

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102221\
 Data File : VY006449.D
 Acq On : 22 Oct 2021 19:09
 Operator : SY/MD
 Sample : M4316-04
 Misc : 4.37G/5ML/MSVOA_Y/SOIL
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 WC-2A-ID

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\82Y102221S.M
 Title : SW846 8260

Signal : TIC: VY006449.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.393	90	94	100	rVB	4327	7482	1.19%	0.194%
2	3.954	342	350	365	rVB	4499	13282	2.11%	0.344%
3	4.722	466	476	486	rBV3	10324	32598	5.19%	0.845%
4	5.759	637	646	656	rBV5	2840	8486	1.35%	0.220%
5	6.704	792	801	812	rBV4	2867	8825	1.40%	0.229%
6	7.722	959	968	974	rBV	79032	187218	29.78%	4.854%
7	7.795	974	980	989	rVB	134747	300094	47.74%	7.780%
8	8.149	1028	1038	1049	rBV	89801	194507	30.94%	5.043%
9	8.331	1061	1068	1077	rVB2	5438	14413	2.29%	0.374%
10	8.691	1119	1127	1136	rBV	221308	431222	68.60%	11.180%
11	9.618	1272	1279	1287	rVB2	8222	15786	2.51%	0.409%
12	9.752	1291	1301	1308	rBV	9464	19718	3.14%	0.511%
13	10.179	1364	1371	1384	rBV	359662	628642	100.00%	16.298%
14	10.581	1431	1437	1442	rBV	6556	12218	1.94%	0.317%
15	11.489	1578	1586	1596	rBV	326839	521914	83.02%	13.531%
16	12.203	1693	1703	1713	rVB5	2931	7536	1.20%	0.195%
17	12.483	1742	1749	1755	rBV	253189	398021	63.31%	10.319%
18	12.648	1769	1776	1783	rVB6	5907	13242	2.11%	0.343%
19	12.812	1797	1803	1807	rBV8	4202	10309	1.64%	0.267%
20	13.068	1837	1845	1849	rBV6	5218	10442	1.66%	0.271%
21	13.282	1872	1880	1889	rBV5	8078	19516	3.10%	0.506%
22	13.428	1897	1904	1910	rBV	297673	464153	73.83%	12.034%
23	13.745	1950	1956	1963	rBV6	15912	29114	4.63%	0.755%
24	14.074	2007	2010	2014	rBV5	6574	8336	1.33%	0.216%
25	14.147	2014	2022	2027	rBV10	9019	22890	3.64%	0.593%
26	14.196	2027	2030	2036	rBV8	6509	13496	2.15%	0.350%
27	14.257	2036	2040	2044	rBV5	17162	35392	5.63%	0.918%
28	14.422	2056	2067	2071	rBV7	19201	47210	7.51%	1.224%
29	14.477	2071	2076	2079	rVV7	7827	13766	2.19%	0.357%
30	14.739	2115	2119	2123	rVB5	13048	20879	3.32%	0.541%
31	14.849	2133	2137	2139	rBV3	10516	16791	2.67%	0.435%
32	14.940	2150	2152	2157	rVB3	15619	20258	3.22%	0.525%
33	15.007	2159	2163	2166	rBV4	13511	21795	3.47%	0.565%
34	15.123	2179	2182	2190	rVB7	18940	40444	6.43%	1.049%
35	15.214	2193	2197	2203	rBV	41178	64545	10.27%	1.673%
36	15.281	2204	2208	2212	rBV6	16866	33570	5.34%	0.870%

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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

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37	15.604	2258	2261	2267	rVB4	28669	51381	8.17%	1.332%
38	16.159	2347	2352	2359	rBV2	36045	65351	10.40%	1.694%
39	16.604	2420	2425	2429	rBV8	14485	32311	5.14%	0.838%

