

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121422\
 Data File : VY011858.D
 Acq On : 14 Dec 2022 20:05
 Operator : KP/MD
 Sample : N6038-11
 Misc : 3.93g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 28 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 RB-34-(1.5-2)

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\82Y120922S.M
 Title : SW846 8260

Signal : TIC: VY011858.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	3.948	339	349	364	rBV	43284	120596	11.22%	1.547%
2	4.716	463	475	491	rBV2	43524	132559	12.33%	1.700%
3	6.984	837	847	859	rBV2	9190	29310	2.73%	0.376%
4	7.716	958	967	972	rBV	45536	106984	9.95%	1.372%
5	7.789	972	979	994	rVB	340448	770804	71.71%	9.886%
6	8.142	1027	1037	1048	rBV	113873	245330	22.82%	3.146%
7	8.691	1118	1127	1140	rBV	522996	1009653	93.93%	12.949%
8	10.179	1363	1371	1379	rBV	389555	674166	62.72%	8.646%
9	10.721	1452	1460	1466	rVB2	8729	15107	1.41%	0.194%
10	11.489	1579	1586	1598	rBV	655906	1074930	100.00%	13.786%
11	11.587	1598	1602	1611	rVB8	4253	10919	1.02%	0.140%
12	11.703	1611	1621	1626	rBV4	6677	16075	1.50%	0.206%
13	12.026	1664	1674	1682	rBV7	6451	18107	1.68%	0.232%
14	12.337	1718	1725	1734	rBV	75944	119692	11.13%	1.535%
15	12.483	1741	1749	1758	rBV2	335807	534444	49.72%	6.854%
16	12.587	1758	1766	1771	rVV2	9368	17445	1.62%	0.224%
17	12.733	1784	1790	1794	rBV2	8458	14466	1.35%	0.186%
18	12.812	1798	1803	1809	rVV3	22758	37819	3.52%	0.485%
19	12.891	1809	1816	1824	rVV	114576	184883	17.20%	2.371%
20	12.971	1824	1829	1837	rVB	7826	13862	1.29%	0.178%
21	13.123	1844	1854	1868	rVB3	22183	51264	4.77%	0.657%
22	13.343	1881	1890	1892	rBV5	13090	26505	2.47%	0.340%
23	13.428	1898	1904	1913	rVB	539314	856761	79.70%	10.988%
24	13.525	1913	1920	1927	rVB	28461	42050	3.91%	0.539%
25	13.629	1933	1937	1940	rBV3	12138	18536	1.72%	0.238%
26	13.666	1940	1943	1952	rVB2	19252	32452	3.02%	0.416%
27	13.751	1952	1957	1961	rBV5	11927	21180	1.97%	0.272%
28	13.885	1975	1979	1981	rVV3	9652	13658	1.27%	0.175%
29	13.916	1981	1984	1988	rVV	11037	15647	1.46%	0.201%
30	13.971	1988	1993	1998	rVB2	25960	42036	3.91%	0.539%
31	14.080	2006	2011	2017	rBV2	19306	31720	2.95%	0.407%
32	14.214	2027	2033	2037	rBV3	11164	18669	1.74%	0.239%
33	14.300	2042	2047	2049	rVV3	14057	23884	2.22%	0.306%
34	14.336	2049	2053	2057	rVB	20477	29651	2.76%	0.380%
35	14.379	2057	2060	2063	rBV3	8465	11338	1.05%	0.145%
36	14.513	2075	2082	2086	rVV6	8255	18689	1.74%	0.240%

