

Data Path : Z:\voasrv\HPCHEM1\MSVOA_D\Data\VD052422\
 Data File : VD073343.D
 Acq On : 25 May 2022 01:23
 Operator : VA/SY
 Sample : N2949-24
 Misc : 5.13G/5.00ml/MSVOA_D/SOIL
 ALS Vial : 32 Sample Multiplier: 1

Instrument :
 MSVOA_D
 ClientSampleId :
 P044-SS004-0006-01

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: VD073343.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.962	507	517	527	rBV3	28630	90655	4.28%	0.654%
2	5.168	545	552	553	rBV2	21146	32496	1.54%	0.234%
3	5.185	553	555	565	rVB	23488	46570	2.20%	0.336%
4	5.997	682	693	700	rBV4	13944	41238	1.95%	0.297%
5	7.185	882	895	909	rBV	36284	111953	5.29%	0.807%
6	7.909	1007	1018	1023	rBV	252064	591160	27.92%	4.264%
7	7.973	1023	1029	1041	rVB2	409328	934369	44.14%	6.739%
8	8.326	1071	1089	1099	rBV3	227583	814971	38.50%	5.878%
9	8.861	1170	1180	1190	rBV	614024	1235732	58.37%	8.912%
10	10.332	1422	1430	1439	rBV	980832	1722105	81.35%	12.420%
11	10.408	1439	1443	1445	rBV5	15737	22677	1.07%	0.164%
12	10.714	1488	1495	1501	rBV2	39731	71714	3.39%	0.517%
13	11.073	1550	1556	1563	rBV2	46888	82391	3.89%	0.594%
14	11.450	1615	1620	1626	rVB3	13426	23154	1.09%	0.167%
15	11.638	1642	1652	1660	rBV	977010	1689351	79.80%	12.184%
16	11.885	1689	1694	1700	rVB	18642	30860	1.46%	0.223%
17	12.079	1722	1727	1730	rBV4	14754	25989	1.23%	0.187%
18	12.250	1749	1756	1762	rBV2	32627	60957	2.88%	0.440%
19	12.620	1808	1819	1826	rVV2	927372	2116983	100.00%	15.268%
20	12.691	1826	1831	1837	rVV3	47004	116370	5.50%	0.839%
21	12.761	1837	1843	1854	rVB	123236	291339	13.76%	2.101%
22	12.967	1868	1878	1883	rBV5	83646	205107	9.69%	1.479%
23	13.014	1884	1886	1895	rVB3	24833	44034	2.08%	0.318%
24	13.126	1895	1905	1906	rBV6	17635	38523	1.82%	0.278%
25	13.202	1908	1918	1930	rVB	202967	413165	19.52%	2.980%
26	13.308	1930	1936	1945	rVB	66338	109751	5.18%	0.792%
27	13.414	1945	1954	1962	rBV	240059	451206	21.31%	3.254%
28	13.491	1962	1967	1968	rVV3	16121	23948	1.13%	0.173%
29	13.561	1969	1979	1984	rVV	1080683	1831863	86.53%	13.212%
30	13.608	1984	1987	1997	rVB	183065	376635	17.79%	2.716%
31	13.773	2008	2015	2021	rBV4	55614	112308	5.31%	0.810%
32	13.832	2021	2025	2031	rVV7	11421	28266	1.34%	0.204%
33	13.920	2035	2040	2043	rVV6	11674	25202	1.19%	0.182%
34	13.949	2043	2045	2052	rVB4	13821	22845	1.08%	0.165%
35	14.085	2064	2068	2074	rBV5	12272	29320	1.38%	0.211%

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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

