

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041123\
 Data File : VY013248.D
 Acq On : 11 Apr 2023 17:23
 Operator : KP/MD
 Sample : 02257-01
 Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 ELI-SOLID-0407

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\82Y041123S.M
 Title : SW846 8260

Signal : TIC: VY013248.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.168	55	57	60	rBV	333	309	2.11%	0.218%
2	2.211	62	64	67	rVV3	471	597	4.08%	0.420%
3	2.838	165	167	169	rBV2	146	154	1.05%	0.108%
4	2.960	185	187	189	rBV2	167	162	1.11%	0.114%
5	3.003	192	194	198	rVB2	295	303	2.07%	0.213%
6	3.107	208	211	214	rVB	177	178	1.22%	0.125%
7	3.168	217	221	224	rBV2	183	274	1.87%	0.193%
8	3.418	260	262	266	rVB2	191	257	1.76%	0.181%
9	3.460	266	269	271	rBV	174	223	1.52%	0.157%
10	3.546	280	283	288	rVB2	125	172	1.17%	0.121%
11	3.948	346	349	353	rBV2	121	167	1.14%	0.118%
12	4.100	371	374	375	rBV2	158	149	1.02%	0.105%
13	4.405	421	424	426	rVB2	166	201	1.37%	0.142%
14	4.625	456	460	461	rBV2	122	147	1.00%	0.104%
15	4.698	468	472	473	rBV	792	868	5.93%	0.611%
16	4.795	485	488	489	rBV	201	205	1.40%	0.144%
17	4.954	511	514	516	rBV2	148	158	1.08%	0.111%
18	5.137	538	544	547	rBV2	92	201	1.37%	0.142%
19	5.423	589	591	594	rVB2	148	153	1.05%	0.108%
20	5.637	624	626	629	rVB	151	157	1.07%	0.111%
21	5.905	668	670	672	rBV2	178	151	1.03%	0.106%
22	6.003	681	686	689	rVB2	223	349	2.38%	0.246%
23	6.301	732	735	737	rVB	214	245	1.67%	0.173%
24	6.332	737	740	745	rBV2	166	315	2.15%	0.222%
25	6.411	750	753	755	rBV	127	157	1.07%	0.111%
26	6.441	755	758	761	rVB2	100	155	1.06%	0.109%
27	6.783	812	814	816	rBV2	166	166	1.13%	0.117%
28	6.954	835	842	843	rBV	522	600	4.10%	0.423%
29	7.124	867	870	871	rBV2	119	148	1.01%	0.104%
30	7.216	882	885	887	rBV2	134	172	1.17%	0.121%
31	7.478	924	928	931	rBV2	235	270	1.84%	0.190%
32	7.716	961	967	973	rBV4	2309	4965	33.92%	3.497%
33	7.789	973	979	987	rVB2	3182	6732	45.99%	4.741%
34	8.014	1014	1016	1018	rBV	209	222	1.52%	0.156%
35	8.094	1026	1029	1030	rVB2	156	155	1.06%	0.109%
36	8.142	1030	1037	1045	rBV	2397	4994	34.11%	3.517%