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37	14.568	2086	2091	2095	rVV3	13746	24700	2.30%	0.317%
38	14.611	2095	2098	2103	rVB	11095	15931	1.48%	0.204%
39	14.684	2103	2110	2116	rBV3	37621	84465	7.86%	1.083%
40	14.836	2130	2135	2139	rBV2	8475	13510	1.26%	0.173%
41	14.946	2148	2153	2162	rBV6	18787	45556	4.24%	0.584%
42	15.056	2165	2171	2181	rVB2	17292	39991	3.72%	0.513%
43	15.239	2190	2201	2207	rBV	182003	312723	29.09%	4.011%
44	15.342	2213	2218	2223	rBV5	10634	20442	1.90%	0.262%
45	15.525	2241	2248	2254	rBV4	10778	21800	2.03%	0.280%
46	15.690	2267	2275	2277	rBV5	8235	17308	1.61%	0.222%
47	15.726	2278	2281	2291	rVB5	12557	23477	2.18%	0.301%
48	16.037	2325	2332	2338	rBV3	7979	16850	1.57%	0.216%
49	16.232	2357	2364	2367	rBV4	9821	21155	1.97%	0.271%
50	16.293	2367	2374	2390	rVB	188801	382381	35.57%	4.904%
51	16.488	2398	2406	2419	rBV	171382	355609	33.08%	4.561%

