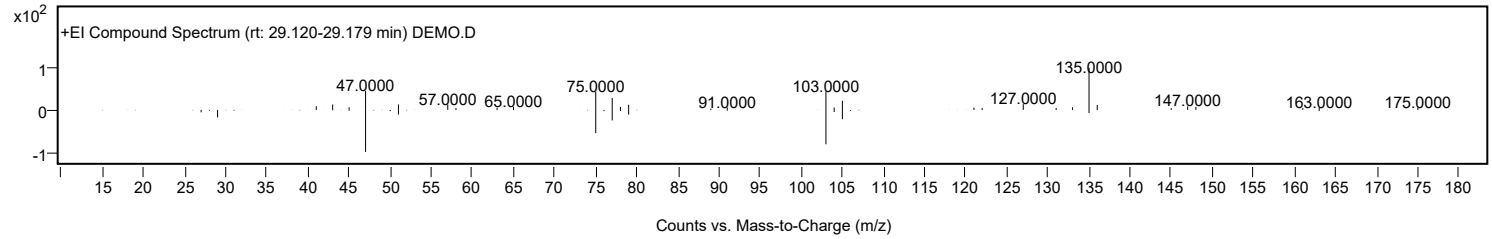
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			59.63			NIST.L

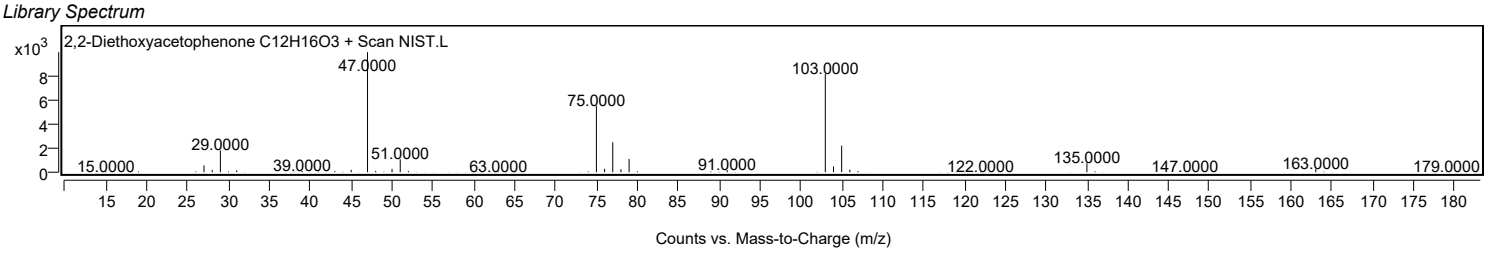
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 78: Amberlyn

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Amberlyn	C16 H28 O	29.573			3738-00-9	LibSearch	74.08	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		74.08			50		

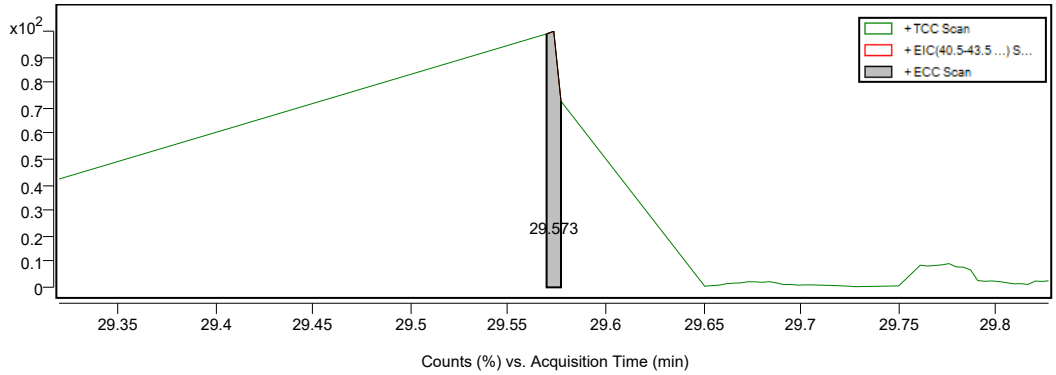
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

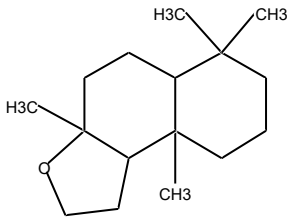
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Amberlyn	C16H28O		LibSearch	29.573			3738-00-9	74.08		
Naphtho[2,1-b]furan, dodecahydro-3a,6,6,9a-tetramethyl-	C16H28O		LibSearch	29.573	2.340		3738-00-9	72.35		
Ambroxan	C16H28O		LibSearch	29.573			6790-58-5	72.00		
Ambroxide	C16H28O		LibSearch	29.573	-9.237		6790-58-5	71.04		
Ambrox	C16H28O		LibSearch	29.573	2.340		100679-85-4	68.55		
Benzene, 1-(1-hydroxyheptyl)-3-[1-(tetrahydropyran-2-yloxy)heptyl]-	C25H42O3		LibSearch	29.573	-19.143		1000196-54-9	55.46		
Heptane, 1,7-dibromo-	C7H14Br2		LibSearch	29.573	7.757		4549-31-9	51.15		
Heptane, 1,7-dibromo-	C7H14Br2		LibSearch	29.573	7.757		4549-31-9	49.26		
Isoascaridole	C10H16O2		LibSearch	29.573			1619-26-7	48.98		
Decane, 1,10-dibromo-	C10H20Br2		LibSearch	29.573	2.773		4101-68-2	48.68		
5-Methylisoxazol-3-amine bis(trifluoroacetate)	C8H4F6N2O3		LibSearch	29.573	11.690		1000373-35-6	48.66		
4,7-Dimethyl-5-decyne-4,7-diol	C12H22O2		LibSearch	29.573	5.990		126-87-4	48.23		
7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(2-methyloxiranyl)-	C10H16O2		LibSearch	29.573	10.773		96-08-2	48.02		
Decane, 1,10-dibromo-	C10H20Br2		LibSearch	29.573	2.773		4101-68-2	47.82		
Glutaric acid, di(2-methoxyphenyl) ester	C19H20O6		LibSearch	29.573	-13.377		1000358-67-4	46.75		
Dill ether	C10H16O		LibSearch	29.573	14.463		74410-10-9	46.62		
Heptane, 1,7-dibromo-	C7H14Br2		LibSearch	29.573	7.757		4549-31-9	46.39		
(1R,2S,4S,5R,7R)-5-isopropyl-1-methyl-3,8-dioxatricyclo[5.1.0.02,4]octane	C10H16O2		LibSearch	29.573	12.723		1000439-66-9	46.27		
3-Tetradecyn-1-ol	C14H26O		LibSearch	29.573	1.690		55182-74-6	46.25		
4-Hexen-1-ol, 2-ethenyl-2,5-dimethyl-	C10H18O		LibSearch	29.573	10.423		50598-21-5	46.19		
Decane, 1,2-dibromo-	C10H20Br2		LibSearch	29.573	3.840		28467-71-2	46.14		
Decane, 1-bromo-	C10H21Br		LibSearch	29.573	7.723		112-29-8	45.95		
7-Oxabicyclo[4.1.0]heptane, 1-methyl-4-(2-methyloxiranyl)-	C10H16O2		LibSearch	29.573	10.773		96-08-2	45.88		
3-Methyl-1-dodecyn-3-ol	C13H24O		LibSearch	29.573	6.190		24424-78-0	45.75		
Cyclopropanemethanol, 2,2,3,3-tetramethyl-	C8H16O		LibSearch	29.573	14.023		2415-96-5	45.73		
Octane, 1,8-dibromo-	C8H16Br2		LibSearch	29.573	6.090		4549-32-0	45.69		
Hexane, 1-bromo-	C6H13Br		LibSearch	29.573	14.340		111-25-1	45.65		
1-Bromo-8-chlorooctane	C8H16BrCl		LibSearch	29.573	7.273		1000438-83-6	45.56		
(1S,2R,4R,7R)-4-Isopropyl-7-methyl-3,8-dioxatricyclo[5.1.0.02,4]octane	C10H16O2		LibSearch	29.573	12.523		1619-26-7	45.45		
1-Bromo-5-methylhexane	C7H15Br		LibSearch	29.573	13.757		35354-37-1	45.42		
Decane, 5,6-bis(2,2-dimethylpropylidene)-, (Z,Z)-	C20H38		LibSearch	29.573	-0.593		73002-85-4	45.42		
Nonane, 1-bromo-	C9H19Br		LibSearch	29.573	9.373		693-58-3	45.27		
Cyclopropanecarboxylic acid, tridec-2-ynyl ester	C17H28O2		LibSearch	29.573	-2.060		1000299-38-2	45.23		
5,9-Methanobenzocyclooctene-1(2H)-one, 3,4,5,6,7,8,9,10-octahydro-3,5-dihydroxy-3,3,7,7,9-pentamethyl-	C18H28O3		LibSearch	29.573	-8.010		54833-46-4	45.16		
Lavandulol	C10H18O		LibSearch	29.573	15.273		498-16-8	45.14		
Bis(2-isopropyl-5-methylcyclohexyl) methylphosphonate (isomer 3)	C21H41O3P		LibSearch	29.573			1000510-36-7	45.02		
2-Pentenoic acid, 3-methyl-5-(2,6,6-trimethyl-1-cyclohexenyl)	C15H24O2		LibSearch	29.573	-1.327		1000196-81-2	44.97		
Deca-2,6-dien-10-al <2,6-dimethyl->	C12H20O		LibSearch	29.573			762-26-5	44.96		
Dimethyl heptenone	C9H16O		LibSearch	29.573			33046-81-0	44.96		
4-Hexen-1-ol, 5-methyl-2-(1-methylethenyl)-, (R)-	C10H18O		LibSearch	29.573	10.473		498-16-8	44.94		
Limonene oxide, cis-	C10H16O		LibSearch	29.573	12.390		13837-75-7	44.89		
Decane, 1-bromo-	C10H21Br		LibSearch	29.573	7.723		112-29-8	44.88		
Dill ether	C10H16O		LibSearch	29.573			74410-10-9	44.86		
Pentadecane, 1-bromo-	C15H31Br		LibSearch	29.573	-0.560		629-72-1	44.83		
p-Cyanophenyl p-(2-butoxyethoxy)benzoate	C20H21NO4		LibSearch	29.573	-14.993		67131-98-0	44.81		
2,6-Heptadienal, 2,4-dimethyl-	C9H14O		LibSearch	29.573	12.657		85136-08-9	44.80		
2,5-Octadiene, 3,4,5,6-tetramethyl-	C12H22		LibSearch	29.573	11.290		247797-85-9	44.79		
2-Bromopropionic acid, cyclopentyl ester	C8H13BrO2		LibSearch	29.573	8.590		149863-74-1	44.73		
Lavandulyl acetate	C12H20O2		LibSearch	29.573	9.873		20777-39-3	44.67		
Sesquilavandulol <(E)->	C15H26O		LibSearch	29.573			120707-27-9	44.67		

Compound Chromatograms (overlaid)

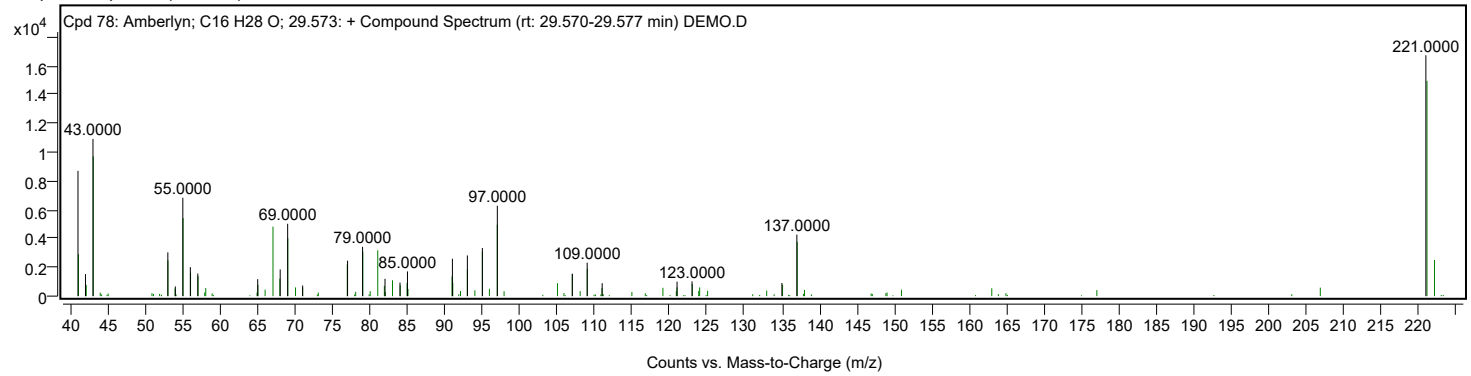


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



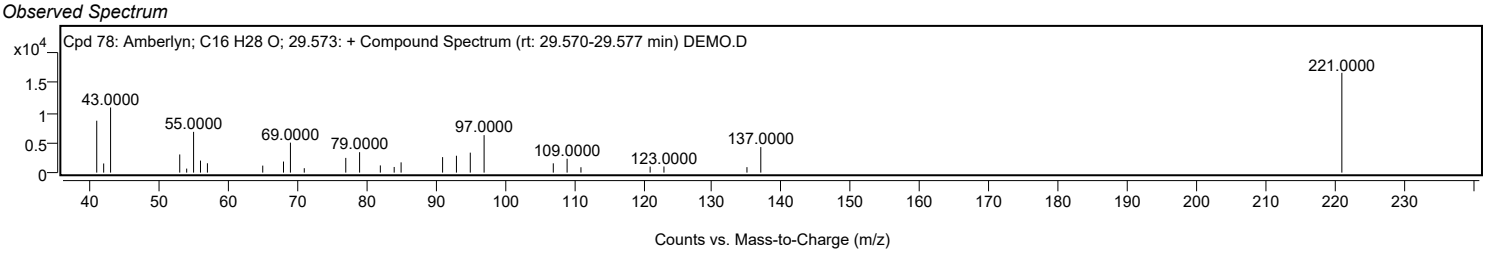
Amberlyn

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			74.08			PWNose.xml

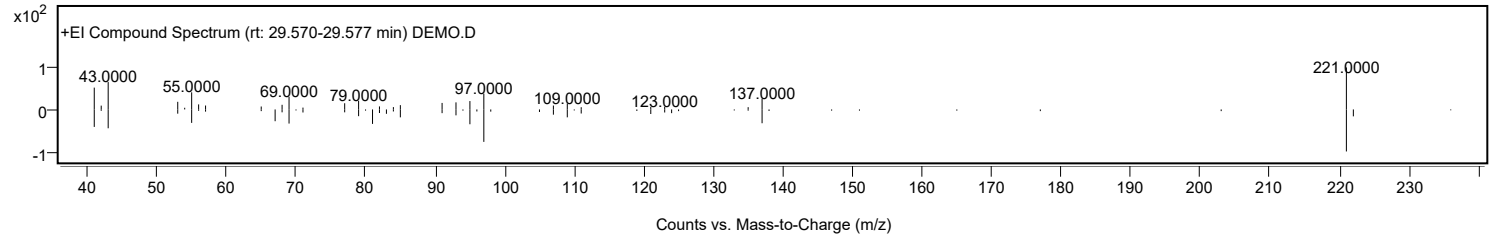
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			74.08			PWNose.xml

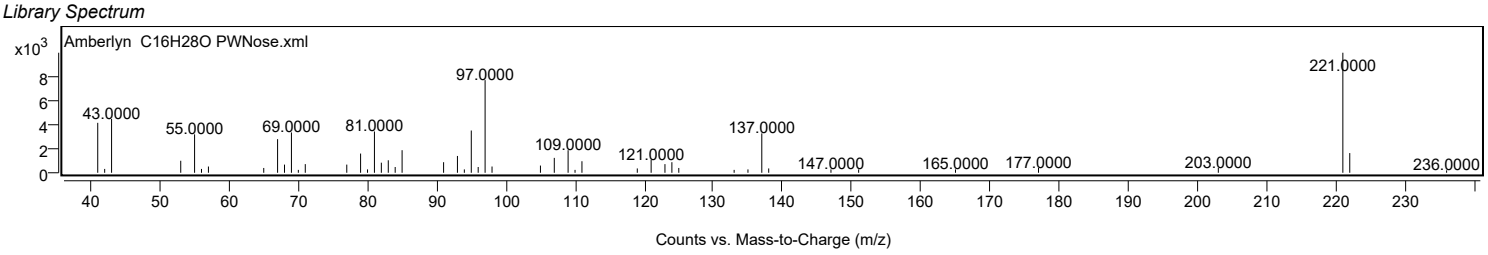
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 79: N-Carboxyethylrhodanine

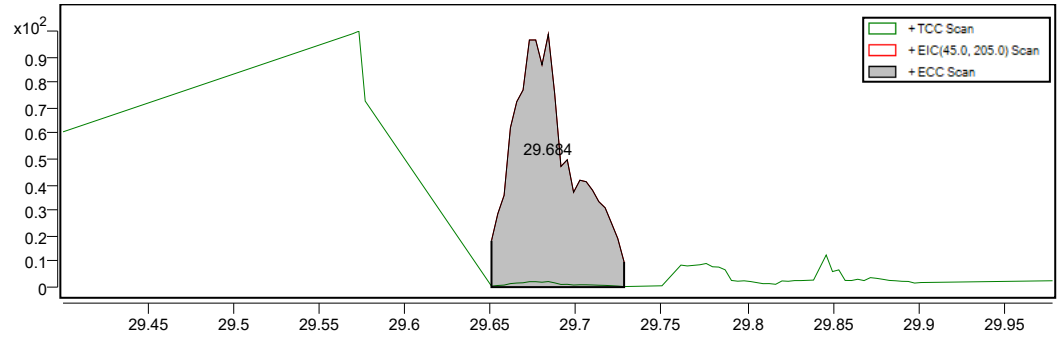
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
N-Carboxyethylrhodanine	C6 H7 N O3 S2	29.684			7025-19-6	LibSearch	20.64	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		20.64			5		

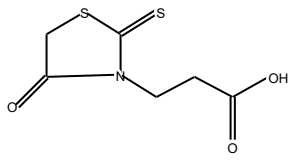
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
N-Carboxyethylrhodanine	C6H7NO3S2		LibSearch	29.684	-2.400		7025-19-6	20.64		
Adenosine, 2',3'-O-di-tert-butyldimethylsilyl-5',5'-dimethyl-	C24H45N5O4Si2		LibSearch	29.684	-23.300		1000127-34-4	14.99		
3-[6-Chloro-1-(3-methoxypropyl)-1,3-benzodiazol-2-yl]prop-2-enoic acid	C14H15ClN2O3		LibSearch	29.684	-10.083		1000459-11-1	13.97		
1,3-Cyclohexanedione, 2-(2-hydroxy-6-oxo-1-cyclohexen-1-yl)-2-(methoxymethyl)-	C14H18O5		LibSearch	29.684	-7.716		29817-42-3	12.43		
2-(7,8-Dimethoxy-1-oxophthalazin-2-yl)butanedioic acid	C14H14N2O7		LibSearch	29.684	-17.516		1000459-40-8	11.17		

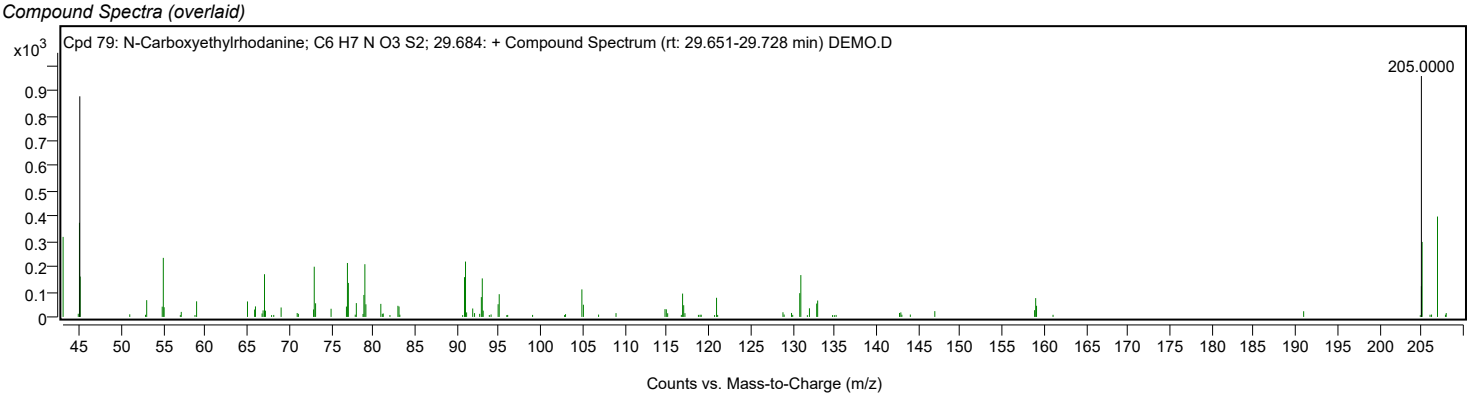
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



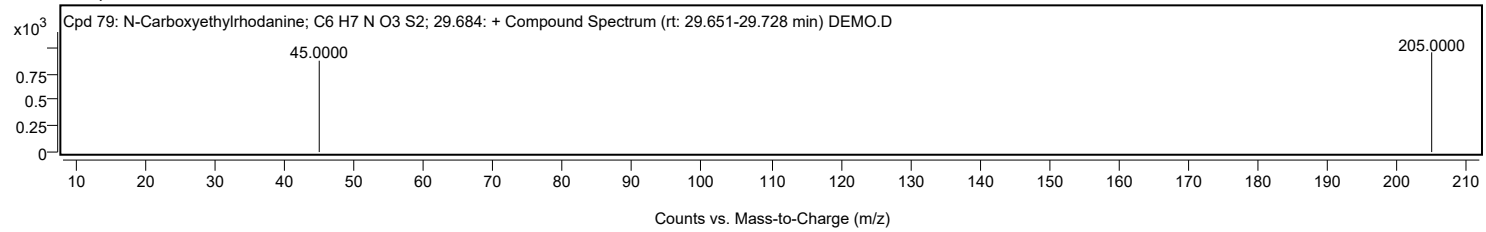
N-Carboxyethylrhodanine

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			20.64			NIST.L

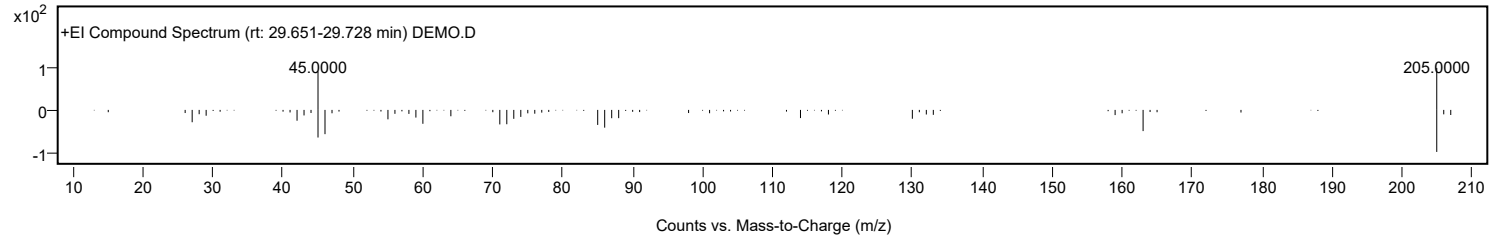
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			20.64			NIST.L

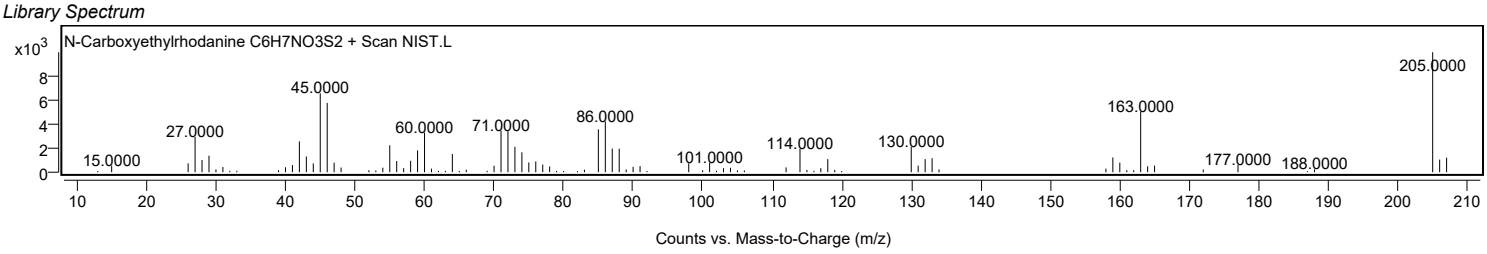
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 80: Hexanethioic acid, S-methyl ester

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Hexanethioic acid, S-methyl ester	C7 H14 O S	29.768			2432-77-1	LibSearch	61.97	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		61.97			50		

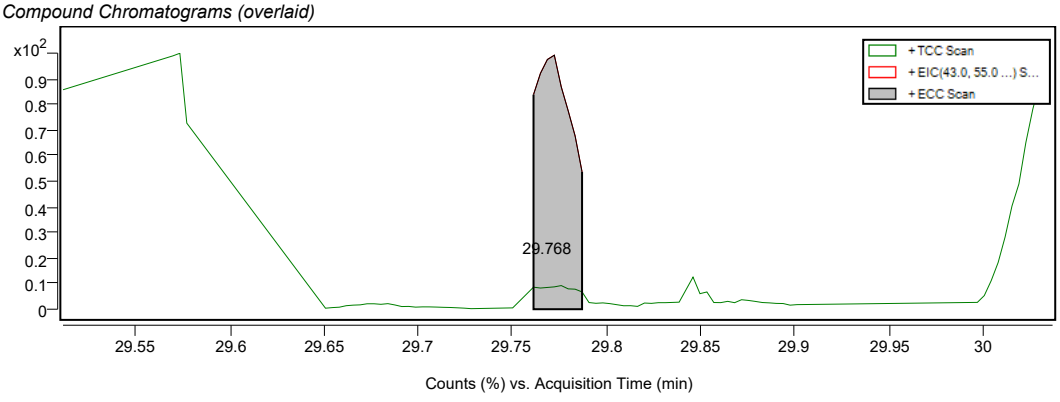
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

