

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY051822\
 Data File : VY008812.D
 Acq On : 18 May 2022 14:33
 Operator : KP/MD
 Sample : N2869-04
 Misc : 5.44g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 P027-SS003-0006-01

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_Y\methods\82Y051722S.M
 Title : SW846 8260

Signal : TIC: VY008812.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.522	109	115	121	rBV4	5434	14937	1.93%	0.287%
2	4.716	465	475	485	rBV4	7349	23486	3.03%	0.451%
3	5.741	634	643	653	rBV3	3346	9323	1.20%	0.179%
4	6.990	837	848	860	rBV	11192	40942	5.29%	0.786%
5	7.716	957	967	973	rBV	114327	266790	34.45%	5.122%
6	7.789	973	979	989	rVB	172615	382098	49.34%	7.335%
7	8.136	1024	1036	1049	rVB2	122043	297100	38.37%	5.704%
8	8.691	1118	1127	1135	rBV	272123	538859	69.58%	10.345%
9	10.179	1364	1371	1379	rBV	472276	774399	100.00%	14.866%
10	10.264	1379	1385	1389	rBV5	4001	9207	1.19%	0.177%
11	10.581	1427	1437	1443	rBV	37454	67404	8.70%	1.294%
12	10.947	1490	1497	1510	rBV	54179	108707	14.04%	2.087%
13	11.319	1553	1558	1563	rVB2	7052	11591	1.50%	0.223%
14	11.490	1578	1586	1595	rBV	445164	701755	90.62%	13.472%
15	11.569	1595	1599	1609	rVB8	4180	10434	1.35%	0.200%
16	11.746	1622	1628	1633	rVB3	5818	9582	1.24%	0.184%
17	11.941	1655	1660	1669	rBV4	5058	11930	1.54%	0.229%
18	12.044	1673	1677	1682	rVV2	8836	13929	1.80%	0.267%
19	12.111	1682	1688	1698	rVB2	9745	16834	2.17%	0.323%
20	12.483	1739	1749	1756	rBV3	374351	753663	97.32%	14.468%
21	12.556	1756	1761	1768	rVV4	11971	29184	3.77%	0.560%
22	12.630	1768	1773	1783	rVB2	30312	69394	8.96%	1.332%
23	12.831	1795	1806	1812	rBV3	25107	58703	7.58%	1.127%
24	12.886	1813	1815	1824	rVB3	6350	10135	1.31%	0.195%
25	12.983	1824	1831	1834	rBV6	3937	8605	1.11%	0.165%
26	13.038	1834	1840	1841	rVV3	10718	16767	2.17%	0.322%
27	13.069	1841	1845	1855	rVB	43292	70345	9.08%	1.350%
28	13.178	1857	1863	1871	rVB	16170	23119	2.99%	0.444%
29	13.282	1871	1880	1889	rBV2	56680	103483	13.36%	1.987%
30	13.428	1894	1904	1909	rVV	406378	644914	83.28%	12.381%
31	13.483	1909	1913	1923	rVB2	37442	80612	10.41%	1.548%
32	13.648	1933	1940	1945	rBV5	12219	21415	2.77%	0.411%
33	13.971	1987	1993	1999	rBV3	4816	9413	1.22%	0.181%

