

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042822\
 Data File : VY008547.D
 Acq On : 28 Apr 2022 14:59
 Operator : KP/MD
 Sample : N2588-03
 Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 MH-2

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\82Y042122S.M
 Title : SW846 8260

Signal : TIC: VY008547.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	4.716	465	475	485	rVB4	2827	8245	2.91%	0.381%
2	6.984	837	847	861	rBV2	5338	21984	7.76%	1.016%
3	7.716	957	967	973	rBV2	41815	100534	35.50%	4.644%
4	7.789	973	979	991	rVB	63769	146236	51.64%	6.755%
5	8.142	1029	1037	1050	rVB2	37096	85376	30.15%	3.944%
6	8.691	1119	1127	1135	rBV	101355	199322	70.39%	9.207%
7	10.179	1364	1371	1382	rBV	167792	283179	100.00%	13.081%
8	10.581	1429	1437	1443	rBV	3504	6701	2.37%	0.310%
9	10.947	1492	1497	1507	rBV	15293	29374	10.37%	1.357%
10	11.319	1551	1558	1566	rVB2	2710	5049	1.78%	0.233%
11	11.489	1580	1586	1597	rVB	164986	265244	93.67%	12.253%
12	12.008	1663	1671	1675	rBV5	1212	3108	1.10%	0.144%
13	12.123	1686	1690	1694	rBV5	1771	3691	1.30%	0.170%
14	12.483	1741	1749	1757	rVB	136950	219265	77.43%	10.129%
15	12.569	1757	1763	1767	rBV6	1374	3706	1.31%	0.171%
16	12.648	1770	1776	1783	rVB7	3577	8624	3.05%	0.398%
17	12.727	1783	1789	1796	rBV7	2319	6770	2.39%	0.313%
18	12.806	1796	1802	1803	rBV5	3804	6796	2.40%	0.314%
19	13.062	1842	1844	1849	rVB5	2119	3242	1.14%	0.150%
20	13.172	1858	1862	1866	rBV7	3141	5934	2.10%	0.274%
21	13.227	1866	1871	1873	rBV6	1956	2921	1.03%	0.135%
22	13.294	1878	1882	1884	rBV4	2596	3427	1.21%	0.158%
23	13.428	1898	1904	1911	rBV	165431	256030	90.41%	11.827%
24	13.568	1922	1927	1930	rBV7	2737	4054	1.43%	0.187%
25	13.751	1951	1957	1962	rBV5	12000	22475	7.94%	1.038%
26	13.806	1962	1966	1969	rVV6	2808	4458	1.57%	0.206%
27	13.855	1969	1974	1979	rVB8	4017	8822	3.12%	0.408%
28	13.940	1982	1988	1989	rBV5	6036	10774	3.80%	0.498%
29	13.971	1990	1993	2002	rVB6	10633	21671	7.65%	1.001%
30	14.080	2006	2011	2015	rBV6	5019	8180	2.89%	0.378%
31	14.147	2018	2022	2026	rVB6	6167	10451	3.69%	0.483%
32	14.202	2027	2031	2035	rVB5	4479	5798	2.05%	0.268%
33	14.257	2035	2040	2046	rBV6	24543	52210	18.44%	2.412%
34	14.379	2056	2060	2062	rBV5	3406	5442	1.92%	0.251%
35	14.422	2063	2067	2072	rBV4	14544	25151	8.88%	1.162%
36	14.550	2085	2088	2090	rBV3	4933	6065	2.14%	0.280%