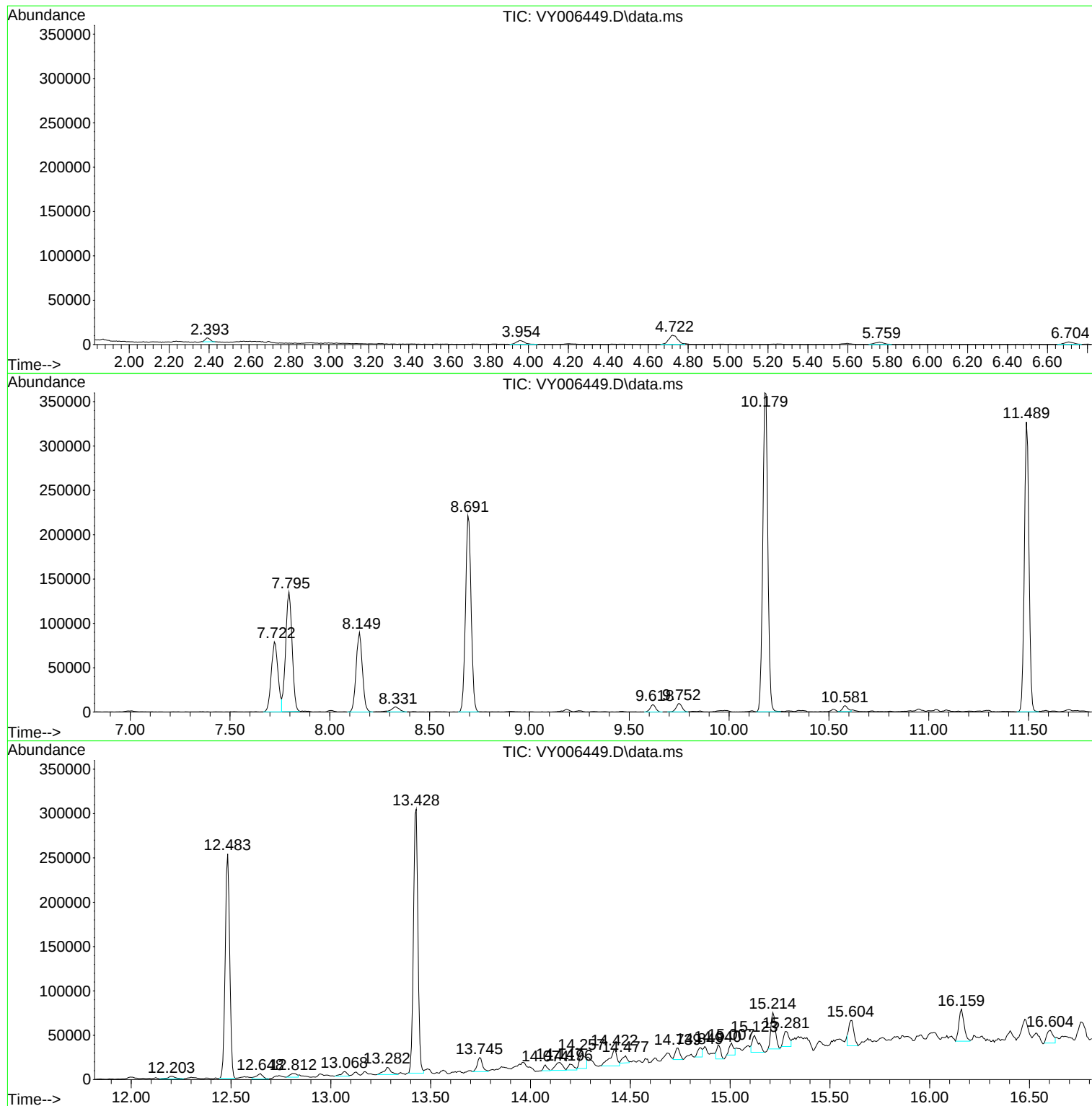
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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



