

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100323\
 Data File : VY015813.D
 Acq On : 03 Oct 2023 18:06
 Operator : SY/MD
 Sample : 04704-01
 Misc : 6.80g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 S-4(0-5)

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\82Y091923S.M
 Title : SW846 8260

Signal : TIC: VY015813.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.381	87	92	98	rVB	6473	11206	1.24%	0.165%
2	3.948	340	349	366	rBV	19298	60503	6.72%	0.891%
3	4.186	380	388	400	rBV	8265	23468	2.61%	0.346%
4	4.710	462	474	488	rBV2	27552	87792	9.75%	1.293%
5	5.740	633	643	656	rBV2	20055	61405	6.82%	0.905%
6	6.990	837	848	861	rBV2	10388	31319	3.48%	0.461%
7	7.710	956	966	972	rBV	120943	284626	31.61%	4.193%
8	7.783	972	978	990	rVB	217176	482884	53.62%	7.114%
9	8.136	1026	1036	1049	rBV	140747	317279	35.23%	4.674%
10	8.685	1116	1126	1138	rBV	336360	654610	72.69%	9.644%
11	10.179	1363	1371	1377	rBV	512560	900519	100.00%	13.267%
12	10.240	1377	1381	1392	rVB	15432	27321	3.03%	0.403%
13	10.575	1430	1436	1445	rBV2	6678	11910	1.32%	0.175%
14	11.489	1576	1586	1595	rBV	480294	797877	88.60%	11.755%
15	11.691	1610	1619	1630	rVB2	7051	19329	2.15%	0.285%
16	12.032	1666	1675	1680	rBV4	10236	24519	2.72%	0.361%
17	12.331	1718	1724	1729	rBV2	16499	28829	3.20%	0.425%
18	12.386	1729	1733	1739	rVB6	5351	9648	1.07%	0.142%
19	12.477	1741	1748	1759	rBV	387997	637256	70.77%	9.389%
20	12.757	1786	1794	1799	rVV2	30780	58563	6.50%	0.863%
21	12.806	1799	1802	1809	rVB4	17775	27543	3.06%	0.406%
22	12.965	1824	1828	1836	rVB4	5064	9509	1.06%	0.140%
23	13.117	1849	1853	1859	rBV2	12131	19499	2.17%	0.287%
24	13.422	1897	1903	1913	rVB	491627	754533	83.79%	11.117%
25	13.526	1913	1920	1932	rBV	479280	766310	85.10%	11.290%
26	13.623	1933	1936	1939	rVV2	14282	22909	2.54%	0.338%
27	13.660	1940	1942	1948	rVB2	11103	14371	1.60%	0.212%
28	13.806	1963	1966	1973	rVB3	9508	19455	2.16%	0.287%
29	13.891	1975	1980	1986	rVV6	7303	19320	2.15%	0.285%
30	13.958	1986	1991	1999	rVB2	61538	104069	11.56%	1.533%
31	14.080	2005	2011	2019	rBV6	9477	22036	2.45%	0.325%
32	14.294	2042	2046	2049	rBV4	5689	10174	1.13%	0.150%
33	14.330	2049	2052	2057	rVB	10651	14394	1.60%	0.212%
34	14.416	2063	2066	2073	rVB7	5911	10739	1.19%	0.158%
35	14.507	2076	2081	2086	rBV8	4401	9113	1.01%	0.134%
36	14.562	2086	2090	2094	rBV5	5567	10083	1.12%	0.149%