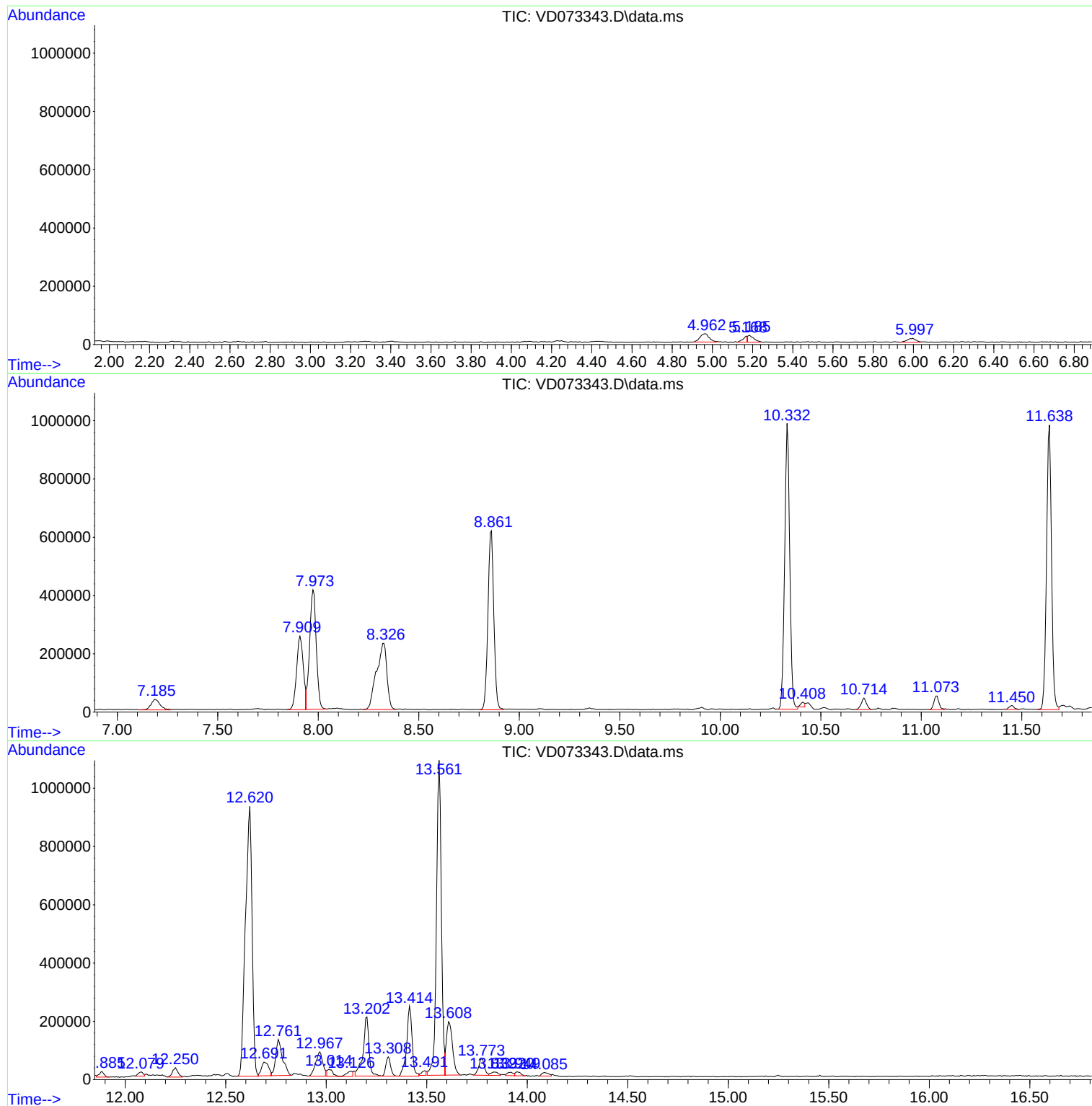
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051922S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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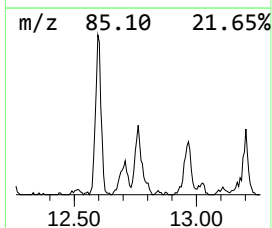
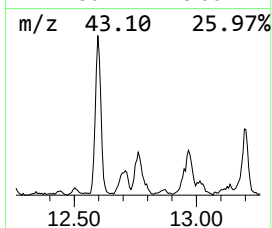
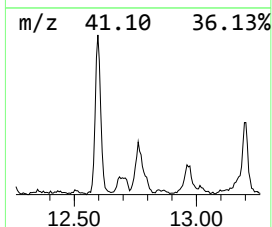