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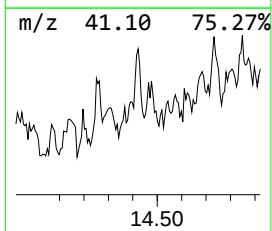
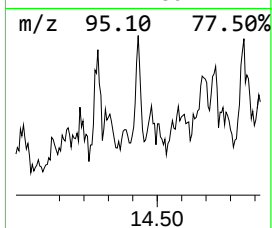
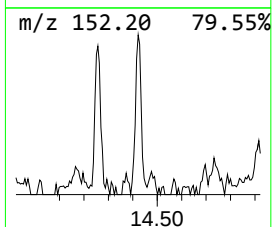
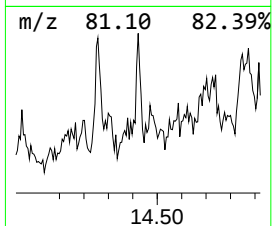
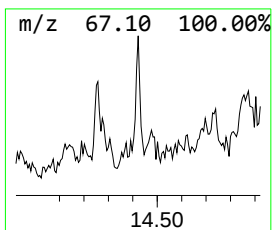
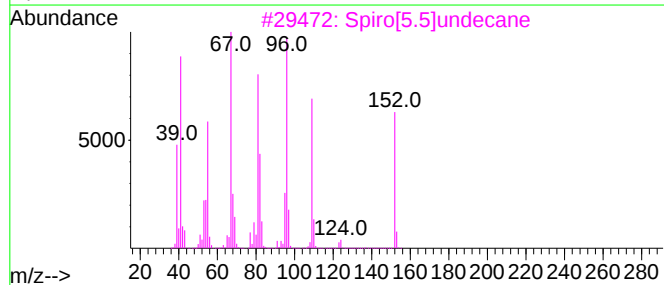
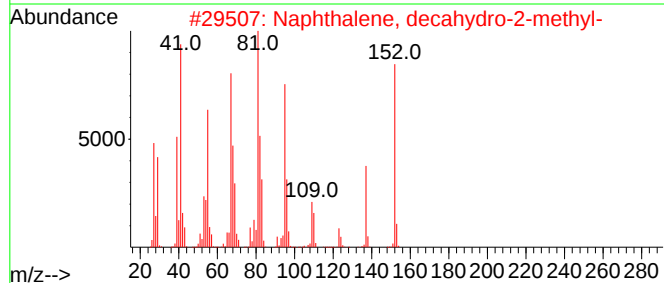
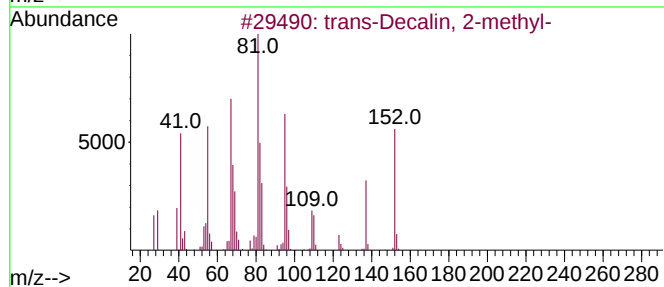
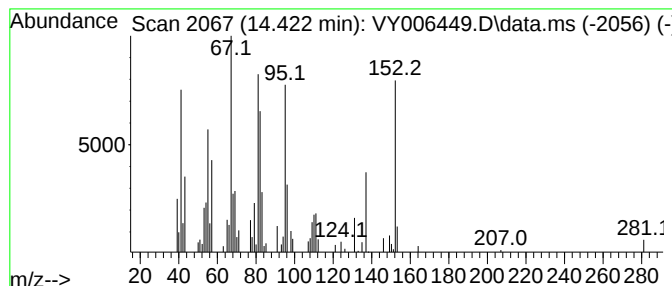
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 2 trans-Decalin, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.422	5.09 ug/l	47210	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	76
2			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	76
3			Spiro[5.5]undecane	152	C11H20	000180-43-8	70
4			Cyclohexanone, 5-methyl-2-(1-met...	152	C10H16O	015932-80-6	52
5			Bicyclo[2.2.1]heptane, 2-methyl-	110	C8H14	015185-11-2	49