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37	14.684	2103	2110	2115	rBV5	34034	77328	8.59%	1.139%
38	14.830	2130	2134	2139	rBV5	9566	15025	1.67%	0.221%
39	15.050	2165	2170	2178	rVB7	9744	24170	2.68%	0.356%
40	15.233	2194	2200	2205	rBV	58216	95369	10.59%	1.405%
41	15.287	2205	2209	2213	rVV3	19402	28484	3.16%	0.420%
42	15.678	2268	2273	2277	rBV8	7272	15534	1.73%	0.229%
43	15.726	2277	2281	2285	rVB5	10405	16374	1.82%	0.241%
44	16.031	2328	2331	2338	rVB7	7642	11488	1.28%	0.169%
45	16.226	2358	2363	2367	rVV7	7526	14097	1.57%	0.208%
46	16.287	2367	2373	2380	rVV2	23094	46249	5.14%	0.681%
47	16.482	2399	2405	2414	rBV	36326	78426	8.71%	1.155%

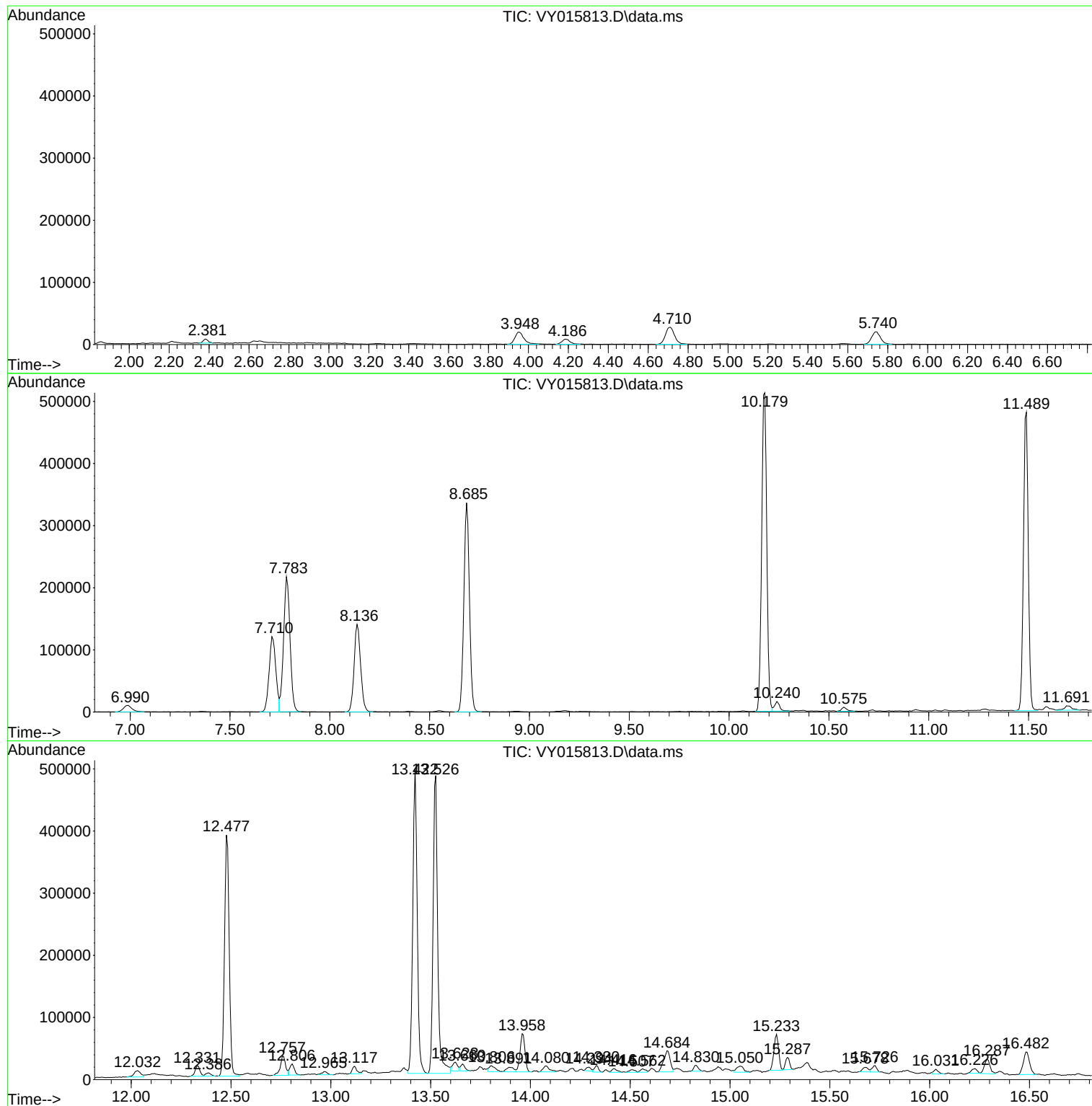
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091923S.M
Quant Title : SW846 8260