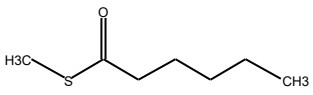
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Hexanethioic acid, S-methyl ester	C7H14OS		LibSearch	29.768	11.368		2432-77-1	61.97		
Pentanoic acid, 2-methyl-, anhydride	C12H22O3		LibSearch	29.768	6.618		63169-61-9	61.58		
Ethyl 4-(ethyloxy)-2-oxobut-3-enoate	C8H12O4		LibSearch	29.768	9.702		1000305-38-2	59.07		
Butanoic acid, 2-(2-cyanoethyl)-2-(2-ethyl-1-oxobutoxy)-3-oxo-, ethyl ester	C15H23NO5		LibSearch	29.768	-4.898		1010460-88-7	57.71		
n-Caproic acid vinyl ester	C8H14O2		LibSearch	29.768	13.535		3050-69-9	57.50		
4H-Imidazol-4-one, 2-amino-1,5-dihydro-	C3H5N3O		LibSearch	29.768	9.285		503-86-6	56.91		
6,7-Dodecanedione	C12H22O2		LibSearch	29.768	5.002		13757-90-9	56.30		
2-Hexanone, 6-bromo-	C6H11BrO		LibSearch	29.768	12.268		10226-29-6	55.98		
Pentanoic acid, 2-methyl-, anhydride	C12H22O3		LibSearch	29.768	6.618		63169-61-9	55.45		
2-Pentene, 5-(pentyloxy)-, (E)-	C10H20O		LibSearch	29.768	11.452		56052-85-8	55.13		
2,5-Dimethyl-2-(2-tetrahydrofuryl)tetrahydrofuran	C10H18O2		LibSearch	29.768	9.535		1010112-55-9	55.02		
Hexanoic acid, anhydride	C12H22O3		LibSearch	29.768	4.485		2051-49-2	54.95		
2,5-Hexanedione	C6H10O2		LibSearch	29.768	14.935		110-13-4	54.93		
Hexanoic acid, anhydride	C12H22O3		LibSearch	29.768	4.485		2051-49-2	54.81		
Hexanoic acid, anhydride	C12H22O3		LibSearch	29.768	4.485		2051-49-2	54.17		
2-Furancarboxylic acid, tetrahydro-3-methyl-5-oxo-	C6H8O4		LibSearch	29.768	8.035		22073-04-7	53.64		
Hexanoic acid, thio-, S-butyl ester	C10H20OS		LibSearch	29.768	6.402		2432-79-3	53.60		
2,3-Octanedione	C8H14O2		LibSearch	29.768	11.635		585-25-1	53.56		
Cyclohexanecarboxylic acid, 1-(2-ethyl-1-oxobutoxy)-2-oxo-, ethyl ester	C15H24O5		LibSearch	29.768	-3.432		1000460-66-2	53.48		
Hexanethioic acid, S-propyl ester	C9H18OS		LibSearch	29.768	8.052		2432-78-2	53.34		
Hexano-dibutyrin	C17H30O6		LibSearch	29.768	-6.048		65235-12-3	53.28		
2-Ethylbutyric acid, 4-nitrophenyl ester	C12H15NO4		LibSearch	29.768	-0.048		1000369-85-5	52.98		
Cyclopentanecarboxylic acid, 1-(2-ethyl-1-oxobutoxy)-2-oxo-, ethyl ester	C14H22O5		LibSearch	29.768	-1.432		1000460-66-4	52.16		
p-Nitrophenyl hexanoate	C12H15NO4		LibSearch	29.768	-1.115		956-75-2	52.07		
Hexanethioic acid, S-ethyl ester	C8H16OS		LibSearch	29.768	9.718		2450-12-6	51.99		
2,5-Hexanedione	C6H10O2		LibSearch	29.768	14.935		110-13-4	51.62		
2-Furancarboxylic acid, tetrahydro-3-methyl-5-oxo-, methyl ester	C7H10O4		LibSearch	29.768	9.535		85547-53-1	51.55		
Hexanoic acid, anhydride	C12H22O3		LibSearch	29.768	4.485		2051-49-2	51.22		
Acetonyl acetone	C6H10O2		LibSearch	29.768	24.288		110-13-4	50.67		
5-Amino-2-methyl-2H-tetrazole	C2H5N5		LibSearch	29.768			6154-04-7	50.23		
Hexanethioic acid, S-heptyl ester	C13H26OS		LibSearch	29.768	1.435		2432-80-6	50.01		
Hexanethioic acid, S-methyl ester	C7H14OS		LibSearch	29.768	11.368		2432-77-1	49.79		
2,5-Hexanedione	C6H10O2		LibSearch	29.768	14.935		110-13-4	49.75		
Hexanoic acid, cyclobutyl ester	C10H18O2		LibSearch	29.768	9.685		1000282-83-1	49.27		
Butyrate <2-ethyl-, allyl->	C9H16O2		LibSearch	29.768			7493-69-8	49.00		
Hexanohydroxamic acid	C6H13NO2		LibSearch	29.768	10.485		4312-93-0	48.85		
2-Pentenoic acid, 4-hydroxy-	C5H8O3		LibSearch	29.768	12.352		28525-83-9	48.72		
3,4-Diamino-1,2,4(4H)-triazole	C2H5N5		LibSearch	29.768	10.935		38104-45-9	48.69		
Hexanoic acid, 1,1-dimethylpropyl ester	C11H22O2		LibSearch	29.768	9.818		116423-69-9	48.64		
Pyrrolidine-2,4-dione	C4H5NO2		LibSearch	29.768	14.202		37772-89-7	48.52		
iso-Amyl levulinate	C10H18O3		LibSearch	29.768	8.868		71172-75-3	48.47		
2,5-Octanedione	C8H14O2		LibSearch	29.768	11.635		3214-41-3	48.00		
2-Ethylbutyric acid, 2-nitrophenyl ester	C12H15NO4		LibSearch	29.768	-0.048		1000369-86-5	47.95		
3,5-Diamino-1,2,4-triazole	C2H5N5		LibSearch	29.768	7.918		1455-77-2	47.86		
4-Heptanone, 3-ethyl-	C9H18O		LibSearch	29.768	13.302		1528-25-2	47.68		
3-Octanone, 2-methyl-	C9H18O		LibSearch	29.768	13.302		923-28-4	47.64		
Hexanoic acid, 2-butenyl ester	C10H18O2		LibSearch	29.768	9.918		94291-54-0	47.58		
Acetic caproic anhydride	C8H14O3		LibSearch	29.768	11.102		92351-84-3	47.53		
Butyric acid, 2,2-dimethyl-, vinyl ester	C8H14O2		LibSearch	29.768	14.952		13170-00-8	47.41		
2-Ethylbutyric acid, 4-cyanophenyl ester	C13H15NO2		LibSearch	29.768	1.902		1000369-61-1	46.78		

Compound Chromatograms (overlaid)

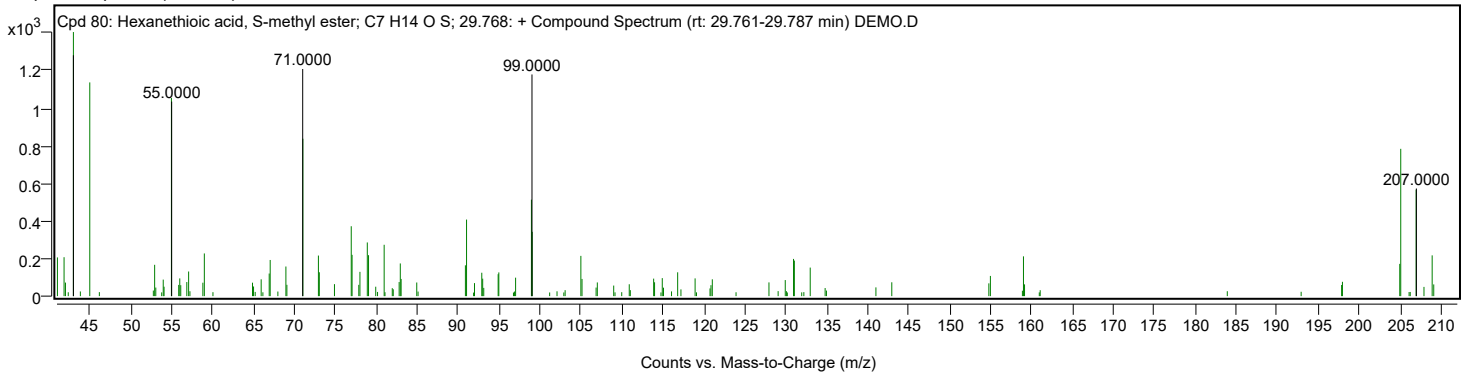


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



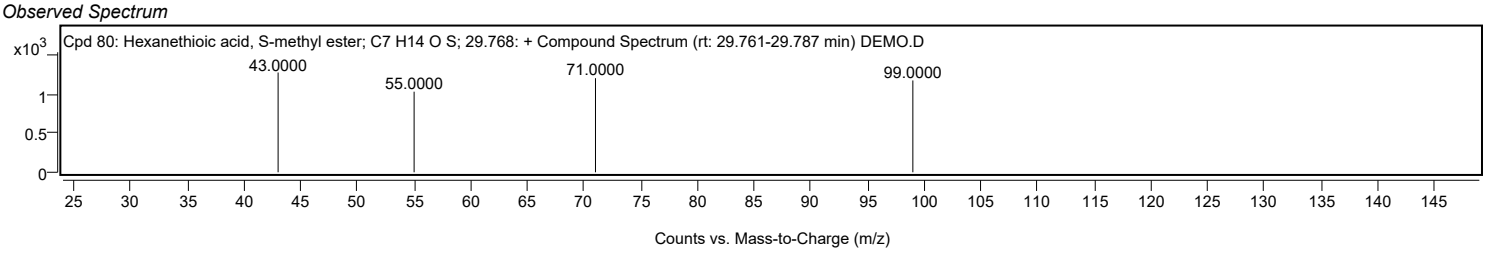
Hexanethioic acid, S-methyl ester

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			61.97			NIST.L

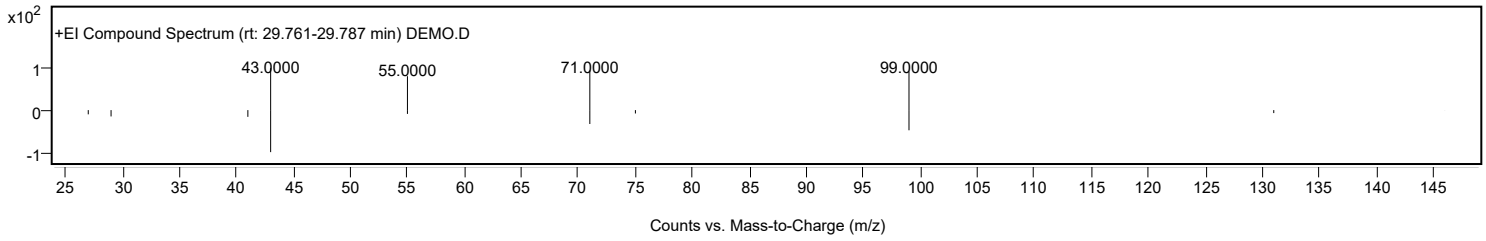
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			61.97			NIST.L

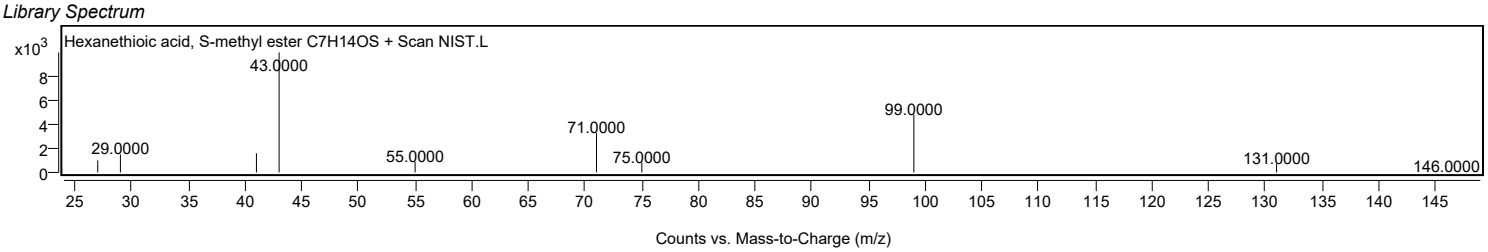
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 81: N-Carboxyethylrhodanine

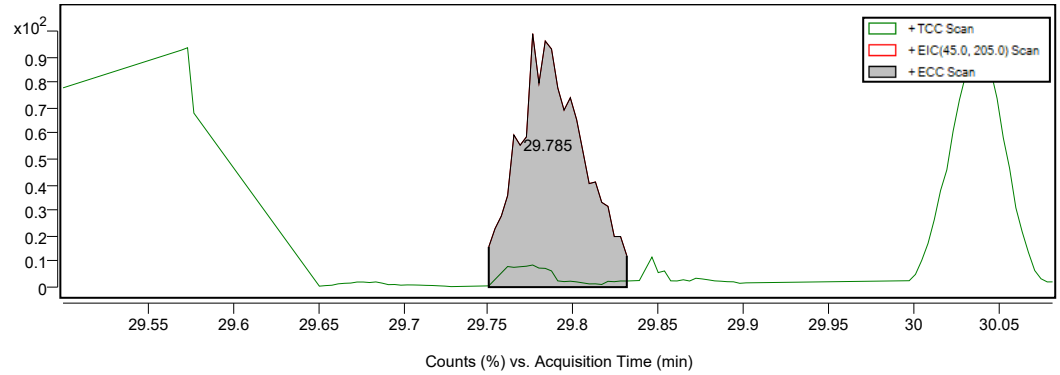
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
N-Carboxyethylrhodanine	C6 H7 N O3 S2	29.785			7025-19-6	LibSearch	20.68	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		20.68			5		

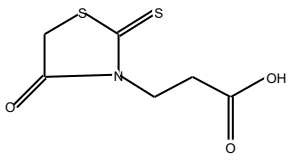
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
N-Carboxyethylrhodanine	C6H7NO3S2		LibSearch	29.785	-2.298		7025-19-6	20.68		
Adenosine, 2',3'-O-di-tert-butyldimethylsilyl-5',5'-dimethyl-	C24H45N5O4Si2		LibSearch	29.785	-23.198		1000127-34-4	15.00		
3-[6-Chloro-1-(3-methoxypropyl)-1,3-benzodiazol-2-yl]prop-2-enoic acid	C14H15ClN2O3		LibSearch	29.785	-9.982		1000459-11-1	14.00		
1,3-Cyclohexanedione, 2-(2-hydroxy-6-oxo-1-cyclohexen-1-yl)-2-(methoxymethyl)-	C14H18O5		LibSearch	29.785	-7.615		29817-42-3	12.44		
2-(7,8-Dimethoxy-1-oxophthalazin-2-yl)butanedioic acid	C14H14N2O7		LibSearch	29.785	-17.415		1000459-40-8	11.19		

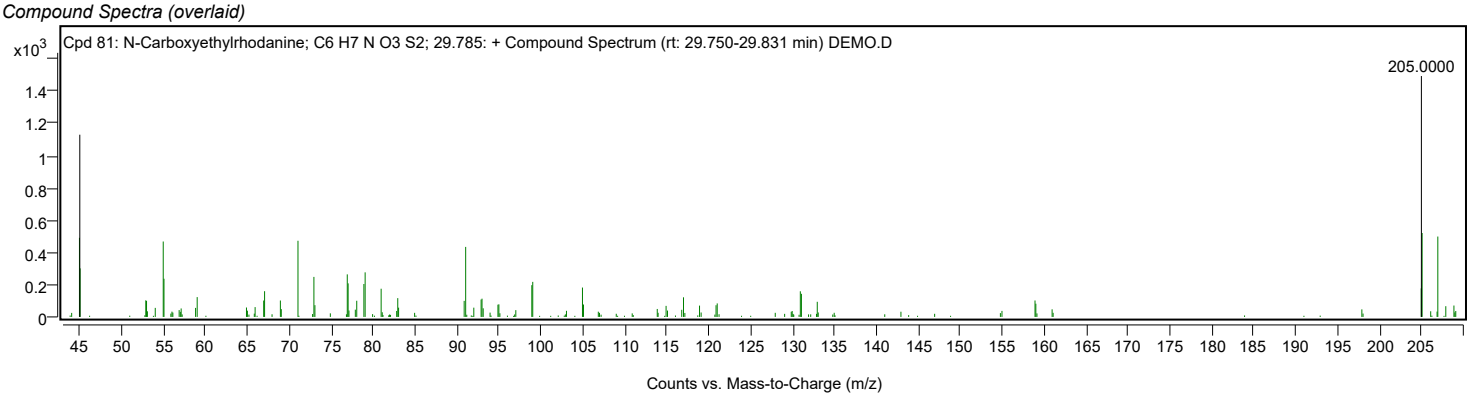
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



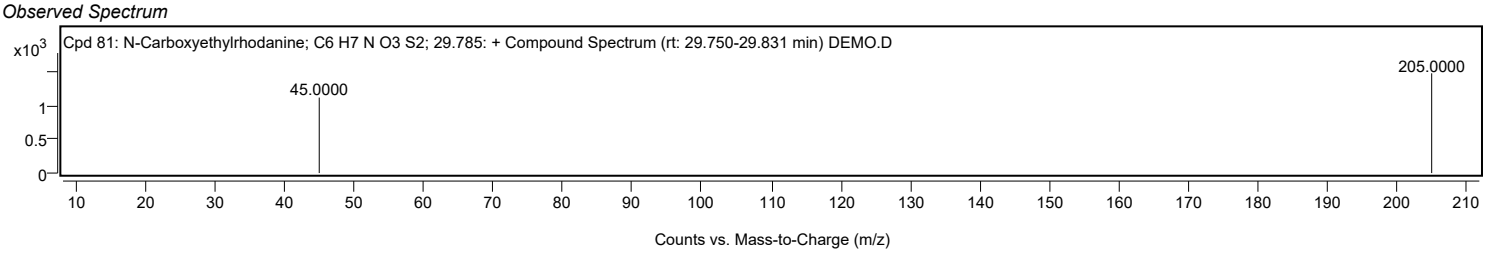
N-Carboxyethylrhodanine

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			20.68			NIST.L

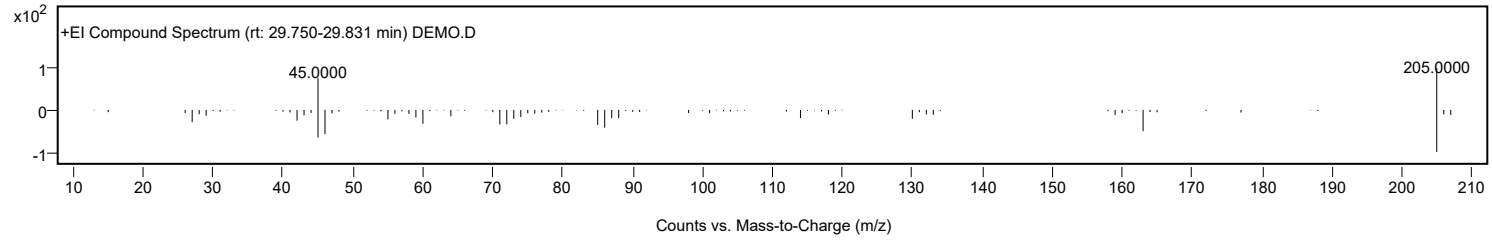
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			20.68			NIST.L

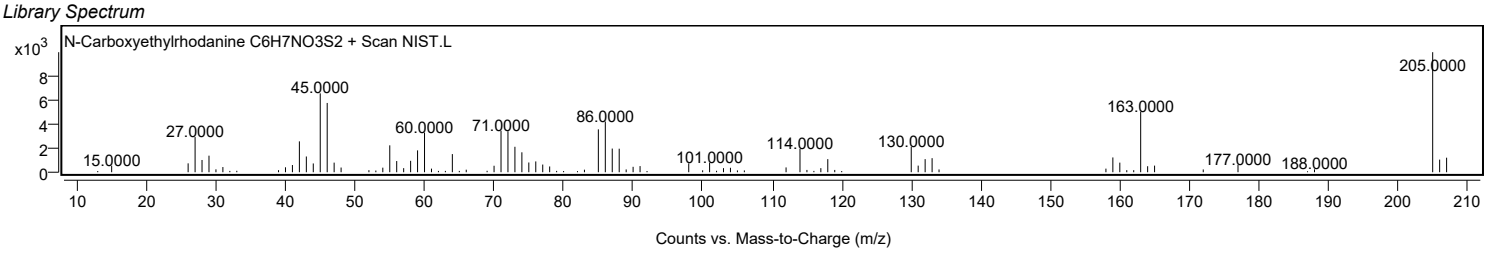
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 82: Nortricyclyl bromide

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Nortricyclyl bromide	C7 H9 Br	29.848			1000342-32-2	LibSearch	43.32	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		43.32			50		

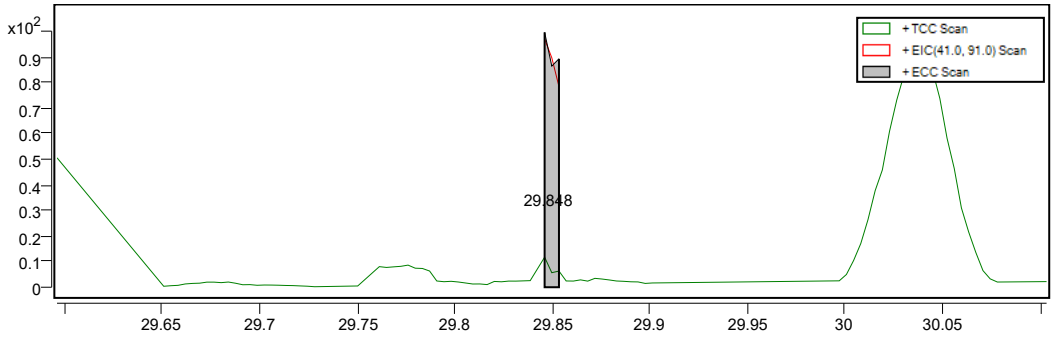
Compound Discovery Report

Agilent | Trusted Answers

Compound ID Table

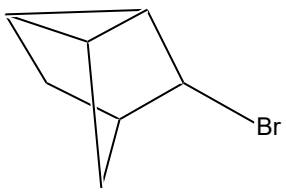
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Nortricyclyl bromide	C7H9Br		LibSearch	29.848	16.865		1000342-32-2	43.32		
Benzeneacetic acid, 2-propenyl ester	C11H12O2		LibSearch	29.848	7.365		1797-74-6	40.94		
Myrcene	C10H16		LibSearch	29.848			123-35-3	39.01		
Thujene<alpha->	C10H16		LibSearch	29.848	24.228		2867-05-2	38.43		
Myrcene	C10H16		LibSearch	29.848	22.418		123-35-3	37.01		
Tricyclo[4.1.0.0(2,4)]heptane, 5-(phenylthio)-, (1.alpha.,2.beta.,4.beta.,5.alpha.,6.alpha.)-	C13H14S		LibSearch	29.848	4.365		71055-11-3	37.00		
1,5-Dimethyl-1,4-cyclohexadiene	C8H12		LibSearch	29.848	15.465		4190-06-1	36.76		
Octane, 1-chloro-	C8H17Cl		LibSearch	29.848	12.481		111-85-3	36.27		
1,4-Cyclohexadiene, 1,2-dimethyl-	C8H12		LibSearch	29.848	15.465		17351-28-9	36.23		
Heptane, 1-chloro-	C7H15Cl		LibSearch	29.848	14.148		629-06-1	36.12		
.beta.-Myrcene	C10H16		LibSearch	29.848	13.881		123-35-3	35.83		
1,4-Dihydro-2-methylbenzoic acid	C8H10O2		LibSearch	29.848	9.998		55886-48-1	35.53		
Pinene<beta->	C10H16		LibSearch	29.848	22.808		127-91-3	34.36		
1-(1-Chloro-2-butoxycyclopropyl)-2-cyclopropylacetylene	C12H17ClO		LibSearch	29.848	6.448		1000222-64-3	34.31		
Bicyclo[3.2.0]hept-2-ene, 4-bromo-	C7H9Br		LibSearch	29.848	13.481		38352-98-6	33.64		
.beta.-Pinene	C10H16		LibSearch	29.848	14.131		127-91-3	33.34		
1,4-DIMETHYL-CYCLOHEXA-1,3-DIENE	C8H12		LibSearch	29.848	15.465		26120-52-5	32.75		
Benzeneacetamide, N-phenyl-	C14H13NO		LibSearch	29.848	-2.919		621-06-7	32.29		
.beta.-Myrcene	C10H16		LibSearch	29.848	13.881		123-35-3	31.74		
.beta.-Pinene	C10H16		LibSearch	29.848	14.131		127-91-3	31.50		
.beta.-Myrcene	C10H16		LibSearch	29.848	13.881		123-35-3	31.32		
Benzene, [[(1-ethenyl-1,5-dimethyl-4-hexenyl)oxy]methyl]-	C17H24O		LibSearch	29.848	0.615		77611-58-6	31.27		
Pyridine, 4-(3-phenylpropyl)-	C14H15N		LibSearch	29.848	2.198		2057-49-0	30.98		
.beta.-Myrcene	C10H16		LibSearch	29.848	13.881		123-35-3	30.25		
Benzene, [[(1-ethenyl-1,5-dimethyl-4-hexenyl)oxy]methyl]-	C17H24O		LibSearch	29.848	0.615		77611-58-6	29.88		
Butanoic acid, 3-methyl-, 1-ethenyl-1,5-dimethyl-4-hexenyl ester	C15H26O2		LibSearch	29.848	4.748		1118-27-0	28.57		
1,3,7-Octatriene, 3,7-dimethyl-	C10H16		LibSearch	29.848	13.881		502-99-8	28.01		
Pyridine, 4-(3-phenylpropyl)-	C14H15N		LibSearch	29.848	2.198		2057-49-0	27.58		
1,5-Octadiyne	C8H10		LibSearch	29.848	15.981		764-74-9	27.17		
3-Picolinium, 1-anilino-, hydroxide, inner salt	C12H12N2		LibSearch	29.848			31382-88-4	27.14		
Methyl m-tolyl carbinol	C9H12O		LibSearch	29.848	10.365		1010342-29-9	26.75		
Geranyl isovalerate	C15H26O2		LibSearch	29.848	3.415		109-20-6	26.31		
2-Cyclohexene-6-carboxylic acid, 3-methyl-1-(5-oxo-3,4-dihydro-2H-pyrrolyl)-, ethyl ester	C14H21NO3		LibSearch	29.848	-3.152		1000138-08-3	26.16		
Bicyclo[3.2.0]hept-2-ene, 5-chloro-	C7H9Cl		LibSearch	29.848	15.598		43011-86-5	26.11		
1,1-Difluoro-2,2-dimethylcyclopropane	C5H8F2		LibSearch	29.848	23.581		335-03-5	26.09		
1-Carboxy-5,5-dimethylcyclohexa-1,3-diene	C9H12O2		LibSearch	29.848	8.781		10321-89-8	25.47		
Linalyl formate	C11H18O2		LibSearch	29.848			115-99-1	25.36		
Artemisia triene	C10H16		LibSearch	29.848			18383-70-5	25.22		
Artemisia triene	C10H16		LibSearch	29.848	24.238		18383-70-5	25.19		
Linalool formate	C11H18O2		LibSearch	29.848	13.428		115-99-1	25.11		
sec-Butyl fluoroformate	C5H9FO2		LibSearch	29.848	19.948		53813-78-8	25.05		
Butanoic acid, 3-methyl-, 1-ethenyl-1,5-dimethyl-4-hexenyl ester	C15H26O2		LibSearch	29.848	4.748		1118-27-0	24.53		
1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (Z,E)-	C15H24		LibSearch	29.848	5.548		26560-14-5	24.45		
2,2-Dichloroethanol, benzyldimethylsilyl ether	C11H16Cl2OSi		LibSearch	29.848	4.465		1000375-56-1	24.19		
Santolina triene	C10H16		LibSearch	29.848	14.948		2153-66-4	23.83		
Linalyl phenylacetate	C18H24O2		LibSearch	29.848	-2.569		7143-69-3	23.71		
3-(1-Benzyl-1H-imidazol-2-yl)-5-phenylisoxazole	C19H15N3O		LibSearch	29.848	-13.502		1000306-59-5	23.63		
1,3,6,10-Dodecatetraene, 3,7,11-trimethyl-, (Z,E)-	C15H24		LibSearch	29.848	5.548		26560-14-5	23.24		
1,4-Cyclohexadien, 6-methyl-3-(1-phenylpropyl)-	C16H20		LibSearch	29.848	1.881		1000149-66-6	23.19		
Linalyl cinnamate	C19H24O2		LibSearch	29.848			78-37-5	23.01		