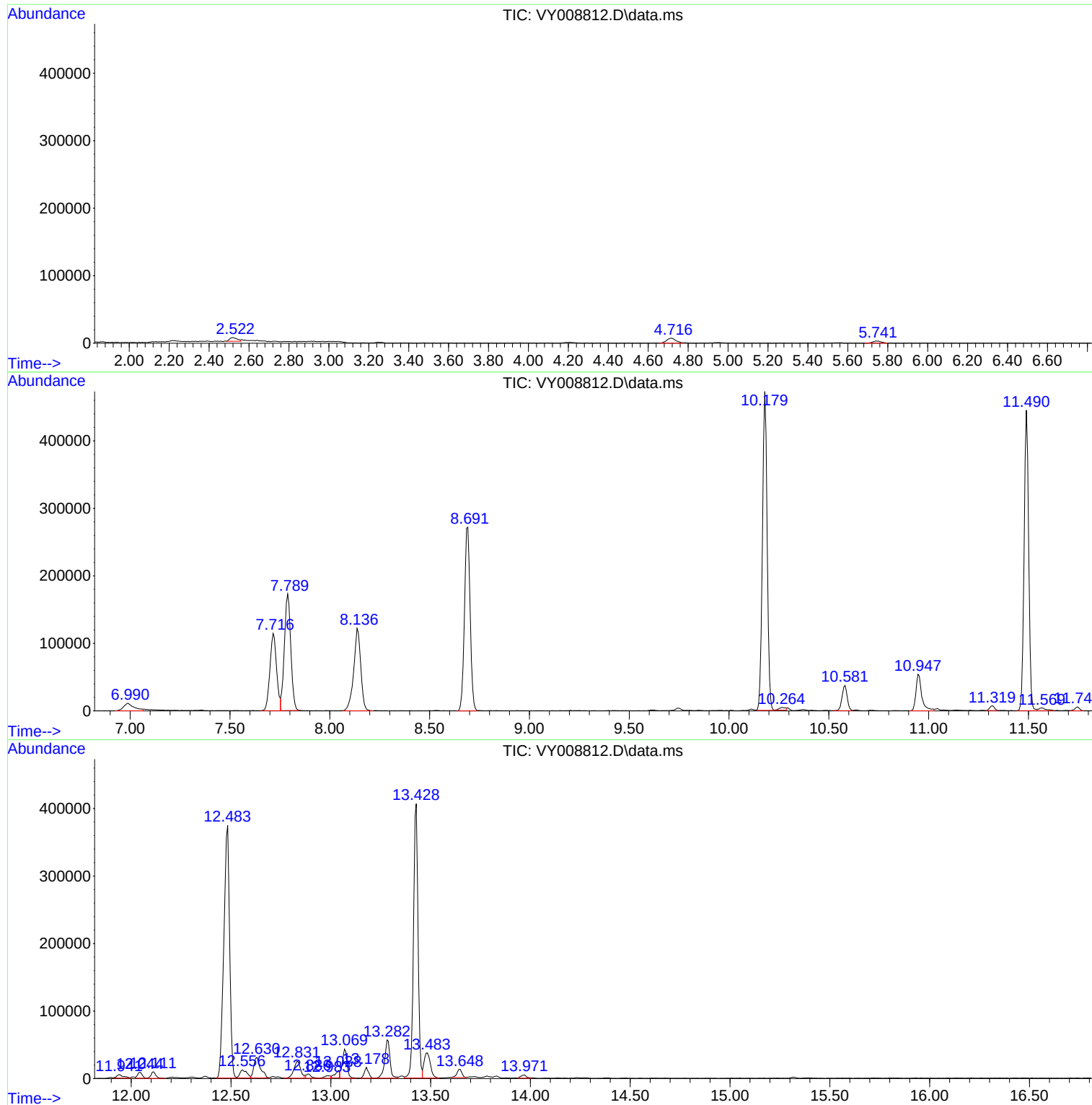
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MSVOA_Y
ClientSampleId :
P027-SS003-0006-01

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051722S.M
Quant Title : SW846 8260