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



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S-4(0-5)

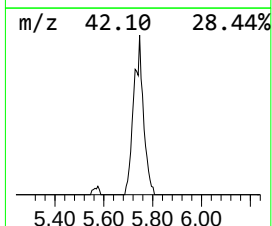
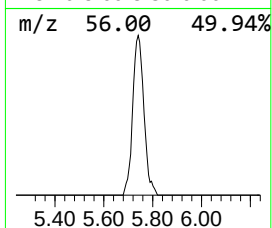
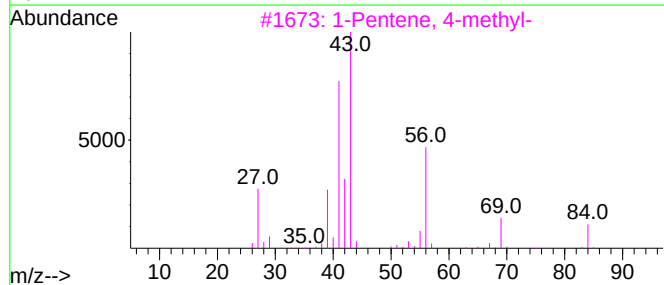
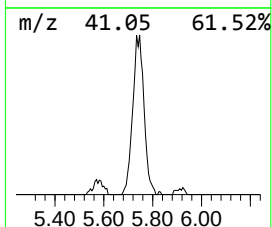
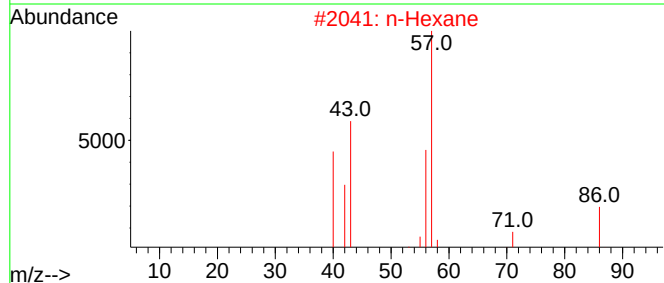
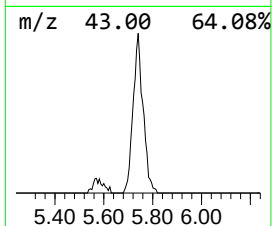
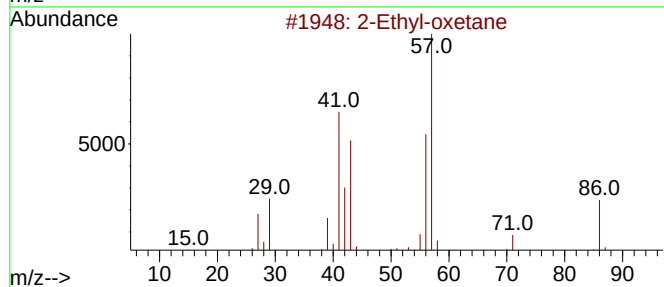
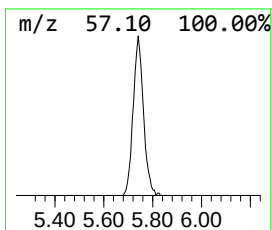
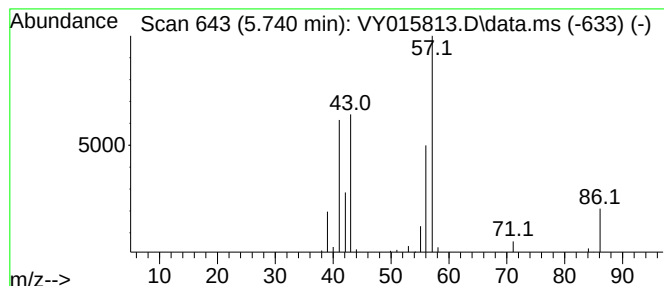
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091923S.M
Quant Title : SW846 8260