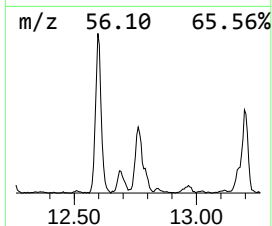
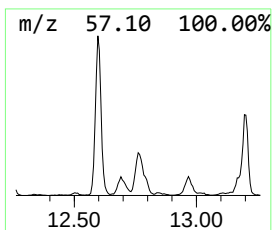
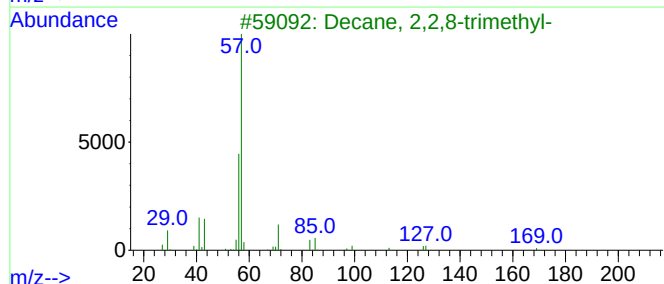
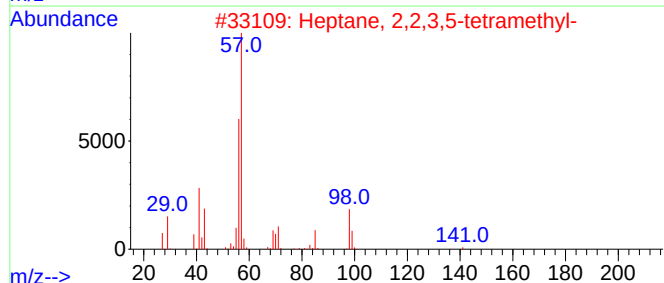
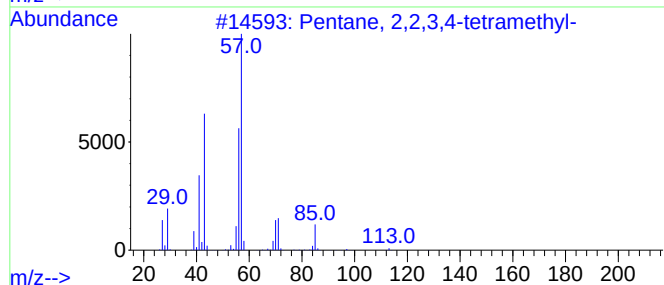
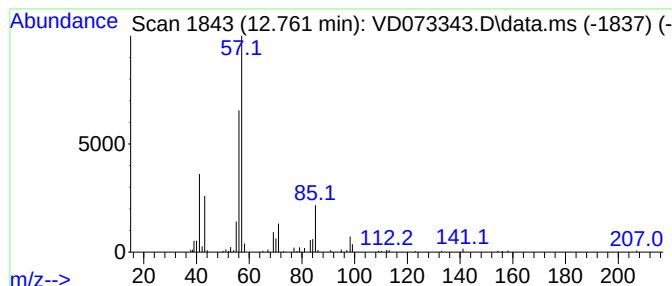
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051922S.M
Quant Title : SW846 8260

