

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052422\
 Data File : VD073344.D
 Acq On : 25 May 2022 01:52
 Operator : VA/SY
 Sample : N2949-25
 Misc : 5.29G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 P044-SS005-0006-01

Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Filtering: 5

Sampling : 1

Min Area: 3 % of largest Peak

Start Thrs: 0.2

Max Peaks: 100

Stop Thrs : 0

Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >

Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051922S.M
 Title : SW846 8260

Signal : TIC: VD073344.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.967	507	518	528	rBV3	25669	86921	4.96%	0.720%
2	5.185	543	555	567	rBV3	17940	61775	3.52%	0.511%
3	5.985	686	691	703	rVB6	13556	40261	2.30%	0.333%
4	7.191	884	896	906	rBV2	35171	97154	5.54%	0.804%
5	7.908	1008	1018	1023	rBV2	249795	593025	33.81%	4.910%
6	7.973	1023	1029	1039	rVB	416872	935170	53.31%	7.742%
7	8.326	1073	1089	1098	rBV3	222974	742565	42.33%	6.148%
8	8.855	1170	1179	1191	rBV	607279	1265952	72.17%	10.480%
9	10.332	1422	1430	1438	rBV	987013	1736121	98.98%	14.373%
10	10.714	1490	1495	1502	rVB2	31400	58416	3.33%	0.484%
11	11.073	1549	1556	1567	rVB2	103316	177846	10.14%	1.472%
12	11.449	1614	1620	1627	rVB3	15254	27632	1.58%	0.229%
13	11.638	1643	1652	1662	rBV	933070	1668075	95.10%	13.810%
14	12.620	1809	1819	1827	rBV2	830461	1461310	83.31%	12.098%
15	12.690	1827	1831	1837	rVV6	13506	32266	1.84%	0.267%
16	12.761	1838	1843	1854	rVB3	43029	97619	5.57%	0.808%
17	12.961	1869	1877	1883	rBV6	33816	95723	5.46%	0.792%
18	13.202	1907	1918	1926	rVB	116038	225041	12.83%	1.863%
19	13.308	1930	1936	1942	rBV	50818	83023	4.73%	0.687%
20	13.414	1944	1954	1963	rBV2	203657	379802	21.65%	3.144%
21	13.485	1963	1966	1969	rVV5	13697	21772	1.24%	0.180%
22	13.561	1969	1979	1984	rVV	1028540	1754066	100.00%	14.521%
23	13.608	1984	1987	1997	rVB2	165484	326201	18.60%	2.701%
24	13.773	2006	2015	2020	rBV3	48254	91151	5.20%	0.755%
25	14.085	2063	2068	2074	rBV2	11020	20240	1.15%	0.168%