Compound Chromatograms (overlaid)

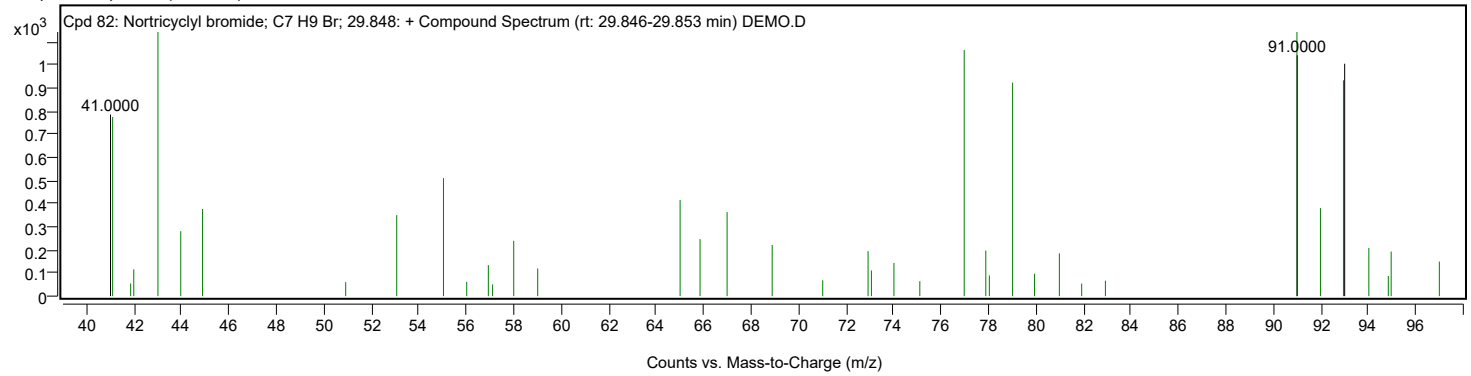


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



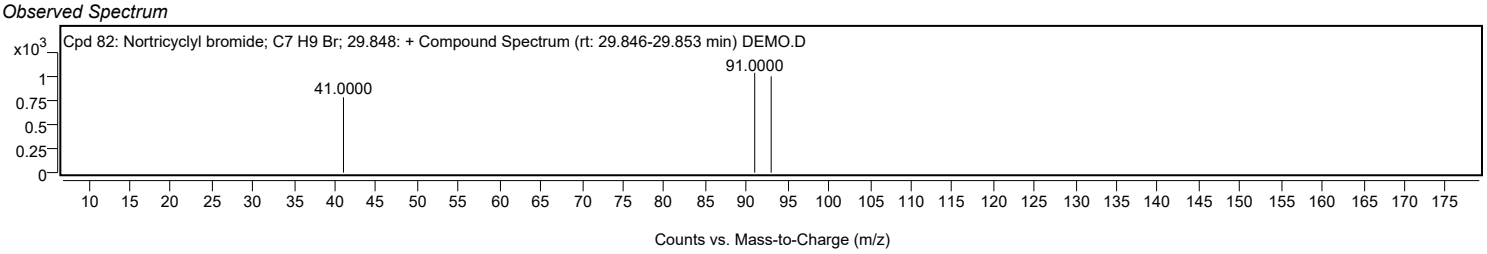
Nortricyclyl bromide

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			43.32			NIST.L

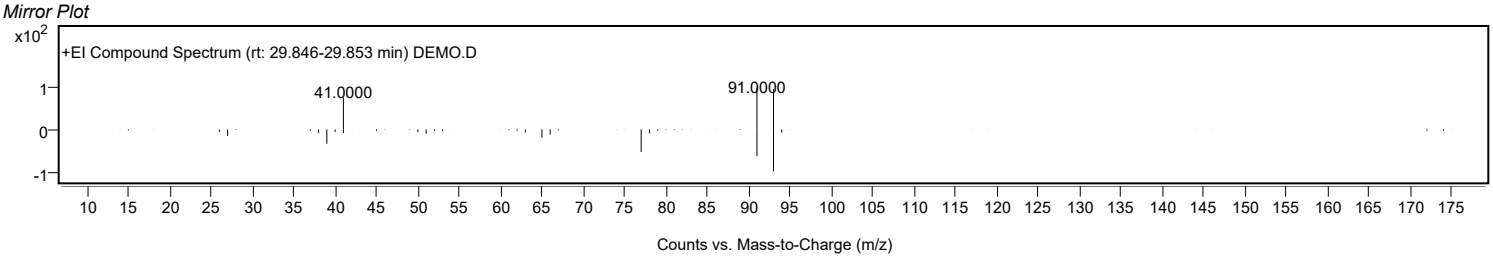
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			43.32			NIST.L

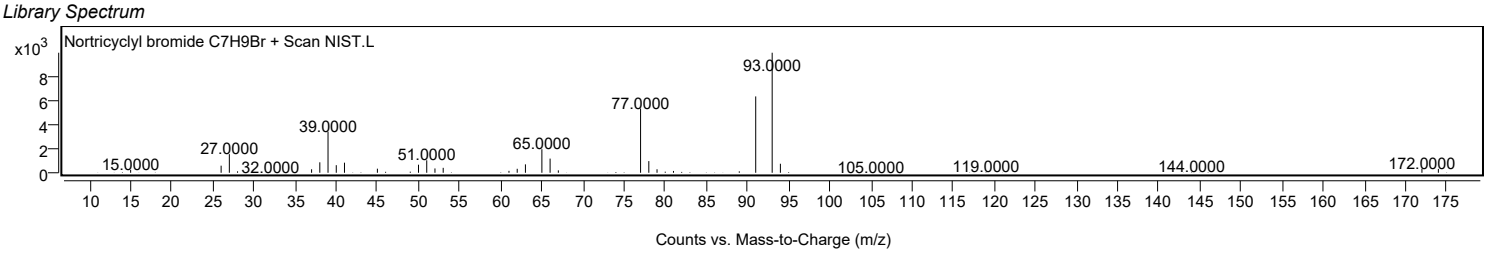
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 83: 3,5-Hexadiyn-2-one

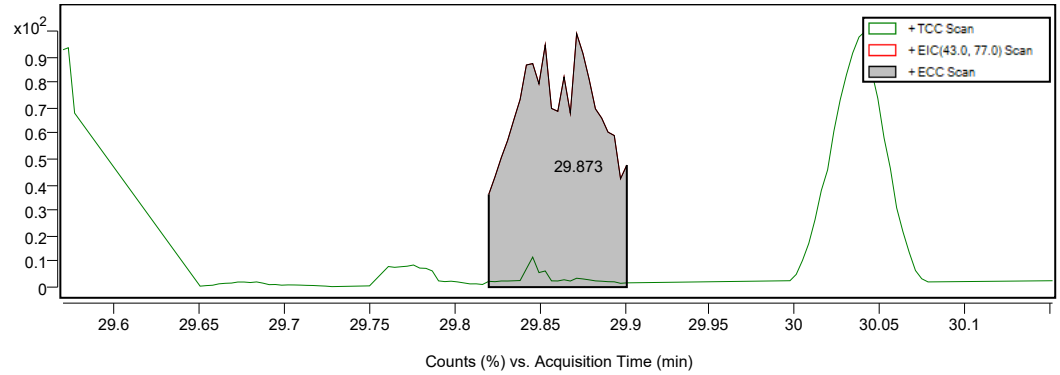
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
3,5-Hexadiyn-2-one	C6 H4 O	29.873			31097-80-0	LibSearch	49.41	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		49.41			50		

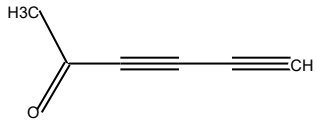
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
3,5-Hexadiyn-2-one	C6H4O		LibSearch	29.873	17.056		31097-80-0	49.41		
2-Propen-1-ol, 3,3-difluoro-, acetate	C5H6F2O2		LibSearch	29.873	19.606		1597-40-6	42.69		
2,2-Difluoroethanol, TMS derivative	C5H12F2OSi		LibSearch	29.873	23.440		1010372-93-9	40.38		
Dimethylphosphinic azide	C2H6N3OP		LibSearch	29.873			58347-13-0	39.91		
1-Butanamine, N-sulfinyl-	C4H9NOS		LibSearch	29.873			13165-70-3	37.95		
ClCH2C(O)OCH(CH3)2	C5H9ClO2		LibSearch	29.873	15.756		105-48-6	36.77		
2,2-Difluoroethanol, TBDMS derivative	C8H18F2OSi		LibSearch	29.873	19.873		1000373-38-9	33.98		
ClCH2C(O)OCH(CH3)2	C5H9ClO2		LibSearch	29.873	15.756		105-48-6	31.52		
Chloroacetic acid, propyl ester	C5H9ClO2		LibSearch	29.873	14.690		5396-24-7	27.91		
Phenyl sulfonyl acetone	C9H10O3S		LibSearch	29.873	2.623		5000-44-2	26.28		
Chloroacetic acid, propyl ester	C5H9ClO2		LibSearch	29.873	14.690		5396-24-7	25.00		
2-Propanone, 1-phenoxy-	C9H10O2		LibSearch	29.873	9.806		621-87-4	24.95		
Phenyl sulfonyl acetone	C9H10O3S		LibSearch	29.873	2.623		5000-44-2	24.47		
2-Propanone, 1-phenoxy-	C9H10O2		LibSearch	29.873	9.806		621-87-4	22.55		
Peroxide, 1,1-dimethylethyl 1-methyl-1-phenylethyl	C13H20O2		LibSearch	29.873	6.990		3457-61-2	22.36		
3-Acetyl-5-phenyl-2-isoxazoline	C11H11NO2		LibSearch	29.873	3.740		1000431-69-6	22.15		
Acetic acid, chloro-, 1-methylbutyl ester	C7H13ClO2		LibSearch	29.873	12.456		90380-52-2	21.00		
Benzenepropanoic acid, .alpha.-(acetyloxy)-3-hydroxy-4-(phenylazo)-, methyl ester, (.+/-.)-	C18H18N2O5		LibSearch	29.873	-14.094		77573-40-1	19.09		
5-Phenyl-thiazolidine	C9H11NS		LibSearch	29.873	4.523		107326-19-2	18.85		
Ethylene, 1-(2-(5-methyl)-furyl)-2-nitro	C7H7NO3		LibSearch	29.873	9.523		1010222-01-4	18.48		
3-Isoxazolecarboxamide, 5-acetyl-4-amino-N-phenyl-	C12H11N3O3		LibSearch	29.873	-8.660		1000350-37-5	17.85		
3-Penten-2-one, 3-(2-furanyl)-	C9H10O2		LibSearch	29.873	10.523		56335-77-4	17.76		
2-Hydroxy-1-phenylhexane-1,5-dione	C12H14O3		LibSearch	29.873	1.123		108574-59-0	16.14		
N-(4-Oxo-2-thioxo-3-thiazolidinyl)acetanilide	C11H10N2O2S2		LibSearch	29.873	-9.177		1000261-00-1	15.65		
Benzenemethanol, 4-bromo-.alpha.-methyl-	C8H9BrO		LibSearch	29.873	6.956		5391-88-8	14.37		
Benzene, (hexylsulfonyl)-	C12H18O2S		LibSearch	29.873	-0.077		16823-63-5	14.10		
Tricyclo[2.2.1.0(3,5)]heptane-2-carboxylic acid, 6-oxo-3-(phenylsulfonyl)-,(r1,trans-2,cis-4)-	C14H12O5S		LibSearch	29.873	-7.844		1010141-76-3	14.06		
5-Benzoyl-2-N-isopropyl-1,3-thiazole-2,4-diamine	C13H15N3OS		LibSearch	29.873	-8.410		1010409-40-4	14.00		
Ethyl 2-(2-chloroacetamido)-3,3,3-trifluoro-2-isopropoxypropionate	C10H15ClF3NO4		LibSearch	29.873	3.723		339352-74-8	13.93		
4-Acetamido-1-phenylpyrazole	C11H11N3O		LibSearch	29.873	-1.427		2590-00-3	13.15		
Benzene, 1-ethyl-2-nitro-	C8H9NO2		LibSearch	29.873	8.390		612-22-6	12.45		
4-Isoxazolecarboxylic acid, 5-methyl-3-phenyl-	C11H9NO3		LibSearch	29.873	0.056		1136-45-4	12.26		
Benzophenone, 2-[N-acetyl-N-methylamino]-5-chloro-	C16H14ClNO2		LibSearch	29.873	-8.377		36271-03-1	11.64		
2-Nitrocumene	C9H11NO2		LibSearch	29.873	7.806		6526-72-3	11.46		
4-(6-Oxabicyclo[3.1.0]hex-1-yl)-but-3-yn-2-one	C9H10O2		LibSearch	29.873	10.940		1000185-32-7	11.29		
6-Methyl-8-phenyl-3,5,7-octatrien-2-one	C15H16O		LibSearch	29.873	1.106		80283-32-5	11.26		
1-(1-Adamantyl)-1-phenylethanol	C18H24O		LibSearch	29.873	-0.427		303797-64-0	11.21		
2,4-Diamino-6,7-dihydro-5,6-diphenyl-7-oxo-5H-pyrrolo[3,4-d]pyrimidine	C18H15N5O		LibSearch	29.873	-23.244		1000214-30-4	10.66		
Acetic acid, 4-acetoxy-2-(2-acetylthioethyl)-5-(7-benzoylamino-3H-pyrazolo[4,3-d]pyrimidin-3-yl)tetrahydrofuran-3-ylmethyl ester	C25H27N5O7S		LibSearch	29.873			1000188-57-6	10.64		
N-(3-Chloro-1,4-dioxonaphthalen-2-yl)-N-phenylacetamide	C18H12ClNO3		LibSearch	29.873	-15.460		4497-73-8	10.39		
Methyl 3-[(5-amino-1-phenyl-1,2,4-triazol-3-yl)amino]-4-methylpent-2-enoate	C15H19N5O2		LibSearch	29.873	-12.327		1000410-75-0	10.07		
N-(2,6-Dimethyl-phenyl)-2-(2-methyl-5-nitro-imidazol-1-yl)-acetamide	C14H16N4O3		LibSearch	29.873	-13.044		333414-54-3	9.87		
Benzofurazan-4,7(4H,7H)-dione, 5-acetylamino-6-phenylamino-	C14H10N4O4		LibSearch	29.873	-17.510		153136-32-4	9.64		
Ethanol, 1-(2-methylene-1-phenylsulfonylcyclopropyl)-	C12H14O3S		LibSearch	29.873	-1.844		1000158-24-4	9.55		
Acetic acid, 13-methyl-3-phenylazo-7,8,9,11,12,13,14,15,16,17-decahydro-6H-cyclopenta[a]phenanthren-17-yl ester	C26H30N2O2		LibSearch	29.873	-19.210		1000203-01-0	9.26		
1-[5-(3-Hydroxy-3-methyl-but-1-ynyl)-thiophen-2-yl]-3-phenyl-propenone	C18H16O2S		LibSearch	29.873	-10.244		1000294-77-9	9.22		
2-Phenyl-4-acetyl-5-chloro-thiazole	C11H8ClNOS		LibSearch	29.873	-1.744		64953-93-1	9.22		
3-Acetylmercaptoethylthio-5-(4-chlorophenyl)-1-phenyltriazol-1,2,4	C18H16ClN3OS2		LibSearch	29.873	-23.377		1010287-03-5	8.99		
2-Oxa-6-azatricyclo[3.3.1.1(3,7)]decan-4-ol, 8-iodo-6-(phenylsulfonyl)-, acetate (ester), (1.alpha.,3.beta.,4.beta.,5.alpha.,7.beta.,8.alpha.)-	C16H18INO5S		LibSearch	29.873	-16.244		50267-29-3	8.90		
2-Diisopropylsilyloxymethyltetrahydrofurane	C11H24O2Si		LibSearch	29.873	9.090		1000279-17-5	8.39		

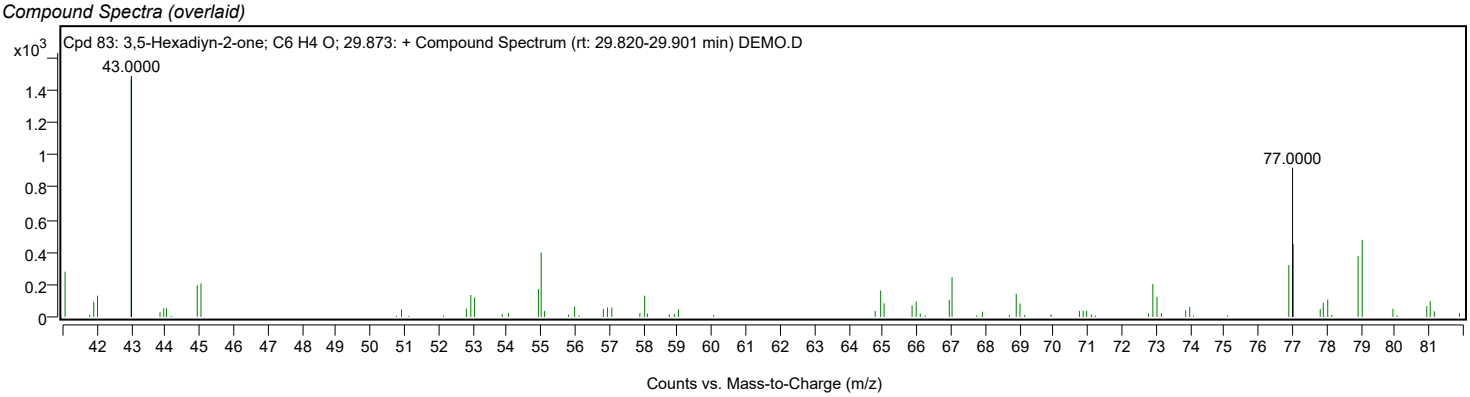
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



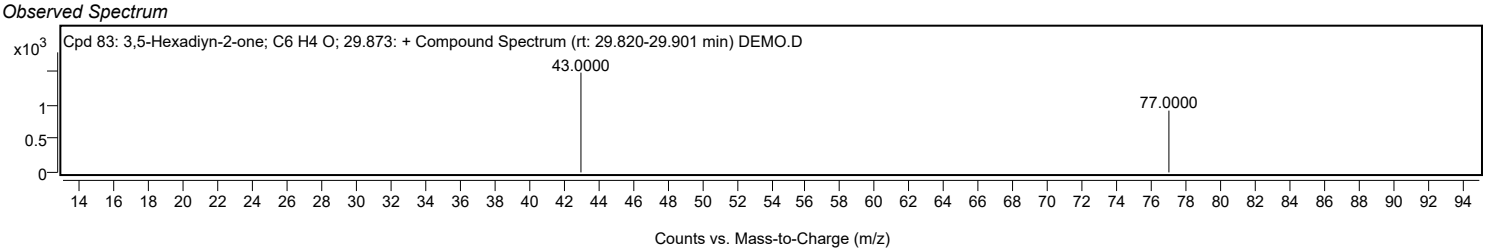
3,5-Hexadiyn-2-one

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			49.41			NIST.L

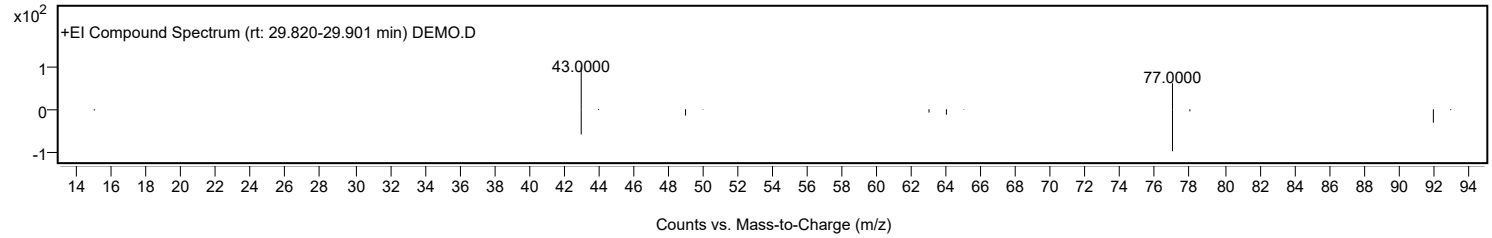
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			49.41			NIST.L

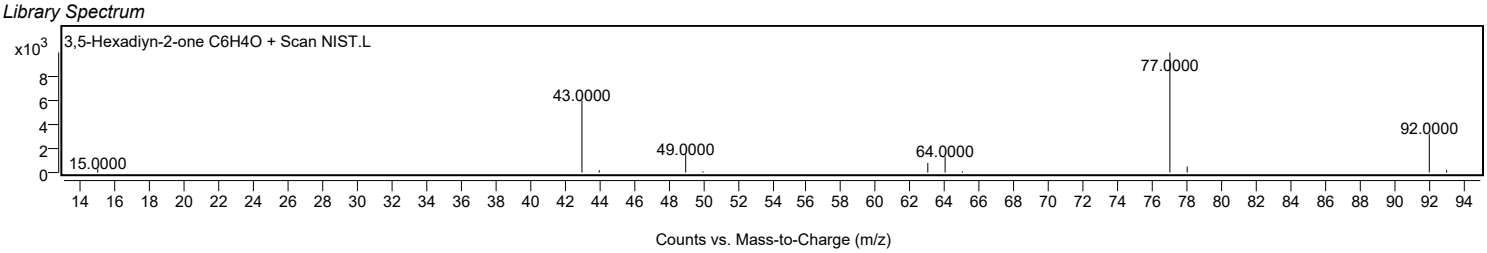
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 84: Galaxolide

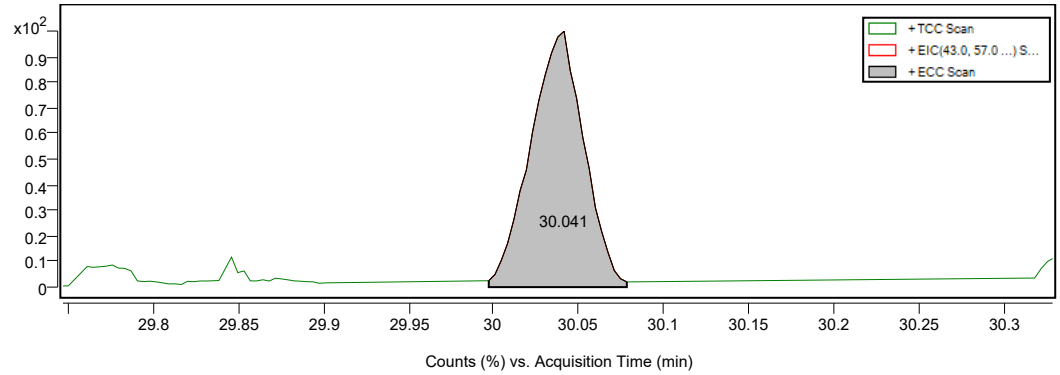
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Galaxolide	C18 H26 O	30.041			1222-05-5	LibSearch	77.71	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		77.71			50		