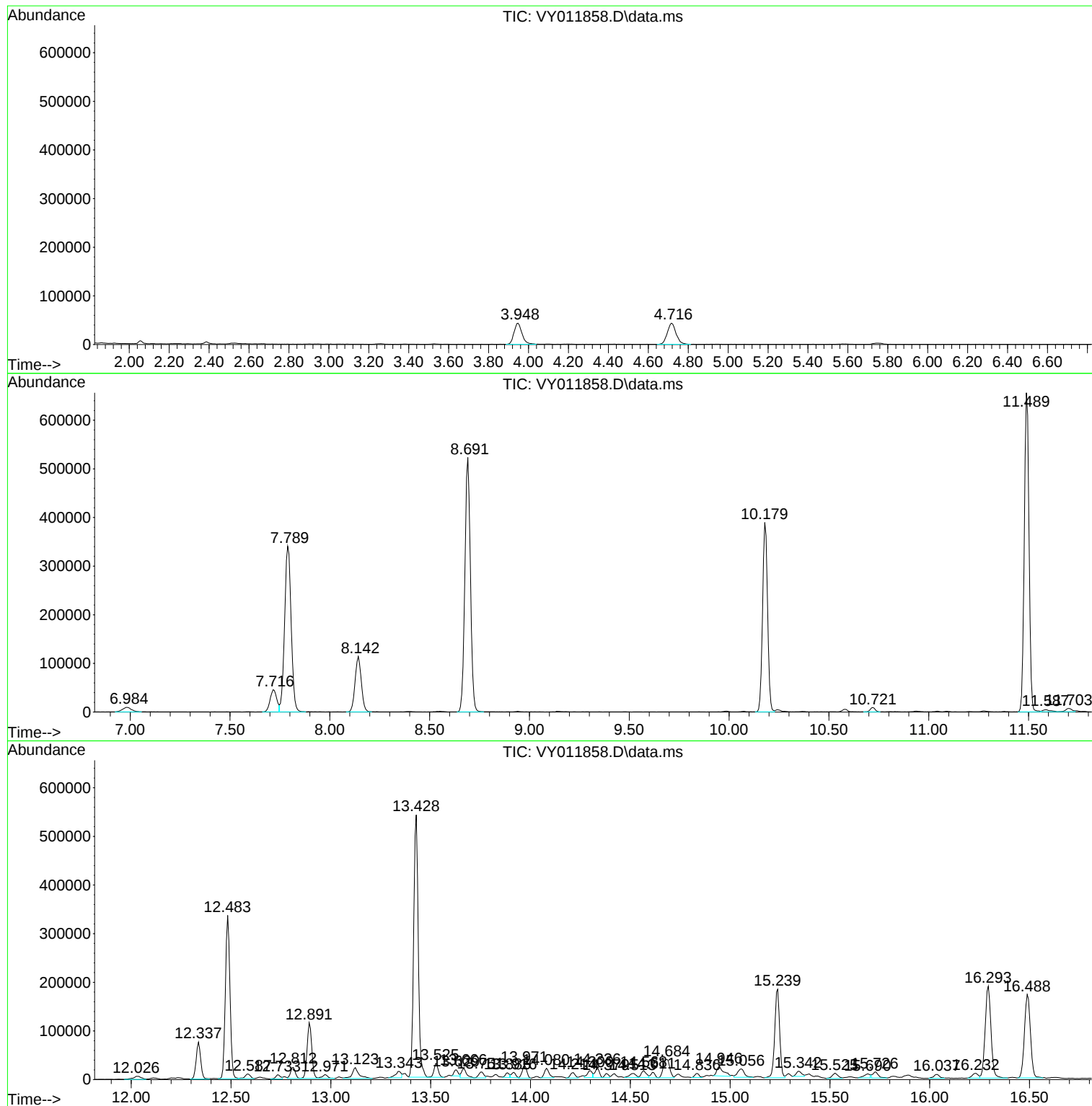
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TIC Library : C:\Database\NIST20.L
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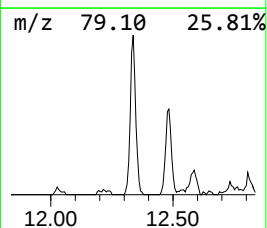
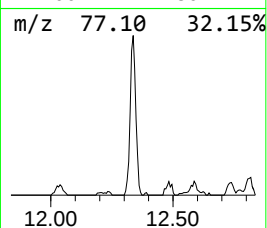
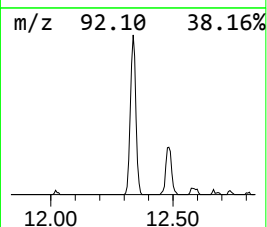