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

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37	14.623	2096	2100	2103	rBV5	6806	10762	3.80%	0.497%
38	14.684	2106	2110	2114	rVV6	14796	26811	9.47%	1.238%
39	14.733	2114	2118	2125	rVB6	20062	36544	12.90%	1.688%
40	14.849	2134	2137	2139	rBV4	6893	7599	2.68%	0.351%
41	14.946	2149	2153	2157	rVB5	13232	19787	6.99%	0.914%
42	15.007	2157	2163	2166	rBV8	7084	14610	5.16%	0.675%
43	15.056	2167	2171	2175	rVV7	6196	11773	4.16%	0.544%
44	15.214	2192	2197	2202	rBV2	26424	44355	15.66%	2.049%
45	15.288	2203	2209	2213	rBV7	9537	20555	7.26%	0.950%
46	15.446	2232	2235	2241	rVB7	6185	11424	4.03%	0.528%
47	15.605	2257	2261	2267	rVB8	15452	27010	9.54%	1.248%
48	16.031	2327	2331	2336	rVB6	11212	17518	6.19%	0.809%
49	16.159	2348	2352	2358	rVB6	12224	22209	7.84%	1.026%
50	16.226	2360	2363	2371	rVB10	5992	10835	3.83%	0.501%
51	16.482	2400	2405	2411	rBV8	9810	22710	8.02%	1.049%

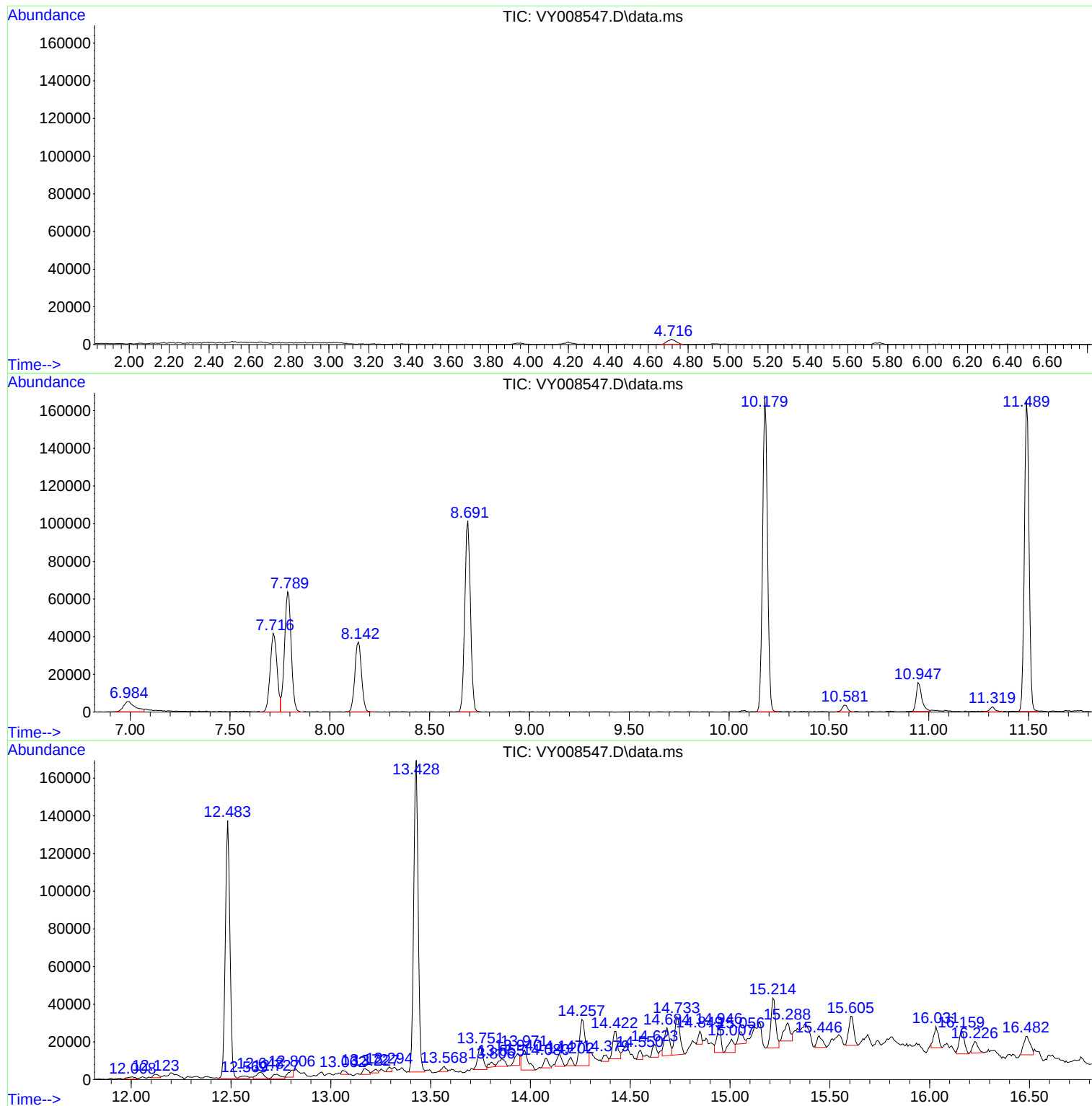
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.M
Quant Title : SW846 8260