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

Peak Number 2 2-Ethyl-oxetane Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.740	6.36 ug/l	61405	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Ethyl-oxetane	86	C5H10O	1010386-40-2	86
2			n-Hexane	86	C6H14	000110-54-3	80
3			1-Pentene, 4-methyl-	84	C6H12	000691-37-2	52
4			Pentane, 2,2,3,4-tetramethyl-	128	C9H20	001186-53-4	47
5			Butane, 2,2,3-trimethyl-	100	C7H16	000464-06-2	40



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-4(0-5)

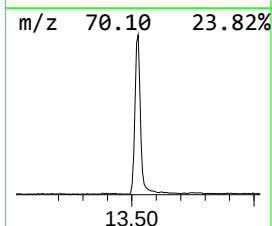
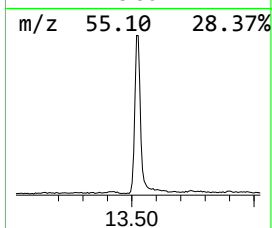
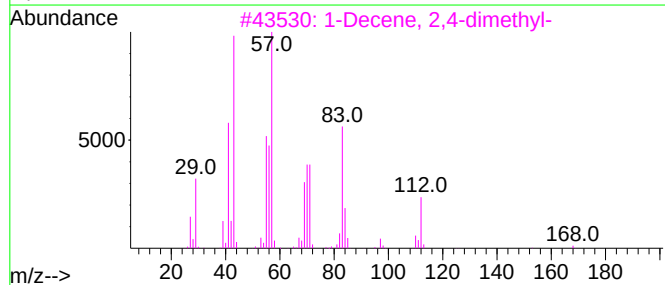
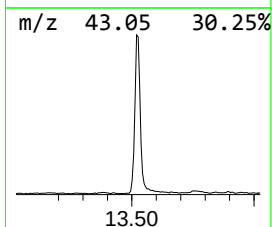
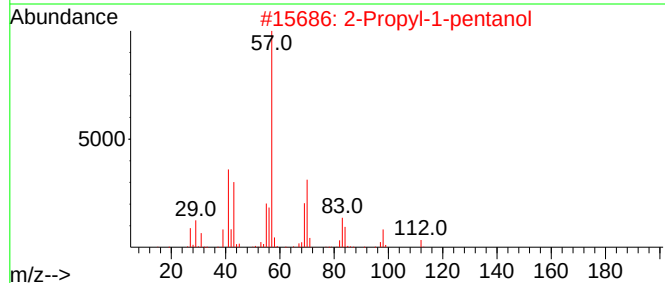
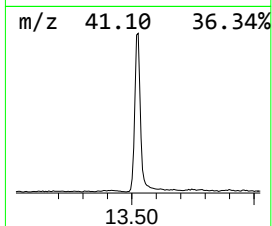
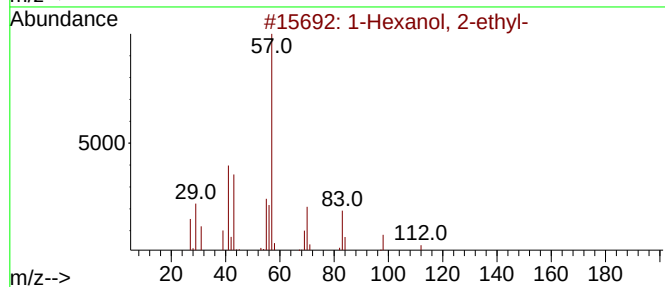
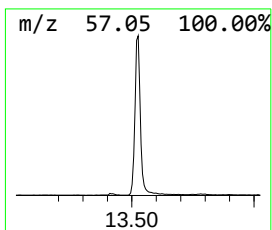
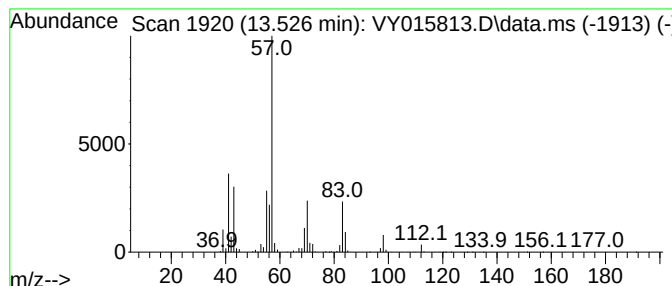
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091923S.M
Quant Title : SW846 8260