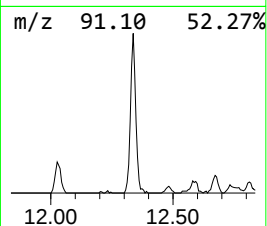
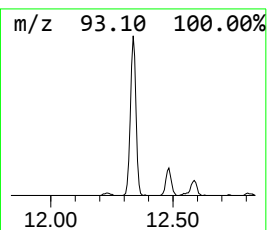
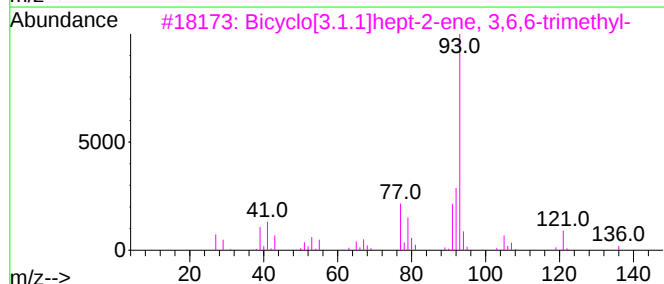
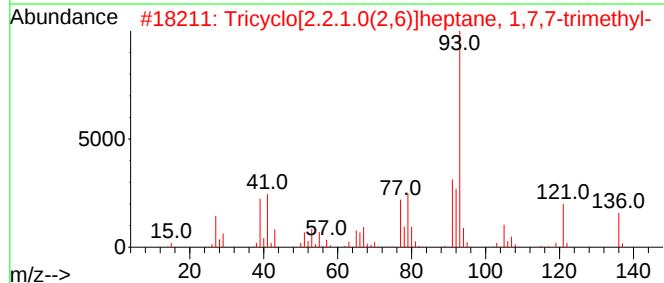
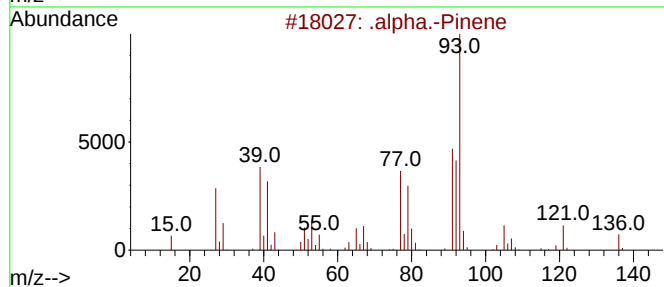
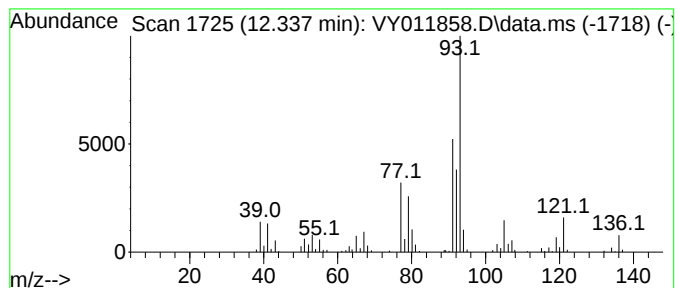
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y120922S.M
Quant Title : SW846 8260