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37	8.222	1048	1050	1054	rBV	152	222	1.52%	0.156%
38	8.289	1057	1061	1066	rBV	130	201	1.37%	0.142%
39	8.575	1107	1108	1111	rVB	226	167	1.14%	0.118%
40	8.612	1111	1114	1116	rBV	168	231	1.58%	0.163%
41	8.691	1120	1127	1135	rVV	4679	9312	63.61%	6.558%
42	8.776	1139	1141	1145	rVV2	149	184	1.26%	0.130%
43	8.831	1148	1150	1154	rVB2	157	148	1.01%	0.104%
44	9.008	1176	1179	1180	rBV	180	174	1.19%	0.123%
45	9.337	1230	1233	1235	rVB2	205	214	1.46%	0.151%
46	9.673	1285	1288	1292	rVB	123	198	1.35%	0.139%
47	10.179	1363	1371	1379	rBV3	6513	12140	82.93%	8.550%
48	10.270	1384	1386	1389	rBV2	140	170	1.16%	0.120%
49	10.337	1394	1397	1400	rBV2	203	291	1.99%	0.205%
50	10.563	1433	1434	1438	rBV2	160	224	1.53%	0.158%
51	10.837	1477	1479	1483	rVB2	147	160	1.09%	0.113%
52	11.489	1581	1586	1592	rBV	6607	9553	65.26%	6.728%
53	11.745	1627	1628	1631	rBV2	176	151	1.03%	0.106%
54	11.922	1656	1657	1658	rBV	311	213	1.46%	0.150%
55	12.038	1662	1676	1677	rBV4	3286	9294	63.49%	6.546%
56	12.270	1712	1714	1717	rVB2	176	177	1.21%	0.125%
57	12.312	1717	1721	1722	rBV	149	174	1.19%	0.123%
58	12.355	1724	1728	1729	rBV4	429	458	3.13%	0.323%
59	12.373	1729	1731	1733	rVV2	386	257	1.76%	0.181%
60	12.483	1744	1749	1759	rVB4	4480	7421	50.69%	5.226%
61	12.648	1773	1776	1780	rBB2	152	195	1.33%	0.137%
62	12.696	1782	1784	1786	rBV2	174	185	1.26%	0.130%
63	12.806	1800	1802	1806	rVB3	199	243	1.66%	0.171%
64	12.885	1812	1815	1816	rBV	370	391	2.67%	0.275%
65	12.953	1816	1826	1837	rVV8	2360	9485	64.79%	6.680%
66	13.050	1838	1842	1843	rVV3	460	678	4.63%	0.478%
67	13.074	1843	1846	1847	rVV3	712	929	6.35%	0.654%
68	13.093	1847	1849	1857	rVB4	862	1691	11.55%	1.191%
69	13.428	1895	1904	1917	rBV4	5747	14639	100.00%	10.310%
70	13.574	1919	1928	1938	rBV8	1593	5015	34.26%	3.532%
71	13.648	1938	1940	1942	rBV2	311	308	2.10%	0.217%
72	13.818	1961	1968	1969	rBV2	1329	1949	13.31%	1.373%
73	13.891	1978	1980	1984	rVB	280	338	2.31%	0.238%
74	13.940	1986	1988	1991	rBV2	201	207	1.41%	0.146%
75	13.965	1991	1992	1996	rBV2	187	196	1.34%	0.138%
76	14.007	1998	1999	2002	rBV	194	208	1.42%	0.146%

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77	14.178	2025	2027	2028	rBV2	476	381	2.60%	0.268%
78	14.208	2028	2032	2037	rVV5	922	1757	12.00%	1.237%
79	14.269	2039	2042	2045	rVB3	742	1191	8.14%	0.839%
80	14.483	2076	2077	2082	rVV2	222	205	1.40%	0.144%
81	14.550	2086	2088	2091	rVV3	129	147	1.00%	0.104%
82	14.647	2102	2104	2106	rBV2	290	279	1.91%	0.196%
83	14.733	2108	2118	2129	rVB4	4032	12453	85.07%	8.770%
84	14.867	2130	2140	2151	rBV3	2996	9477	64.74%	6.674%
85	15.019	2163	2165	2167	rBV	146	181	1.24%	0.127%
86	15.111	2175	2180	2181	rBV2	406	534	3.65%	0.376%
87	15.172	2188	2190	2191	rBV2	212	152	1.04%	0.107%
88	15.208	2194	2196	2198	rBV	236	170	1.16%	0.120%
89	15.318	2213	2214	2219	rVB2	288	211	1.44%	0.149%
90	15.422	2230	2231	2233	rBV2	229	195	1.33%	0.137%
91	15.531	2247	2249	2250	rVB2	255	148	1.01%	0.104%
92	15.562	2252	2254	2257	rBV2	345	244	1.67%	0.172%
93	15.629	2263	2265	2269	rBV2	139	174	1.19%	0.123%
94	15.793	2289	2292	2293	rBV	139	164	1.12%	0.116%
95	15.964	2318	2320	2321	rBV	212	167	1.14%	0.118%
96	16.178	2353	2355	2359	rBV2	177	188	1.28%	0.132%
97	16.360	2383	2385	2386	rVB2	341	181	1.24%	0.127%
98	16.397	2389	2391	2393	rBV2	227	168	1.15%	0.118%

