

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042423\
 Data File : VY013421.D
 Acq On : 25 Apr 2023 02:17
 Operator : KP/MD
 Sample : 02427-02
 Misc : 3.95g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 41 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 20230287-24-1

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\82Y042423S.M

Title : SW846 8260

Signal : TIC: VY013421.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.863	3	7	14	rVB2	34358	51615	5.23%	0.693%
2	2.217	59	65	69	rBV	20605	38874	3.94%	0.522%
3	3.253	228	235	243	rVB4	5344	12510	1.27%	0.168%
4	3.954	339	350	360	rBV2	51537	170201	17.25%	2.286%
5	4.198	380	390	402	rBV	50497	138625	14.05%	1.862%
6	4.716	463	475	490	rBV2	18519	60982	6.18%	0.819%
7	6.990	837	848	866	rBV3	21178	73151	7.41%	0.983%
8	7.716	956	967	973	rBV	148165	355390	36.01%	4.774%
9	7.789	973	979	990	rVB	244649	550232	55.76%	7.391%
10	8.143	1028	1037	1050	rBV	156963	356342	36.11%	4.786%
11	8.545	1097	1103	1109	rBV6	4992	10064	1.02%	0.135%
12	8.691	1118	1127	1139	rBV	367183	733944	74.37%	9.858%
13	8.929	1158	1166	1173	rBV4	4893	11360	1.15%	0.153%
14	9.185	1195	1208	1214	rBV8	4523	13766	1.39%	0.185%
15	10.179	1363	1371	1380	rBV	581563	986863	100.00%	13.256%
16	11.087	1514	1520	1525	rVB4	6294	10200	1.03%	0.137%
17	11.489	1578	1586	1595	rBV	540398	871301	88.29%	11.703%
18	11.685	1612	1618	1624	rBV8	6404	17834	1.81%	0.240%
19	11.739	1624	1627	1639	rVB10	8655	21798	2.21%	0.293%
20	11.995	1662	1669	1677	rBV10	10536	35931	3.64%	0.483%
21	12.209	1694	1704	1705	rBV9	16621	36096	3.66%	0.485%
22	12.233	1705	1708	1713	rVB2	28404	41583	4.21%	0.559%
23	12.319	1713	1722	1727	rBV8	10687	29128	2.95%	0.391%
24	12.483	1741	1749	1755	rBV3	432008	743454	75.34%	9.986%
25	12.569	1755	1763	1767	rBV8	13532	34464	3.49%	0.463%
26	12.642	1768	1775	1781	rVB7	35090	86297	8.74%	1.159%
27	12.733	1781	1790	1796	rBV8	20215	65319	6.62%	0.877%
28	12.812	1796	1803	1804	rVV5	24345	50965	5.16%	0.685%
29	12.831	1804	1806	1817	rVB6	30529	68329	6.92%	0.918%
30	12.953	1822	1826	1828	rVV5	9511	12228	1.24%	0.164%
31	13.068	1837	1845	1850	rBV2	40457	72803	7.38%	0.978%
32	13.129	1851	1855	1858	rVB4	7320	10277	1.04%	0.138%
33	13.172	1858	1862	1867	rBV3	20710	41789	4.23%	0.561%
34	13.282	1872	1880	1885	rBV2	70059	133532	13.53%	1.794%
35	13.422	1896	1903	1909	rBV	491923	784772	79.52%	10.541%
36	13.477	1909	1912	1919	rVB	55419	106746	10.82%	1.434%