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

Peak Number 1 .alpha.-Pinene Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.337	5.57 ug/l	119692	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			.alpha.-Pinene	136	C10H16	000080-56-8	94
2			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000508-32-7	91
3			Bicyclo[3.1.1]hept-2-ene, 3,6,6-...	136	C10H16	004889-83-2	91
4			(1R)-2,6,6-Trimethylbicyclo[3.1....	136	C10H16	007785-70-8	91
5			.gamma.-Terpinene	136	C10H16	000099-85-4	90



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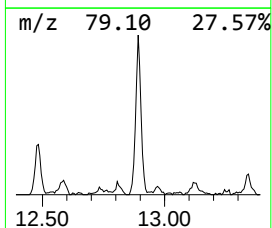
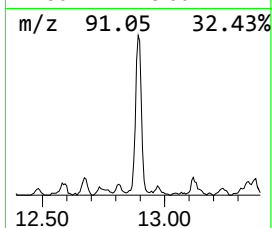
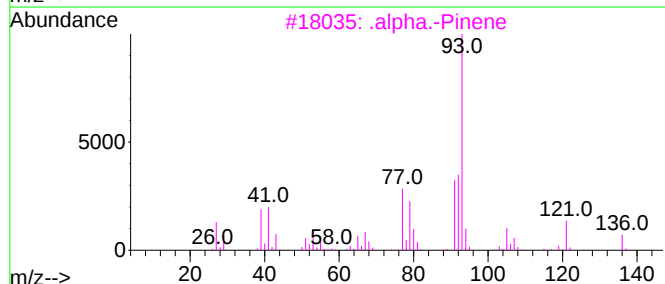
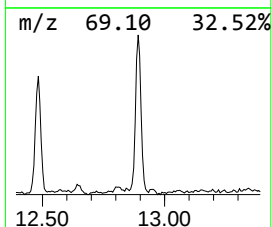
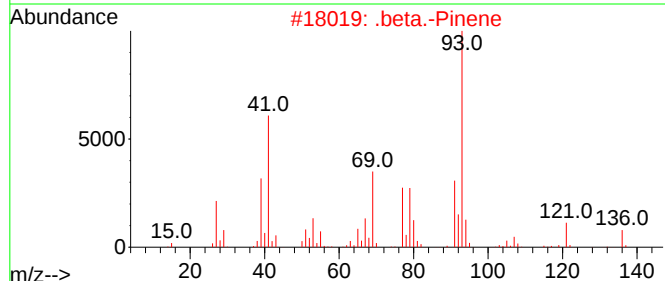
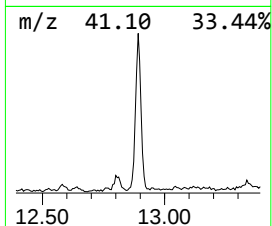
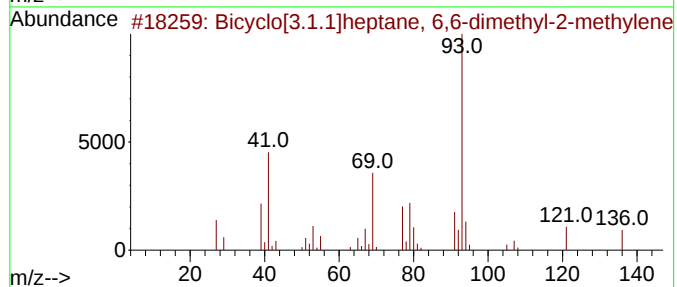
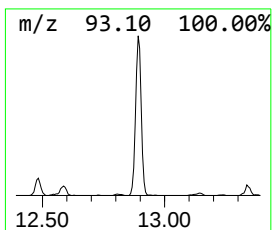
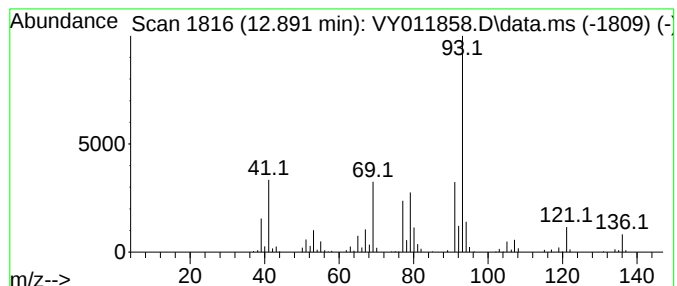
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y120922S.M
Quant Title : SW846 8260