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



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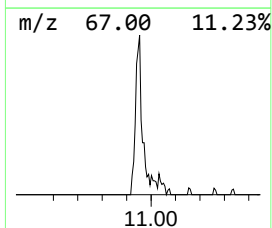
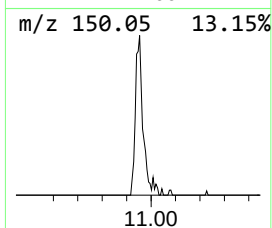
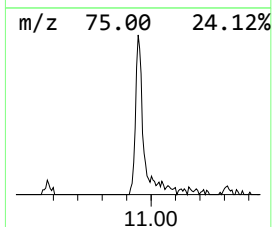
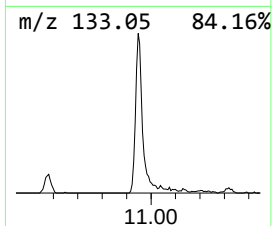
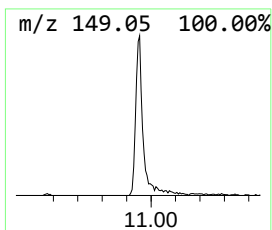
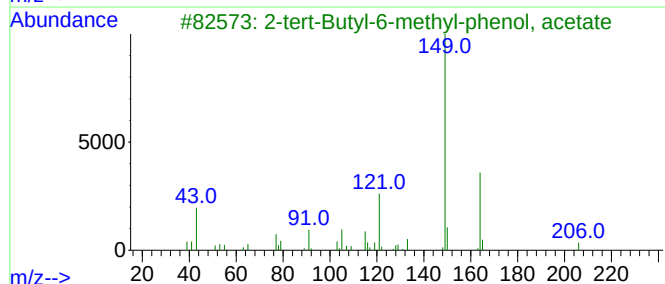
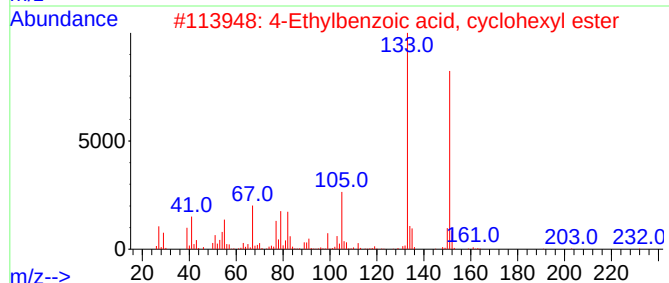
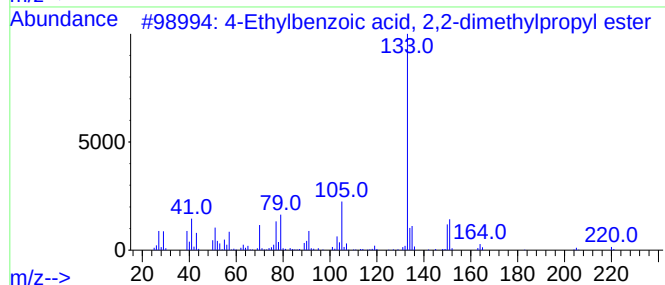
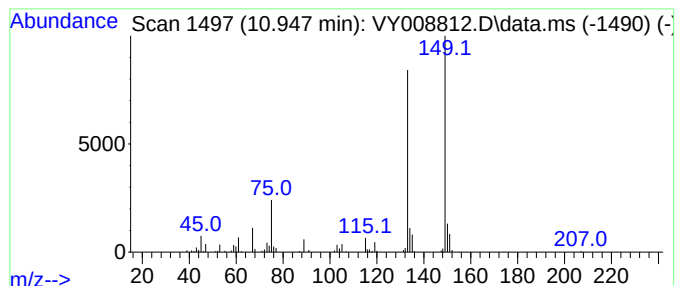
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051722S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown10.947 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	7.75 ug/l	108707	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Ethylbenzoic acid, 2,2-dimethy...	220	C14H20O2	1000293-49-5	25
2			4-Ethylbenzoic acid, cyclohexyl ...	232	C15H20O2	1000293-32-1	25
3			2-tert-Butyl-6-methyl-phenol, ac...	206	C13H18O2	125829-28-9	25
4			1H-Benzotriazole, 5-methoxy-	149	C7H7N3O	027799-91-3	25
5			Benzenamine, 2-cyclopropyl-	133	C9H11N	1000327-33-3	25



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ClientSampleId :
P027-SS003-0006-01