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

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37	13.568	1923	1927	1930	rVB5	15800	22332	2.26%	0.300%
38	13.635	1931	1938	1943	rBV4	29932	70373	7.13%	0.945%
39	13.745	1951	1956	1960	rBV4	25895	41900	4.25%	0.563%
40	13.965	1986	1992	2002	rVB	84295	171625	17.39%	2.305%
41	14.141	2017	2021	2027	rVB9	14810	31968	3.24%	0.429%
42	14.202	2027	2031	2035	rBV7	8931	15007	1.52%	0.202%
43	14.251	2035	2039	2044	rBV7	22099	43330	4.39%	0.582%
44	14.391	2056	2062	2064	rBV6	13457	28399	2.88%	0.381%
45	14.416	2064	2066	2070	rVB4	19929	28020	2.84%	0.376%
46	14.733	2114	2118	2124	rVB9	18848	30348	3.08%	0.408%
47	14.843	2134	2136	2141	rBV6	9675	13855	1.40%	0.186%
48	14.940	2148	2152	2156	rVB7	11166	17184	1.74%	0.231%
49	15.001	2158	2162	2166	rBV7	8349	19063	1.93%	0.256%
50	15.117	2178	2181	2189	rVB9	13330	28783	2.92%	0.387%
51	15.598	2257	2260	2267	rVB7	16745	30339	3.07%	0.408%
52	16.013	2326	2328	2337	rVB9	7924	13604	1.38%	0.183%

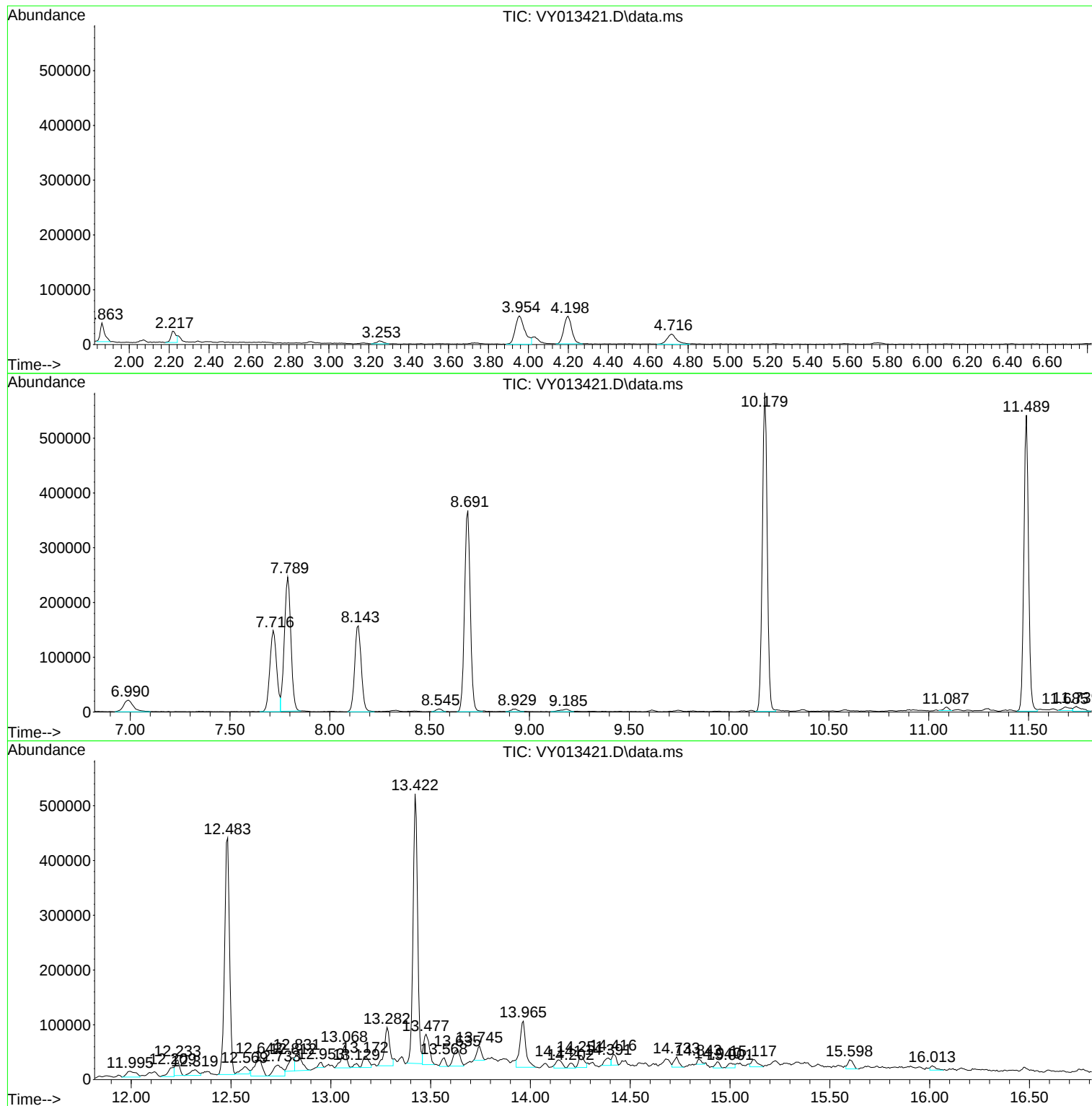
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ClientSampleId :
20230287-24-1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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