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Instrument :
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ClientSampleId :
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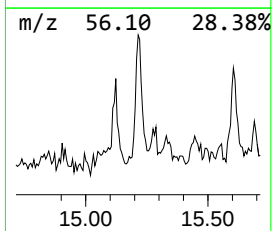
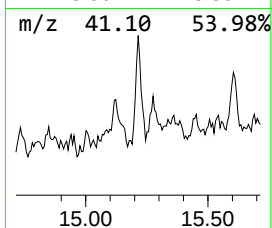
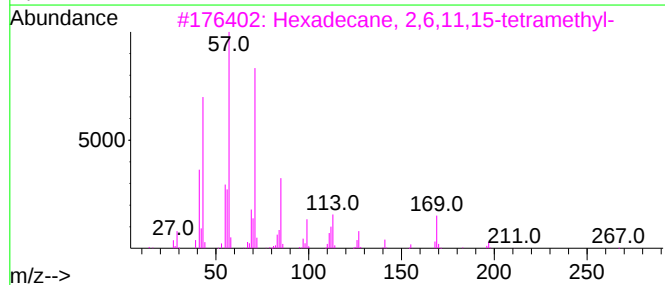
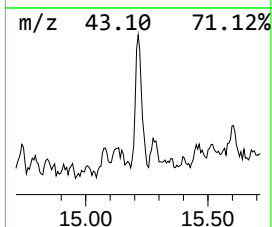
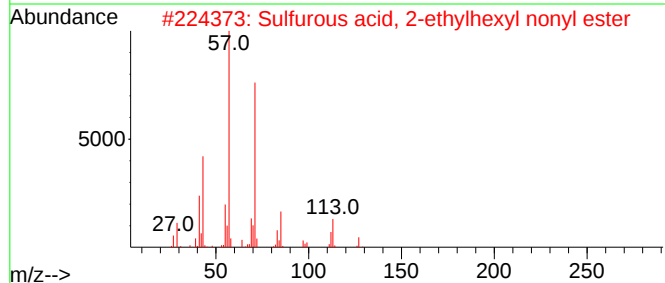
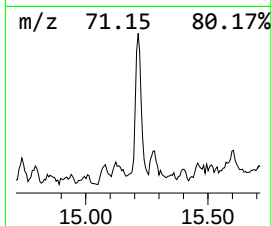
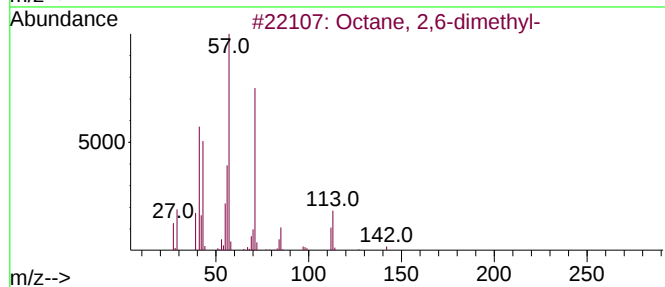
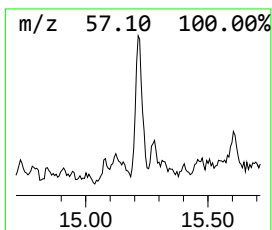
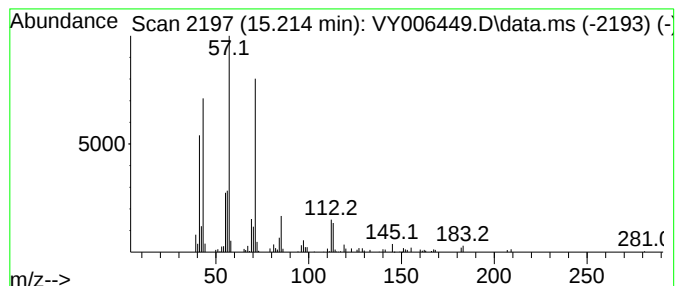
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Peak Number 3 Octane, 2,6-dimethyl- Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.214	6.95 ug/l	64545	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	86
2			Sulfurous acid, 2-ethylhexyl non...	320	C17H36O3S	1010309-19-2	83
3			Hexadecane, 2,6,11,15-tetramethyl-	282	C20H42	000504-44-9	80
4			Sulfurous acid, decyl 2-ethylhex...	334	C18H38O3S	1000309-19-3	64
5			Carbonic acid, dodecyl 2-ethylhe...	342	C21H42O3	1000383-13-9	59