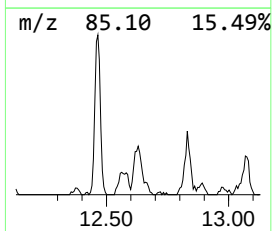
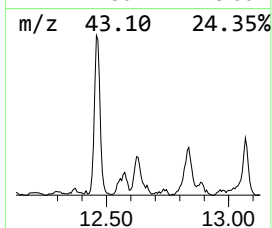
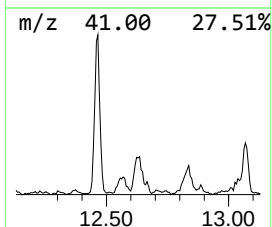
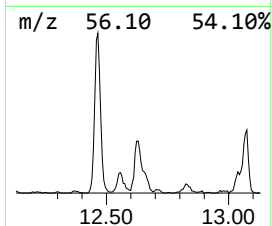
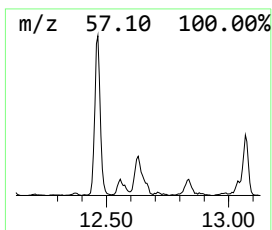
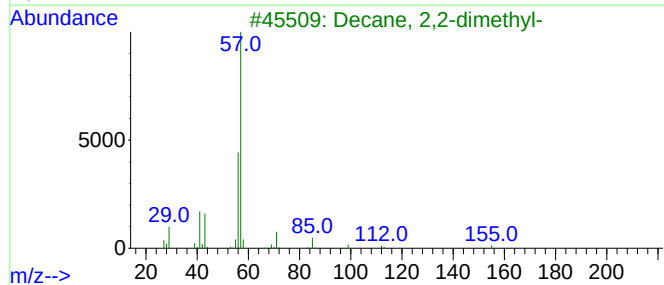
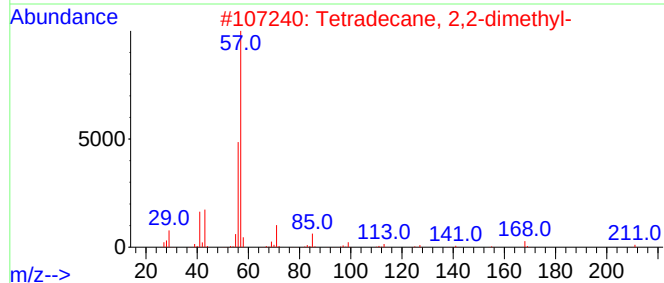
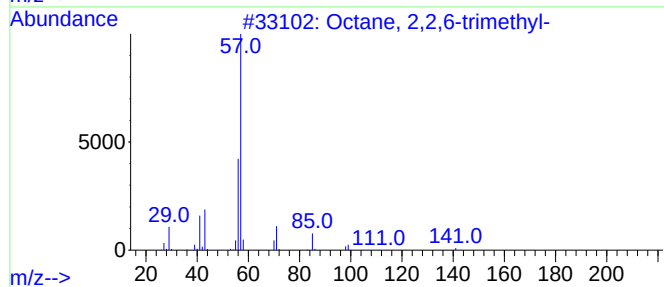
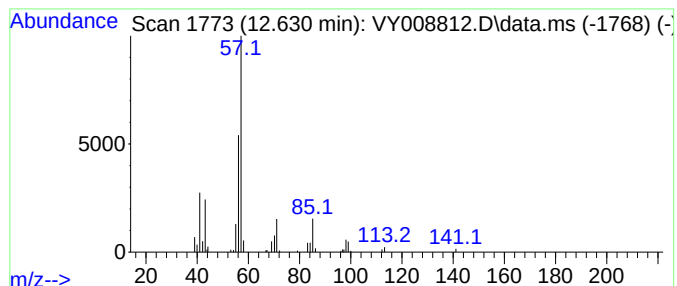
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y051722S.M
Quant Title : SW846 8260

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

Peak Number 3 Octane, 2,2,6-trimethyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.630	5.38 ug/l	69394	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	72
2			Tetradecane, 2,2-dimethyl-	226	C16H34	059222-86-5	72
3			Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	72
4			Decane, 2,2,9-trimethyl-	184	C13H28	062238-00-0	72
5			Dodecane, 2,2,11,11-tetramethyl-	226	C16H34	127204-12-0	72