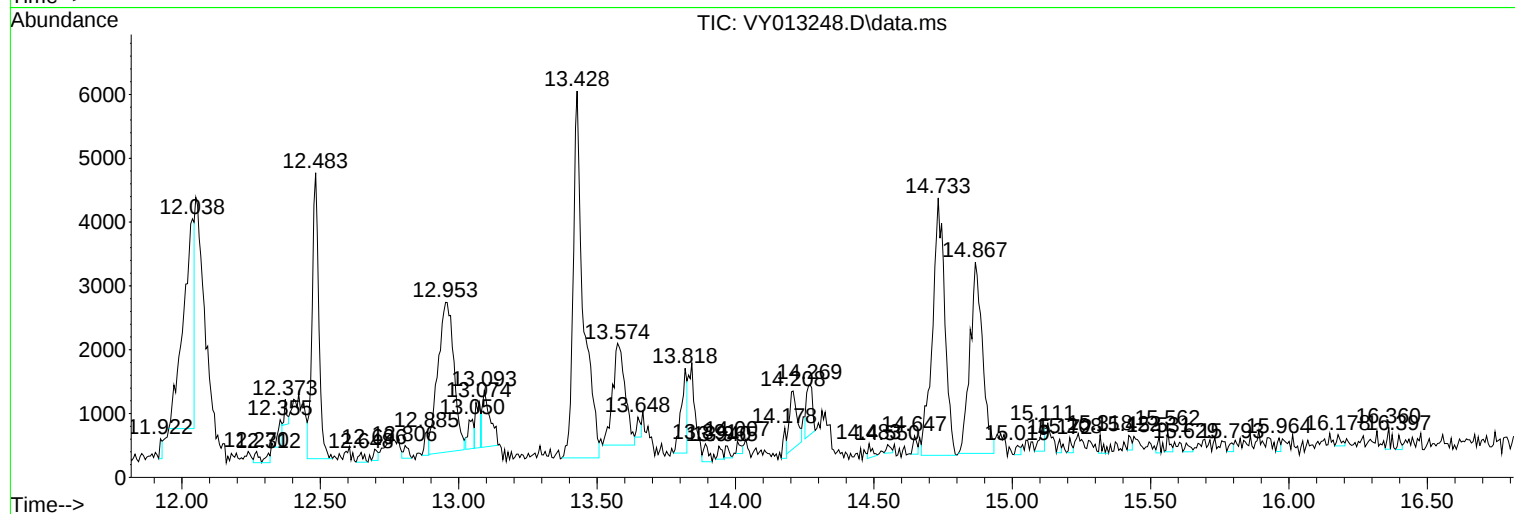
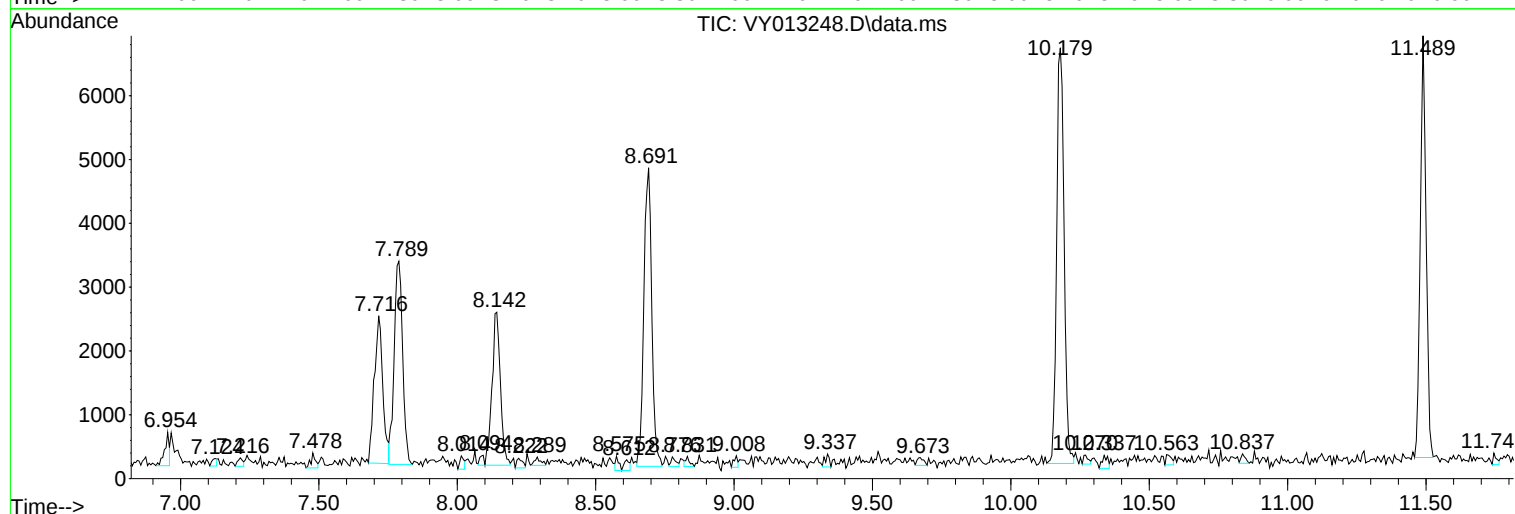