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

Peak Number 2 Pentane, 2,2,3,4-tetramethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.761	7.95 ug/l	291339	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	50
2			Heptane, 2,2,3,5-tetramethyl-	156	C11H24	061868-42-6	50
3			Decane, 2,2,8-trimethyl-	184	C13H28	062238-01-1	50
4			2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	45
5			Pentane, 3-methyl-	86	C6H14	000096-14-0	43



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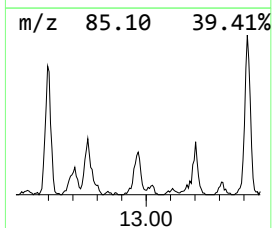
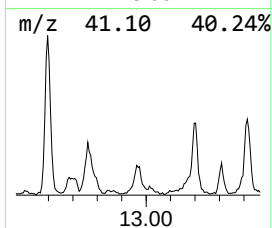
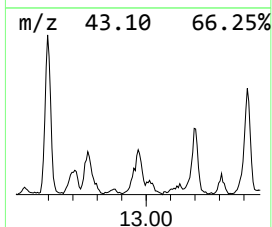
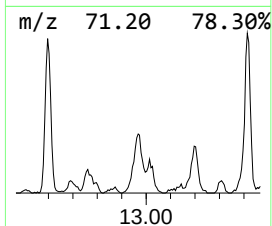
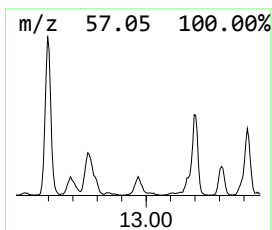
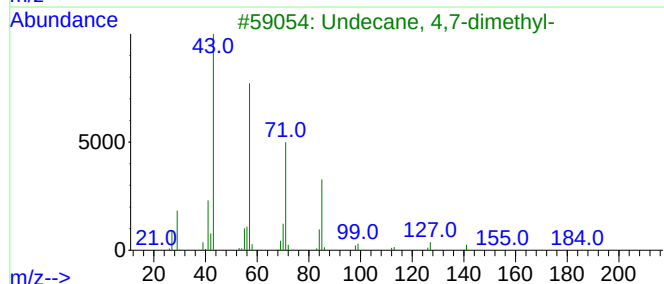
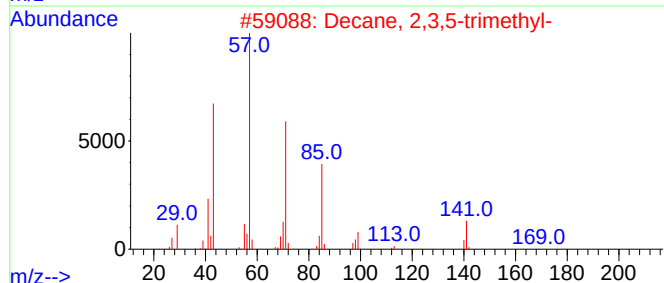
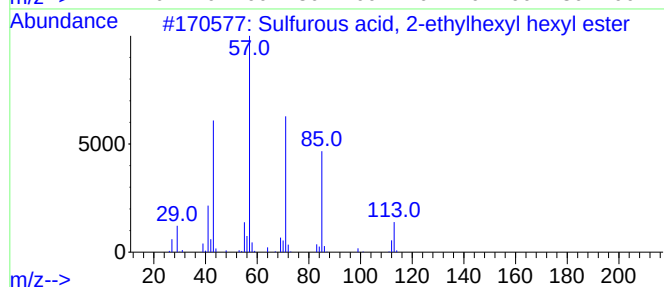
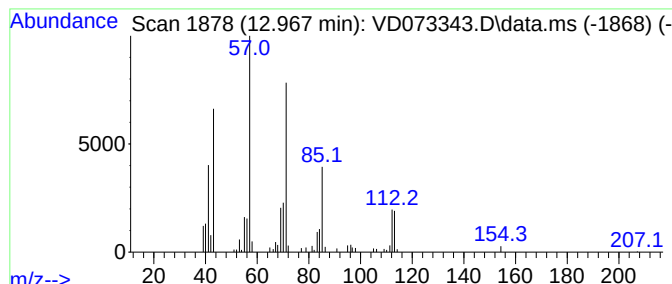
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_D\Method\82D051922S.M
Quant Title : SW846 8260

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

Peak Number 3 Sulfurous acid, 2-ethylhexy... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.967	5.60 ug/l	205107	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	59
2			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	53
3			Undecane, 4,7-dimethyl-	184	C13H28	017301-32-5	53
4			Carbonic acid, eicosyl vinyl ester	368	C23H44O3	1000382-54-3	53
5			Sulfurous acid, nonyl 2-propyl e...	250	C12H26O3S	1000309-12-0	52