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



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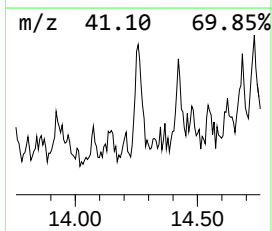
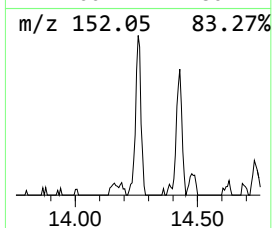
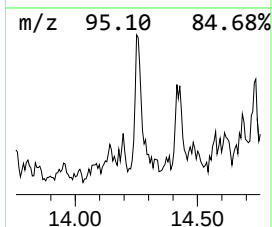
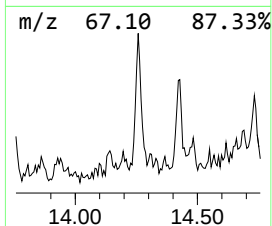
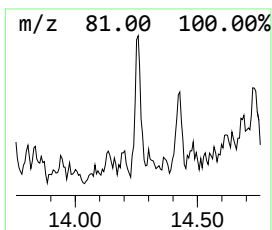
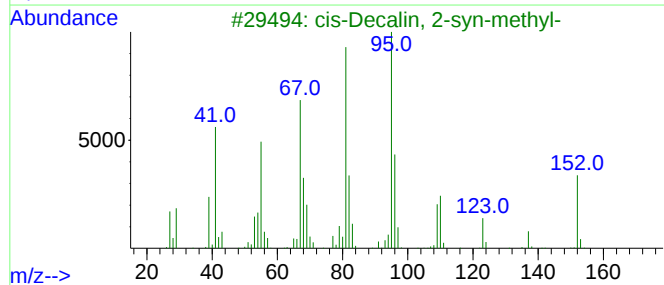
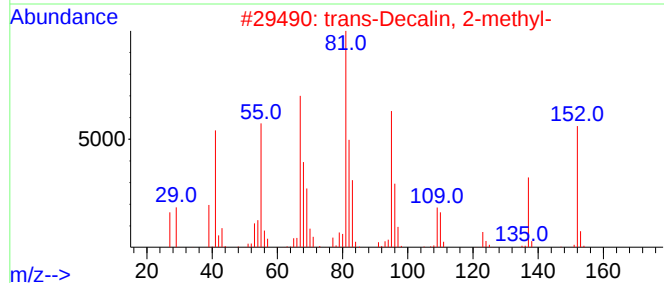
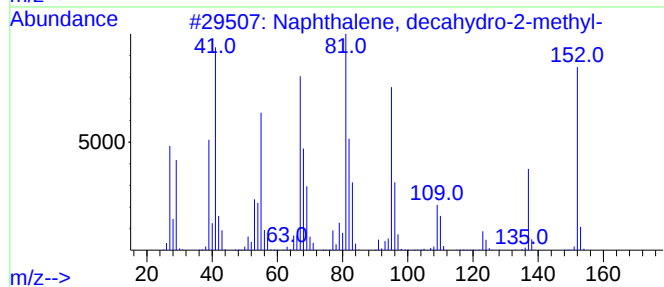
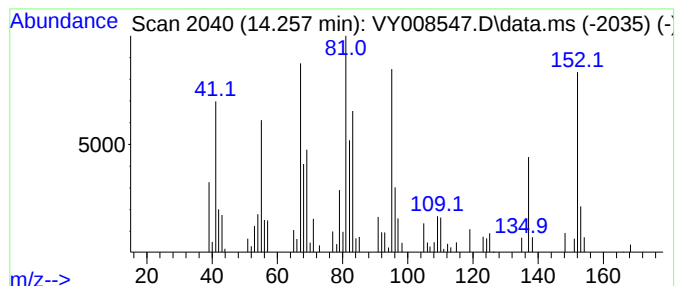
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.M
Quant Title : SW846 8260