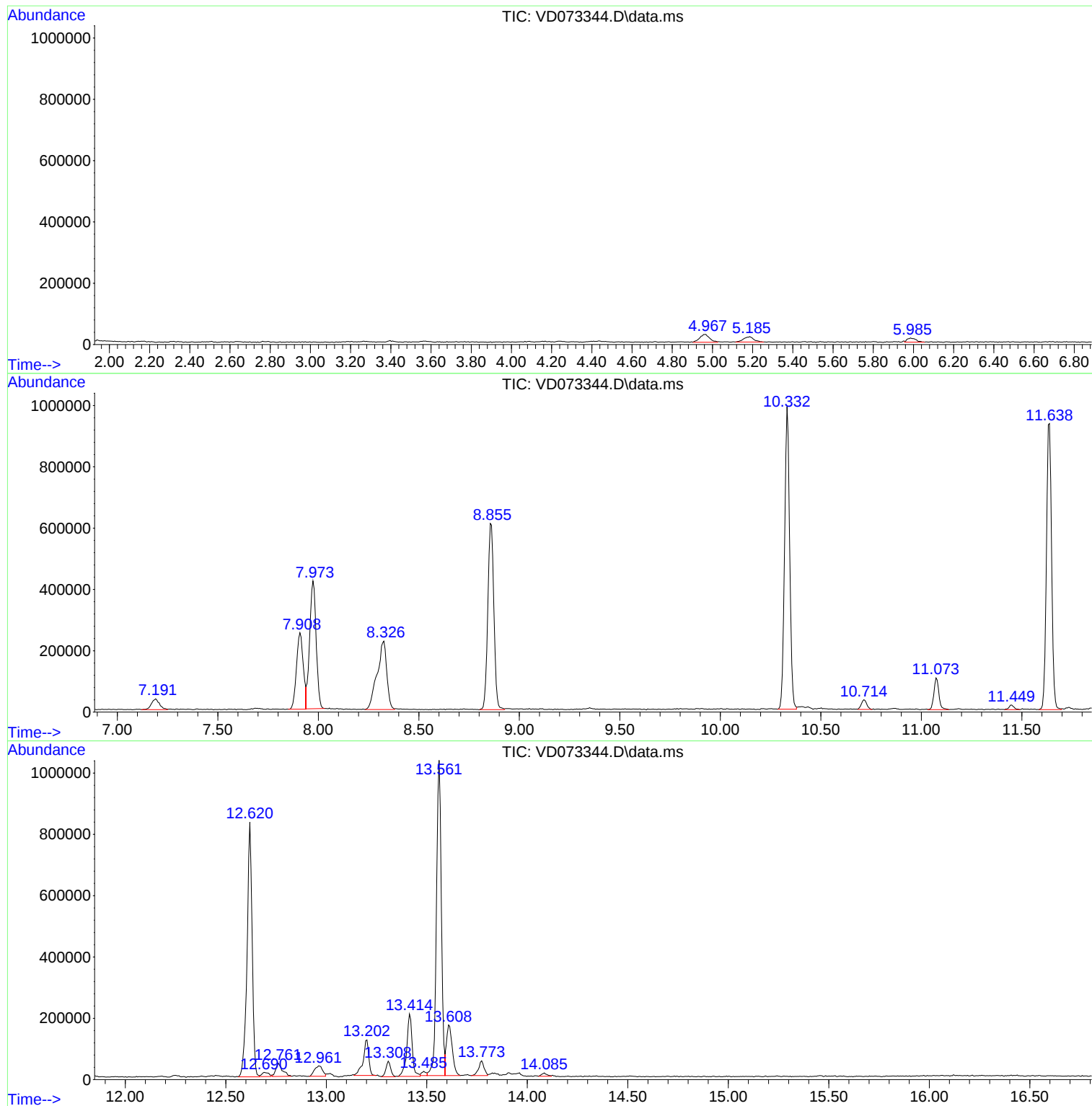
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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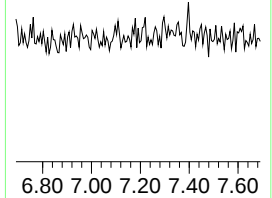
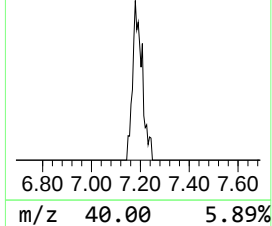
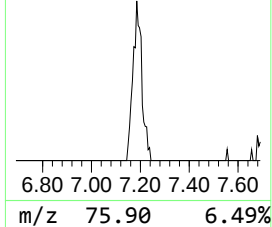
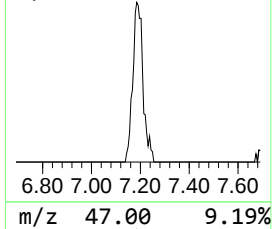
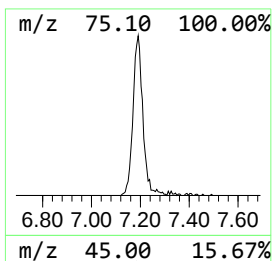
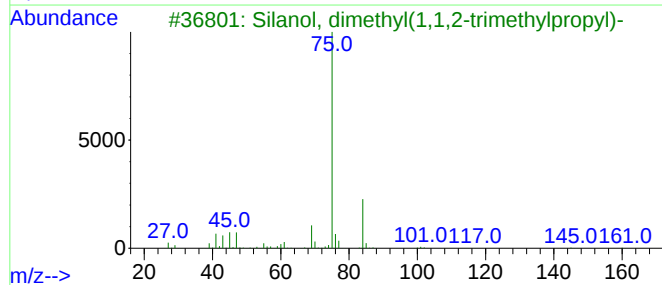