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

Peak Number 3 1-Hexanol, 2-ethyl- Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.526	50.78 ug/l	766310	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	90
2			2-Propyl-1-pentanol	130	C8H18O	058175-57-8	50
3			1-Decene, 2,4-dimethyl-	168	C12H24	055170-80-4	50
4			Chloroacetic acid, 2-ethylhexyl ...	206	C10H19ClO2	005345-58-4	45
5			Heptane, 1,1'-oxybis-	214	C14H30O	000629-64-1	43



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ALS Vial : 20 Sample Multiplier: 1

Instrument :
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ClientSampleId :
S-4(0-5)

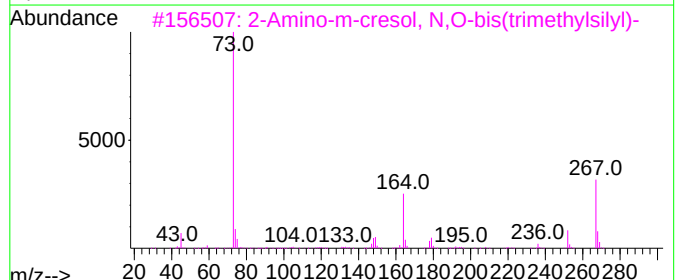
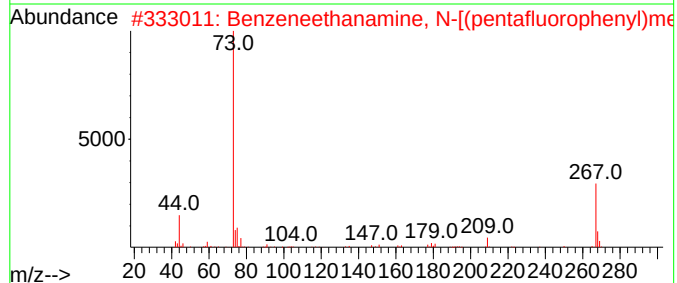
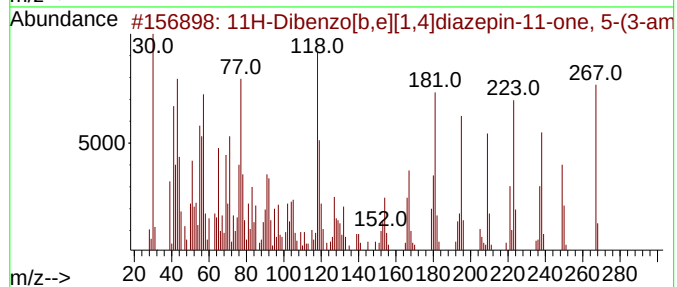
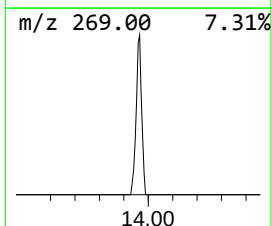
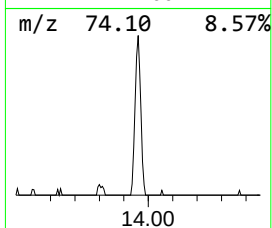
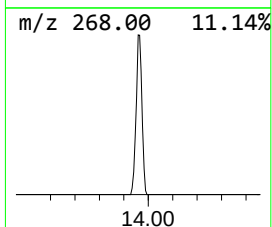
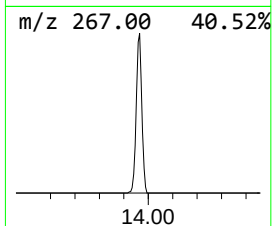
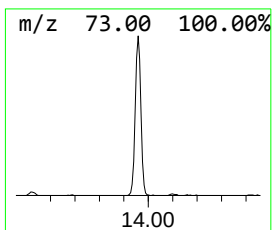
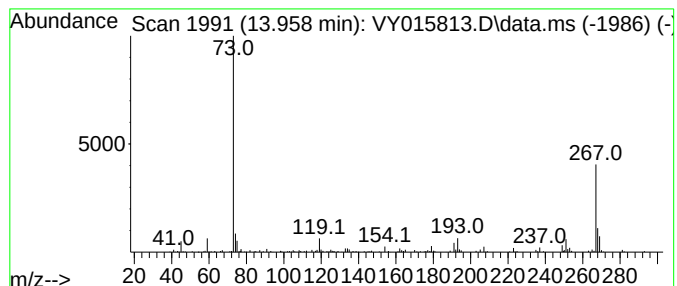
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091923S.M
Quant Title : SW846 8260