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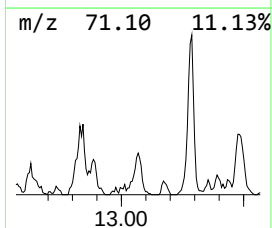
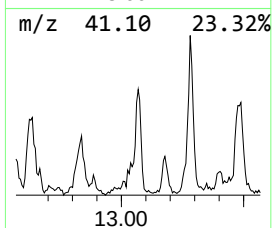
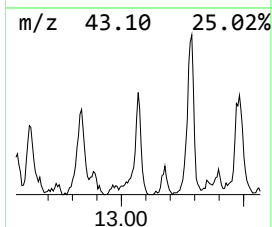
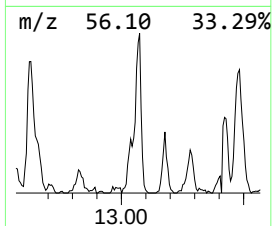
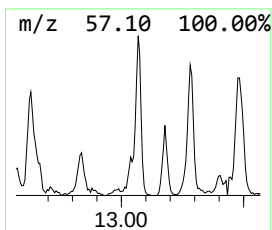
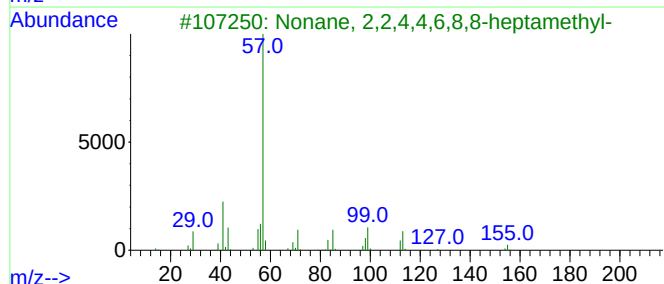
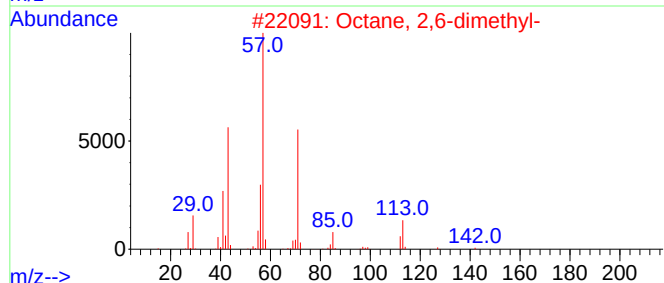
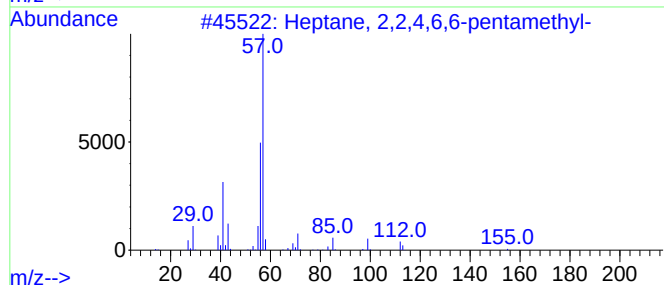
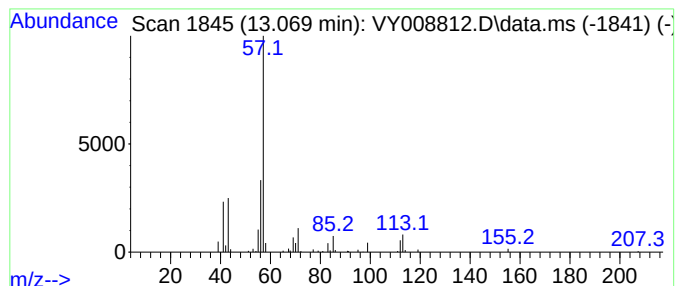
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Quant Title : SW846 8260

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

Peak Number 4 Heptane, 2,2,4,6,6-pentamet... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.069	5.45 ug/l	70345	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	72
2			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
3			Nonane, 2,2,4,4,6,8,8-heptamethyl-	226	C16H34	004390-04-9	59
4			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	59
5			Decane, 2,2-dimethyl-	170	C12H26	017302-37-3	59