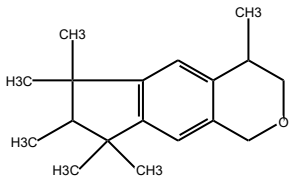
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Galaxolide	C18H26O		LibSearch	30.041			1222-05-5	77.71		
Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-	C18H26O		LibSearch	30.041	-1.842		1222-05-5	76.39		
Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-	C18H26O		LibSearch	30.041	-1.842		1222-05-5	73.52		
7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin	C18H26O		LibSearch	30.041	-3.242		88-29-9	69.46		
Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-	C18H26O		LibSearch	30.041	-1.842		1222-05-5	68.34		
7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin	C18H26O		LibSearch	30.041	-3.242		88-29-9	67.94		
Cyclopenta[g]-2-benzopyran, 1,3,4,6,7,8-hexahydro-4,6,6,7,8,8-hexamethyl-	C18H26O		LibSearch	30.041	-1.842		1222-05-5	67.65		
7-Acetyl-6-ethyl-1,1,4,4-tetramethyltetralin	C18H26O		LibSearch	30.041	-3.242		88-29-9	66.81		
Tonalid	C18H26O		LibSearch	30.041	-2.609		21145-77-7	62.86		
Acetic acid, 2-[3-oxo-1H-imidazo[1,2-a][1,3]benzimidazol-2(3H)-yliden]-, methyl ester	C12H9N3O3		LibSearch	30.041	-7.826		1000337-79-9	58.39		
Tetralide	C18H26O		LibSearch	30.041			21145-77-7	57.93		
Brayelin	C15H14O4		LibSearch	30.041	-5.876		6054-10-0	56.01		
9-Oxabicyclo[3.3.1]nonan-3-ol, 7-[(trityloxy)methyl]	C28H30O3		LibSearch	30.041	-25.442		1000197-53-9	55.61		
Isoxazole, 4,5-dihydro-3-methyl-4-(4-diethylaminobenzylidene)-5-oxo-	C15H18N2O2		LibSearch	30.041	-5.842		328002-66-0	55.26		
Tonalid	C18H26O		LibSearch	30.041	-2.609		21145-77-7	55.07		
Luvangetin	C15H14O4		LibSearch	30.041	-5.876		483-92-1	54.93		
Peucedanin	C15H14O4		LibSearch	30.041	-4.976		133-26-6	54.39		
1,3-Pentanediol, 2-methylene-5-triphenylmethoxy-	C25H26O3		LibSearch	30.041	-21.626		1000197-32-3	54.18		
4-Isoxazolidinamine, 3-oxo-N-(p-tosyl)-2-trityl-	C29H26N2O4S		LibSearch	30.041	-41.576		1000256-00-1	53.68		
1,6-Ditritylfrutcose triacetate	C50H46O9		LibSearch	30.041	-67.942		1000128-02-3	53.27		
1-Pentanol, 5,5,5-triphenyl-	C23H24O		LibSearch	30.041	-14.876		2294-95-3	52.78		
.beta.-Alanine, N-hydroxy-N-[2,3-O-(1-methylethylidene)-5-O-(triphenylmethyl)-.beta.-d-ribofuranosyl]-, methyl ester	C31H35NO7		LibSearch	30.041	-30.976		64018-66-2	51.87		
4-cyano-3-fluorophenyl 4-(4-butylcyclohexyl)benzoate	C24H26FNO2		LibSearch	30.041	-18.626		92118-83-7	51.62		
Brayelin	C15H14O4		LibSearch	30.041	-5.876		6054-10-0	51.47		
1-Dimethylphenylsilyloxy-4-methoxybenzene	C15H18O2Si		LibSearch	30.041	1.024		1000307-90-7	51.28		
2,7-Anhydro-1-trityl-l-galacto-heptulofuranose	C26H26O6		LibSearch	30.041	-28.909		1000126-10-4	50.76		
Benzene, 1,1',1"-ethylidynetris-	C20H18		LibSearch	30.041	-5.876		5271-39-6	50.51		
Lyxofuranose, 5-O-trityl-, triacetate	C30H30O8		LibSearch	30.041	-32.342		103419-92-7	50.35		
6-Trityl-d-galactose tetraacetate	C33H34O10		LibSearch	30.041	-38.692		1000126-10-5	50.28		
Epistephamiersine	C21H27NO6		LibSearch	30.041	-14.492		52389-15-8	50.25		
1-Tritylaziridine-2-carbothioic acid, S-phenyl ester	C28H23NOS		LibSearch	30.041	-28.759		1000191-60-9	50.20		
Xanthoxyletin	C15H14O4		LibSearch	30.041	-5.876		84-99-1	49.99		
2-Octanone, 4-methyl-1,1,1-triphenyl-	C27H30O		LibSearch	30.041	-18.659		72152-22-8	49.85		
1,1,1-triphenyl-2-decanone	C28H32O		LibSearch	30.041	-21.392		72152-27-3	49.82		
Benzene, 1,1',1"-[(cyclohexyloxy)methylidyne]tris-	C25H26O		LibSearch	30.041	-16.476		20705-40-2	49.31		
5-Undecen-2-one, 4-methyl-1,1,1-triphenyl-	C30H34O		LibSearch	30.041	-23.759		1000197-51-8	49.11		
6-Acetyl-5-methoxy-2,7-dimethyl-1,4-naphthoguinone	C15H14O4		LibSearch	30.041	-7.159		960-64-5	48.99		
.alpha.-d-Lyxofuranose, 1-O-acetyl-2,3-O-ethylboranediyl-5-O-trityl-	C28H29BO6		LibSearch	30.041			1000152-13-1	48.90		
Methyl 6-trityl-.beta.-d-galactopyranoside	C26H28O6		LibSearch	30.041	-29.642		1000126-15-8	48.85		
6-O-Triphenylmethyl-.beta.-D-glucopyranose	C26H28O6		LibSearch	30.041	-29.642		1000197-32-5	48.62		
1-Trityl-4-formylimidazole	C23H18N2O		LibSearch	30.041	-18.742		33016-47-6	48.52		
.alpha.-d-Glucopyranoside, methyl 6-O-(triphenylmethyl)-, triacetate	C32H34O9		LibSearch	30.041	-36.626		18031-49-7	48.51		
4-[5-Chloro-2-hydroxybenzylideneamino]-2-tritylisoxazolidin-3-one	C29H23ClN2O3		LibSearch	30.041	-39.859		16561-89-0	48.49		
.alpha.-D-Glucofuranosidurono-6,3-lactone, phenyl-2,5-di-O-acetyl-1-thio-	C16H16O7S		LibSearch	30.041	-13.576		1000163-78-5	48.35		
Benzoic acid, 4-(4-butylcyclohexyl)-, 2,3-dicyano-4-(pentyloxy)phenyl ester	C30H36N2O3		LibSearch	30.041	-33.442		75941-91-2	48.22		
3-(Triphenylmethyl)-5-oxazolidinone	C22H19NO2		LibSearch	30.041	-17.842		1010432-52-9	48.20		
Benzoic acid, 4-(4-butylcyclohexyl)-, 4-butoxy-2,3-dicyanophenyl ester	C29H34N2O3		LibSearch	30.041	-31.792		75941-90-1	48.17		
2-Methyl-4-quinolinecarboxamide, TMS derivative	C14H18N2OSi		LibSearch	30.041	-4.292		1010479-15-1	48.06		
Imidazole, 4-iodo-1-triphenylmethyl-	C22H17IN2		LibSearch	30.041	-20.859		96797-15-8	48.03		
3-Hydroxy-2,4-dimethyl-5-trityloxy-pentanoic acid, methyl ester	C27H30O4		LibSearch	30.041	-22.092		102736-47-0	47.93		

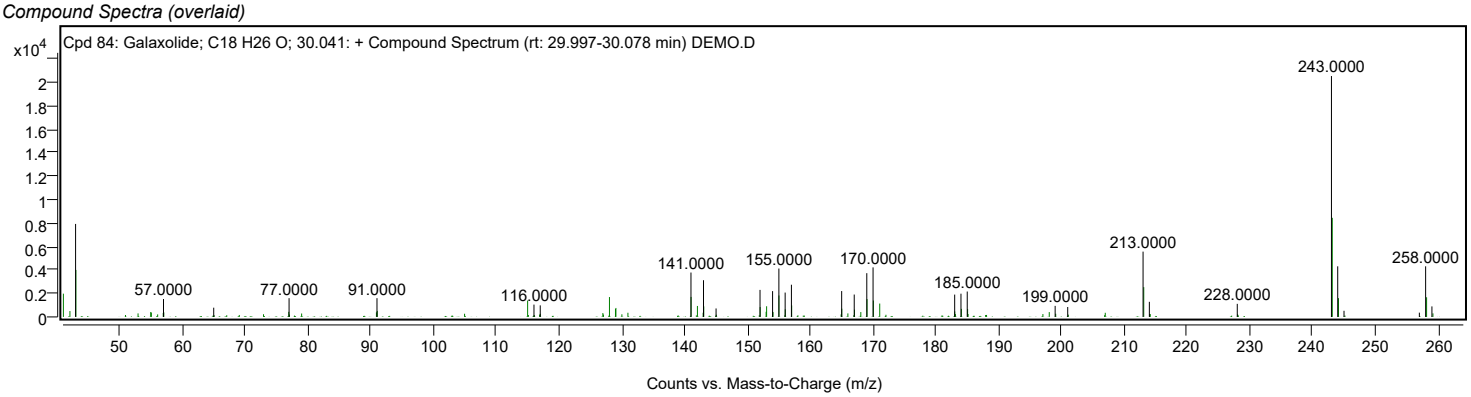
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



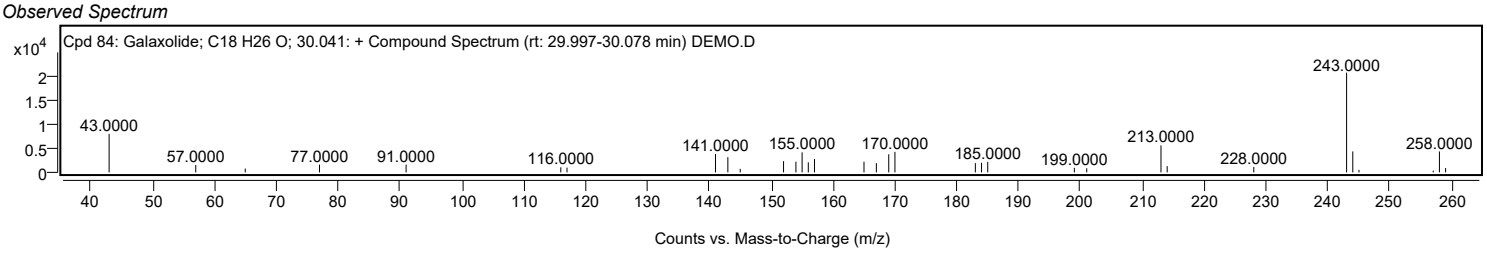
Galaxolide

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			77.71			PWNose.xml

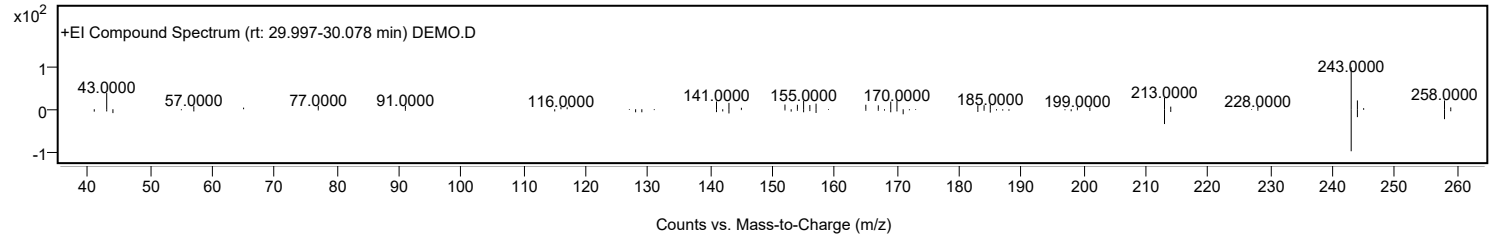
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			77.71			PWNose.xml

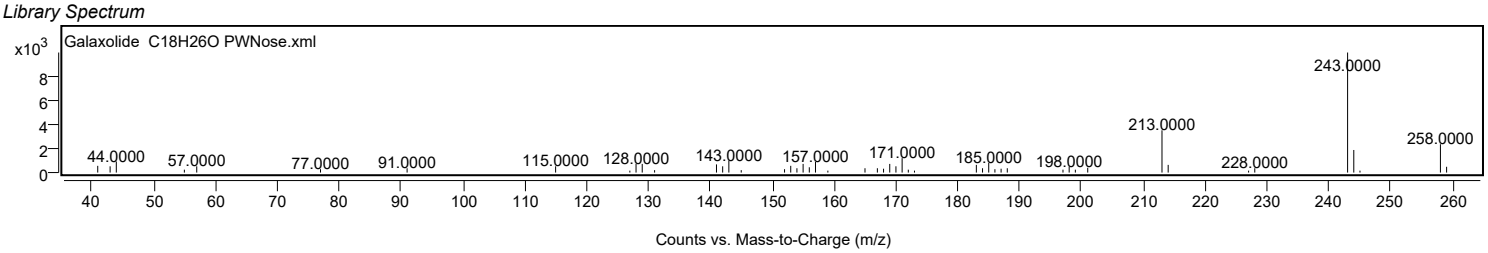
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 85: Hexylacetylene

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Hexylacetylene	C8 H14	30.347			629-05-0	LibSearch	71.62	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		71.62			50		

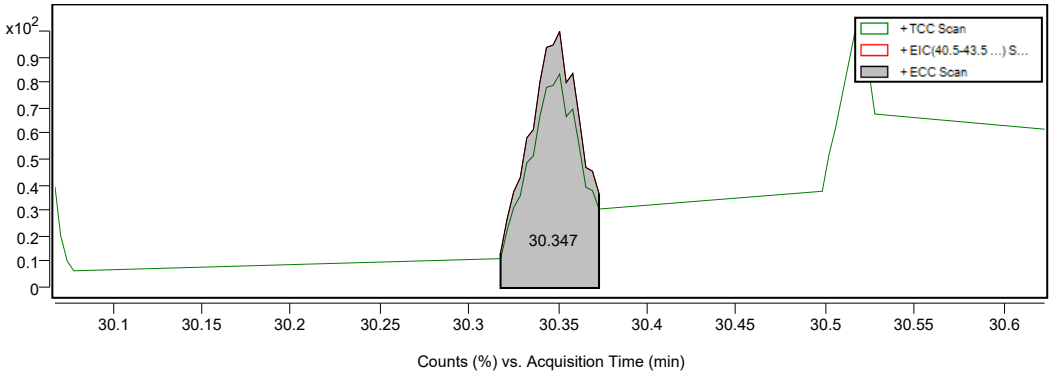
Compound Discovery Report

Agilent | Trusted Answers

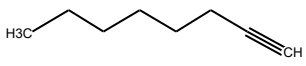
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Hexylacetylene	C8H14		LibSearch	30.347			629-05-0	71.62		
3-Octyne	C8H14		LibSearch	30.347	16.447		15232-76-5	69.28		
3,4-Octadiene	C8H14		LibSearch	30.347			34511-01-8	68.52		
2,3-Nonadiene	C9H16		LibSearch	30.347			22433-34-7	68.03		
Octylacetylene	C10H18		LibSearch	30.347			764-93-2	67.71		
Salvene<Z->	C9H16		LibSearch	30.347	26.337		33746-70-2	67.54		
Spiropentane, propyl-	C8H14		LibSearch	30.347	17.447		6191-88-4	67.32		
Undecyne<1->	C11H20		LibSearch	30.347	17.897		2243-98-3	67.10		
1-Octyne	C8H14		LibSearch	30.347	16.781		629-05-0	66.93		
Oct-(5Z)-enol	C8H16O		LibSearch	30.347			64275-73-6	66.16		
Undecyne <1->	C11H20		LibSearch	30.347			2243-98-3	65.77		
1,5-Hexadiene, 2,5-dimethyl-	C8H14		LibSearch	30.347	17.831		627-58-7	65.70		
1-Undecyne	C11H20		LibSearch	30.347	11.814		2243-98-3	65.62		
1,1'-Bicyclopropyl, 1,1'-dimethyl-	C8H14		LibSearch	30.347	17.531		59020-33-6	65.59		
1-Nonyne	C9H16		LibSearch	30.347	15.114		3452-09-3	65.48		
3-Octyne, 5-methyl-	C9H16		LibSearch	30.347	15.864		62108-33-2	65.43		
3,4-Octadiene, 7-methyl-	C9H16		LibSearch	30.347			37050-05-8	65.41		
3,4-Nonadiene	C9H16		LibSearch	30.347			37050-03-6	65.26		
3,4-Octadiene, 7-methyl-	C9H16		LibSearch	30.347			37050-05-8	65.15		
1,4-Hexadiene, 2,5-dimethyl-	C8H14		LibSearch	30.347	17.531		927-97-9	65.07		
3-Octyne	C8H14		LibSearch	30.347	16.447		15232-76-5	65.01		
1-Octyne	C8H14		LibSearch	30.347	16.781		629-05-0	64.90		
Cyclopropene, 1-butyl-2-ethyl-	C9H16		LibSearch	30.347	15.031		50915-91-8	64.83		
3-Octyne	C8H14		LibSearch	30.347	16.447		15232-76-5	64.82		
3-Nonyne	C9H16		LibSearch	30.347	14.797		20184-89-8	64.76		
1-Nonyne	C9H16		LibSearch	30.347	15.114		3452-09-3	64.68		
Cyclopropane, (2-methylenebutyl)-	C8H14		LibSearch	30.347	17.247		74685-56-6	64.68		
2-Nonyne	C9H16		LibSearch	30.347	14.797		19447-29-1	64.66		
1,4-Heptadiene, 3-methyl-	C8H14		LibSearch	30.347	17.847		1603-01-6	64.55		
3-Nonyne	C9H16		LibSearch	30.347	14.797		20184-89-8	64.53		
Bicyclo[7.1.0]decane	C10H18		LibSearch	30.347	11.997		286-76-0	64.53		
Pentylacetylene	C7H12		LibSearch	30.347			628-71-7	64.32		
3,4-Octadiene, 7-methyl-	C9H16		LibSearch	30.347			37050-05-8	64.22		
Oct-(3Z)-enol	C8H16O		LibSearch	30.347			20125-84-2	64.08		
1,4-Pentadiene, 3-propyl-	C8H14		LibSearch	30.347	18.131		996-83-8	64.08		
Octenol<5Z->	C8H16O		LibSearch	30.347	20.147		64275-73-6	64.05		
Non-(6Z)-enol	C9H18O		LibSearch	30.347			35854-86-5	64.01		
Propanoic acid <2-oxo-, (3Z)-hexenyl-> ester	C9H14O3		LibSearch	30.347			68133-76-6	63.95		
2-Methyl-1,5-heptadiene (c,t)	C8H14		LibSearch	30.347	17.147		6766-54-7	63.94		
Bicyclo[2.1.0]pentane, 1,4-dimethyl-	C7H12		LibSearch	30.347	19.531		17065-18-8	63.90		
1-Octyne	C8H14		LibSearch	30.347	16.781		629-05-0	63.81		
Nonenol<6Z->	C9H18O		LibSearch	30.347	16.087		35854-86-5	63.77		
1-Nonyne	C9H16		LibSearch	30.347	15.114		3452-09-3	63.71		
3-Nonyne	C9H16		LibSearch	30.347	14.797		20184-89-8	63.64		
4-Nonyne	C9H16		LibSearch	30.347	14.797		20184-91-2	63.64		
3-Octyne	C8H14		LibSearch	30.347	16.447		15232-76-5	63.61		
3-Octyne, 2-methyl-	C9H16		LibSearch	30.347	15.864		55402-15-8	63.54		
2-Methyl-1,5-heptadiene (c,t)	C8H14		LibSearch	30.347	17.147		6766-54-7	63.39		
Hexenyl pyruvate<3Z->	C9H14O3		LibSearch	30.347	15.357		68133-76-6	63.35		
Hepten-1-ol<4Z->	C7H14O		LibSearch	30.347	23.717		6191-71-5	63.27		

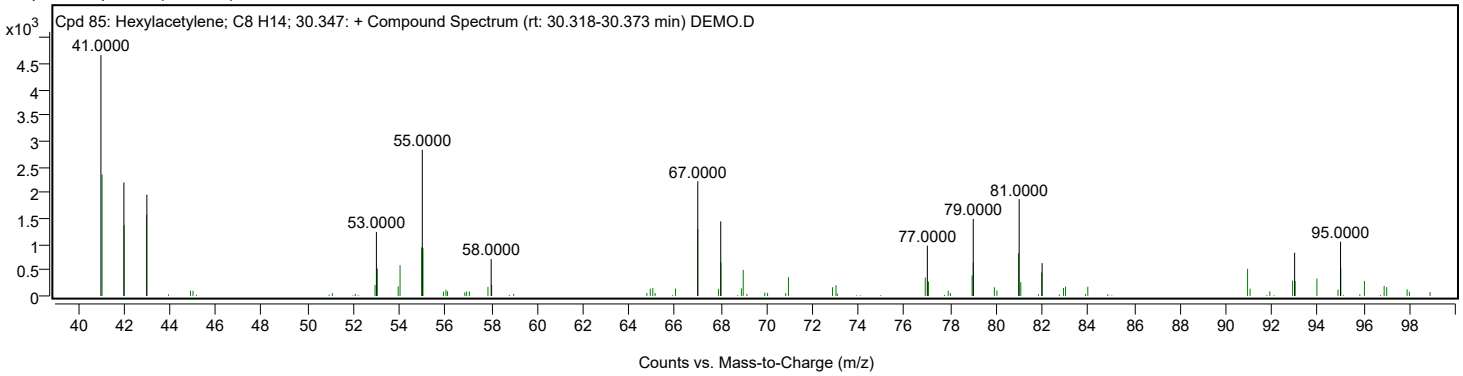
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



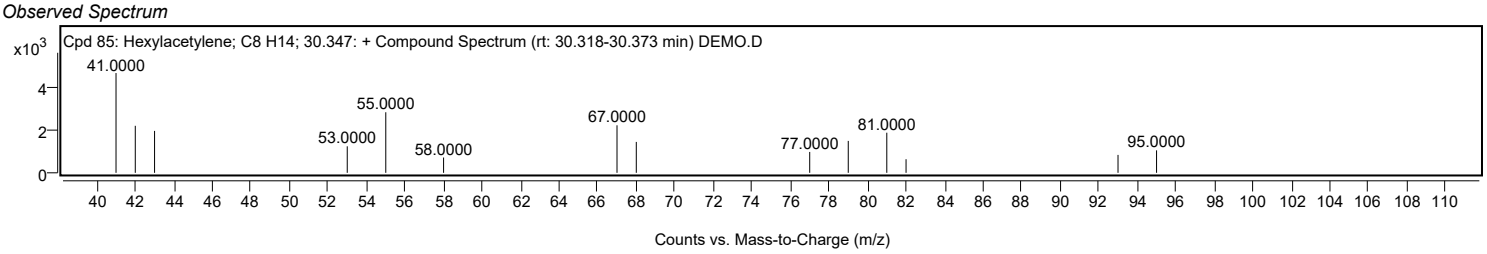
Hexylacetylene

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			71.62			PWNose.xml

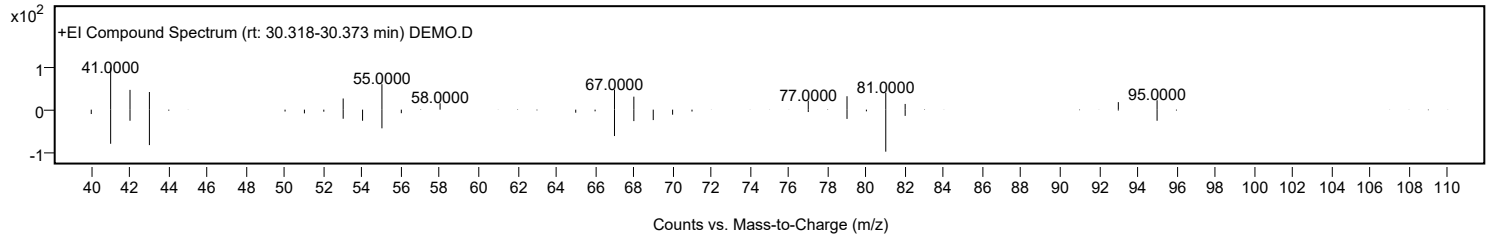
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			71.62			PWNose.xml

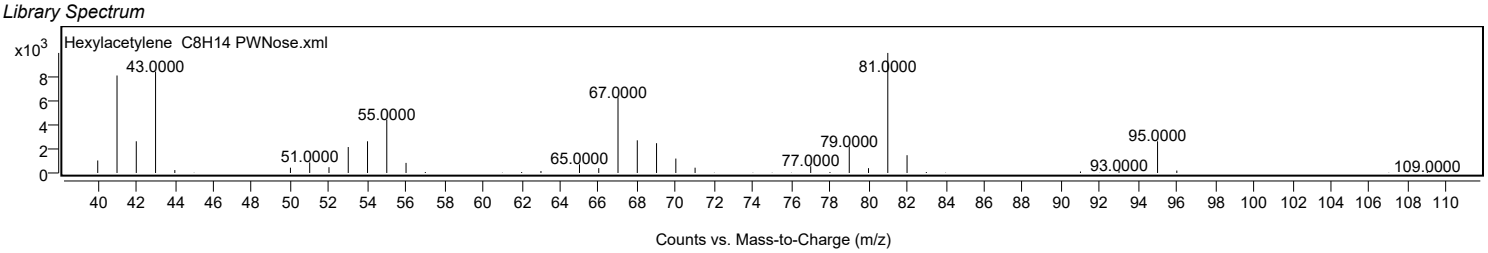
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 86: Cyclopentanemethanol