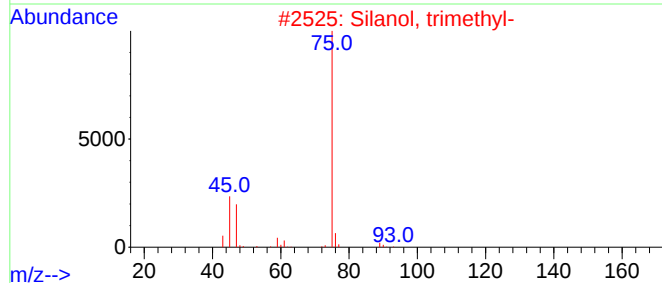
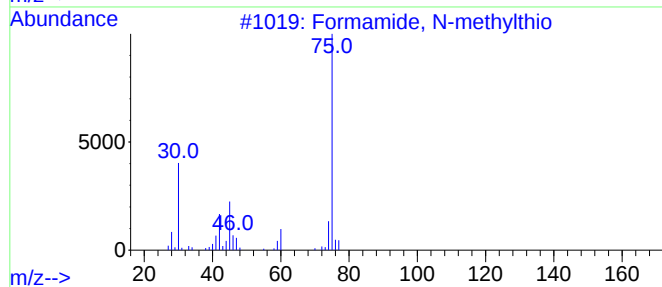
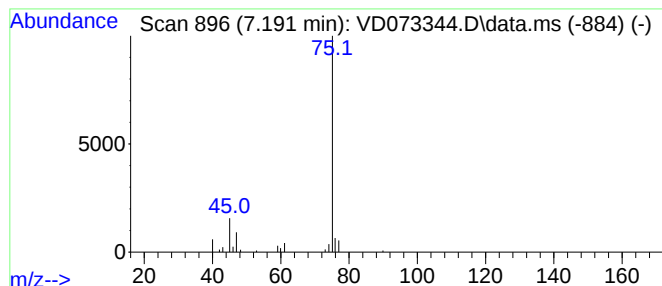
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051922S.M
Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 1 Formamide, N-methylthio Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
7.191	5.19 ug/l	97154	Pentafluorobenzene	7.973