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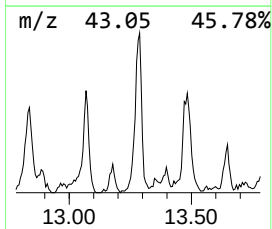
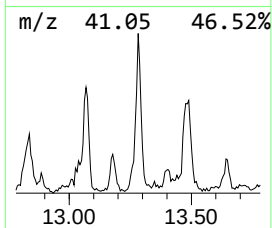
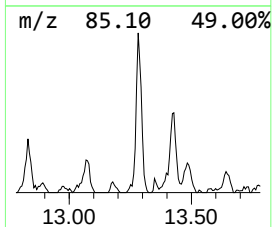
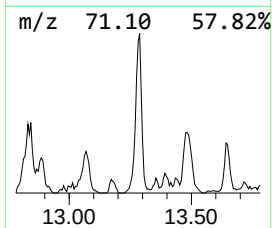
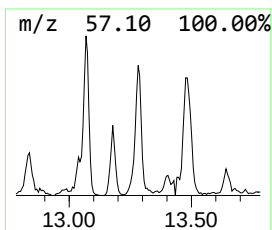
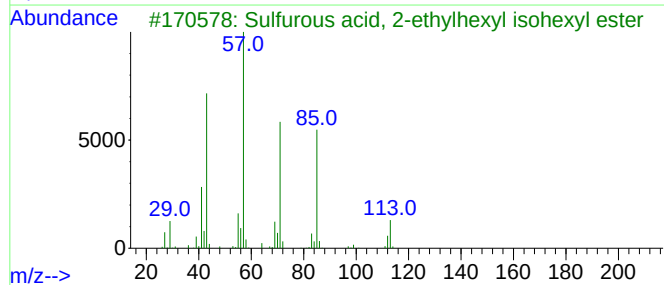
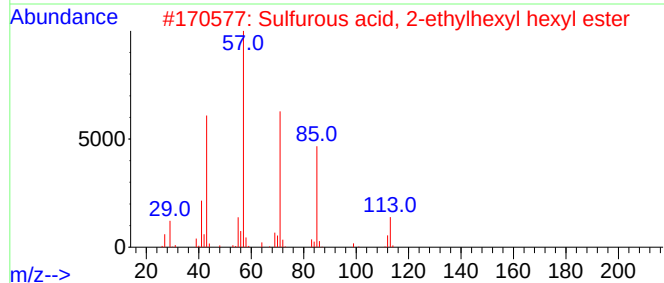
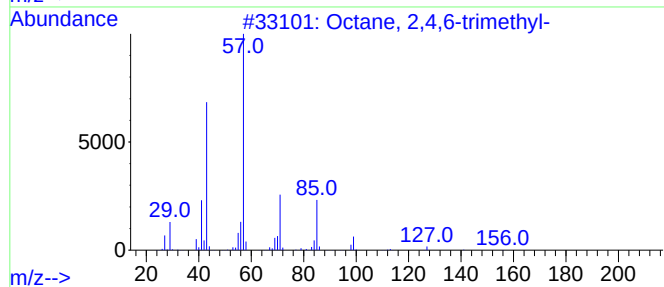
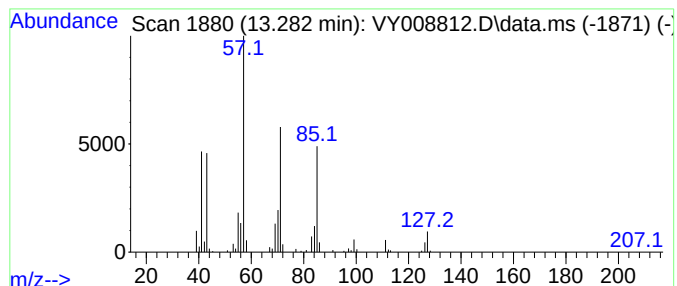
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TIC Library : C:\Database\NIST20.L
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Peak Number 5 Octane, 2,4,6-trimethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	8.02 ug/l	103483	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,4,6-trimethyl-	156	C11H24	062016-37-9	59
2			Sulfurous acid, 2-ethylhexyl hex...	278	C14H30O3S	1000309-20-2	53
3			Sulfurous acid, 2-ethylhexyl iso...	278	C14H30O3S	1000309-19-0	53
4			Hexadecane	226	C16H34	000544-76-3	47
5			Succinic acid, hex-4-yn-3-yl tet...	282	C15H22O5	1000390-71-7	47