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

Peak Number 3 Naphthalene, decahydro-2-me... Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.257	10.20 ug/l	52210	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, decahydro-2-methyl-	152	C11H20	002958-76-1	93
2			trans-Decalin, 2-methyl-	152	C11H20	1000152-47-3	91
3			cis-Decalin, 2-syn-methyl-	152	C11H20	1000155-85-6	74
4			Bicyclo[3.3.2]decan-9-one	152	C10H16O	028054-91-3	72
5			Bicyclo[2.2.1]heptan-2-one, 1,7,...	152	C10H16O	000464-48-2	68



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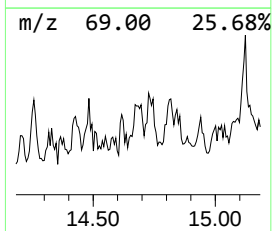
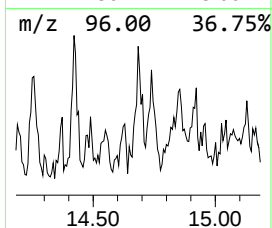
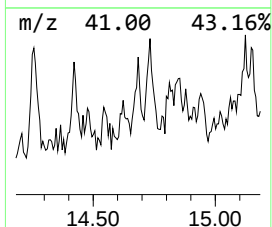
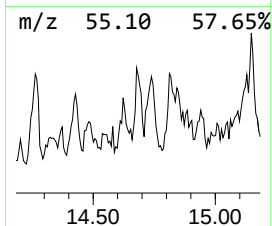
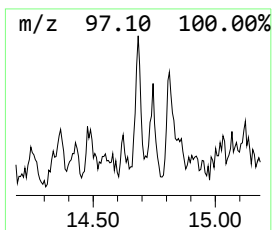
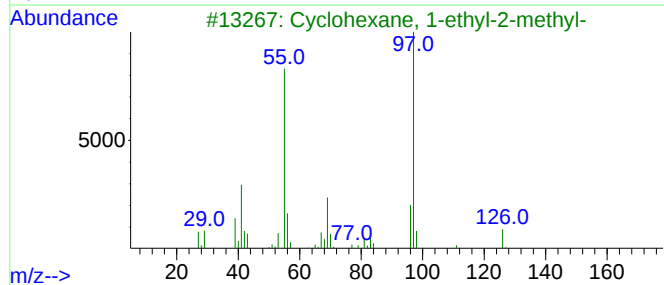
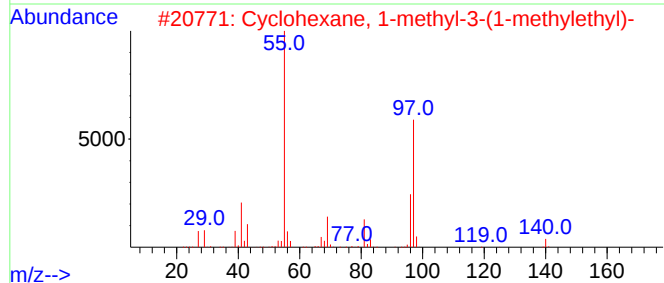
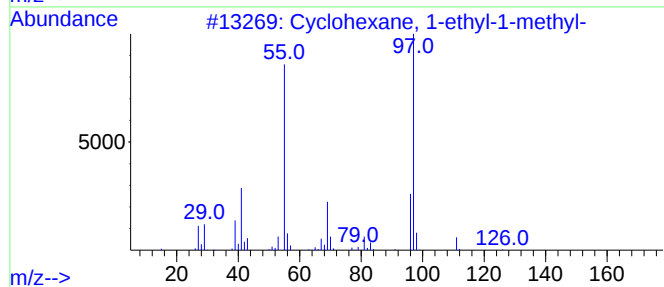
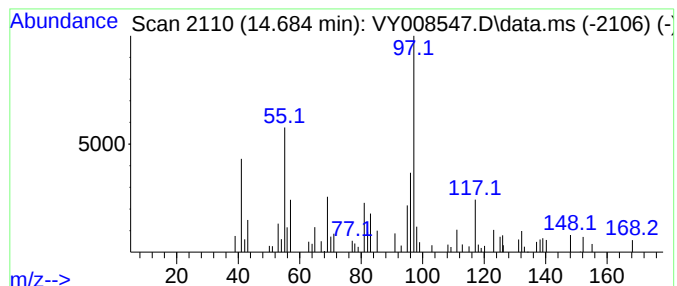
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 unknown14.684 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.684	5.24 ug/l	26811	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexane, 1-ethyl-1-methyl-	126	C9H18	004926-90-3	47
2			Cyclohexane, 1-methyl-3-(1-methy...	140	C10H20	016580-24-8	46
3			Cyclohexane, 1-ethyl-2-methyl-	126	C9H18	003728-54-9	46
4			1H-Pyrazole, 5-ethyl-4,5-dihydro...	126	C7H14N2	021981-22-6	46
5			m-Menthane, (1S,3S)-(+)-	140	C10H20	013837-67-7	43