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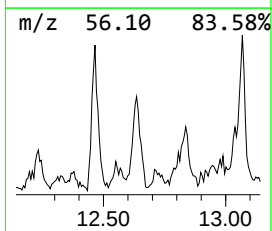
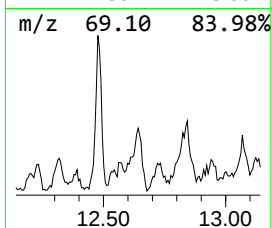
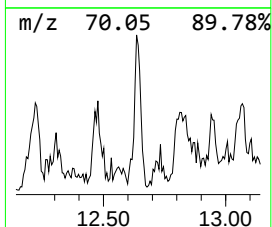
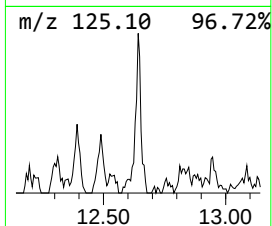
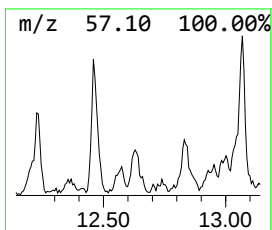
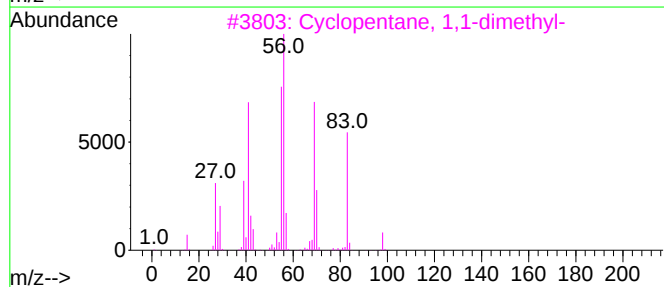
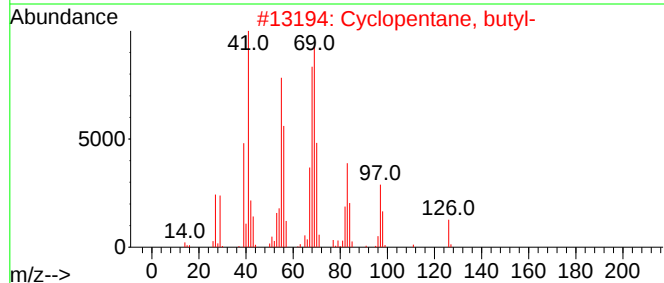
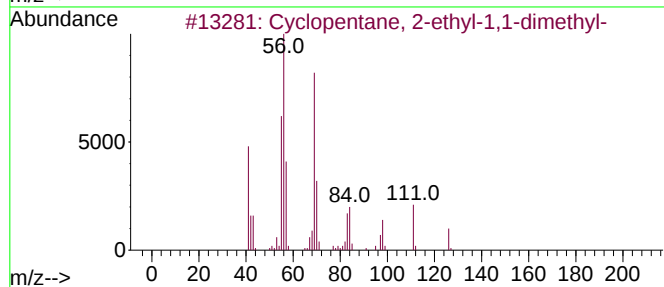
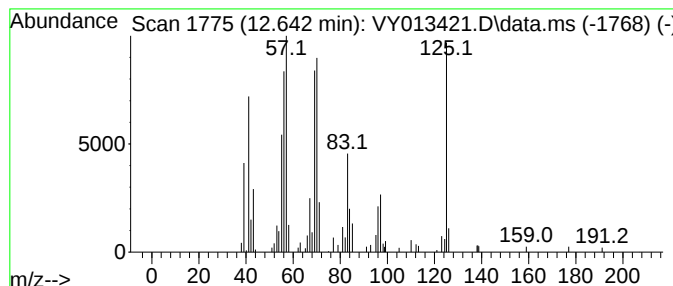
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.642 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.642	5.50 ug/l	86297	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclopentane, 2-ethyl-1,1-dimethyl-	126	C9H18	054549-80-3	43
2			Cyclopentane, butyl-	126	C9H18	002040-95-1	42
3			Cyclopentane, 1,1-dimethyl-	98	C7H14	001638-26-2	25
4			2,2-Dimethyl-3-heptene trans	126	C9H18	019550-75-5	22
5			2-Amino-4-hydroxy-6-methylpyrimi...	125	C5H7N3O	003977-29-5	14