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

Peak Number 2 Bicyclo[3.1.1]heptane, 6,6-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.892	10.79 ug/l	184883	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[3.1.1]heptane, 6,6-dimet...	136	C10H16	018172-67-3	97
2			.beta.-Pinene	136	C10H16	000127-91-3	96
3			.alpha.-Pinene	136	C10H16	000080-56-8	91
4			Bicyclo[3.1.0]hexane, 4-methylen...	136	C10H16	003387-41-5	87
5			Tricyclo[2.2.1.0(2,6)]heptane, 1...	136	C10H16	000488-97-1	83



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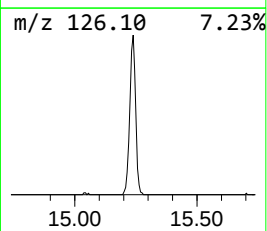
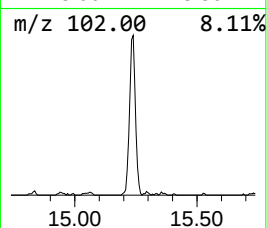
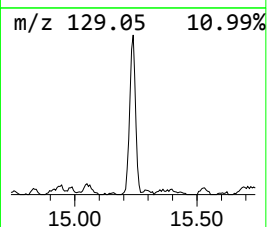
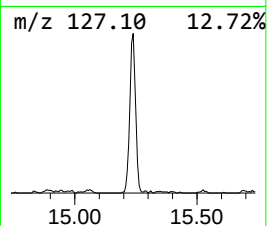
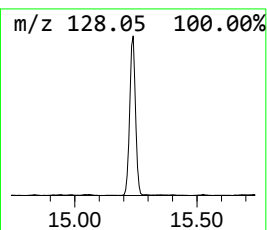
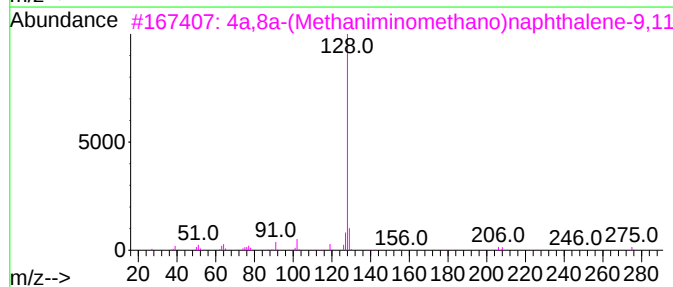
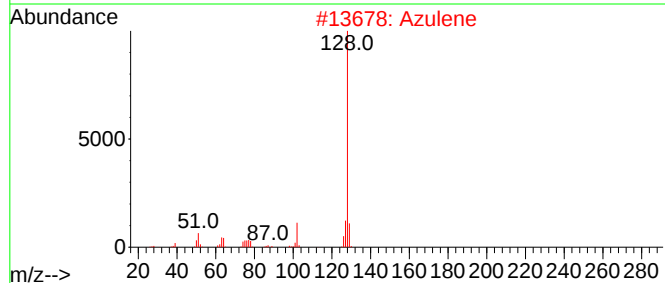
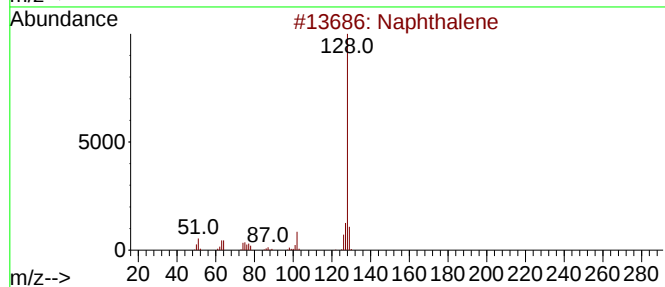
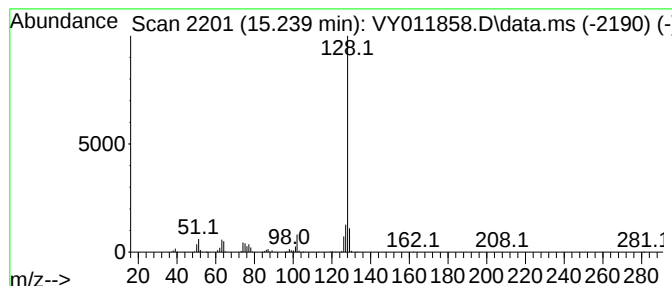
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y120922S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 3 Azulene Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.239	18.25 ug/l	312723	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene	128	C10H8	000091-20-3	95
2			Azulene	128	C10H8	000275-51-4	93
3			4a,8a-(Methaniminomethano)naphth...	275	C18H13NO2	069915-10-2	78
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