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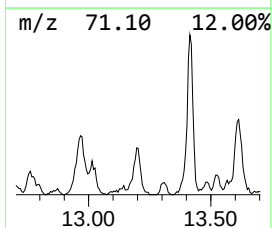
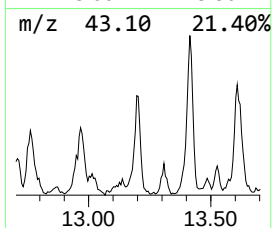
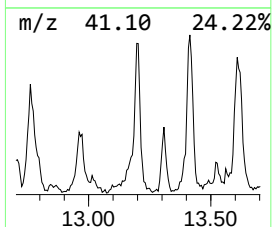
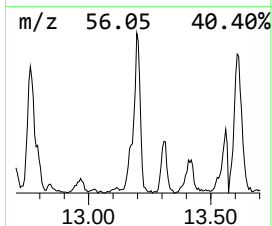
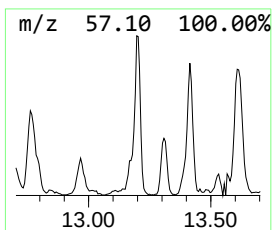
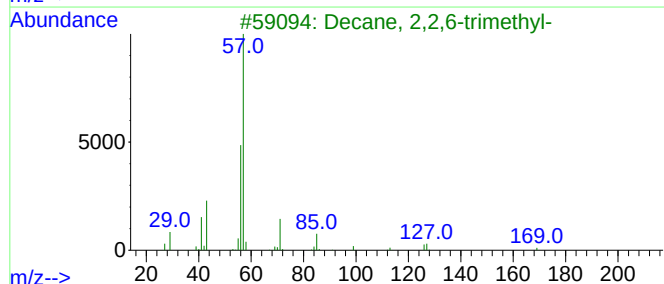
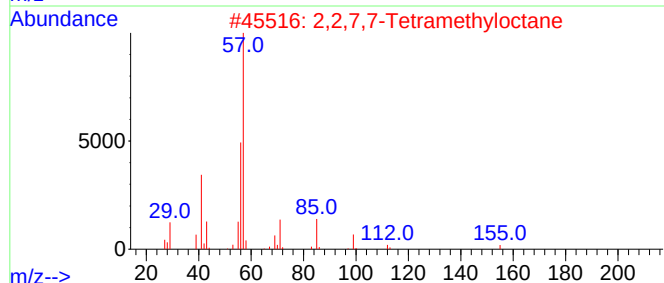
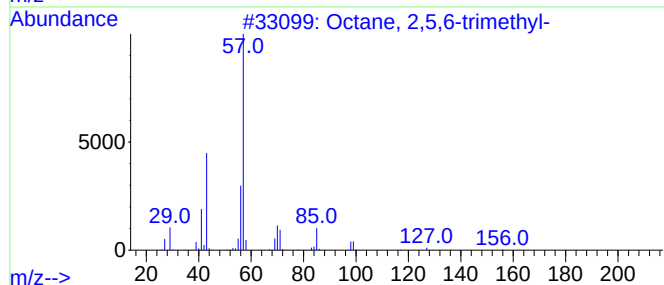
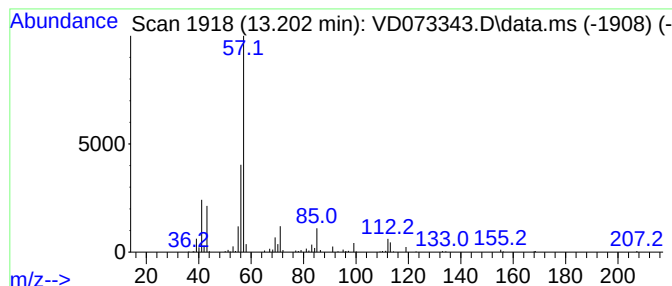
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Octane, 2,5,6-trimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.202	11.28 ug/l	413165	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,5,6-trimethyl-	156	C11H24	062016-14-2	80
2			2,2,7,7-Tetramethyloctane	170	C12H26	001071-31-4	72
3			Decane, 2,2,6-trimethyl-	184	C13H28	062237-97-2	64
4			Decane, 2,2,7-trimethyl-	184	C13H28	062237-99-4	64
5			Octane, 2,2-dimethyl-	142	C10H22	015869-87-1	59