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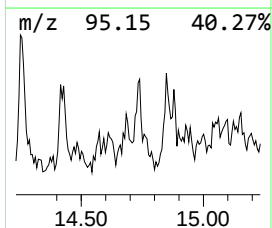
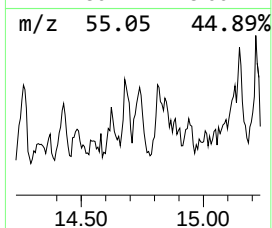
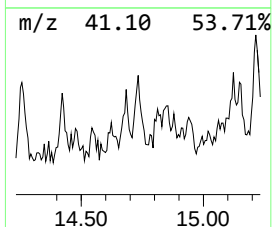
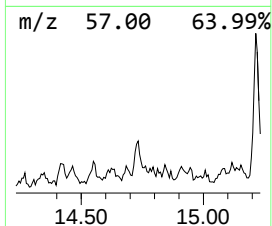
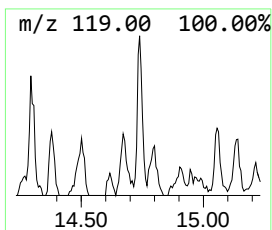
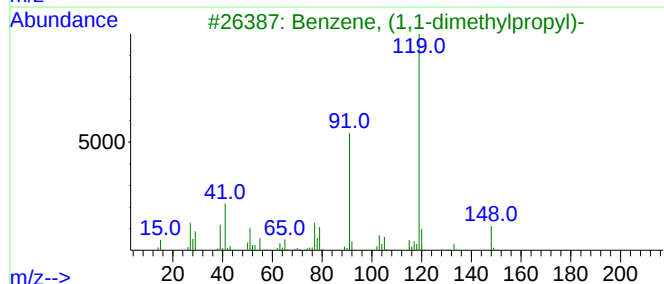
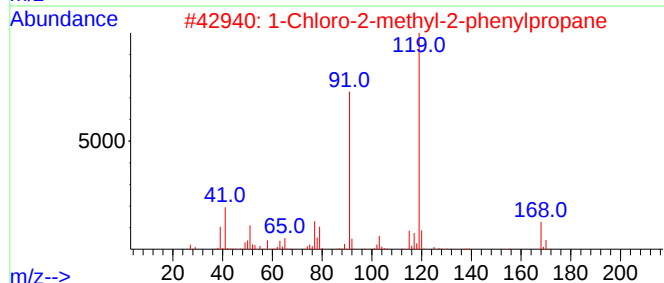
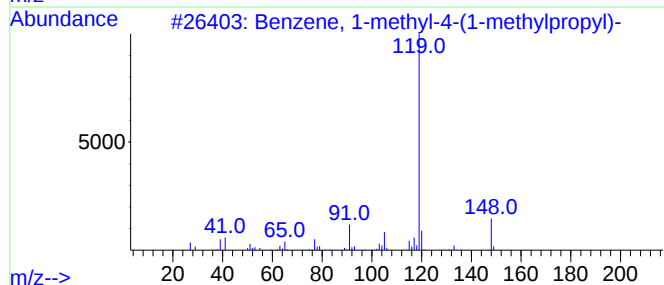
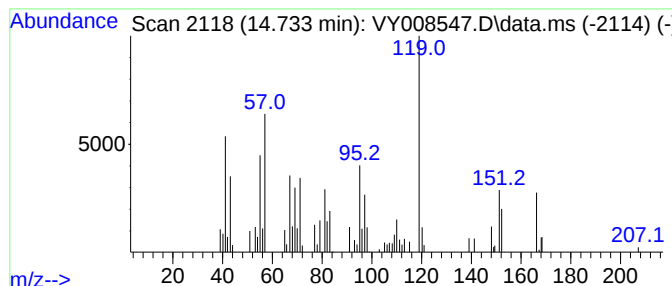
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.M
Quant Title : SW846 8260