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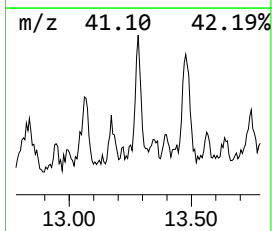
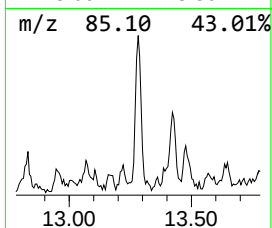
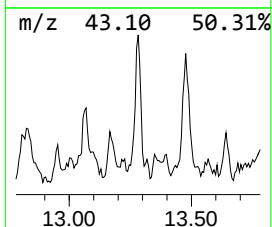
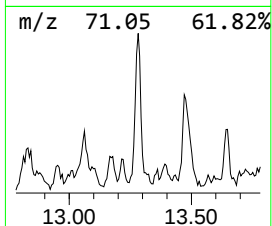
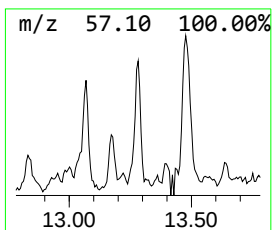
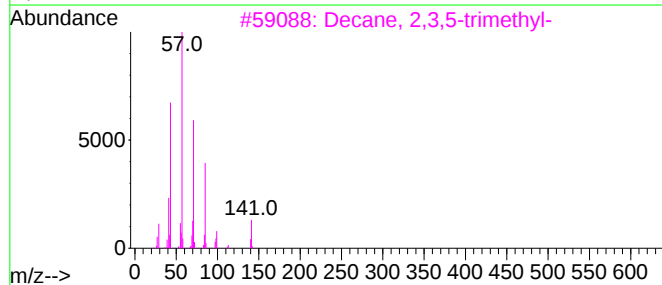
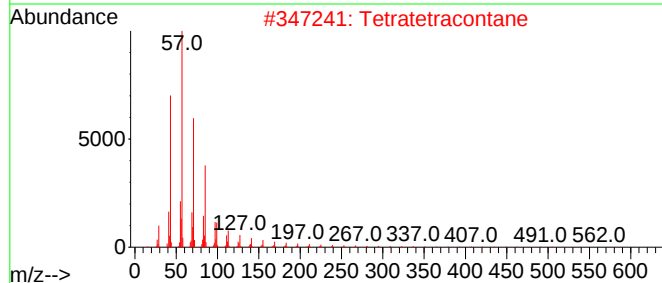
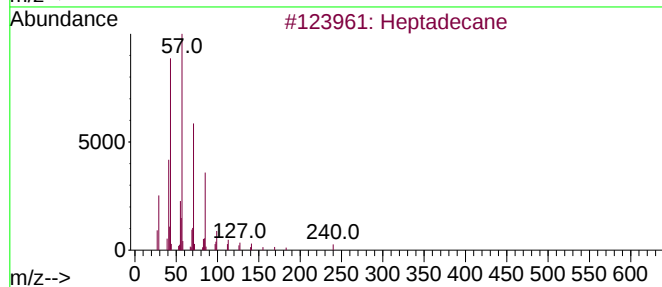
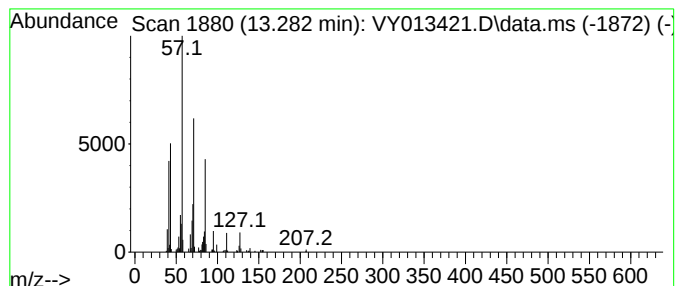
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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