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Cyclopentanemethanol	C6 H12 O	30.506			3637-61-4	LibSearch	61.41	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		61.41			50		

Compound Discovery Report

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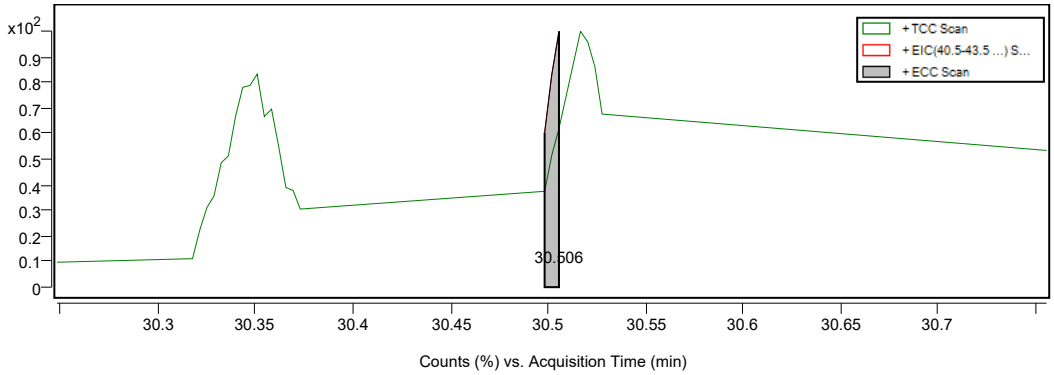
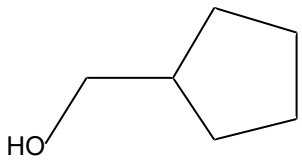
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Cyclopentanemethanol	C6H12O		LibSearch	30.506	15.456		3637-61-4	61.41		
Hex-(3Z)-enyl formate	C7H12O2		LibSearch	30.506			33467-73-1	60.47		
But-(2E)-enoic acid <hex-(3Z)-enyl-> ester	C10H16O2		LibSearch	30.506			65405-80-3	59.34		
Cyclopentanemethanol	C6H12O		LibSearch	30.506	15.456		3637-61-4	59.20		
Montaverdi	C10H16O2		LibSearch	30.506			188570-78-7	59.08		
Hex-(3E)-enyl acetate	C8H14O2		LibSearch	30.506			3681-82-1	58.56		
1,1'-Carbonyldiimidazole	C7H6N4O		LibSearch	30.506	6.422		530-62-1	58.45		
Hexenyl acetate<3Z->	C8H14O2		LibSearch	30.506	22.576		3681-71-8	58.18		
Hex-(3Z)-enyl acetate	C8H14O2		LibSearch	30.506			3681-71-8	58.01		
Hexenyl acetate<3E->	C8H14O2		LibSearch	30.506	22.666		3681-82-1	57.92		
1,1'-Carbonyldiimidazole	C7H6N4O		LibSearch	30.506	6.422		530-62-1	57.60		
Cyclopentane, 2-propenyl-	C8H14		LibSearch	30.506	16.339		3524-75-2	57.23		
Pent-2-enoic acid <2-methyl-, hex-(3Z)-enyl-> ester	C12H20O2		LibSearch	30.506			76649-17-7	57.03		
4-Hexen-1-ol, acetate	C8H14O2		LibSearch	30.506	13.972		72237-36-6	56.97		
4-Hexen-1-ol, acetate	C8H14O2		LibSearch	30.506	13.972		72237-36-6	56.97		
Oct-(5Z)-enol	C8H16O		LibSearch	30.506			64275-73-6	56.79		
3-Cyclopentyl-1-propanol	C8H16O		LibSearch	30.506	12.139		767-05-5	56.59		
3-Hexen-1-ol, acetate, (E)-	C8H14O2		LibSearch	30.506	13.972		3681-82-1	56.30		
Salvene<Z->	C9H16		LibSearch	30.506	26.496		33746-70-2	56.24		
Cyclopentanemethanol	C6H12O		LibSearch	30.506	15.456		3637-61-4	56.17		
1H-Pyrazole, 1-acetyl-	C5H6N2O		LibSearch	30.506	14.672		10199-64-1	56.15		
3-Hexen-1-ol, acetate, (Z)-	C8H14O2		LibSearch	30.506	13.972		3681-71-8	56.00		
3-Hexen-1-ol, acetate, (Z)-	C8H14O2		LibSearch	30.506	13.972		3681-71-8	55.93		
Propanenitrile, 2,2-dimethyl-	C5H9N		LibSearch	30.506	19.189		630-18-2	55.93		
Hexylacetylene	C8H14		LibSearch	30.506			629-05-0	55.66		
Cyclopentane, nitro-	C5H9NO2		LibSearch	30.506	14.789		2562-38-1	55.63		
Hexenyl 2-methyl-2-pentenoate<3Z->	C12H20O2		LibSearch	30.506	5.896		76649-17-7	55.58		
Salvene <Z->	C9H16		LibSearch	30.506			33746-70-2	55.38		
Hexenyl formate<3Z->	C7H12O2		LibSearch	30.506	25.186		33467-73-1	55.16		
3-Hexen-1-ol, formate, (Z)-	C7H12O2		LibSearch	30.506	14.022		33467-73-1	55.06		
trans-3-Hexen-1-ol, trifluoroacetate	C8H11F3O2		LibSearch	30.506	16.739		1000352-31-0	54.98		
Hex-(3Z)-enol	C6H12O		LibSearch	30.506			928-96-1	54.96		
3-Hexen-1-ol, acetate, (Z)-	C8H14O2		LibSearch	30.506	13.972		3681-71-8	54.92		
1,5-Heptadiene, 2,6-dimethyl-	C9H16		LibSearch	30.506	16.039		6709-39-3	54.88		
Cyclopentene, 1-methyl-	C6H10		LibSearch	30.506	19.322		693-89-0	54.87		
1H-Pyrazole	C3H4N2		LibSearch	30.506	16.656		288-13-1	54.75		
2,3-Nonadiene	C9H16		LibSearch	30.506			22433-34-7	54.73		
4-Hexen-1-ol, acetate	C8H14O2		LibSearch	30.506	13.972		72237-36-6	54.42		
Cyclopropane, 2-(1,1-dimethyl-2-propenyl)-1,1-dimethyl-	C10H18		LibSearch	30.506	16.189		81051-15-2	54.35		
2-Butenoic acid, 3-hexenyl ester, (E,Z)-	C10H16O2		LibSearch	30.506	10.522		65405-80-3	54.31		
3-Hexen-1-ol, formate, (Z)-	C7H12O2		LibSearch	30.506	14.022		33467-73-1	54.25		
Hex-(3E)-enol	C6H12O		LibSearch	30.506			928-97-2	54.16		
3-Cyclopentyl-1-propanol	C8H16O		LibSearch	30.506	12.139		767-05-5	54.06		
3-Cyclopentyl-1-propanol	C8H16O		LibSearch	30.506	12.139		767-05-5	54.04		
1-But-1-enylaziridine	C6H11N		LibSearch	30.506	17.522		1000195-06-7	54.04		
4-Hexen-1-ol, acetate, (Z)-	C8H14O2		LibSearch	30.506	13.972		42125-17-7	53.98		
(Z)-Hex-3-en-1-yl propyl carbonate	C10H18O3		LibSearch	30.506	9.406		1000372-80-5	53.80		
Cyclopentane, 2-propenyl-	C8H14		LibSearch	30.506	16.339		3524-75-2	53.77		
Cyclopropane, 1,1-dimethyl-2-(1-methyl-2-propenyl)-	C9H16		LibSearch	30.506	17.506		74779-84-3	53.52		
Cyclopentane, nitro-	C5H9NO2		LibSearch	30.506	14.789		2562-38-1	53.52		

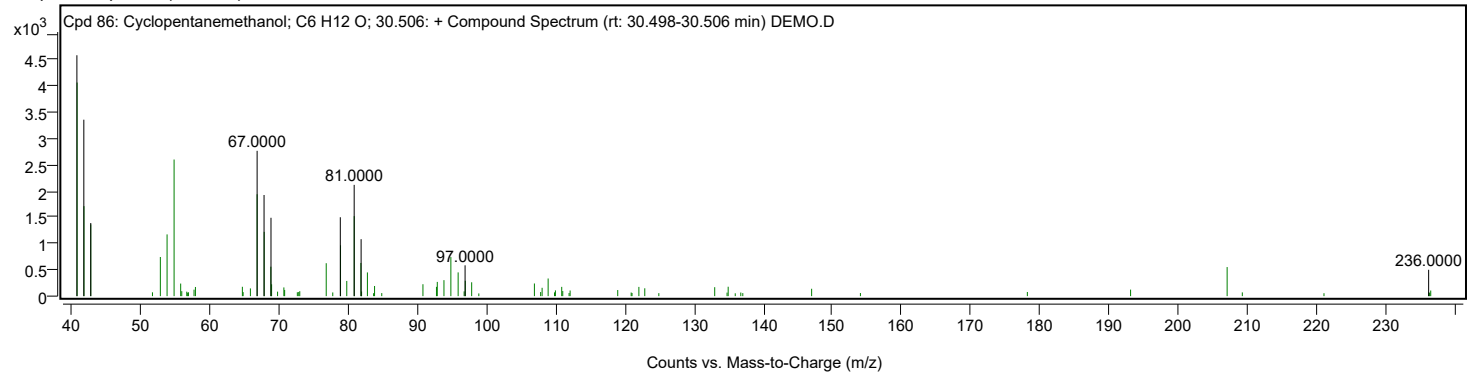
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



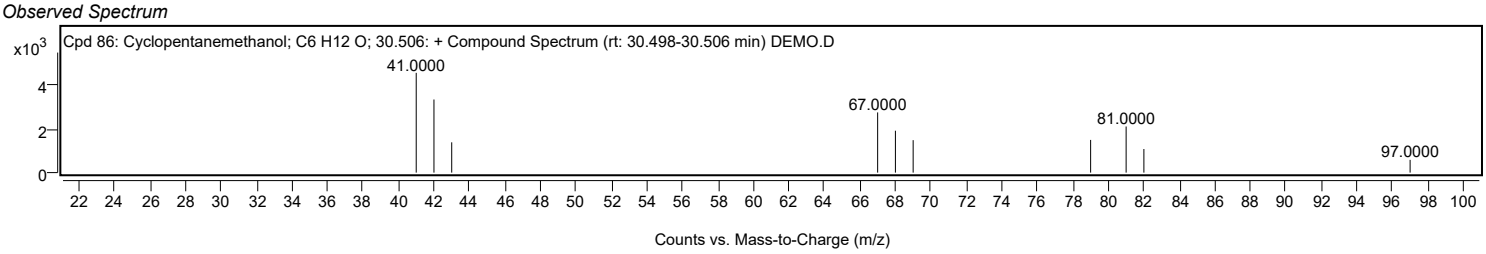
Cyclopentanemethanol

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			61.41			NIST.L

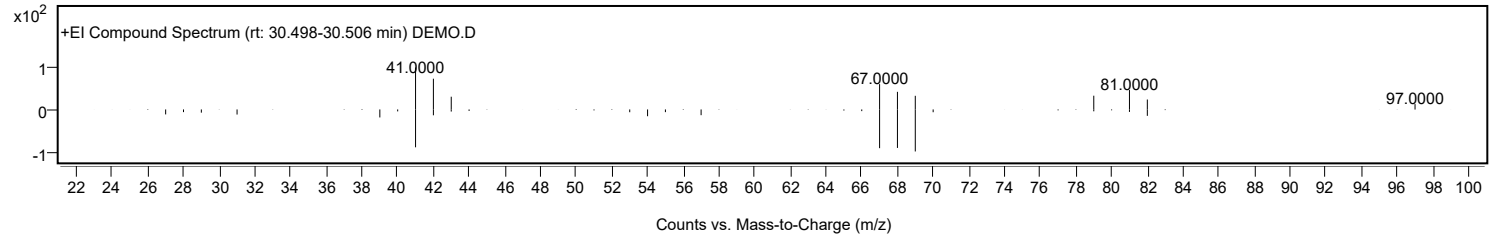
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			61.41			NIST.L

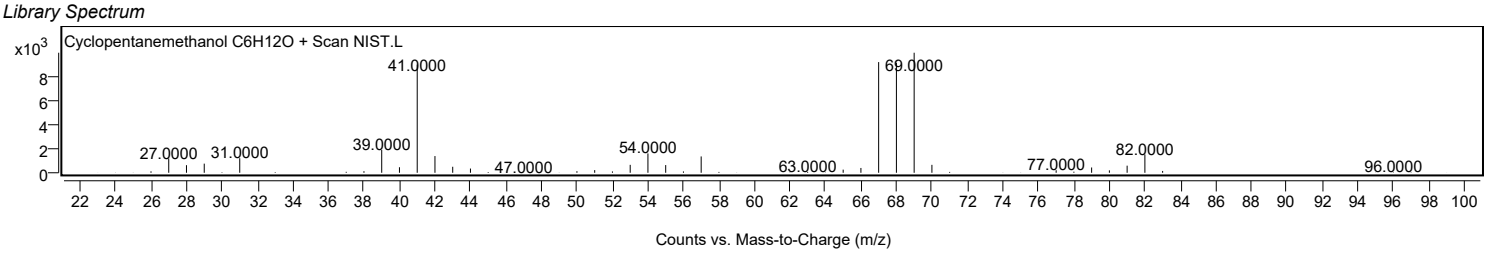
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 87: Hexylacetylene

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Hexylacetylene	C8 H14	30.517			629-05-0	LibSearch	74.61	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		74.61			50		

Compound Discovery Report

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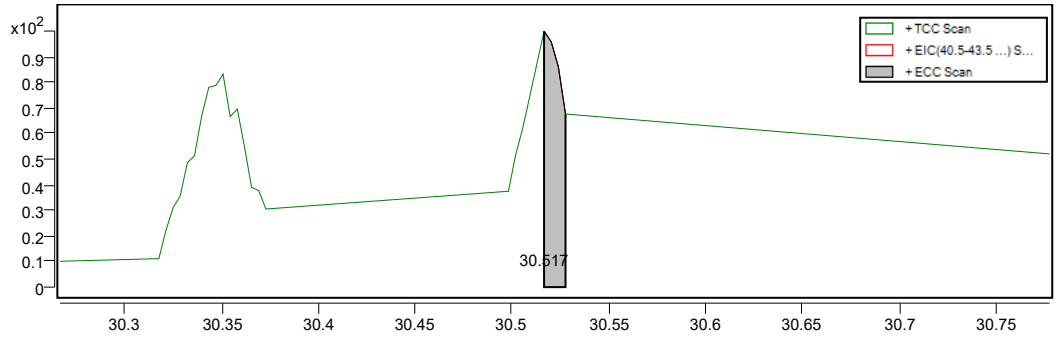
Compound ID Table

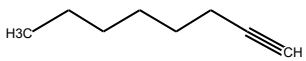
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Hexylacetylene	C8H14		LibSearch	30.517			629-05-0	74.61		
Spiropentane, butyl-	C9H16		LibSearch	30.517	15.967		6191-90-8	72.67		
1,7-Octadiene	C8H14		LibSearch	30.517	17.233		3710-30-3	72.34		
1,1'-Bicyclopropyl, 1,1'-dimethyl-	C8H14		LibSearch	30.517	17.700		59020-33-6	72.31		
Ethane, 1,2-dicyclopropyl-	C8H14		LibSearch	30.517	16.850		37520-11-9	71.93		
Cyclohexanemethanol, 4-methyl-, cis-	C8H16O		LibSearch	30.517	12.450		3937-48-2	71.85		
Undecyne<1->	C11H20		LibSearch	30.517	18.067		2243-98-3	71.84		
1,6-Heptadiene, 3-methyl-	C8H14		LibSearch	30.517	18.300		50871-05-1	71.61		
1,7-Octadiene	C8H14		LibSearch	30.517	17.233		3710-30-3	71.60		
1-Octyne	C8H14		LibSearch	30.517	16.950		629-05-0	71.50		
Bicyclo[4.1.0]heptane, 3-methyl-	C8H14		LibSearch	30.517	17.133		41977-47-3	71.24		
1,6-Octadiene, (E)-	C8H14		LibSearch	30.517	16.933		19036-81-8	71.24		
Ethane, 1,2-dicyclopropyl-	C8H14		LibSearch	30.517	16.850		37520-11-9	71.02		
1,6-Octadiene	C8H14		LibSearch	30.517	16.933		3710-41-6	70.89		
1-Undecyne	C11H20		LibSearch	30.517	11.983		2243-98-3	70.52		
Octylacetylene	C10H18		LibSearch	30.517			764-93-2	70.50		
Oct-(3Z)-enol	C8H16O		LibSearch	30.517			20125-84-2	70.33		
Spiropentane, propyl-	C8H14		LibSearch	30.517	17.617		6191-88-4	70.13		
Nonen-1-ol<3Z->	C9H18O		LibSearch	30.517	16.777		10340-23-5	70.11		
Bicyclo[4.1.0]heptane, 2-methyl-	C8H14		LibSearch	30.517	17.133		41977-46-2	70.11		
Oct-(5Z)-enol	C8H16O		LibSearch	30.517			64275-73-6	70.07		
Undecyne <1->	C11H20		LibSearch	30.517			2243-98-3	70.07		
Non-(6Z)-enol	C9H18O		LibSearch	30.517			35854-86-5	70.06		
Dec-9-en-1-ol	C10H20O		LibSearch	30.517	11.947		13019-22-2	70.01		
Bicyclo[7.1.0]decane	C10H18		LibSearch	30.517	12.167		286-76-0	69.98		
1-Octyne	C8H14		LibSearch	30.517	16.950		629-05-0	69.94		
Nonenol<6Z->	C9H18O		LibSearch	30.517	16.257		35854-86-5	69.93		
1,10-Undecadiene	C11H20		LibSearch	30.517	12.267		13688-67-0	69.62		
1,9-Decadiene	C10H18		LibSearch	30.517	13.933		1647-16-1	69.50		
2-Nonyne	C9H16		LibSearch	30.517	14.967		19447-29-1	69.46		
Cyclopropane, (2-methylenebutyl)-	C8H14		LibSearch	30.517	17.417		74685-56-6	69.36		
1,9-Decadiene	C10H18		LibSearch	30.517	13.933		1647-16-1	69.35		
Citronellene <beta->	C10H18		LibSearch	30.517			2436-90-0	69.26		
Octen-1-ol<3Z->	C8H16O		LibSearch	30.517	20.997		20125-84-2	69.19		
1-Undecyne	C11H20		LibSearch	30.517	11.983		2243-98-3	69.12		
1,7-Octadiene	C8H14		LibSearch	30.517	17.233		3710-30-3	69.03		
1-Nonyne	C9H16		LibSearch	30.517	15.283		3452-09-3	68.98		
1,8-Nonadiene	C9H16		LibSearch	30.517	15.583		4900-30-5	68.93		
1,9-Decadiene	C10H18		LibSearch	30.517	13.933		1647-16-1	68.71		
1,2-Nonadiene	C9H16		LibSearch	30.517			22433-33-6	68.70		
1-Tetradecyne	C14H26		LibSearch	30.517	7.000		765-10-6	68.62		
1,6-Octadiene, 3,7-dimethyl-, (S)-	C10H18		LibSearch	30.517	15.083		10281-55-7	68.59		
2-Octyne	C8H14		LibSearch	30.517	16.617		2809-67-8	68.56		
cis,cis-2,7-Nonadiene	C9H16		LibSearch	30.517	14.983		36901-84-5	68.55		
Citronellene<beta->	C10H18		LibSearch	30.517	24.367		2436-90-0	68.53		
1-Octyne	C8H14		LibSearch	30.517	16.950		629-05-0	68.51		
Decen-1-ol<4E->	C10H20O		LibSearch	30.517	12.137		10339-62-5	68.43		
Octenol<5Z->	C8H16O		LibSearch	30.517	20.317		64275-73-6	68.39		
Decen-1-ol <(4E)->	C10H20O		LibSearch	30.517			10339-62-5	68.32		
3-Octyne	C8H14		LibSearch	30.517	16.617		15232-76-5	68.22		

Compound Chromatograms (overlaid)

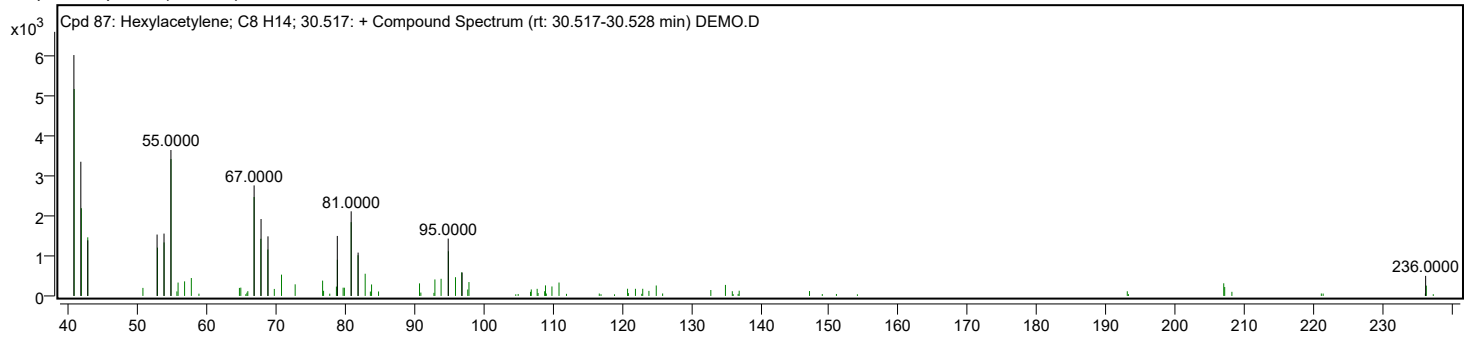


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



Counts vs. Mass-to-Charge (m/z)

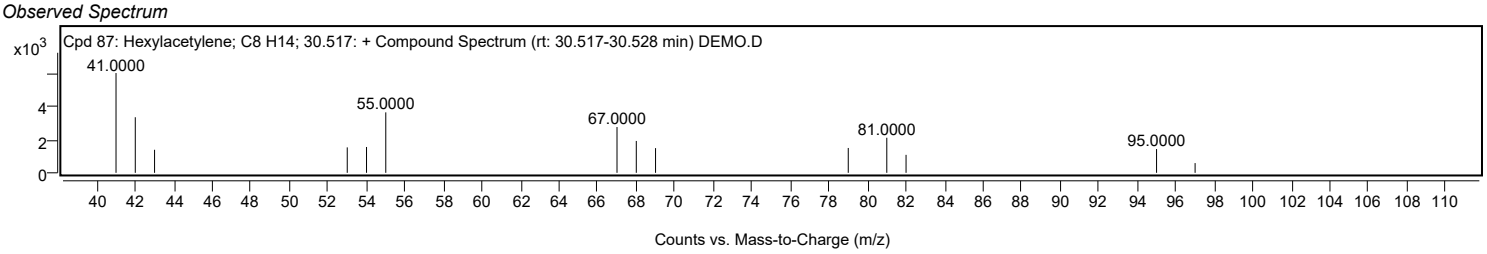
Hexylacetylene

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			74.61			PWNose.xml

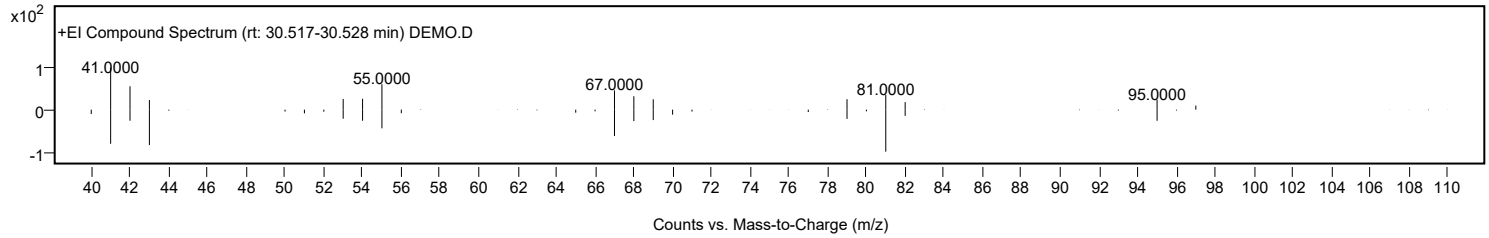
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			74.61			PWNose.xml

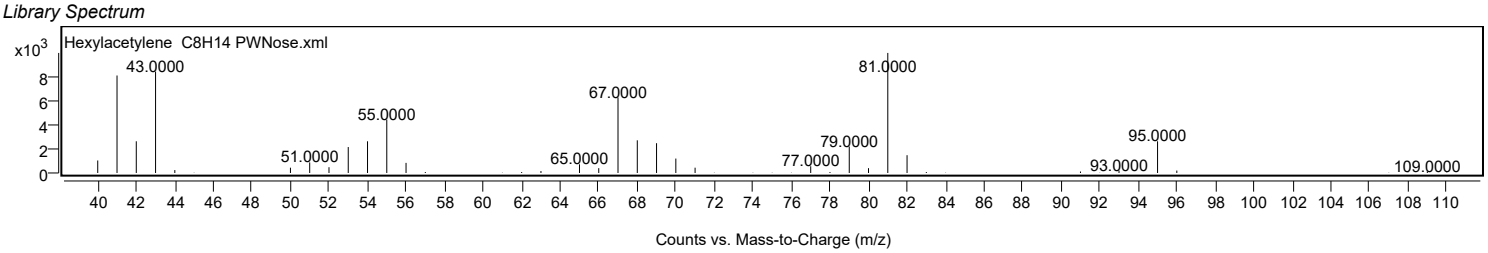
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 88: Undecyne<1->