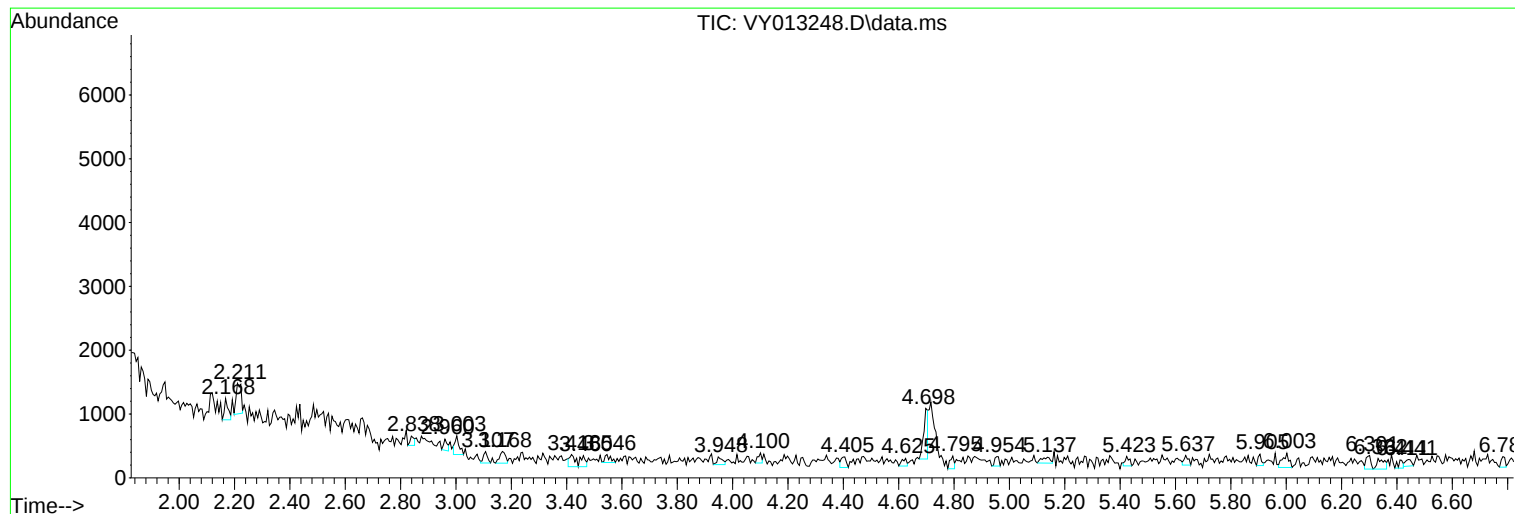
Sum of corrected areas: 141989