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Formamide, N-methylthio	75	C2H5NS	018952-41-5	72
2			Silanol, trimethyl-	90	C3H10OSi	001066-40-6	72
3			Silanol, dimethyl(1,1,2-trimethyl...	160	C8H20OSi	055644-10-5	56
4			Ethanethioamide	75	C2H5NS	000062-55-5	9
5			Chloromethyl cyanide	75	C2H2ClN	000107-14-2	9



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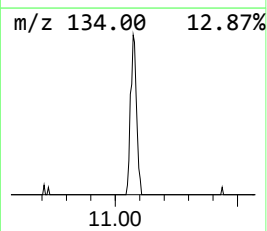
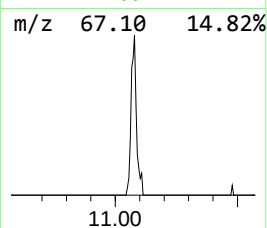
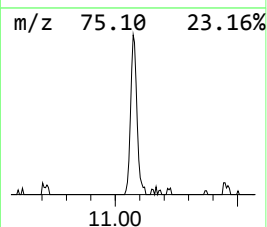
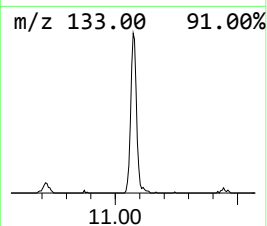
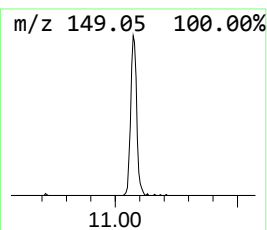
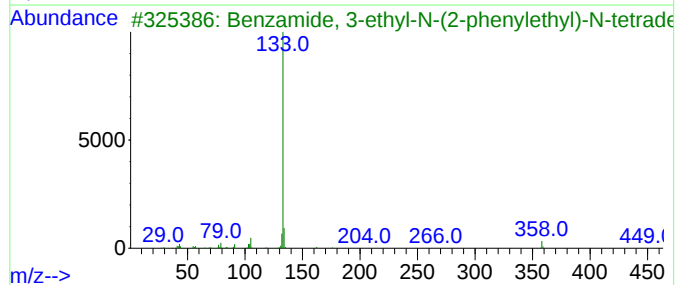
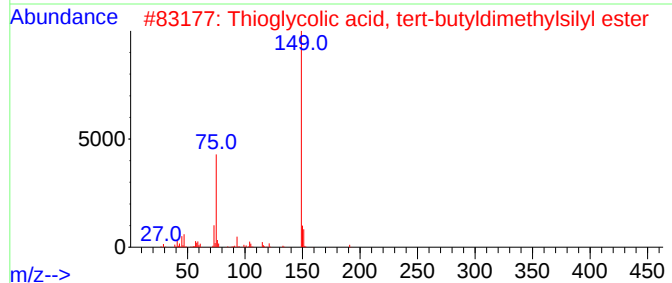
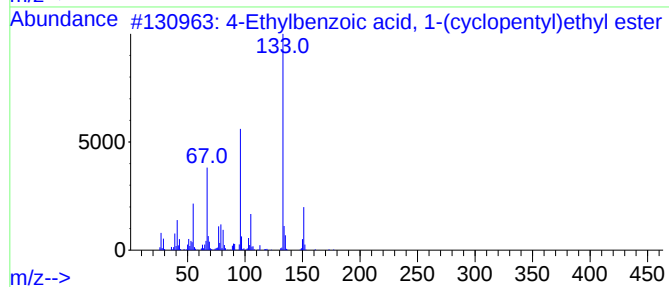
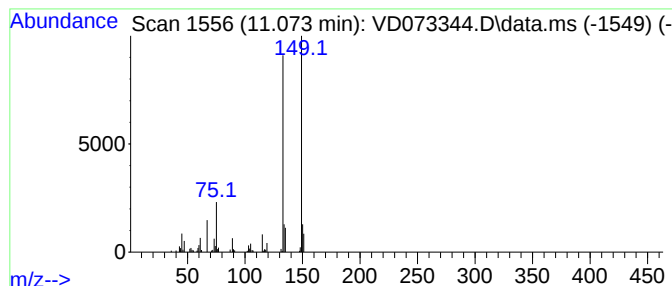
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Quant Title : SW846 8260

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Peak Number 2 unknown11.073 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.073	5.33 ug/l	177846	Chlorobenzene-d5	11.638

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Ethylbenzoic acid, 1-(cyclopentyl)ethyl ester	246	C16H22O2	1010293-32-2	35
2			Thioglycolic acid, tert-butyl dimethylsilyl ester	206	C8H18O2SSi	1000476-01-2	35
3			Benzamide, 3-ethyl-N-(2-phenylethyl)-N-tetradecyl	449	C31H47NO	1000451-43-2	27
4			Silane, diethoxydimethyl-	148	C6H16O2Si	000078-62-6	25
5			1H-Indole-3-thiol	149	C8H7NS	000480-94-4	17