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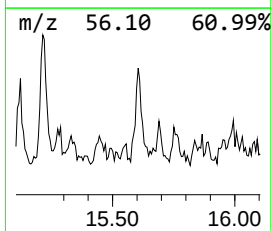
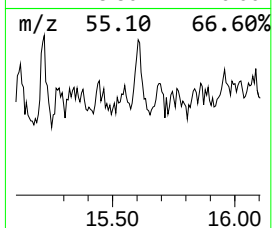
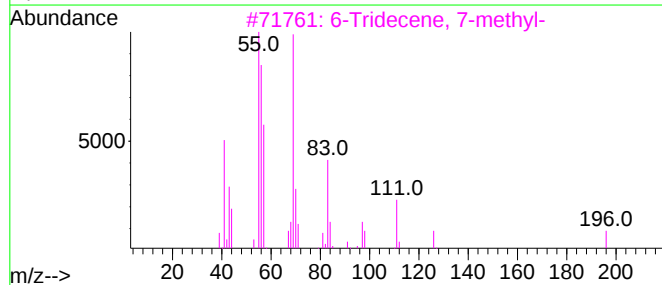
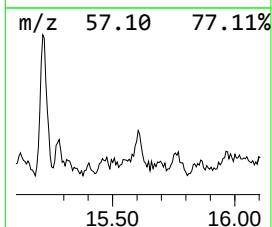
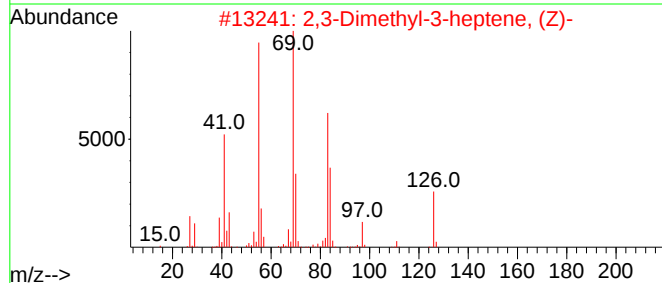
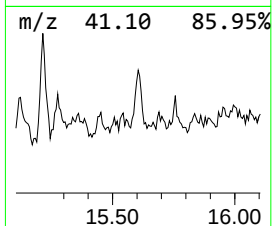
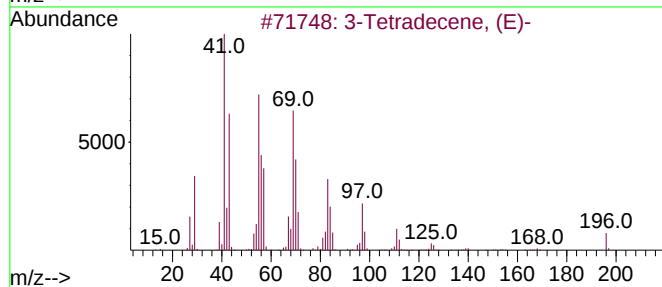
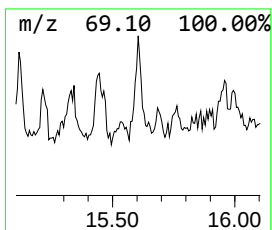
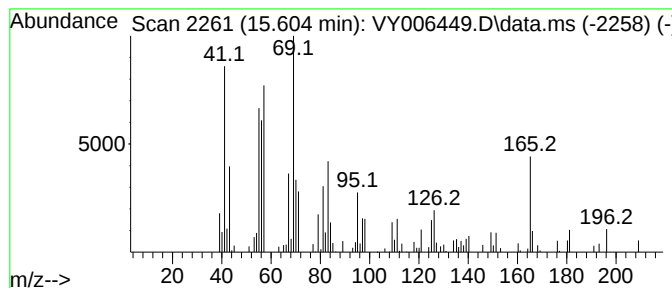
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y102221S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown15.605 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.605	5.53 ug/l	51381	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Tetradecene, (E)-	196	C14H28	041446-68-8	49
2			2,3-Dimethyl-3-heptene, (Z)-	126	C9H18	059643-73-1	43
3			6-Tridecene, 7-methyl-	196	C14H28	024949-42-6	43
4			2-Methyl-2-octene	126	C9H18	016993-86-5	43
5			4,8-Dimethylnona-3,8-dien-2-one	166	C11H18O	872858-42-9	38