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

Peak Number 5 unknown14.733 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	7.14 ug/l	36544	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 1-methyl-4-(1-methylpro...	148	C11H16	001595-16-0	27
2			1-Chloro-2-methyl-2-phenylpropane	168	C10H13Cl	000515-40-2	27
3			Benzene, (1,1-dimethylpropyl)-	148	C11H16	002049-95-8	27
4			o-Toluic acid, 1-(cyclopentyl)et...	232	C15H20O2	1000293-34-7	25
5			p-Toluic acid, 5-tridecyl ester	318	C21H34O2	1000299-80-5	16



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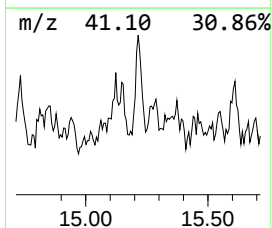
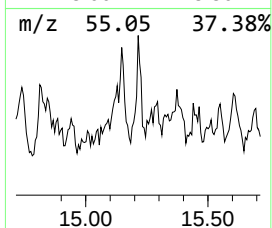
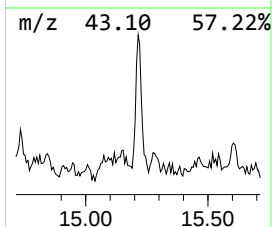
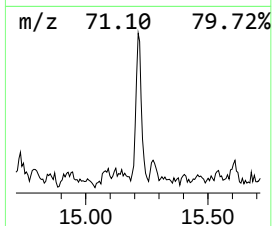
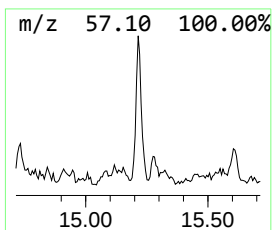
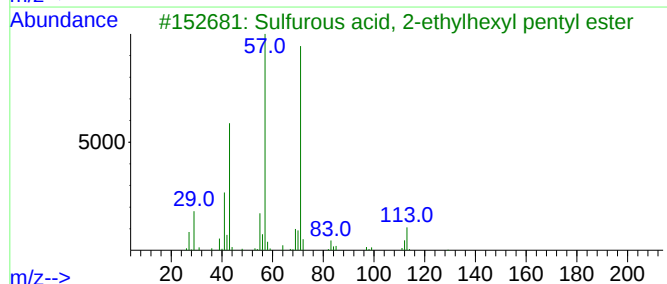
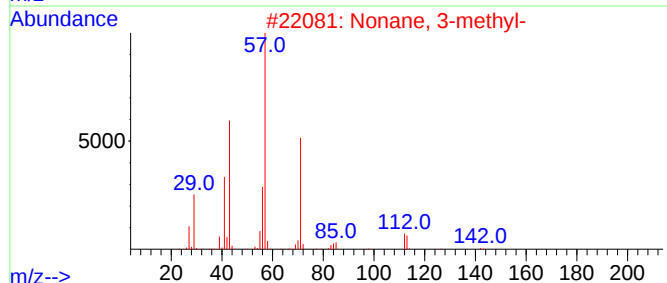
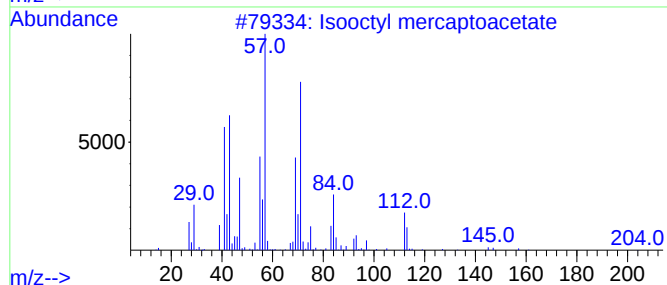
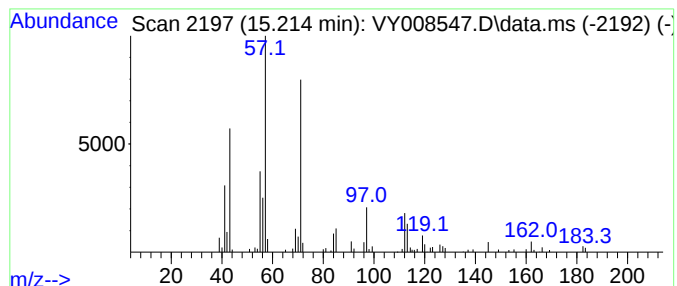
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.M
Quant Title : SW846 8260

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

Peak Number 6 Isooctyl mercaptoacetate Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.214	8.66 ug/l	44355	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Isooctyl mercaptoacetate	204	C10H20O2S	025103-09-7	64
2			Nonane, 3-methyl-	142	C10H22	005911-04-6	59
3			Sulfurous acid, 2-ethylhexyl pen...	264	C13H28O3S	1000309-18-9	50
4			Heptane, 2,4-dimethyl-	128	C9H20	002213-23-2	50
5			6-Methyl-2-heptanol, 2-methylpro...	200	C12H24O2	1000447-36-7	50