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

Peak Number 4 11H-Dibenzo[b,e][1,4]diazep... Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.959	6.90 ug/l	104069	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	91
2			Benzeneethanamine, N-[(pentaflu...	475	C21H26F5NO2Si2	055429-85-1	64
3			2-Amino-m-cresol, N,O-bis(trimet...	267	C13H25NOSi2	1000449-77-1	59
4			5-(3-Pyridinyl)-1,3,4-thiadiazol...	267	C10H13N3S2Si	1000471-43-6	50
5			4-(2-Fluorophenyl)-2,3-dihydro-1...	267	C12H14FNOSSi	1000504-37-6	50



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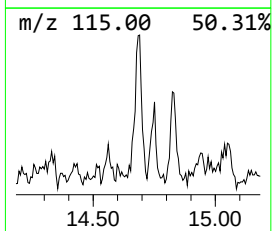
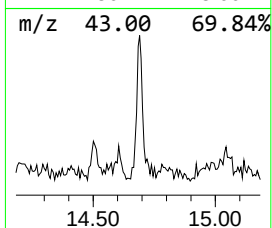
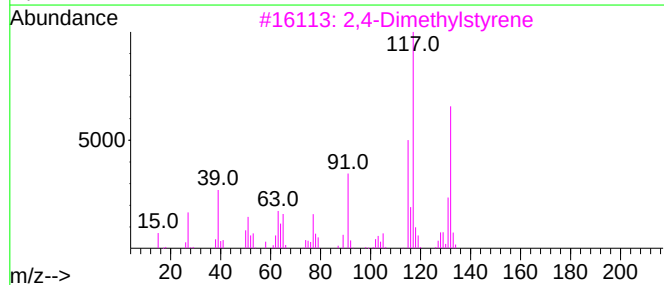
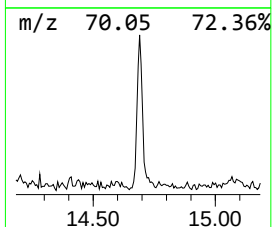
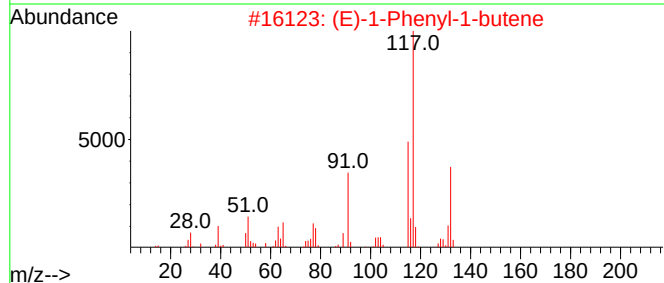
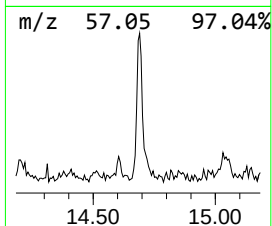