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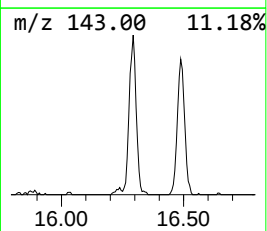
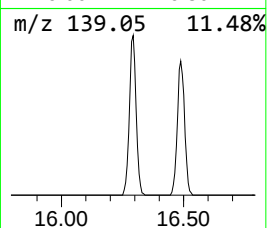
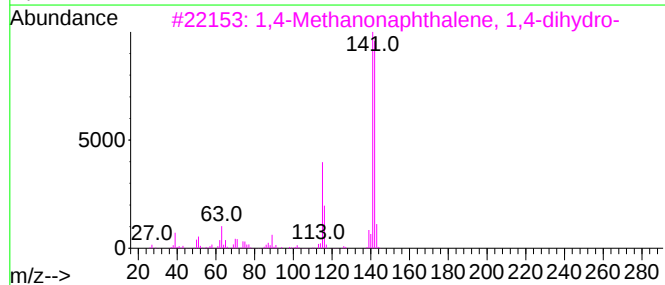
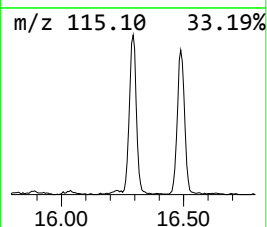
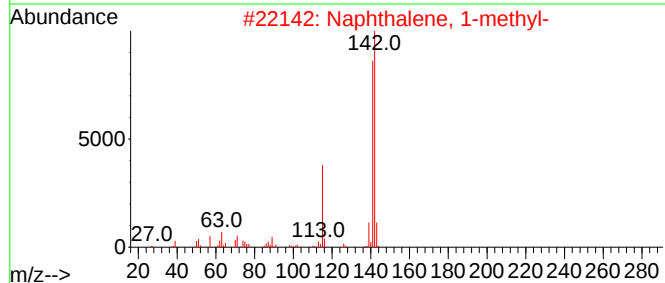
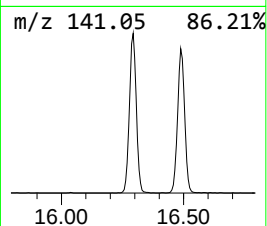
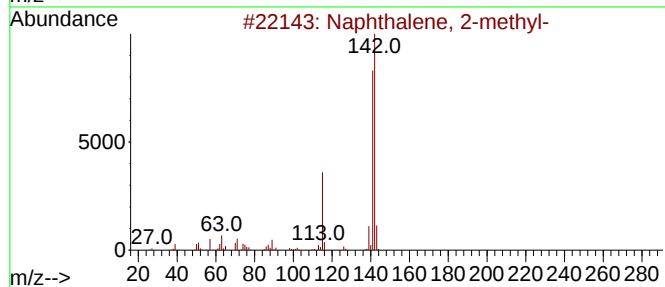
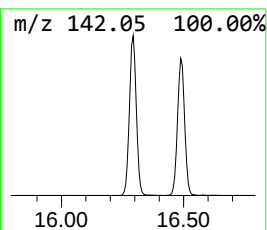
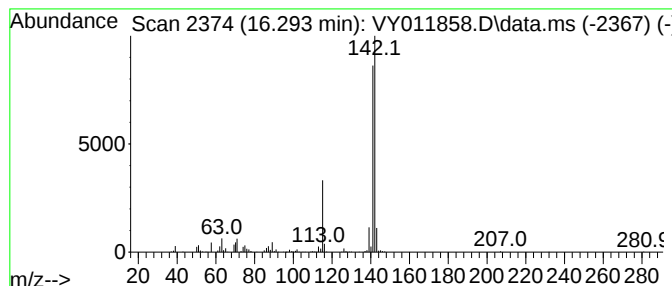
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Quant Title : SW846 8260

TIC Library : C:\Database\NIST20.L
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Peak Number 4 1,4-Methanonaphthalene, 1,4... Concentration Rank 1

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16.293	22.32 ug/l	382381	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
4			Benzocycloheptatriene	142	C11H10	000264-09-5	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	72