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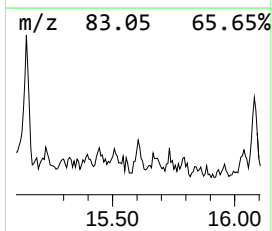
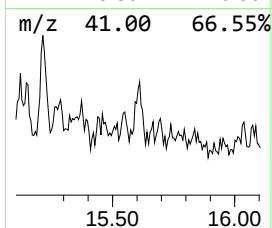
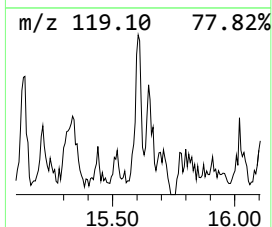
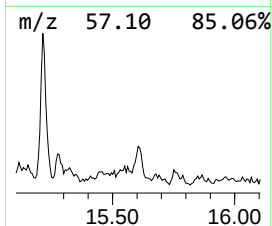
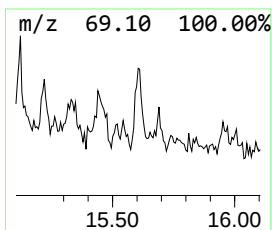
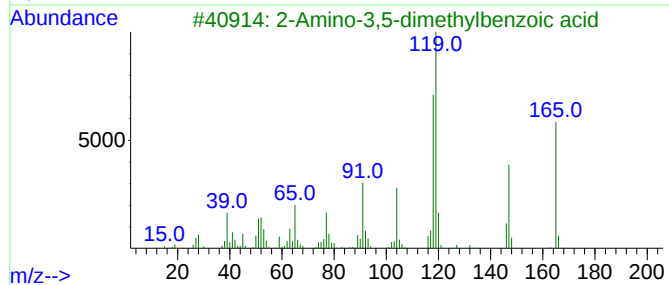
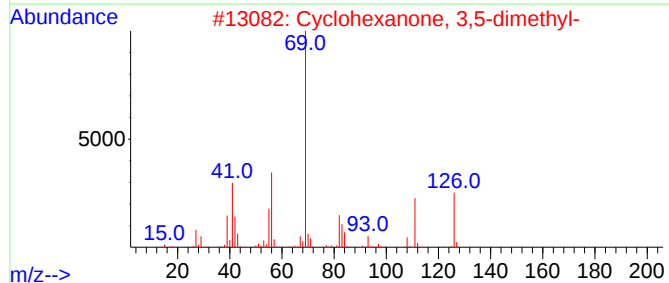
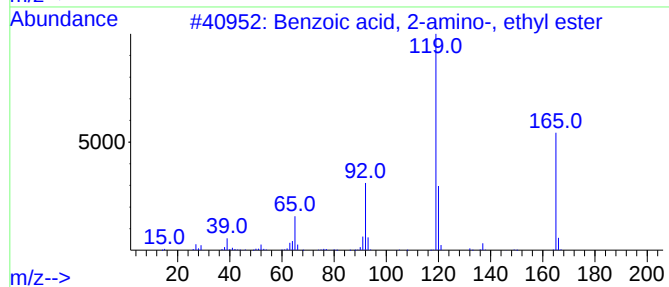
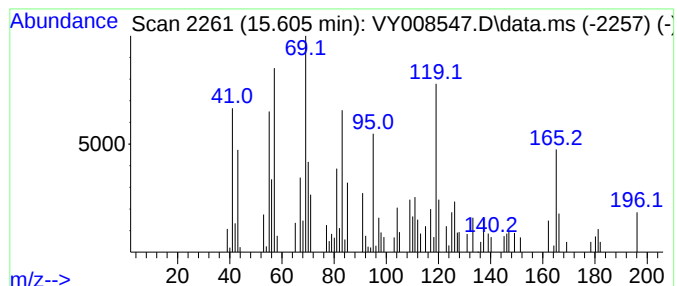
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.M
Quant Title : SW846 8260

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

Peak Number 7 unknown15.605 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.605	5.27 ug/l	27010	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzoic acid, 2-amino-, ethyl ester	165	C9H11NO2	000087-25-2	27
2			Cyclohexanone, 3,5-dimethyl-	126	C8H14O	002320-30-1	25
3			2-Amino-3,5-dimethylbenzoic acid	165	C9H11NO2	014438-32-5	25
4			3,4-Dimethyl cyclohexanone	126	C8H14O	005465-09-8	18
5			3-Heptene, 2,6-dimethyl-	126	C9H18	002738-18-3	18



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY042822\
Data File : VY008547.D
Acq On : 28 Apr 2022 14:59
Operator : KP/MD
Sample : N2588-03
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
MH-2

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y042122S.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
Naphthalene, de...	14.257	10.2	ug/l	52210	4	13.428	256030	50.0
unknown14.684	14.684	5.2	ug/l	26811	4	13.428	256030	50.0
unknown14.733	14.733	7.1	ug/l	36544	4	13.428	256030	50.0
Isooctyl mercap...	15.214	8.7	ug/l	44355	4	13.428	256030	50.0
unknown15.605	15.605	5.3	ug/l	27010	4	13.428	256030	50.0