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Undecyne<1->	C11 H20	31.540			2243-98-3	LibSearch	87.43	Chrom Decon	PWNose.xml

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		87.43			50		

Compound Discovery Report

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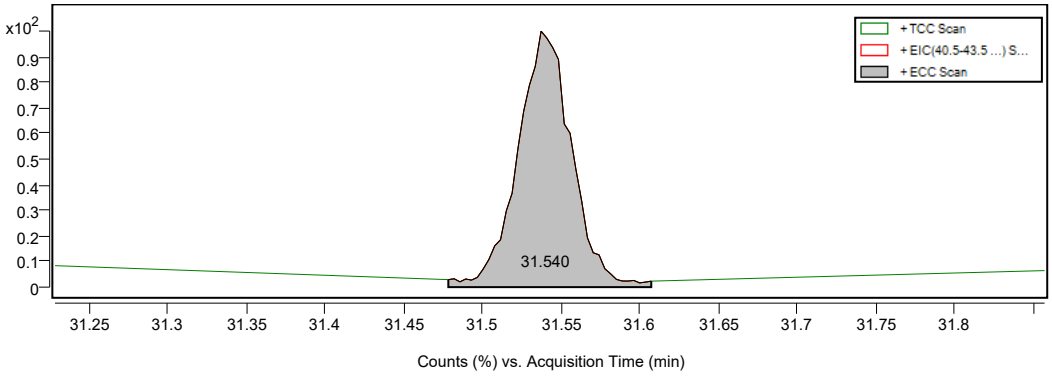
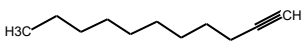
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Undecyne<1->	C11H20		LibSearch	31.540	19.090		2243-98-3	87.43		
Dec-9-en-1-ol	C10H20O		LibSearch	31.540			13019-22-2	87.21		
Octylacetylene	C10H18		LibSearch	31.540			764-93-2	86.86		
Dec-9-en-1-ol	C10H20O		LibSearch	31.540	12.970		13019-22-2	86.80		
Undecyne <1->	C11H20		LibSearch	31.540			2243-98-3	86.70		
Dec-(5Z)-en-1-ol	C10H20O		LibSearch	31.540			51652-47-2	86.69		
Dec-(5E)-en-1-ol	C10H20O		LibSearch	31.540			56578-18-8	86.67		
Dodec-(9Z)-en-1-ol	C12H24O		LibSearch	31.540			35148-18-6	86.62		
1,11-Dodecadiene	C12H22		LibSearch	31.540	11.640		5876-87-9	86.58		
Decen-1-ol<4Z->	C10H20O		LibSearch	31.540	13.300		57074-37-0	86.41		
1,9-Decadiene	C10H18		LibSearch	31.540	14.957		1647-16-1	86.30		
Bicyclo[4.2.0.]octane, 6,7-dimethyl	C10H18		LibSearch	31.540	15.140		1000063-19-2	86.24		
Dodec-(7E)-en-1-yl acetate	C14H26O2		LibSearch	31.540			16695-41-3	86.20		
Dec-9-enyl acetate	C12H22O2		LibSearch	31.540			50816-18-7	86.17		
2-Decyne	C10H18		LibSearch	31.540	14.323		2384-70-5	86.05		
8-Dodecenol	C12H24O		LibSearch	31.540	7.123		42513-42-8	85.74		
1-Tridecyne	C13H24		LibSearch	31.540	9.690		26186-02-7	85.68		
Undecenol <10->	C11H22O		LibSearch	31.540			112-43-6	85.57		
4,5-Nonadiene	C9H16		LibSearch	31.540			821-74-9	85.57		
Tetradec-(7Z)-en-1-ol acetate	C16H30O2		LibSearch	31.540			16974-10-0	85.52		
1-Pentadecyne	C15H28		LibSearch	31.540	6.373		765-13-9	85.51		
Dodec-(8Z)-en-1-ol	C12H24O		LibSearch	31.540			40642-40-8	85.49		
Spiropentane, butyl-	C9H16		LibSearch	31.540	16.990		6191-90-8	85.46		
Undecenol<10->	C11H22O		LibSearch	31.540	8.640		112-43-6	85.43		
Non-(6Z)-enol	C9H18O		LibSearch	31.540			35854-86-5	85.42		
4-Cyclohexyl-1-butanol	C10H20O		LibSearch	31.540	9.523		4441-57-0	85.42		
Cyclodecene, (Z)-	C10H18		LibSearch	31.540	11.857		935-31-9	85.36		
1,11-Dodecadiene	C12H22		LibSearch	31.540	11.640		5876-87-9	85.31		
Dec-(4Z)-en-1-ol	C10H20O		LibSearch	31.540			57074-37-0	85.29		
1,10-Undecadiene	C11H20		LibSearch	31.540	13.290		13688-67-0	85.17		
1,12-Tridecadiene	C13H24		LibSearch	31.540	9.973		21964-48-7	85.15		
1,10-Undecadiene	C11H20		LibSearch	31.540	13.290		13688-67-0	85.11		
1-Dodecyne	C12H22		LibSearch	31.540	11.340		765-03-7	85.07		
1-Dodecyne	C12H22		LibSearch	31.540	11.340		765-03-7	85.04		
(3R,3aS,6R,7[a]R)-Perhydro-3,6-dimethyl-benzo-[b]-furan-2-one	C10H16O2		LibSearch	31.540			92015-65-1	84.78		
Hexylidencyclohexane	C12H22		LibSearch	31.540	9.857		10201-62-4	84.71		
6-Dodecyne	C12H22		LibSearch	31.540	11.023		6975-99-1	84.61		
6-Dodecyne	C12H22		LibSearch	31.540	11.023		6975-99-1	84.58		
Cyclodecene, (Z)-	C10H18		LibSearch	31.540	11.857		935-31-9	84.53		
Cyclohexaneethanol <2->	C8H16O		LibSearch	31.540			4442-79-9	84.44		
1,8-Nonadiene	C9H16		LibSearch	31.540	16.607		4900-30-5	84.41		
7-Tetradecyne	C14H26		LibSearch	31.540	7.707		35216-11-6	84.39		
3-Tetradecyne	C14H26		LibSearch	31.540	7.707		60212-32-0	84.38		
Cycloundecene (Z)	C11H20		LibSearch	31.540	9.857		13151-61-6	84.35		
1,9-Decadiene	C10H18		LibSearch	31.540	14.957		1647-16-1	84.35		
1-Tridecyne	C13H24		LibSearch	31.540	9.690		26186-02-7	84.34		
Decen-1-ol<4E->	C10H20O		LibSearch	31.540	13.160		10339-62-5	84.30		
1-Dodecyne	C12H22		LibSearch	31.540	11.340		765-03-7	84.26		
Nonenol<6Z->	C9H18O		LibSearch	31.540	17.280		35854-86-5	84.26		
1,11-Dodecadiene	C12H22		LibSearch	31.540	11.640		5876-87-9	84.23		

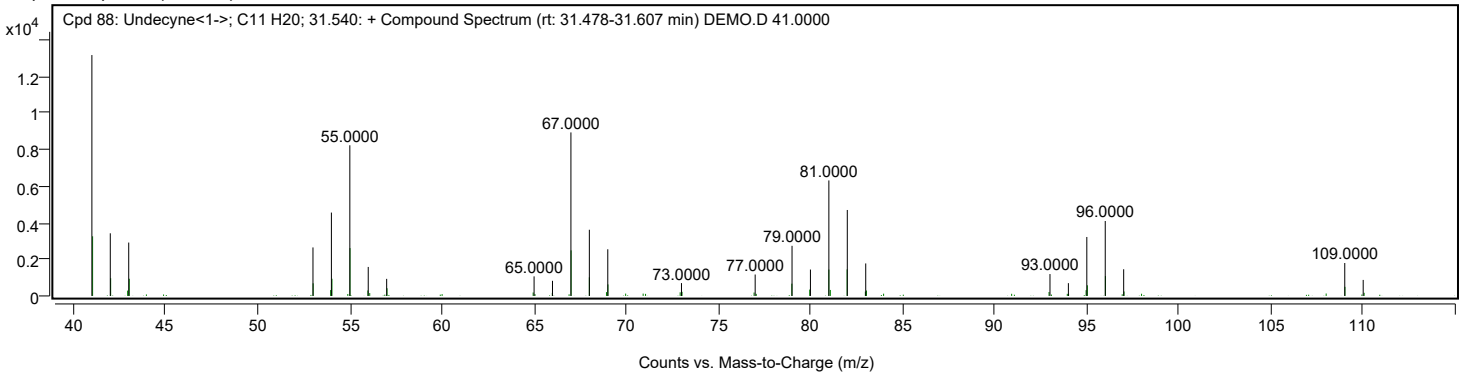
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



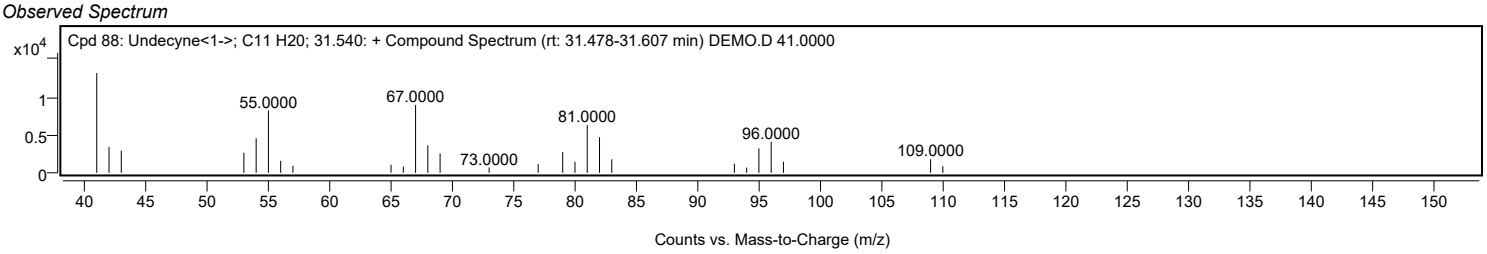
Undecyne<1->

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			87.43			PWNose.xml

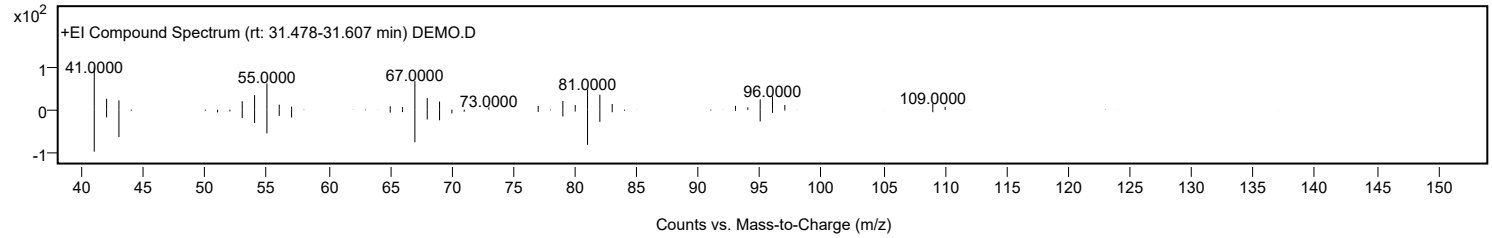
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			87.43			PWNose.xml

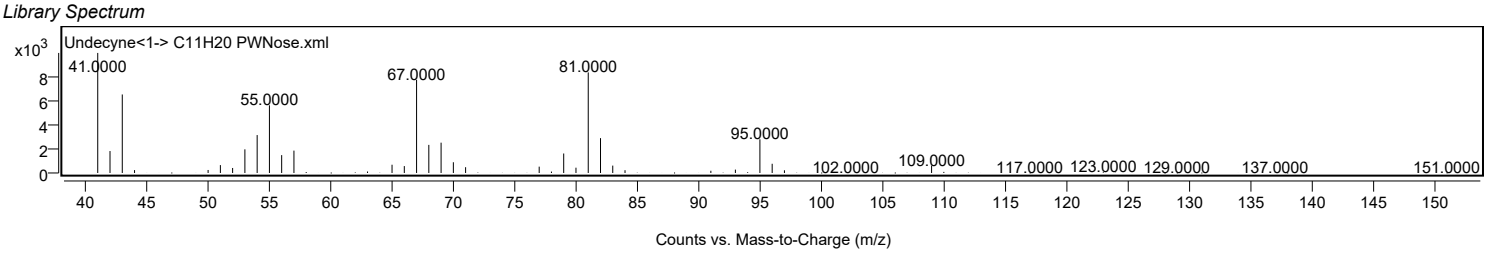
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 89: Ethylene brassylate

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Ethylene brassylate	C15 H26 O4	32.820			105-95-3	LibSearch	95.19	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		95.19			50		

Compound Discovery Report

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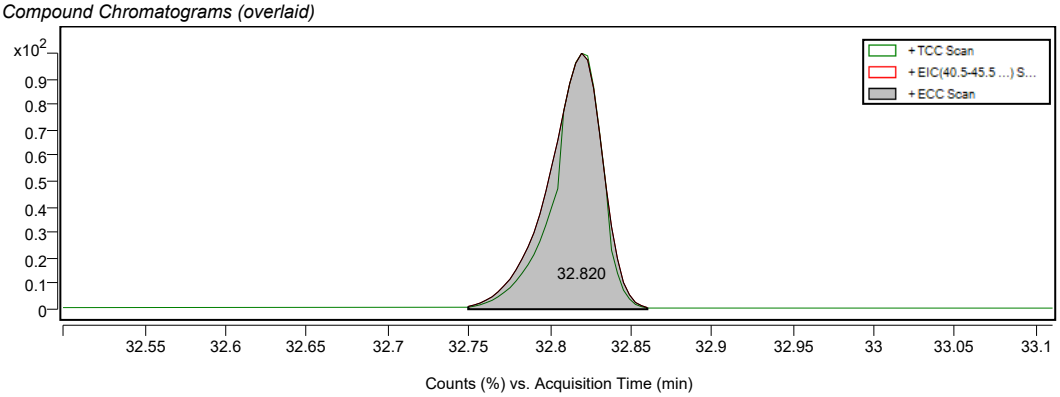
Compound ID Table

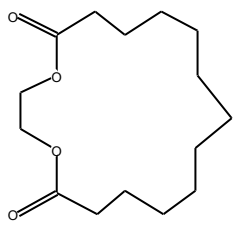
Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Ethylene brassylate	C15H26O4		LibSearch	32.820	-8.664		105-95-3	95.19		
Ethylene brassylate	C15H26O4		LibSearch	32.820	-15.000		105-95-3	94.75		
Ethylene brassylate	C15H26O4		LibSearch	32.820	-8.664		105-95-3	91.73		
Ethylene brassylate	C15H26O4		LibSearch	32.820	-8.664		105-95-3	91.61		
Ethylene brassylate	C15H26O4		LibSearch	32.820			105-95-3	84.86		
E-9-Tetradecenoic acid	C14H26O2		LibSearch	32.820	3.203		50286-30-1	72.26		
Z-8-Methyl-9-tetradecenoic acid	C15H28O2		LibSearch	32.820	2.603		1000130-84-5	72.19		
Myristoleic acid	C14H26O2		LibSearch	32.820	3.203		544-64-9	71.81		
Z-7-Tetradecenoic acid	C14H26O2		LibSearch	32.820	3.203		1000130-98-4	71.74		
Myristoyl chloride	C14H27ClO		LibSearch	32.820	4.070		112-64-1	71.40		
E-11-Tetradecenoic acid	C14H26O2		LibSearch	32.820	3.203		1000130-96-2	71.25		
7-Methyl-Z-tetradecen-1-ol acetate	C17H32O2		LibSearch	32.820	2.453		1000130-99-6	70.93		
Z-11-Tetradecenoic acid	C14H26O2		LibSearch	32.820	3.203		1000130-83-3	70.86		
13-Bromotetradecanoic acid	C14H27BrO2		LibSearch	32.820	-0.530		1000099-12-8	70.79		
Z-11-Pentadecenol	C15H30O		LibSearch	32.820	3.436		1000130-77-0	70.28		
1,4-Dioxacyclohexadecane-5,16-dione	C14H24O4		LibSearch	32.820	-6.664		54982-83-1	69.81		
E-8-Methyl-7-dodecen-1-ol acetate	C15H28O2		LibSearch	32.820	5.070		1000131-32-2	69.77		
Cyclic ethylene dodecanedioate	C14H24O4		LibSearch	32.820			54982-83-1	69.71		
9-Methyl-Z-10-pentadecen-1-ol	C16H32O		LibSearch	32.820	2.853		1000131-00-7	69.08		
Oxacyclotetradecan-2-one, 13-methyl-	C14H26O2		LibSearch	32.820	0.070		57092-32-7	68.31		
Hexadecane-1,2-diol	C16H34O2		LibSearch	32.820	-0.797		6920-24-7	68.29		
Oxacyclohexadecane-2,13-dione	C15H26O3		LibSearch	32.820	-5.764		38223-29-9	68.20		
trans-Traumatic acid	C12H20O4		LibSearch	32.820	0.570		6402-36-4	68.18		
Z-10-Tetradecen-1-ol acetate	C16H30O2		LibSearch	32.820	3.036		1010130-99-3	67.96		
.alpha.-Pyrrolidone, 5-[5,5-dimethoxy-1-hexyl]-N-methyl-	C13H25NO3		LibSearch	32.820	3.753		1000125-91-9	67.96		
Oxacyclododecan-2-one	C11H20O2		LibSearch	32.820	5.086		1725-03-7	67.79		
Myristoleic acid	C14H26O2		LibSearch	32.820	3.203		544-64-9	67.70		
Myristoleic acid	C14H26O2		LibSearch	32.820	3.203		544-64-9	67.70		
13-Tetradecenal	C14H26O		LibSearch	32.820	6.303		85896-31-7	67.57		
Cyclohexadecanolide	C16H30O2		LibSearch	32.820	-12.250		109-29-5	67.44		
Oxacyclododecan-2-one	C11H20O2		LibSearch	32.820	5.086		1725-03-7	67.32		
10-Undecenoyl chloride	C11H19ClO		LibSearch	32.820	9.203		38460-95-6	67.28		
Oxacyclotetradecan-2-one, 14-methyl-	C14H26O2		LibSearch	32.820	0.070		27198-63-6	67.24		
12-Hydroxydodecanoic acid	C12H24O3		LibSearch	32.820	2.603		505-95-3	67.16		
Z-9-Pentadecenol	C15H30O		LibSearch	32.820	3.436		1000130-76-9	67.14		
7-Methyl-Z,Z-8,10-hexadecadien-1-ol acetate	C19H34O2		LibSearch	32.820	-0.997		1000130-88-6	67.06		
Oxacyclotetradecan-2-one	C13H24O2		LibSearch	32.820	1.086		1725-04-8	67.04		
Cyclopentadecanone, 2-hydroxy-	C15H28O2		LibSearch	32.820	-3.147		4727-18-8	66.92		
Cyclopentadecanolide	C15H28O2		LibSearch	32.820	-8.740		106-02-5	66.88		
Z-11-Pentadecenal	C15H28O		LibSearch	32.820	4.336		1010130-84-6	66.82		
(E)-Hexadec-9-enoic acid	C16H30O2		LibSearch	32.820	-0.114		10030-73-6	66.74		
13-Octadecenal, (Z)-	C18H34O		LibSearch	32.820	-0.630		58594-45-9	66.70		
12-Methyl-E,E-2,13-octadecadien-1-ol	C19H36O		LibSearch	32.820	-2.247		1010130-90-4	66.59		
Fumaric acid, 4-octyl 2-chloro-6-fluorophenyl ester	C18H22ClFO4		LibSearch	32.820	-5.847		1000405-62-4	66.45		
Undecanoyl chloride	C11H21ClO		LibSearch	32.820	9.036		17746-05-3	66.44		
cis-7-Hexadecenoic acid	C16H30O2		LibSearch	32.820	-0.114		2416-19-5	66.38		
Octadecanedioic acid	C18H34O4		LibSearch	32.820	-9.230		871-70-5	66.14		
E-2-Hexadecacen-1-ol	C16H32O		LibSearch	32.820	1.786		1010131-10-1	66.10		
2H-Pyran-2-one, tetrahydro-6-nonyl-	C14H26O2		LibSearch	32.820	2.803		2721-22-4	66.05		
3,11-Tetradecadien-1-ol	C14H26O		LibSearch	32.820	4.953		1000131-36-2	65.97		

Compound Chromatograms (overlaid)

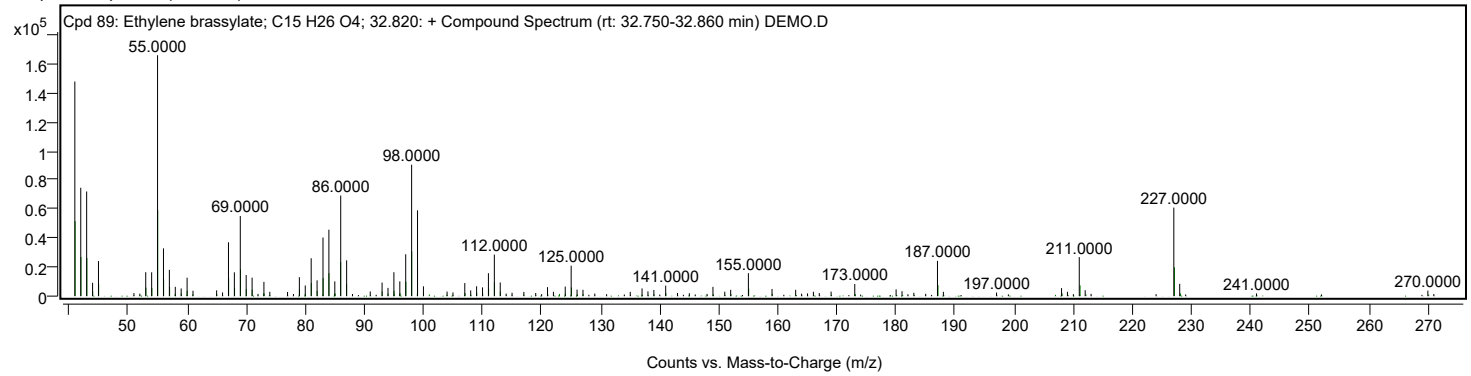


Counts (%) vs. Acquisition Time (min)

Structure



Compound Spectra (overlaid)



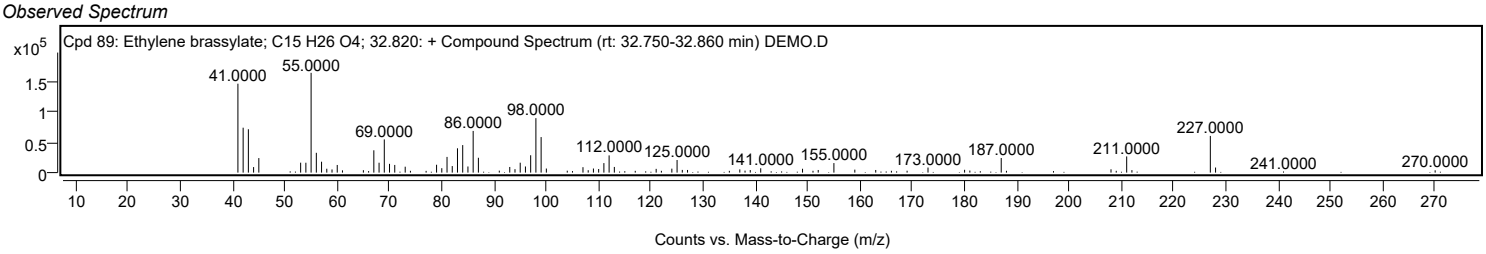
Ethylene brassylate

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			95.19			NIST.L

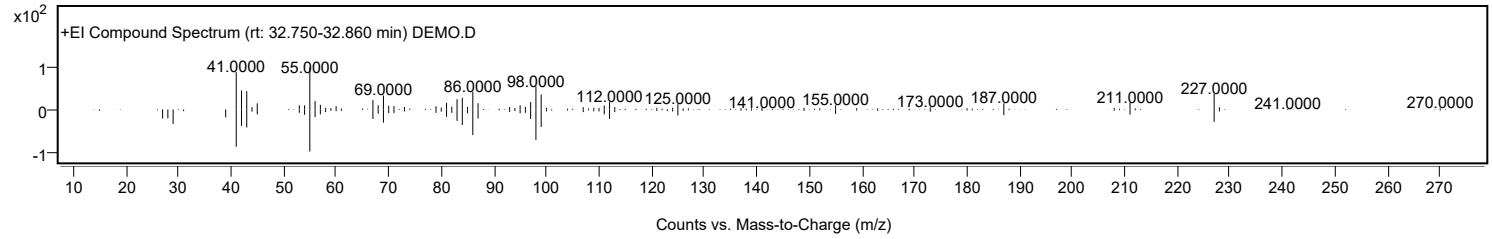
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			95.19			NIST.L

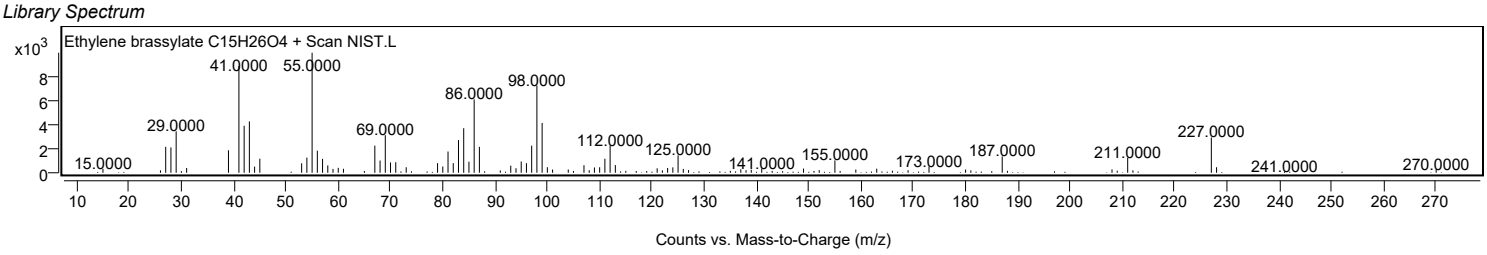
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 90: 2,6-Nonadienal, 3,7-dimethyl-