Peak Number 3 Heptadecane Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.282	8.51 ug/l	133532	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Heptadecane	240	C17H36	000629-78-7	59
2			Tetratetracontane	619	C44H90	007098-22-8	59
3			Decane, 2,3,5-trimethyl-	184	C13H28	062238-11-3	59
4			Decane, 2,4-dimethyl-	170	C12H26	002801-84-5	53
5			Undecane, 4,7-dimethyl-	184	C13H28	017301-32-5	53



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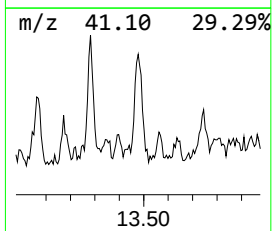
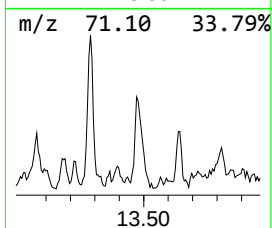
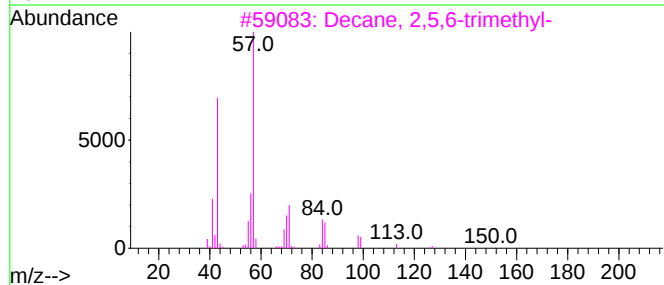
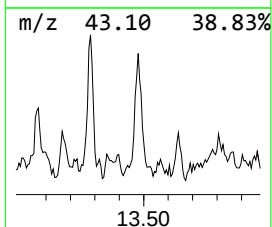
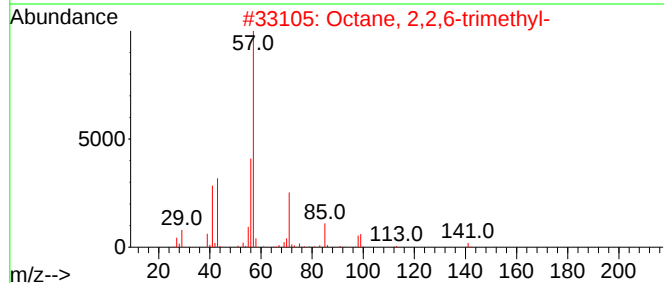
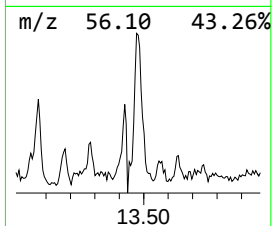
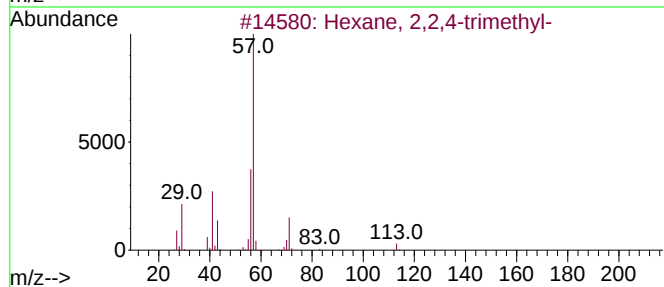
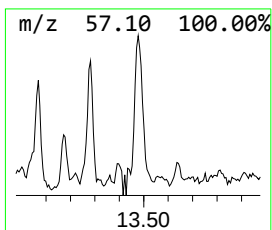
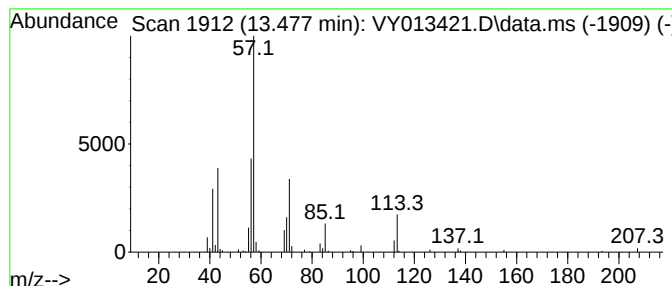
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042423S.M
Quant Title : SW846 8260

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

Peak Number 4 Hexane, 2,2,4-trimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.477	6.80 ug/l	106746	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Hexane, 2,2,4-trimethyl-	128	C9H20	016747-26-5	59
2			Octane, 2,2,6-trimethyl-	156	C11H24	062016-28-8	59
3			Decane, 2,5,6-trimethyl-	184	C13H28	062108-23-0	53
4			Hexane, 2,2,5,5-tetramethyl-	142	C10H22	001071-81-4	50
5			Sulfurous acid, butyl 2-ethylhex...	250	C12H26O3S	1000309-18-8	47