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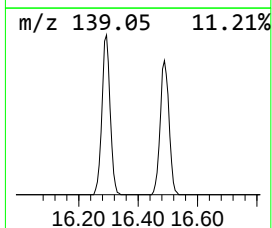
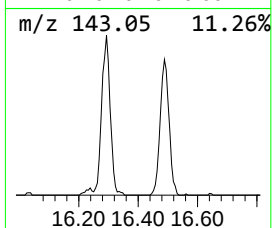
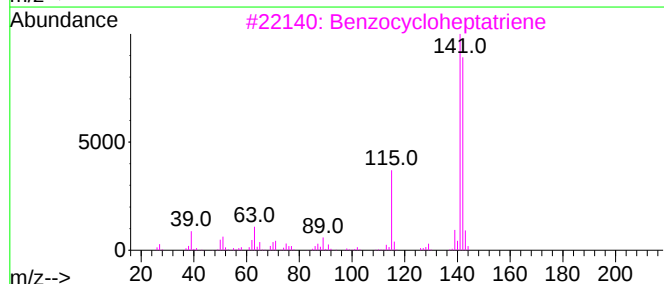
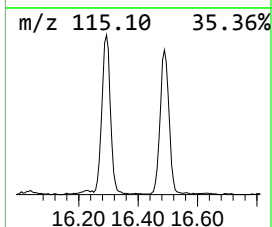
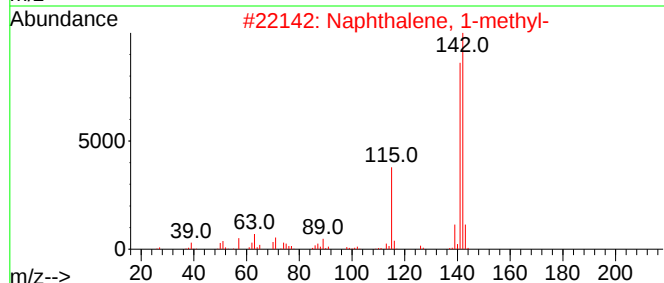
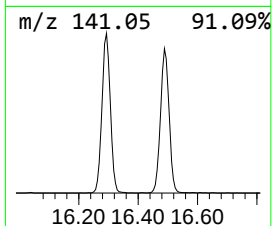
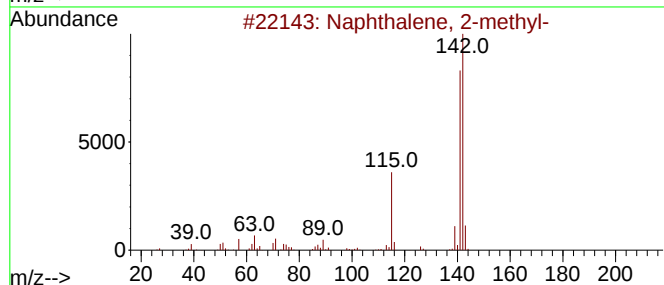
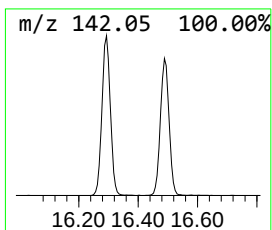
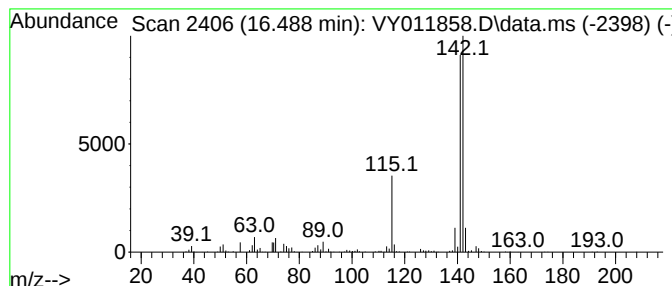
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y120922S.M
Quant Title : SW846 8260

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

Peak Number 5 Benzocycloheptatriene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.488	20.75 ug/l	355609	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2-methyl-	142	C11H10	000091-57-6	96
2			Naphthalene, 1-methyl-	142	C11H10	000090-12-0	96
3			Benzocycloheptatriene	142	C11H10	000264-09-5	91
4			1,4-Methanonaphthalene, 1,4-dihy...	142	C11H10	004453-90-1	91
5			1H-Indene, 1-ethylidene-	142	C11H10	002471-83-2	47



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY121422\
Data File : VY011858.D
Acq On : 14 Dec 2022 20:05
Operator : KP/MD
Sample : N6038-11
Misc : 3.93g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 28 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
RB-34-(1.5-2)

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y120922S.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
.alpha.-Pinene	12.337	5.6	ug/l	119692	3	11.489	1074930	50.0
Bicyclo[3.1.1]h...	12.892	10.8	ug/l	184883	4	13.428	856761	50.0
Azulene	15.239	18.3	ug/l	312723	4	13.428	856761	50.0
1,4-Methanonaph...	16.293	22.3	ug/l	382381	4	13.428	856761	50.0
Benzocyclohepta...	16.488	20.8	ug/l	355609	4	13.428	856761	50.0