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
2,6-Nonadienal, 3,7-dimethyl-	C11 H18 O	32.830			41448-29-7	LibSearch	45.84	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		45.84			50		

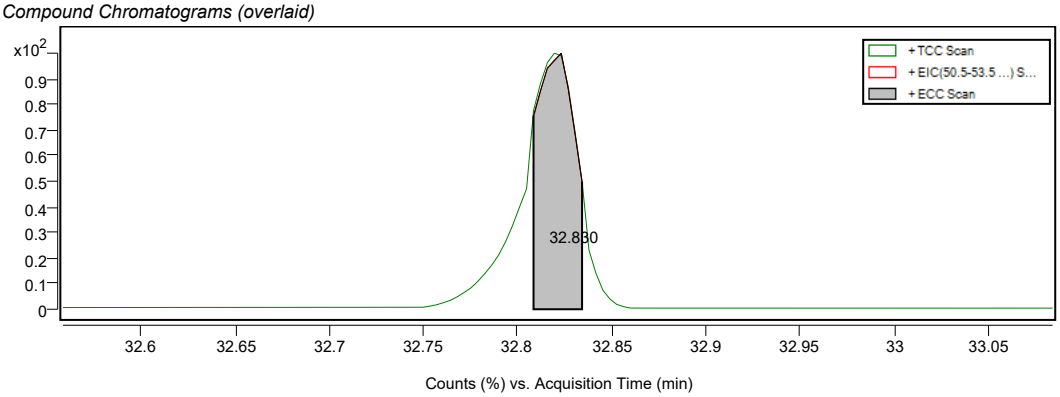
Compound Discovery Report

Agilent | Trusted Answers

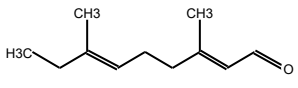
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
2,6-Nonadienal, 3,7-dimethyl-	C11H18O		LibSearch	32.830	11.613		41448-29-7	45.84		
Ethylene brassylate	C15H26O4		LibSearch	32.830	-14.990		105-95-3	44.05		
(1,2-Dichlorotrifluoroethyl)cyclohexane	C8H11Cl2F3		LibSearch	32.830	17.097		219904-98-0	43.85		
3-Hexen-1-ol, 2,5-dimethyl-, formate,(Z)-	C9H16O2		LibSearch	32.830	15.163		1000132-12-3	42.00		
Succinic acid, tridec-2-yn-1-yl trans-hex-3-en-1-yl ester	C23H38O4		LibSearch	32.830	-11.620		1000391-12-6	41.93		
1,2-Benzenediol, O-dichloroacetyl-O'-(3-methylbut-2-enoyl)-	C13H12Cl2O4		LibSearch	32.830	-1.653		1000330-46-9	41.87		
Cyclohexane, (2-nitro-2-propenyl)-	C9H15NO2		LibSearch	32.830	10.697		80255-17-0	41.80		
Cyclobutanecarboxylic acid, but-3-yn-2-yl ester	C10H14O2		LibSearch	32.830	13.530		1000299-12-8	41.57		
8-Tetradecen-1-ol acetate	C16H30O2		LibSearch	32.830	3.047		1000131-36-0	41.51		
Binapacryl	C15H18N2O6		LibSearch	32.830	-8.537		485-31-4	41.28		
Binapacryl	C15H18N2O6		LibSearch	32.830	-8.537		485-31-4	41.23		
2-Butenoic acid, 2-methyl-, 2-methyl-2-propenyl ester, (E)-	C9H14O2		LibSearch	32.830	15.580		61692-82-8	41.19		
Artemisia ketone	C10H16O		LibSearch	32.830	22.950		546-49-6	41.17		
Butane-1,1-dicarbonitrile, 1-cyclohexyl-3-methyl-	C13H20N2		LibSearch	32.830	4.180		1000164-70-2	41.14		
3-Methyl-2-butenoic acid, 2-bromo-4-fluorophenyl ester	C11H10BrFO2		LibSearch	32.830	5.530		1000293-62-2	41.03		
2(5H)-Furanone, 5-(2-methyl-2-propenyl)-	C8H10O2		LibSearch	32.830	13.930		1000155-86-2	40.95		
2H-1,2,3-Triazol-4-amine, 2-cyclohexyl-5-nitro-, 1-oxide	C8H13N5O3		LibSearch	32.830			252555-91-2	40.88		
2-Cyclohexylpiperidine	C11H21N		LibSearch	32.830	8.047		56528-77-9	40.78		
(-)-trans-Isopiperitenol	C10H16O		LibSearch	32.830	12.730		74410-00-7	40.73		
3,7-Decadiene, 2,9-dimethyl-	C12H22		LibSearch	32.830	14.463		74630-13-0	40.68		
Cyclohexane, bromo-	C6H11Br		LibSearch	32.830	16.547		108-85-0	40.49		
Oxalic acid, dicyclohexyl ester	C14H22O4		LibSearch	32.830	1.597		1000309-30-9	40.37		
Fumaric acid, 4-octyl 2-chloro-6-fluorophenyl ester	C18H22ClFO4		LibSearch	32.830	-5.837		1000405-62-4	40.28		
Cyclobutanecarboxylic acid, 4-nitrophenyl ester	C11H11NO4		LibSearch	32.830	3.213		1000307-44-2	40.04		
Propanedinitrile, dicyclohexyl-	C15H22N2		LibSearch	32.830	-1.253		74764-28-6	40.03		
[1,1'-Bicyclopentyl]-2-one	C10H16O		LibSearch	32.830	11.613		4884-24-6	39.95		
Methyl (11R,12R,13S)-(Z)-12,13-epoxy-11-methoxy-9-octadecenoate	C20H36O4		LibSearch	32.830	-4.637		88335-39-1	39.80		
1,5-Octadiene, 7-methyl-3-(1-methylethyl)-	C12H22		LibSearch	32.830	15.830		74630-12-9	39.72		
3,3-Diethoxy-1-propyne	C7H12O2		LibSearch	32.830	19.447		10160-87-9	39.66		
1,2,4-Triazaspiro[4.5]decane-3-thione, 2,7,7,9-tetramethyl-	C11H21N3S		LibSearch	32.830	-0.870		1000277-45-9	39.56		
3-Methylbut-2-enoic acid, 4-nitrophenyl ester	C11H11NO4		LibSearch	32.830	3.847		1000307-59-8	39.47		
Cyclohexane, bromo-	C6H11Br		LibSearch	32.830	16.547		108-85-0	39.46		
9-(Acryloyloxy)nonyl acrylate	C15H24O4		LibSearch	32.830	2.380		107481-28-7	39.44		
3-Methyl-2-butenoic acid, cyclobutyl ester	C9H14O2		LibSearch	32.830	14.647		1000282-89-1	39.43		
3-Methyl-2-butenoic acid, 2-methyloct-5-yn-4-yl ester	C14H22O2		LibSearch	32.830	8.597		1000299-31-3	39.43		
2-Cyclopentylcyclopentanone	C10H16O		LibSearch	32.830			4884-24-6	39.41		
1,5-Heptadien-4-one, 3,3,6-trimethyl-	C10H16O		LibSearch	32.830	15.463		546-49-6	39.29		
3,3-Diethoxy-1-propyne	C7H12O2		LibSearch	32.830	19.447		10160-87-9	39.29		
Shyobunol	C15H26O		LibSearch	32.830	-3.480		35727-45-8	39.29		
Cyclohexane, 2-propenyl-	C9H16		LibSearch	32.830	16.680		2114-42-3	39.24		
Hasmigone <(E)->	C11H18O		LibSearch	32.830			68133-74-4	39.21		
Isocitronellol	C10H20O		LibSearch	32.830	14.930		18479-52-2	39.17		
Hasmigone <(Z)->	C11H18O		LibSearch	32.830			34687-46-2	39.16		
Cyclobutanecarboxylic acid, tridec-2-ynyl ester	C18H30O2		LibSearch	32.830	-0.803		1010299-13-7	39.13		
2H-Benzocyclohepten-2-one, decahydro-9a-methyl-, trans-	C12H20O		LibSearch	32.830	8.397		55103-67-8	39.13		
Oxalic acid, cyclohexyl ethyl ester	C10H16O4		LibSearch	32.830	9.280		1000309-30-2	39.12		
Fumaric acid, 2-octyl 2-chloro-6-fluorophenyl ester	C18H22ClFO4		LibSearch	32.830	-5.837		1000405-58-9	39.10		
Cyclohexane, bromo-	C6H11Br		LibSearch	32.830	16.547		108-85-0	39.09		
Penten-3-one	C5H8O		LibSearch	32.830			1629-58-9	39.07		
Hexane, 1,6-dibromo-	C6H12Br2		LibSearch	32.830	12.663		629-03-8	39.06		

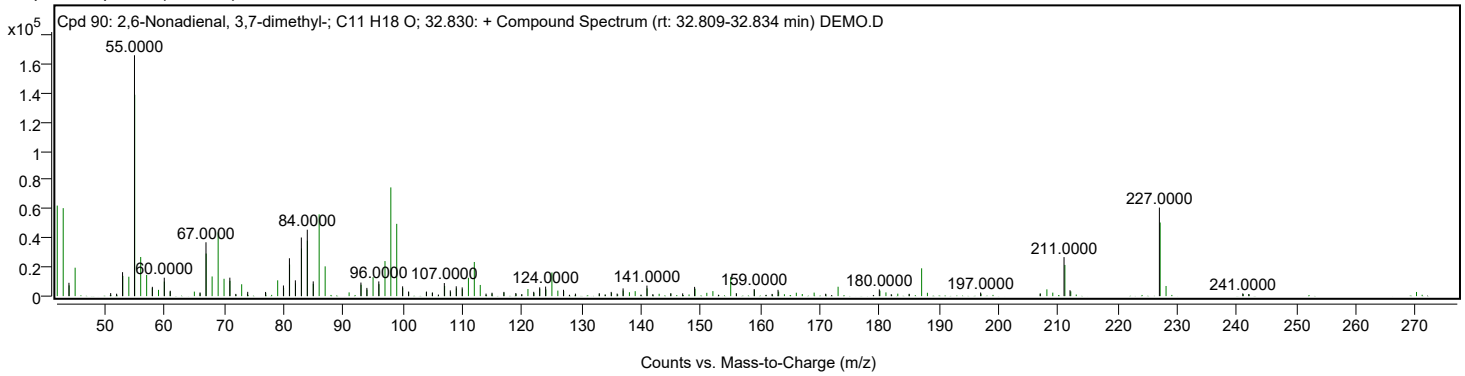
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



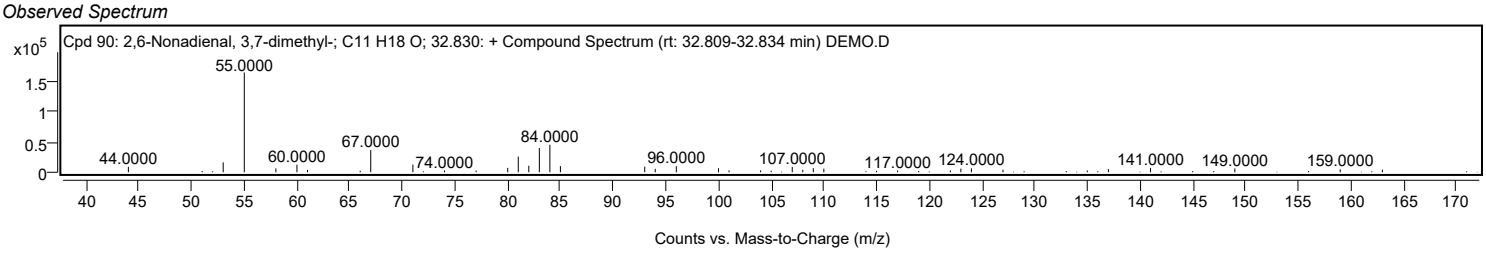
2,6-Nonadienal, 3,7-dimethyl-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			45.84			NIST.L

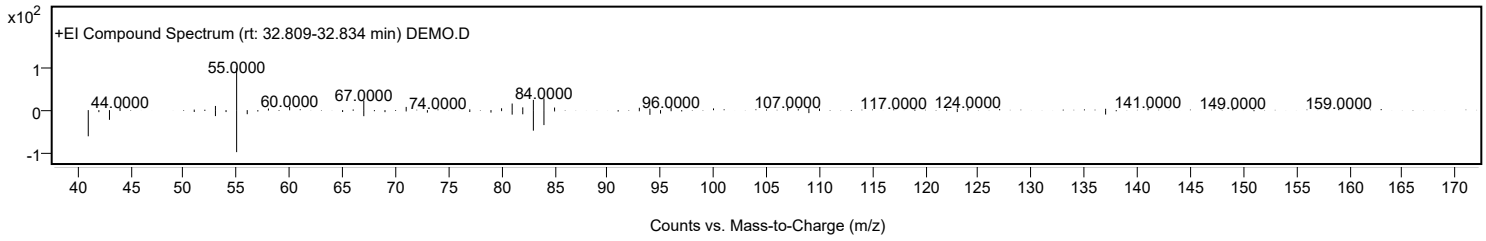
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			45.84			NIST.L

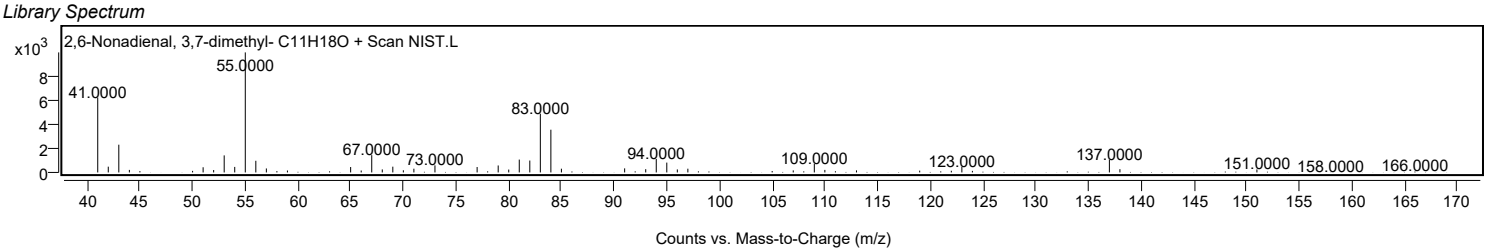
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 91: 2-Methyl-5-nitrobenzimidazole

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
2-Methyl-5-nitrobenzimidazole	C8 H7 N3 O2	38.536			1792-40-1	LibSearch	36.11	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		36.11			3		

Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
2-Methyl-5-nitrobenzimidazole	C8H7N3O2		LibSearch	38.536	9.253		1792-40-1	36.11		
2H-Indazole, 2-methyl-4-nitro-	C8H7N3O2		LibSearch	38.536	13.703		26120-44-5	34.37		
Picrolonic acid	C10H8N4O5		LibSearch	38.536	-0.497		550-74-3	24.22		

Compound Discovery Report

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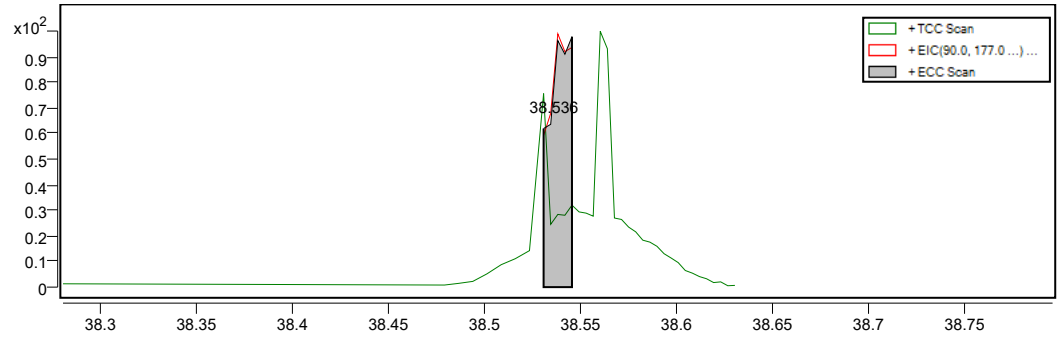
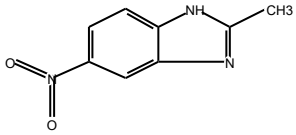
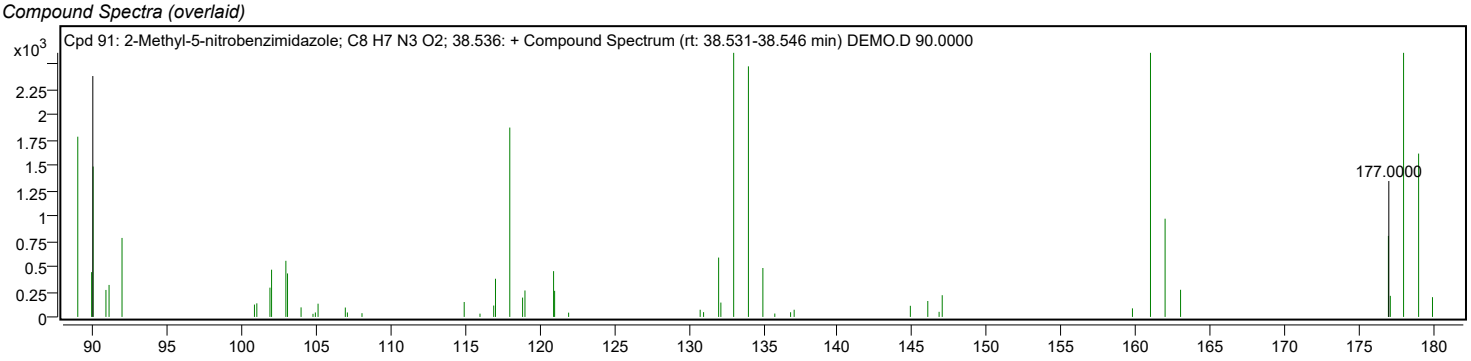
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



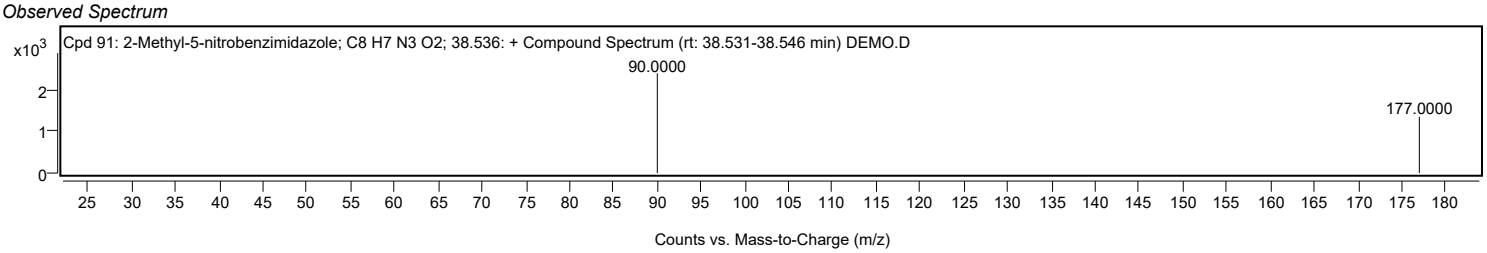
2-Methyl-5-nitrobenzimidazole

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			36.11			NIST.L

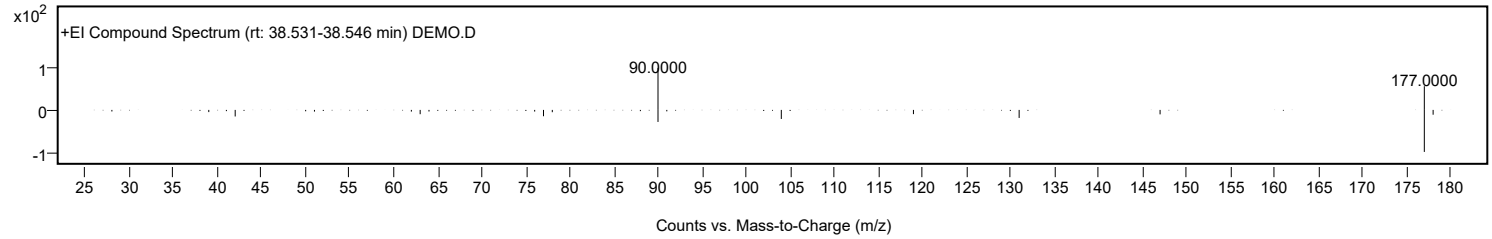
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			36.11			NIST.L

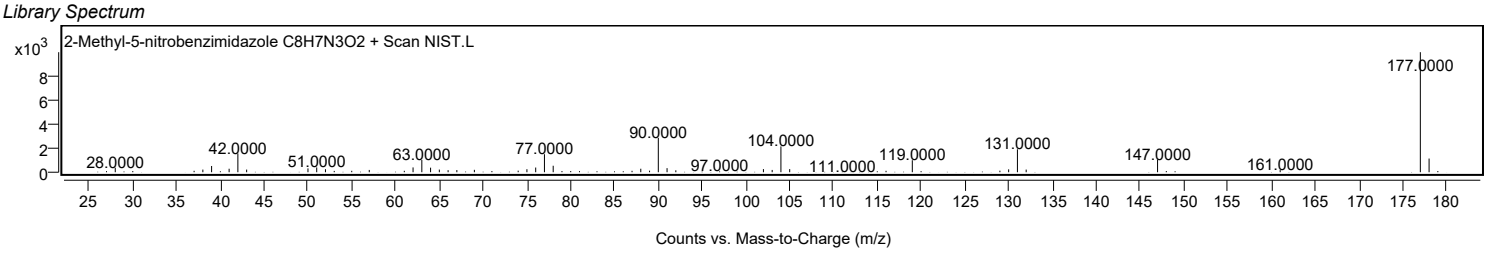
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 92: Benzene, 1-isocyano-3-methoxy-

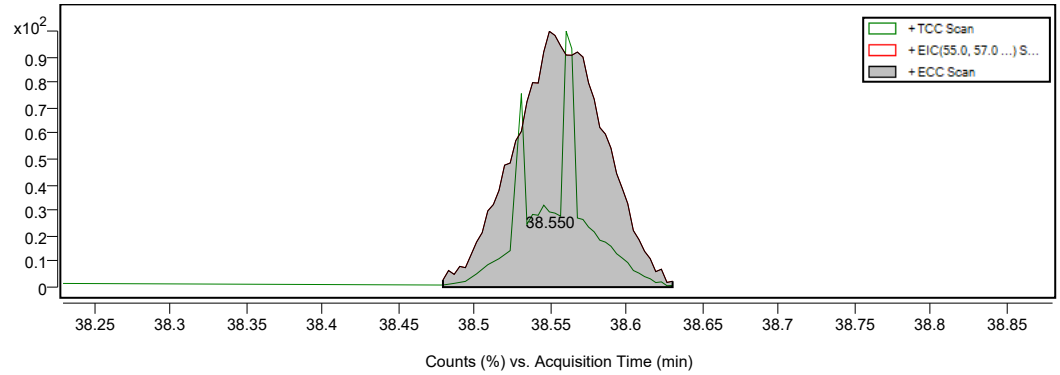
Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Benzene, 1-isocyano-3-methoxy-	C8 H7 N O	38.550			20600-55-9	LibSearch	51.42	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		51.42			50		