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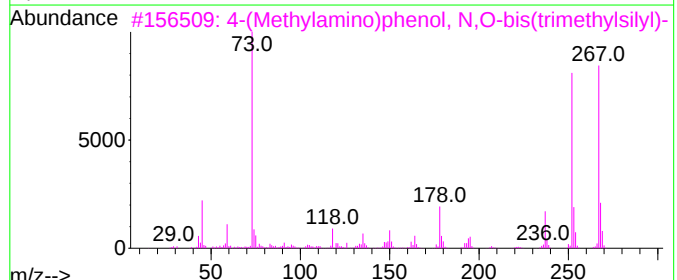
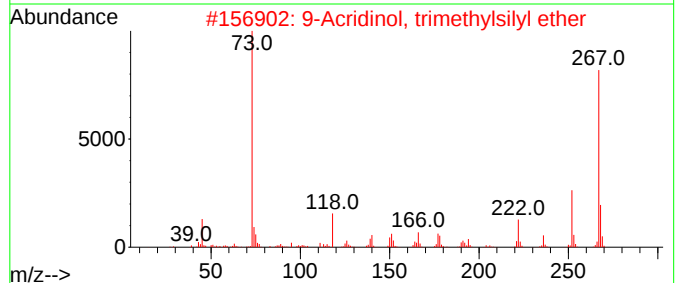
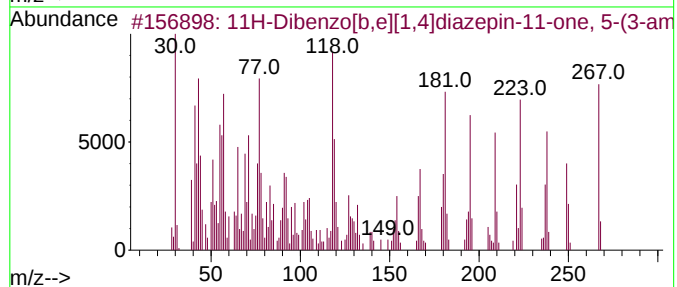
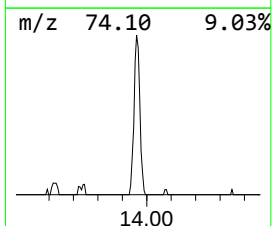
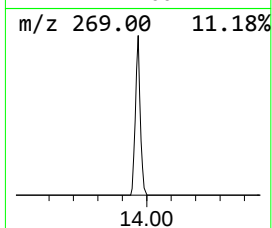
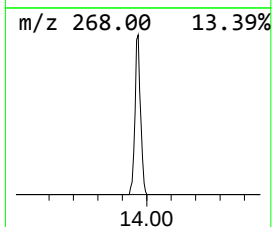
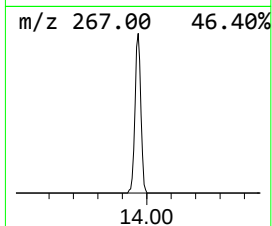
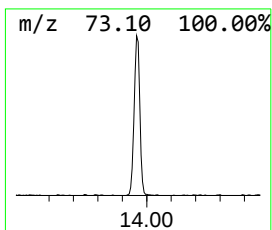
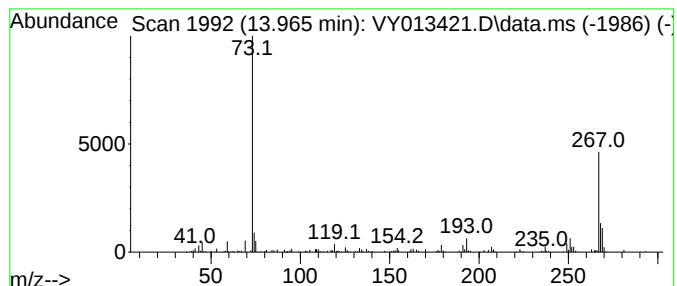
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Quant Title : SW846 8260

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

Peak Number 5 11H-Dibenzo[b,e][1,4]diazep... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	10.93 ug/l	171625	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			11H-Dibenzo[b,e][1,4]diazepin-11...	267	C16H17N3O	013450-73-2	53
2			9-Acridinol, trimethylsilyl ether	267	C16H17NOSi	1000463-65-5	53
3			4-(Methylamino)phenol, N,O-bis(t...	267	C13H25NOSi2	1000471-13-0	50
4			Benzeneethanamine, N-methyl-.bet...	311	C15H29N02Si2	029522-18-7	42
5			2-[(Trimethylsilyl)oxy]-2-{4-[(t...	297	C14H27N02Si2	1000473-27-9	38



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown12.642	12.642	5.5	ug/l	86297	4	13.422	784772	50.0
Heptadecane	13.282	8.5	ug/l	133532	4	13.422	784772	50.0
Hexane, 2,2,4-t...	13.477	6.8	ug/l	106746	4	13.422	784772	50.0
11H-Dibenzo[b,e...	13.965	10.9	ug/l	171625	4	13.422	784772	50.0