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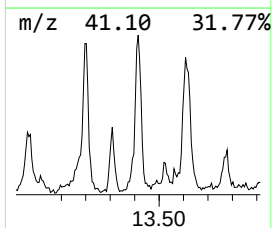
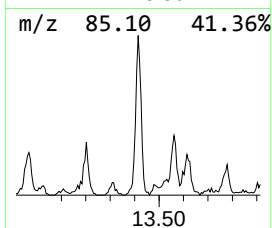
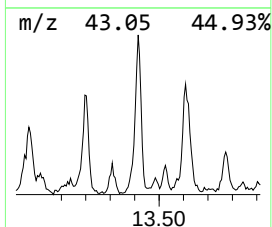
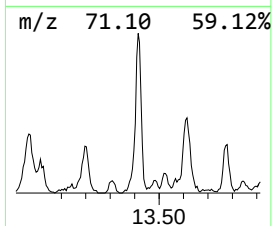
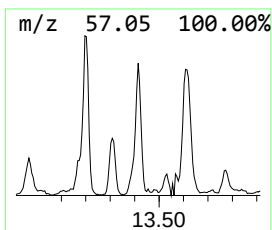
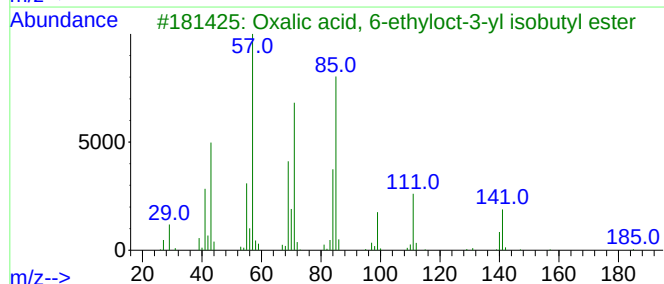
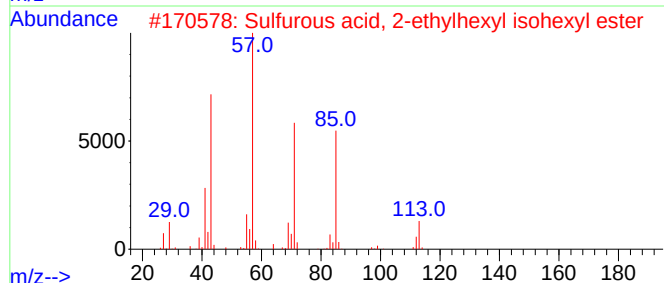
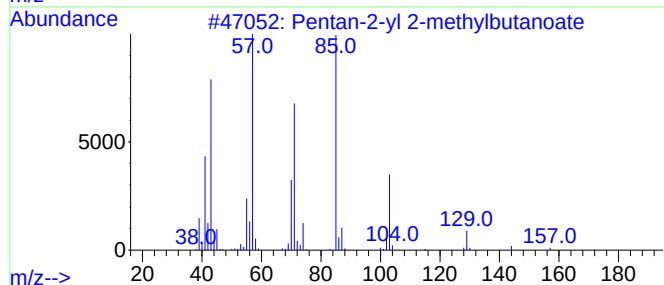
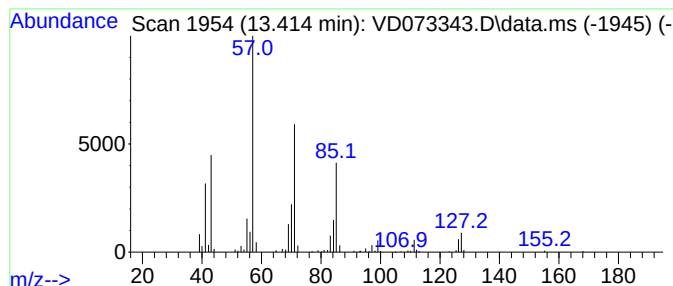
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Pentan-2-yl 2-methylbutanoate Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.414	12.32 ug/l	451206	1,4-Dichlorobenzene-d4	13.561

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentan-2-yl 2-methylbutanoate	172	C10H20O2	1000372-71-7	59
2			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	59
3			Oxalic acid, 6-ethyloct-3-yl iso...	286	C16H30O4	1010309-34-1	50
4			Nonane, 5-butyl-	184	C13H28	017312-63-9	50
5			Undecane, 4,6-dimethyl-	184	C13H28	017312-82-2	50



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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Pentane, 2,2,3,...	12.761	8.0	ug/l	291339	4	13.561	1831860	50.0
Sulfurous acid,...	12.967	5.6	ug/l	205107	4	13.561	1831860	50.0
Octane, 2,5,6-t...	13.202	11.3	ug/l	413165	4	13.561	1831860	50.0
Pentan-2-yl 2-m...	13.414	12.3	ug/l	451206	4	13.561	1831860	50.0