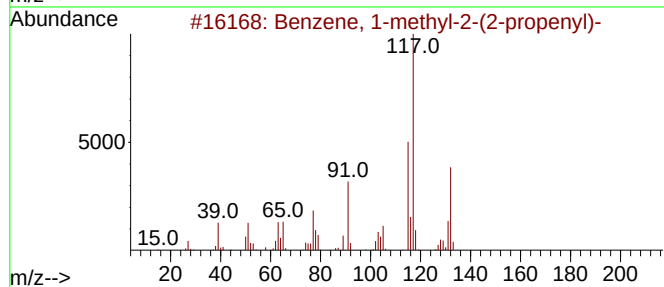
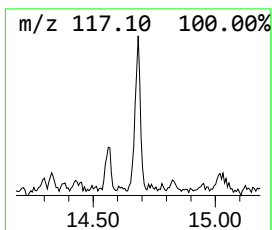
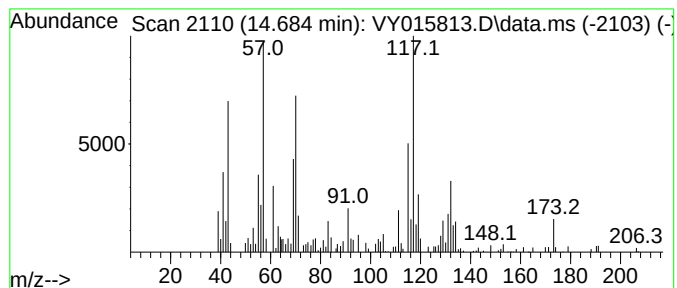
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Quant Title : SW846 8260

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

Peak Number 5 Benzene, 1-methyl-2-(2-prop... Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.684	5.12 ug/l	77328	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-2-(2-propenyl)-	132	C10H12	001587-04-8	86
2			(E)-1-Phenyl-1-butene	132	C10H12	001005-64-7	50
3			2,4-Dimethylstyrene	132	C10H12	002234-20-0	50
4			Benzene, (2-methyl-1-propenyl)-	132	C10H12	000768-49-0	50
5			Cyclopropane, 1-methyl-1-phenyl-	132	C10H12	002214-14-4	45



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Instrument :
MSVOA_Y
ClientSampleId :
S-4(0-5)