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041123S.M
Quant Title : SW846 8260

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



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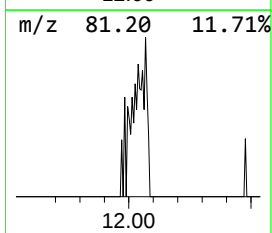
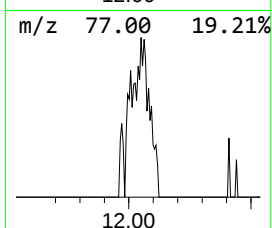
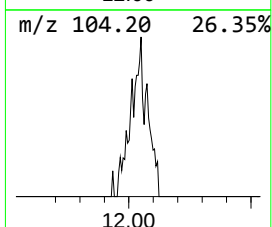
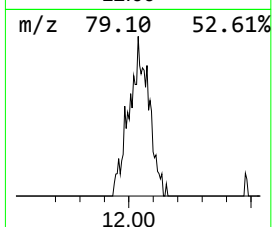
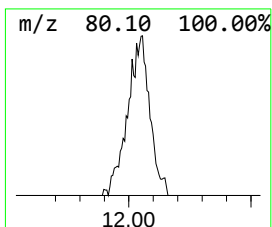
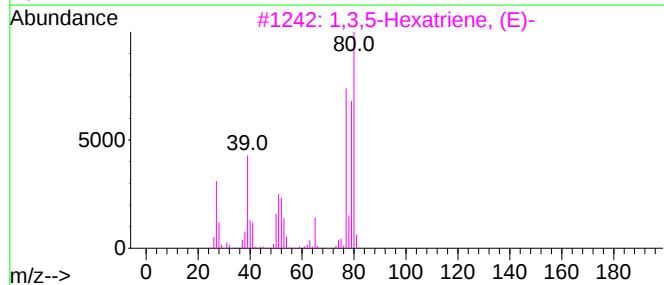
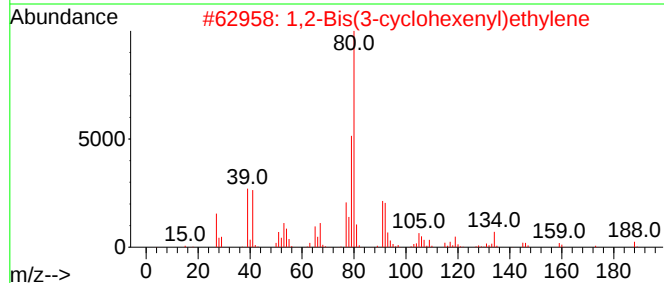
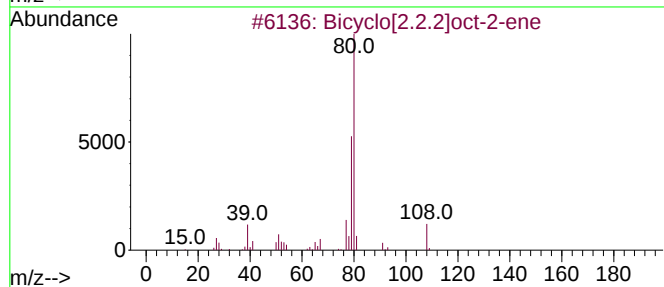
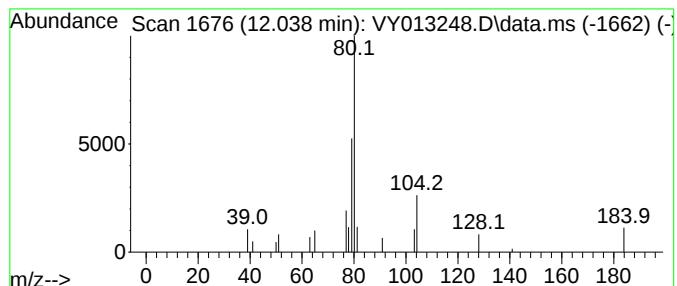
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041123S.M
Quant Title : SW846 8260