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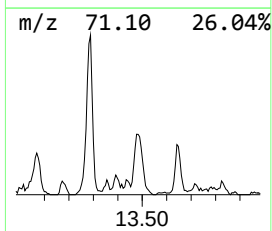
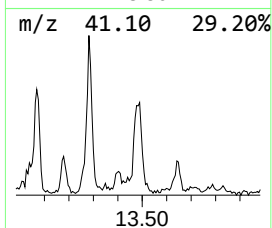
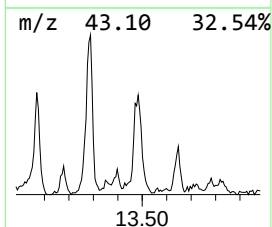
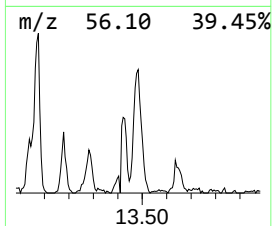
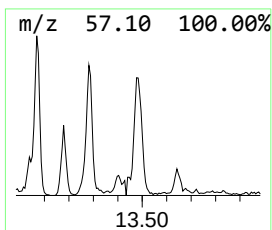
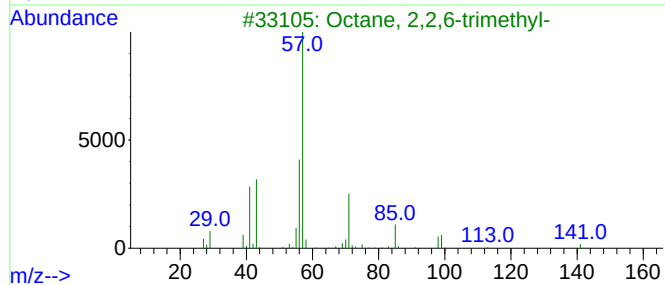
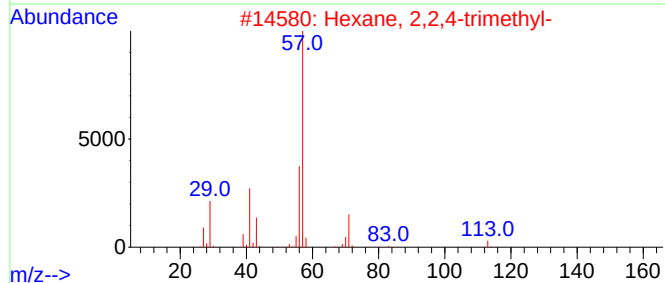
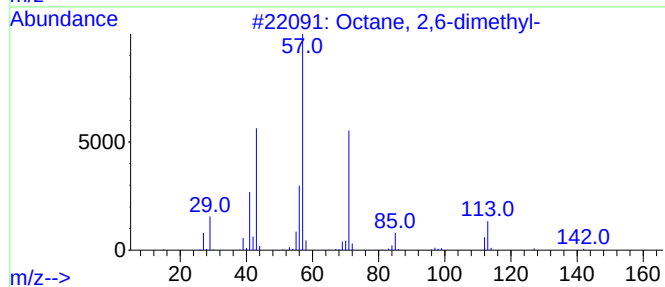
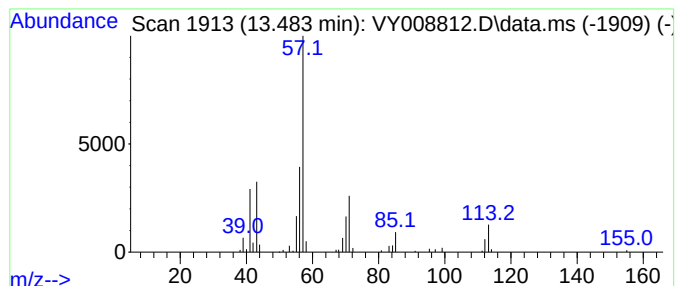
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Quant Title : SW846 8260

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

Peak Number 6 Octane, 2,6-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.483	6.25 ug/l	80612	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Octane, 2,6-dimethyl-	142	C10H22	002051-30-1	64
2			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	64
3			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	59
4			Heptane, 2,2,4,6,6-pentamethyl-	170	C12H26	013475-82-6	53
5			Pentane, 3-ethyl-2,2-dimethyl-	128	C9H20	016747-32-3	50



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Quant Title : SW846 8260

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown10.947	10.947	7.8	ug/l	108707	3	11.490	701755	50.0
Octane, 2,2,6-t...	12.630	5.4	ug/l	69394	4	13.428	644914	50.0
Heptane, 2,2,4,...	13.069	5.5	ug/l	70345	4	13.428	644914	50.0
Octane, 2,4,6-t...	13.282	8.0	ug/l	103483	4	13.428	644914	50.0
Octane, 2,6-dim...	13.483	6.3	ug/l	80612	4	13.428	644914	50.0