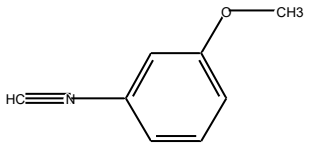
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Benzene, 1-isocyano-3-methoxy-	C8H7NO		LibSearch	38.550			20600-55-9	51.42		
Benzonitrile, 4-methoxy-	C8H7NO		LibSearch	38.550	19.433		874-90-8	47.55		
Benzene, 1-isocyano-4-methoxy-	C8H7NO		LibSearch	38.550			10349-38-9	46.73		
m-Methoxybenzontrile	C8H7NO		LibSearch	38.550	19.433		1527-89-5	44.82		
4-Ethylbenzoic acid, 3-fluorophenyl ester	C15H13FO2		LibSearch	38.550	8.200		1000331-31-0	43.22		
Benzoic acid, 4-ethyl-, 4-cyanophenyl ester	C16H13NO2		LibSearch	38.550	3.150		56131-48-7	42.78		
4-Ethylbenzoic acid, 4-nitrophenyl ester	C15H13NO4		LibSearch	38.550	1.183		1000307-12-7	42.65		
4-Ethylbenzoic acid, 2,3-dichlorophenyl ester	C15H12Cl2O2		LibSearch	38.550	1.783		1000331-31-5	42.63		
4-Ethylbenzoic acid, 2-formyl-4,6-dichlorophenyl ester	C16H12Cl2O3		LibSearch	38.550	-3.250		1010331-31-6	42.45		
1,2-Benzenediol, O-(4-ethylbenzoyl)-O'-methoxycarbonyl-	C17H16O5		LibSearch	38.550	0.183		1000330-50-2	42.17		
6-[4-Methoxyphenyl]-N-methyl-1,2,4,5-tetrazin-3-amine	C10H11N5O		LibSearch	38.550	7.833		72115-81-2	42.12		
m-Methoxybenzontrile	C8H7NO		LibSearch	38.550	19.433		1527-89-5	42.10		
4-Ethylbenzoic acid, 2-fluorophenyl ester	C15H13FO2		LibSearch	38.550	8.200		1000325-73-3	42.03		
1,2-Benzenediol, o-(4-ethylbenzoyl)-	C15H14O3		LibSearch	38.550	4.100		1000325-96-6	41.34		
4-Ethylbenzoic acid, 3,4-dichlorophenyl ester	C15H12Cl2O2		LibSearch	38.550	1.783		1000307-12-6	41.16		
4-Ethyl-N-(4H-1,2,4-triazol-4-yl)benzamide, N-methyl-	C12H14N4O		LibSearch	38.550	6.233		1000492-25-7	40.97		
Benzonitrile, 4-methoxy-	C8H7NO		LibSearch	38.550	19.433		874-90-8	40.95		
1,2-Benzenediol, o-(2-bromopropionyl)-o'-(4-ethylbenzoyl)-	C18H17BrO4		LibSearch	38.550	-4.083		1000325-97-0	40.95		
4-Ethylbenzoic acid, 3-chlorophenyl ester	C15H13ClO2		LibSearch	38.550	4.783		1010325-73-4	40.95		
Benzoic acid, 4-ethyl-, 4-cyanophenyl ester	C16H13NO2		LibSearch	38.550	3.150		56131-48-7	40.88		
2H-Benzotriazole, 2-methyl-	C7H7N3		LibSearch	38.550	19.283		16584-00-2	40.77		
4-Ethylbenzoic acid, 2-methylphenyl ester	C16H16O2		LibSearch	38.550	5.883		1000293-61-2	40.71		
4-Ethylbenzoic acid, anhydride	C18H18O3		LibSearch	38.550	0.300		1000419-67-6	40.68		
1,2-Benzenediol, O-(4-ethylbenzoyl)-O'-propargyloxycarbonyl-	C19H16O5		LibSearch	38.550	-3.100		1000329-75-1	40.64		
4-Ethylbenzoic acid, 4-chlorophenyl ester	C15H13ClO2		LibSearch	38.550	4.783		1000307-12-2	40.57		
1,3-Benzenediol, O-(4-ethylbenzoyl)-O'-propargyloxycarbonyl-	C19H16O5		LibSearch	38.550	-3.100		1000345-53-3	40.53		
4-Ethylbenzoic acid, 2,5-dichlorophenyl ester	C15H12Cl2O2		LibSearch	38.550	1.783		1000325-73-5	40.46		
Propanoic acid, 2,2-dimethyl-, cesium salt	C5H9CsO2		LibSearch	38.550			20442-70-0	40.42		
1,3-Benzenediol, o-(4-ethylbenzoyl)-o'-propionyl-	C18H18O4		LibSearch	38.550	-0.217		1000330-82-9	40.25		
4-Ethylbenzoic acid, tridec-2-ynyl ester	C22H32O2		LibSearch	38.550	-2.833		1000292-54-9	40.16		
Carbonic acid, methyl ester, ester with p-hydroxybenzonitrile	C9H7NO3		LibSearch	38.550	14.983		17175-18-7	40.15		
1,2-Benzenediol, o-(2-chloropropionyl)-o'-(4-ethylbenzoyl)-	C18H17ClO4		LibSearch	38.550	-2.567		1000325-96-9	40.10		
Benzonitrile, 4-methoxy-	C8H7NO		LibSearch	38.550	19.433		874-90-8	39.40		
1,3,4-Thiadiazole-2(3H)-thione, 5-amino-	C2H3N3S2		LibSearch	38.550	16.750		2349-67-9	39.26		
6H-1,2,5-Oxadiazine-6-thione, 4,5-dihydro-3-(p-methoxyphenyl)-	C10H10N2O2S		LibSearch	38.550	4.633		33406-09-6	38.69		
4-Ethylbenzoic acid, 2,4,6-trichlorophenyl ester	C15H11Cl3O2		LibSearch	38.550	-1.217		1000325-73-6	38.48		
Silane, diethoxydimethyl-	C6H16O2Si		LibSearch	38.550	27.233		78-62-6	38.45		
4-Ethylbenzoic acid, phenyl ester	C15H14O2		LibSearch	38.550	7.767		118388-89-9	38.35		
4-Ethylbenzoic acid, 3-methylphenyl ester	C16H16O2		LibSearch	38.550	5.883		1000307-12-1	38.24		
Carbonic acid, methyl ester, ester with m-hydroxybenzonitrile	C9H7NO3		LibSearch	38.550	14.983		17175-19-8	38.21		
Benzonitrile, 4-methoxy-	C8H7NO		LibSearch	38.550	19.433		874-90-8	37.94		
o-Methoxybenzonitrile	C8H7NO		LibSearch	38.550	19.433		6609-56-9	37.59		
Benzene, 1-isocyano-2-methoxy-	C8H7NO		LibSearch	38.550			20771-60-2	37.15		
Borinic acid, diethyl-, phenyl ester	C10H15BO		LibSearch	38.550			74685-90-8	37.00		
1H-2-Benzopyran-1-carboxylic acid, 3,4-dihydro-, ethyl ester	C12H14O3		LibSearch	38.550	12.167		1000362-46-9	36.34		
1-Propanone, 2-chloro-1-(4-ethylphenyl)-2-methyl-	C12H15ClO		LibSearch	38.550	13.333		55012-69-6	36.34		
o-Methoxybenzonitrile	C8H7NO		LibSearch	38.550	19.433		6609-56-9	36.17		
Silane, diethoxydimethyl-	C6H16O2Si		LibSearch	38.550	27.233		78-62-6	36.08		
Propan-1-one, 1-(1,2,3,4-tetrahydro-1-quinolyl)-	C12H15NO		LibSearch	38.550	11.650		38461-44-8	35.55		
2,5-Pyrrolidinedione, 1-[(3,4-dimethylbenzoyl)oxy]-	C13H13NO4		LibSearch	38.550	2.583		1000306-84-7	35.39		

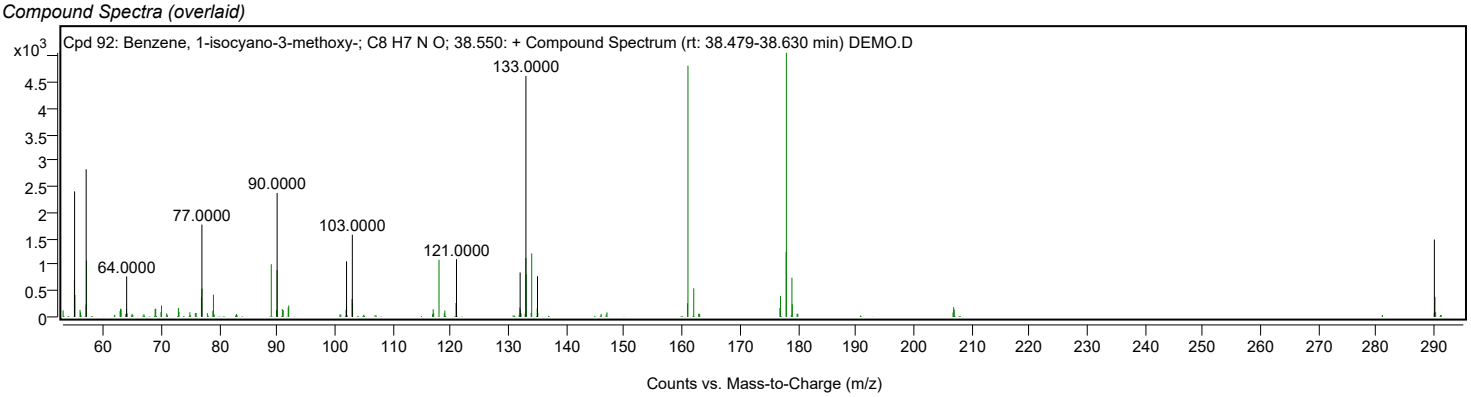
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



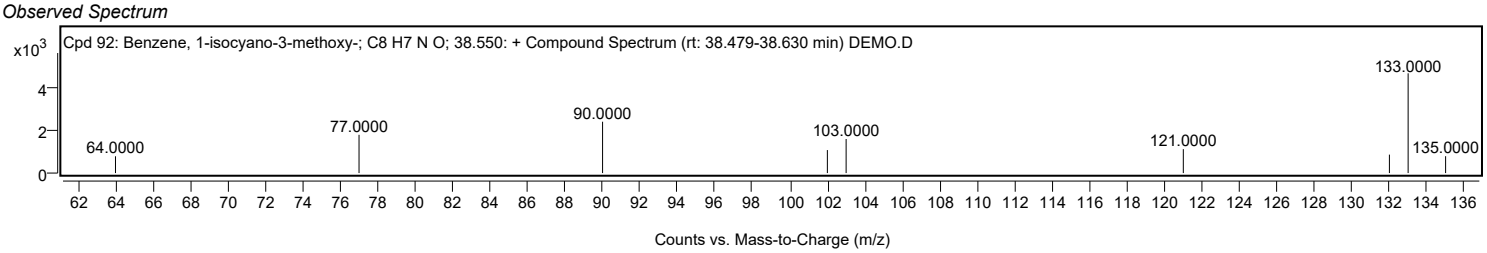
Benzene, 1-isocyano-3-methoxy-

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			51.42			NIST.L

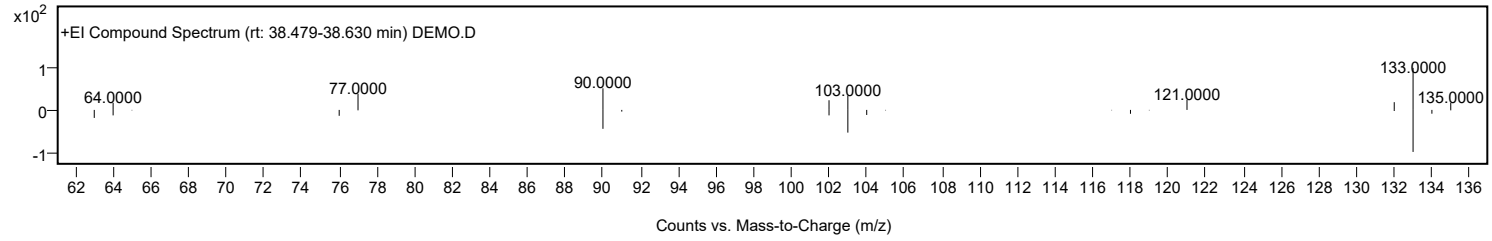
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			51.42			NIST.L

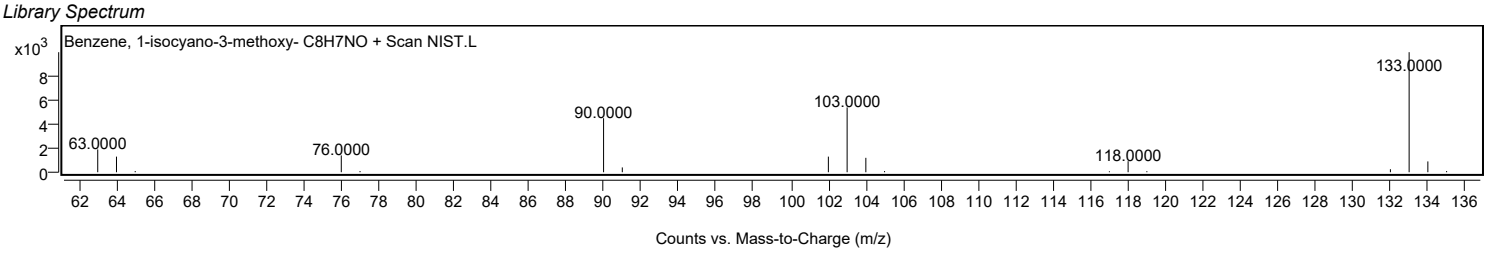
Observed Spectrum



Mirror Plot



Library Spectrum



Cpd. 93: Cinoxate

Name	Formula	RT	RI	Mass	CAS	ID Source	Score	Algorithm	Lib/DB
Cinoxate	C14 H18 O4	38.564			104-28-9	LibSearch	71.97	Chrom Decon	NIST.L

Species	m/z	Score (Lib)	Num Spectra	Score (DB)	Hits	Score (MFG)	Score (RT)
		71.97			50		

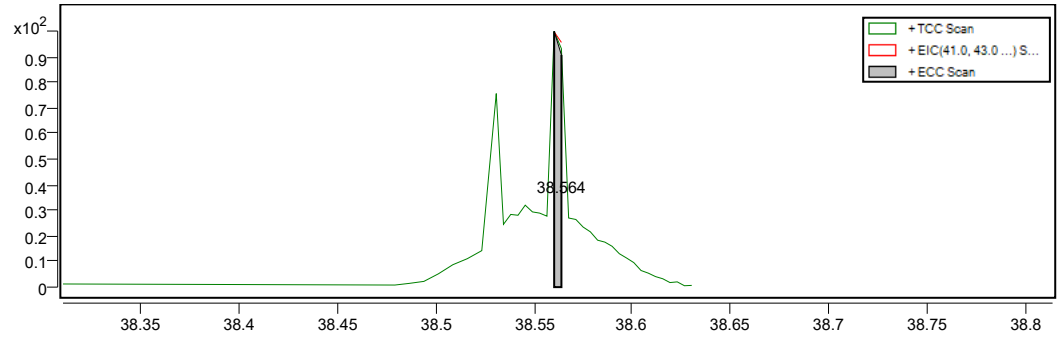
Compound ID Table

Name	Formula	Species	ID Source	RT	RT Diff	Mass	CAS	Score	Score (DB)	Score (MFG)
Cinoxate	C14H18O4		LibSearch	38.564	8.064		104-28-9	71.97		
2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester	C18H26O3		LibSearch	38.564	3.764		5466-77-3	69.60		
Cinnamate <para-methoxy-, octyl->	C18H26O3		LibSearch	38.564			5466-77-3	68.08		
2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester	C18H26O3		LibSearch	38.564	3.764		5466-77-3	67.74		
2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester	C18H26O3		LibSearch	38.564	3.764		5466-77-3	67.14		
Benzo[b]thiophene-3-carboxylic acid	C9H6O2S		LibSearch	38.564	11.631		5381-25-9	66.40		
2-Ethylhexyl trans-4-methoxycinnamate	C18H26O3		LibSearch	38.564	3.764		83834-59-7	65.70		
Cinoxate	C14H18O4		LibSearch	38.564	8.064		104-28-9	65.37		
Benzo(b)thiophene-6-carboxylic acid	C9H6O2S		LibSearch	38.564	11.247		6179-26-6	64.83		
Cinoxate	C14H18O4		LibSearch	38.564	8.064		104-28-9	64.74		
2-Propenoic acid, 3-(4-methoxyphenyl)-, 2-ethylhexyl ester	C18H26O3		LibSearch	38.564	3.764		5466-77-3	64.21		
Cinnamate <4-methoxy-, isopentyl->	C15H20O3		LibSearch	38.564			71617-10-2	63.99		
benzo[b]thiophene-5-carboxylic acid	C9H6O2S		LibSearch	38.564	11.247		1000404-77-7	60.48		
2-Propenoic acid, 3-(4-methoxyphenyl)-	C10H10O3		LibSearch	38.564	12.797		830-09-1	60.18		
Cinoxate	C14H18O4		LibSearch	38.564	8.064		104-28-9	60.10		
Thianaphthene-2-carboxylic acid	C9H6O2S		LibSearch	38.564	11.631		6314-28-9	58.72		
4-Buthylbenzoic acid, 6-chlorohexyl ester	C17H25ClO2		LibSearch	38.564	1.997		1000331-29-7	54.52		
2,4-Dithiocinammic acid	C9H8O2S2		LibSearch	38.564	5.314		1000128-93-6	54.17		
4-Butylbenzoic acid, pentyl ester	C16H24O2		LibSearch	38.564	7.414		1000292-32-1	53.92		
4-Butylbenzoic acid, octyl ester	C19H30O2		LibSearch	38.564	2.431		128434-87-7	53.56		
2-Propenoic acid, 3-(4-methoxyphenyl)-, (E)-	C10H10O3		LibSearch	38.564	12.797		943-89-5	53.39		
4-Butylbenzoic acid, 8-chlorooctyl ester	C19H29ClO2		LibSearch	38.564	-1.319		1000354-32-2	53.38		
4-Butylbenzoic acid, heptyl ester	C18H28O2		LibSearch	38.564	4.097		1000292-32-2	53.36		
p-Methoxycinnamic acid, geranyl ester	C20H26O3		LibSearch	38.564	-0.119		1000196-51-5	53.35		
4-Butylbenzoic acid, hexyl ester	C17H26O2		LibSearch	38.564	5.747		1000292-32-3	53.13		
4-Butylbenzoic acid, undecyl ester	C22H36O2		LibSearch	38.564	-2.536		1000292-21-0	52.89		
4-Butylbenzoic acid, nonyl ester	C20H32O2		LibSearch	38.564	0.781		1000292-20-6	52.88		
2-Oxo-2,3-dihydro-1H-benzimidazole-5-carboxylic acid	C8H6N2O3		LibSearch	38.564	8.147		23814-14-4	52.88		
4-Butylbenzoic acid, decyl ester	C21H34O2		LibSearch	38.564	-0.869		1000292-32-5	52.80		
4-Butylbenzoic acid, tridecyl ester	C24H40O2		LibSearch	38.564	-5.853		1000292-32-6	52.36		
2-Propenoic acid, 3-(4-methoxyphenyl)-	C10H10O3		LibSearch	38.564	12.797		830-09-1	51.97		
4-Butylbenzoic acid, tetradecyl ester	C25H42O2		LibSearch	38.564	-7.503		1000292-32-7	51.79		
4-Butylbenzoic acid, 2-methylbutyl ester	C16H24O2		LibSearch	38.564	8.481		1010331-29-2	51.48		
(+)-Norreticuline, 4'-O-demethyl-6'-methyl-	C18H21NO4		LibSearch	38.564	-11.603		89240-89-1	51.08		
4-Butylbenzoic acid, pentadecyl ester	C26H44O2		LibSearch	38.564	-9.153		1000292-32-8	51.06		
4-Butylbenzoic acid, heptadecyl ester	C28H48O2		LibSearch	38.564	-12.469		1000292-21-3	50.67		
2-Propenoic acid, 3-(4-methoxyphenyl)-	C10H10O3		LibSearch	38.564	12.797		830-09-1	50.65		
4-Butylbenzoic acid, hexadecyl ester	C27H46O2		LibSearch	38.564	-10.819		1010292-32-9	50.64		
4-Butylbenzoic acid, 2-methylpentyl ester	C17H26O2		LibSearch	38.564	6.814		1000354-16-5	49.75		
4-Butylbenzoic acid, octadecyl ester	C29H50O2		LibSearch	38.564	-14.136		1010292-33-0	49.63		
trans-2-Methoxycinnamic acid, isohexyl ester	C16H22O3		LibSearch	38.564	7.081		1000439-07-8	48.94		
Thiazolidine-2-carbohydrazide, 3-(2-methylphenyl)-	C11H15N3OS		LibSearch	38.564	1.147		103856-32-2	48.71		
7-Isoquinolinol, 1,2,3,4-tetrahydro-1-[(4-hydroxyphenyl)methyl]-6-methoxy-, (S)-	C17H19NO3		LibSearch	38.564	-6.053		486-39-5	48.52		
2-Propenoic acid, 3-(4-methoxyphenyl)-	C10H10O3		LibSearch	38.564	12.797		830-09-1	48.07		
1,2,3,4-Tetrahydroisoquinoline, 7-hydroxy-6-methoxy-1-(5-hydroxy-4-methoxy-2-methylbenzyl)-	C19H23NO4		LibSearch	38.564	-11.086		89300-64-1	47.93		
7-Isoquinolinol, 1,2,3,4-tetrahydro-6-methoxy-1-salicyl-	C17H19NO3		LibSearch	38.564	-6.053		24656-61-9	46.82		
3-Methoxycinnamic acid	C10H10O3		LibSearch	38.564	12.797		6099-04-3	46.80		
Benzoic acid, 4-(2-propenyloxy)-, ester with 1,1'-bicyclohexyl-4,4'-diol (2:1)	C32H38O6		LibSearch	38.564	-26.436		1000112-37-2	46.78		
4-Butylbenzoic acid, 2-methylpropyl ester	C15H22O2		LibSearch	38.564	10.131		1000293-52-2	46.63		
4-tert-Butyl-N-cyclooctylbenzamide	C19H29NO		LibSearch	38.564	-1.769		298230-88-3	46.52		

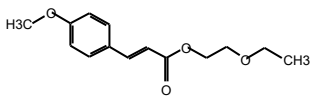
Compound Discovery Report

Agilent | Trusted Answers

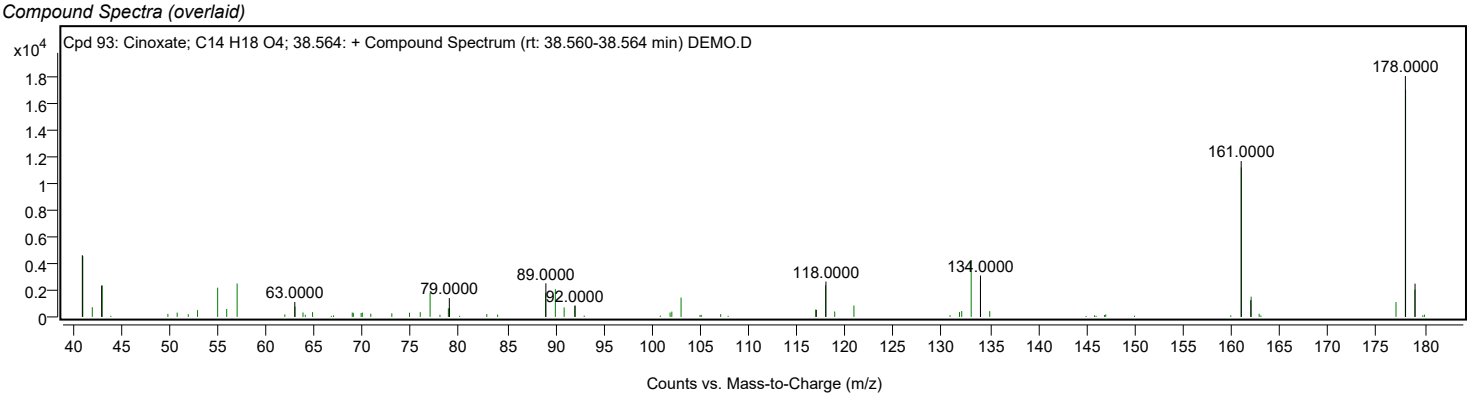
Compound Chromatograms (overlaid)



Structure



Compound Spectra (overlaid)



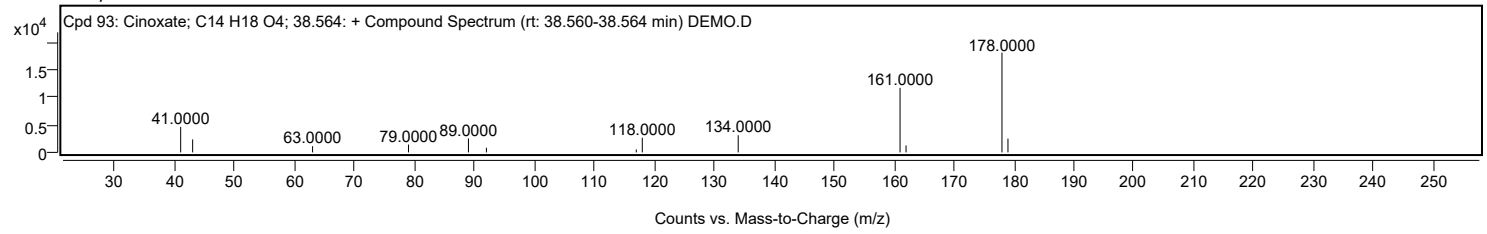
Cinoxate

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			71.97			NIST.L

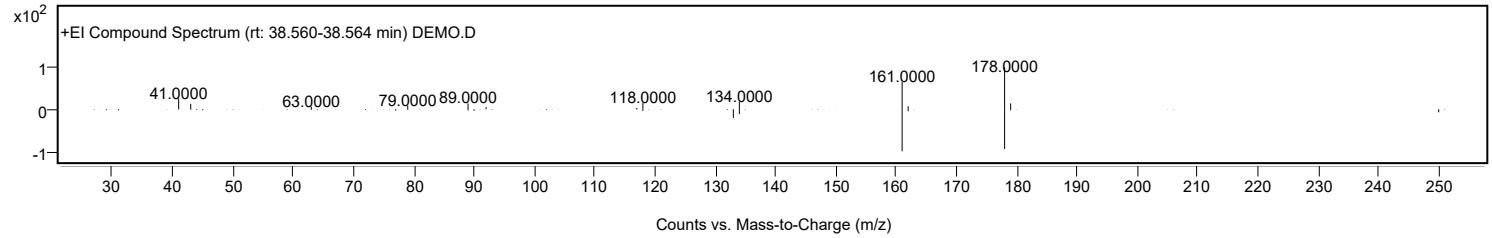
Library Match Details

m/z (prec.)	Species	CE	Score (Lib)	Score (Fwd)	Score (Rev)	Lib/DB
			71.97			NIST.L

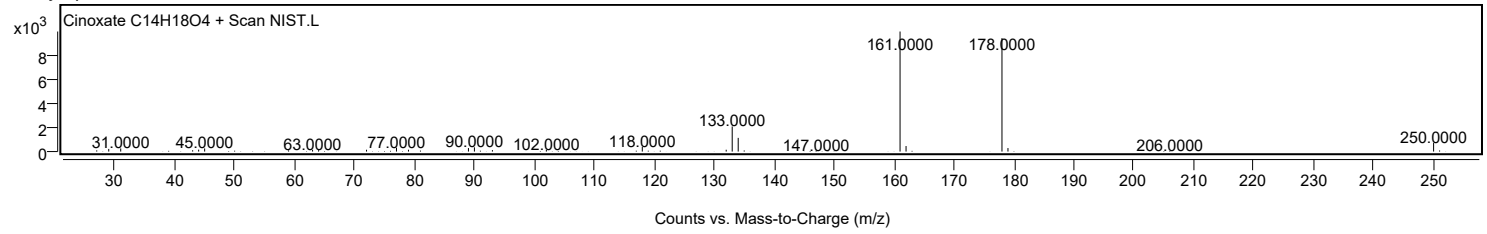
Observed Spectrum



Mirror Plot



Library Spectrum



MassHunter Qual 10.0
(End of Report)