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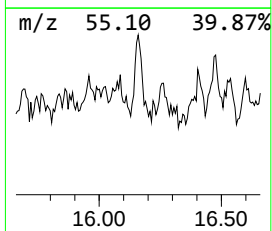
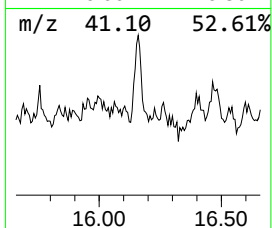
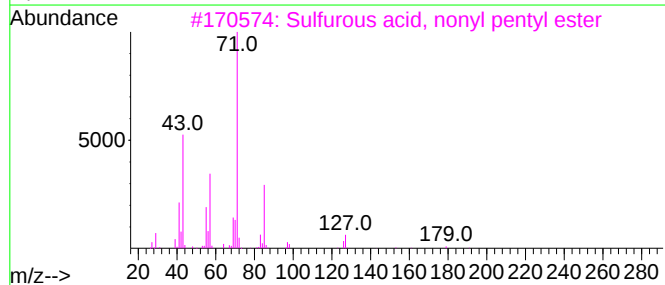
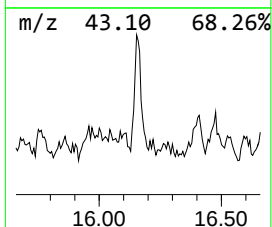
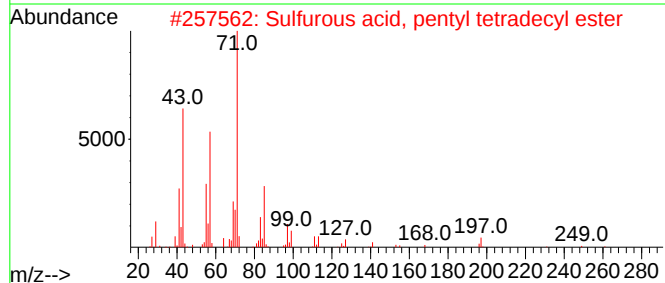
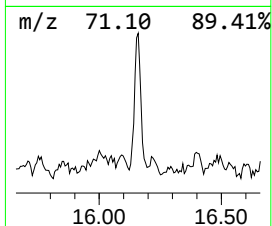
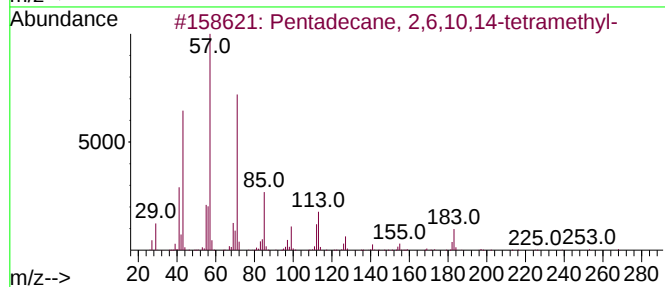
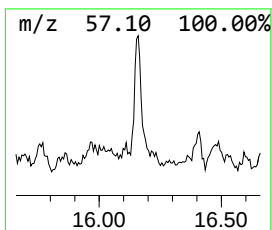
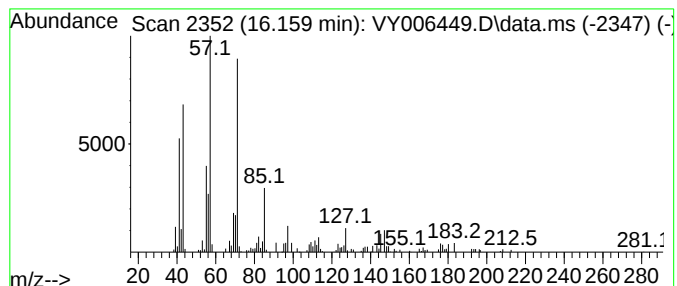
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Peak Number 5 Pentadecane, 2,6,10,14-tetr... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.159	7.04 ug/l	65351	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Pentadecane, 2,6,10,14-tetramethyl-	268	C19H40	001921-70-6	72
2			Sulfurous acid, pentyl tetradecy...	348	C19H40O3S	1010309-14-7	59
3			Sulfurous acid, nonyl pentyl ester	278	C14H30O3S	1000309-14-2	53
4			Sulfurous acid, 2-ethylhexyl oct...	446	C26H54O3S	1000309-20-1	53
5			Dodecane, 2,6,11-trimethyl-	212	C15H32	031295-56-4	53



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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
trans-Decalin, ...	14.422	5.1	ug/l	47210	4	13.428	464153	50.0
Octane, 2,6-dim...	15.214	7.0	ug/l	64545	4	13.428	464153	50.0
unknown15.605	15.605	5.5	ug/l	51381	4	13.428	464153	50.0
Pentadecane, 2,...	16.159	7.0	ug/l	65351	4	13.428	464153	50.0