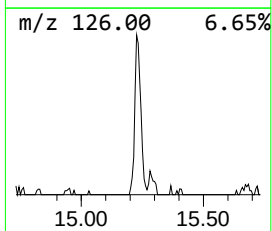
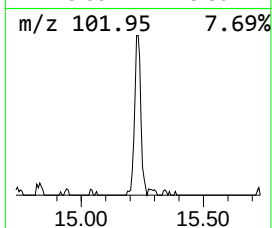
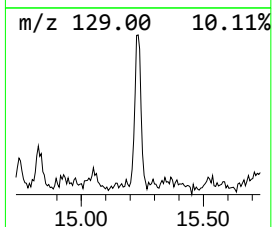
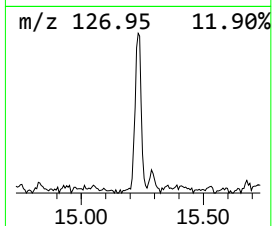
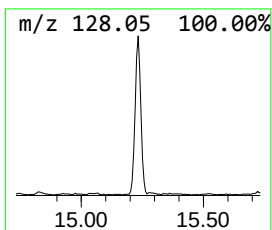
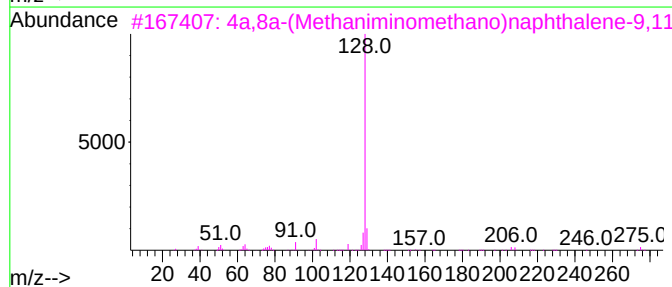
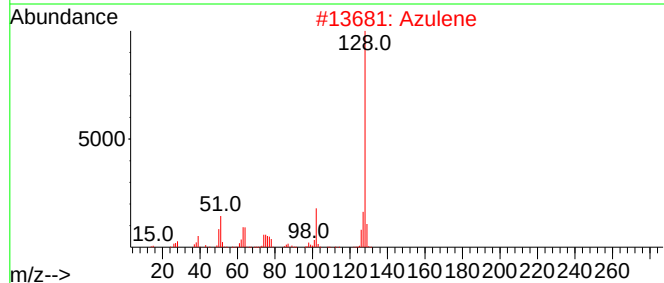
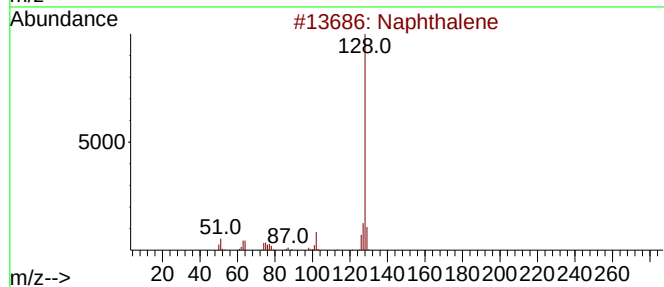
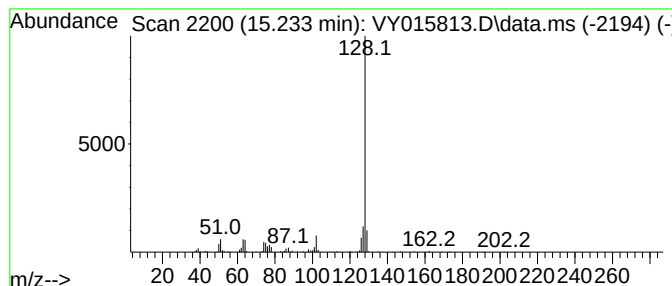
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091923S.M
Quant Title : SW846 8260

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

Peak Number 6 Azulene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.233	6.32 ug/l	95369	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	91
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	64
4			1,3-Dicyanobenzene	128	C8H4N2	000626-17-5	59
5			[4.2.2]Propella-2,4,7,9-tetraene	128	C10H8	088090-34-0	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY100323\
Data File : VY015813.D
Acq On : 03 Oct 2023 18:06
Operator : SY/MD
Sample : 04704-01
Misc : 6.80g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
S-4(0-5)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y091923S.M
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
2-Ethyl-oxetane	5.740	6.4	ug/l	61405	1	7.783	482884	50.0
1-Hexanol, 2-et...	13.526	50.8	ug/l	766310	4	13.422	754533	50.0
11H-Dibenzo[b,e...	13.959	6.9	ug/l	104069	4	13.422	754533	50.0
Benzene, 1-meth...	14.684	5.1	ug/l	77328	4	13.422	754533	50.0
Azulene	15.233	6.3	ug/l	95369	4	13.422	754533	50.0