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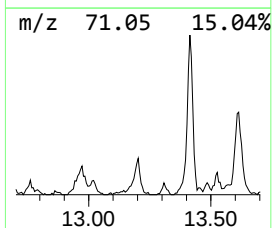
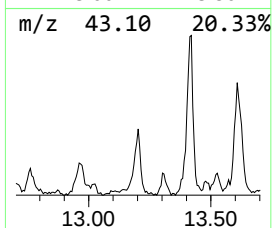
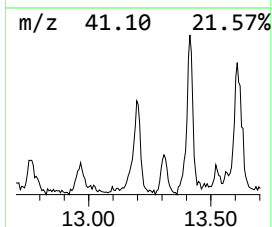
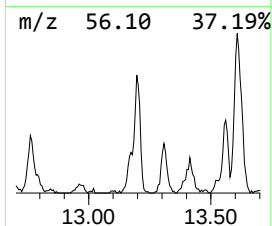
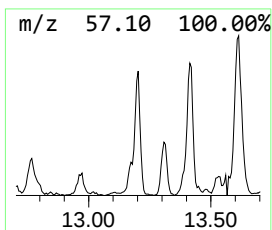
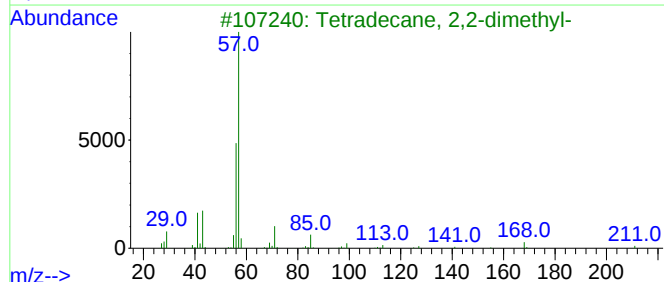
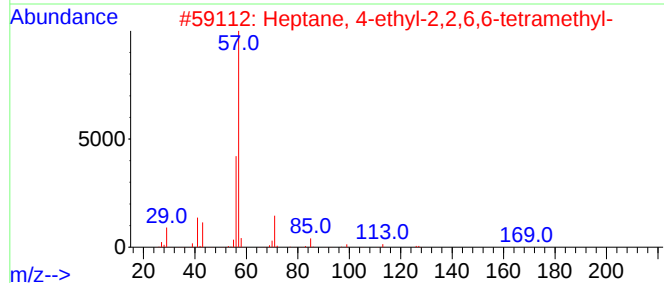
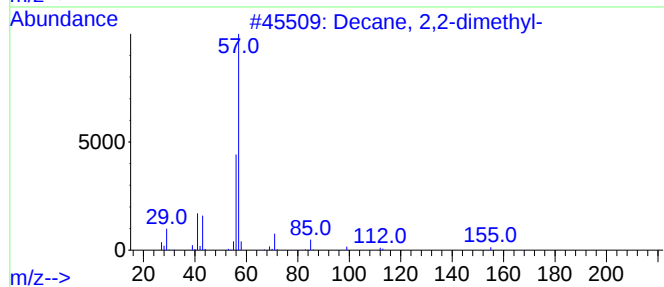
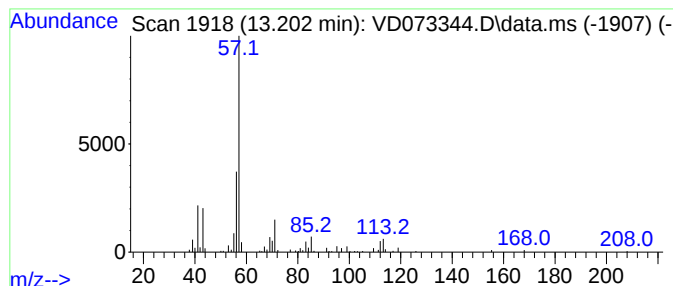
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Peak Number 3 Decane, 2,2-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.202	6.41 ug/l	225041	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	64
2			Heptane, 4-ethyl-2,2,6,6-tetrame...	184	C13H28	062108-31-0	59
3			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	59
4			Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	53
5			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	53



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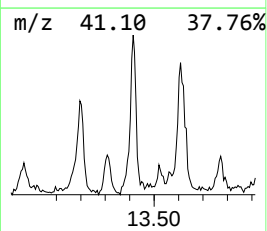
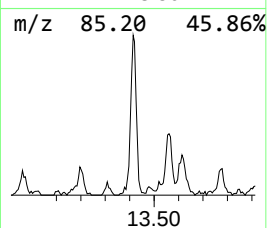
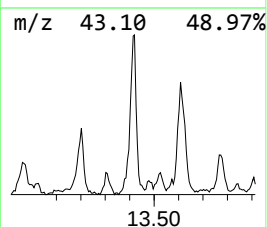
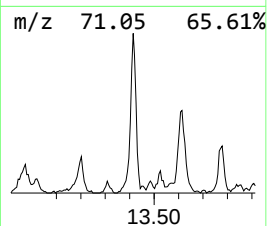
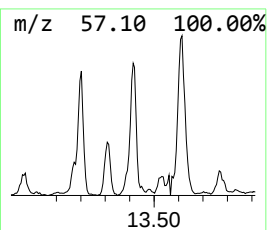
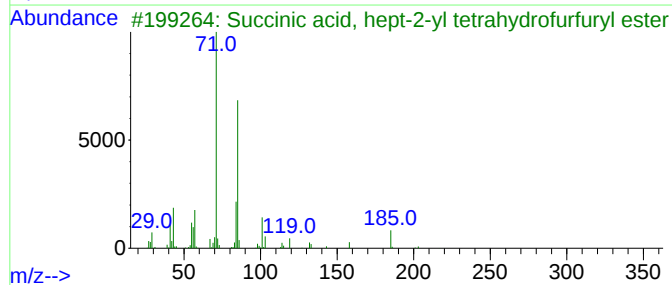
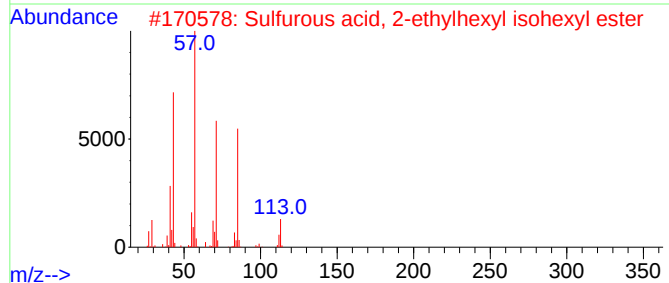
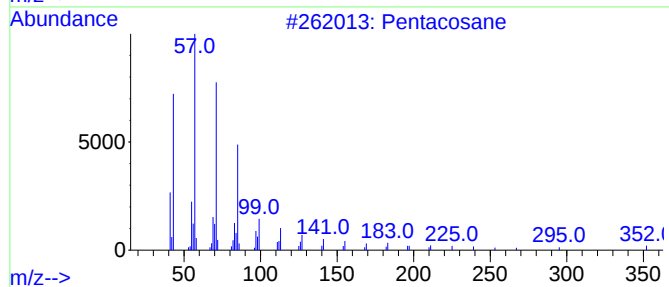
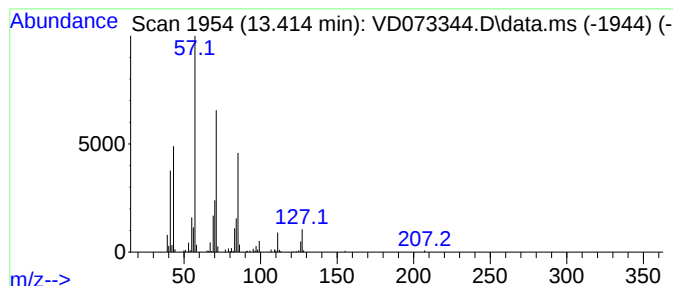
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Peak Number 4 Pentacosane Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.414	10.83 ug/l	379802	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentacosane	352	C25H52	000629-99-2	64
2			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	53
3			Succinic acid, hept-2-yl tetrahy...	300	C16H28O5	1000390-71-8	50
4			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	50
5			Nonane, 5-methyl-5-propyl-	184	C13H28	017312-75-3	50



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Formamide, N-me...	7.191	5.2	ug/l	97154	1	7.973	935170	50.0
unknown11.073	11.073	5.3	ug/l	177846	3	11.638	1668080	50.0
Decane, 2,2-dim...	13.202	6.4	ug/l	225041	4	13.561	1754070	50.0
Pentacosane	13.414	10.8	ug/l	379802	4	13.561	1754070	50.0