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

Peak Number 1 Bicyclo[2.2.2]oct-2-ene Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.038	48.64 ug/l	9294	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Bicyclo[2.2.2]oct-2-ene	108	C8H12	000931-64-6	78
2			1,2-Bis(3-cyclohexenyl)ethylene	188	C14H20	017527-28-5	78
3			1,3,5-Hexatriene, (E)-	80	C6H8	000821-07-8	72
4			1-Penten-3-yne, 2-methyl-	80	C6H8	000926-55-6	72
5			4,7-Methanoisobenzofuran-1,3-dio...	178	C10H10O3	000117-40-8	72



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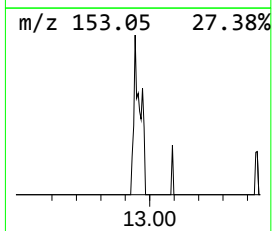
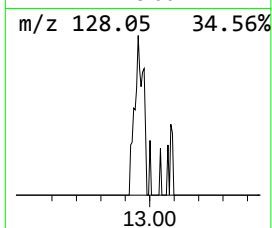
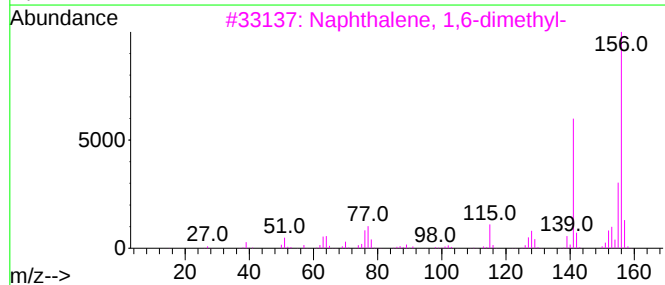
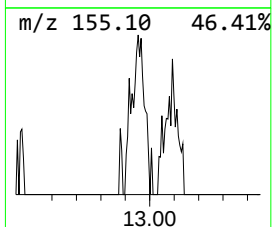
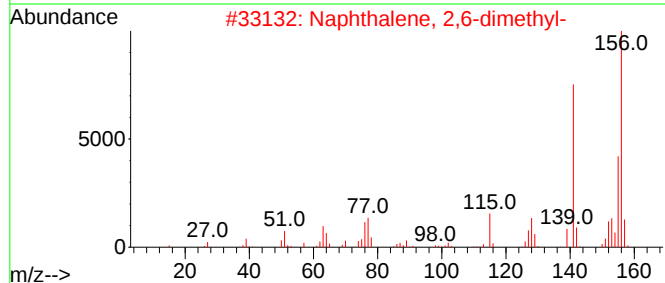
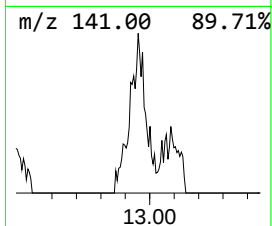
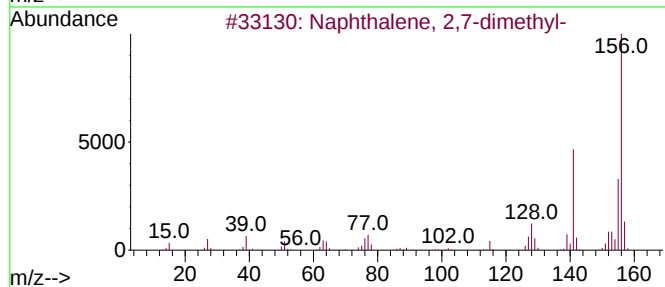
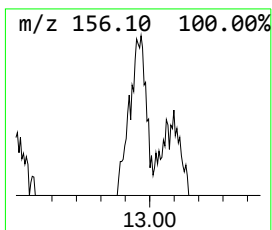
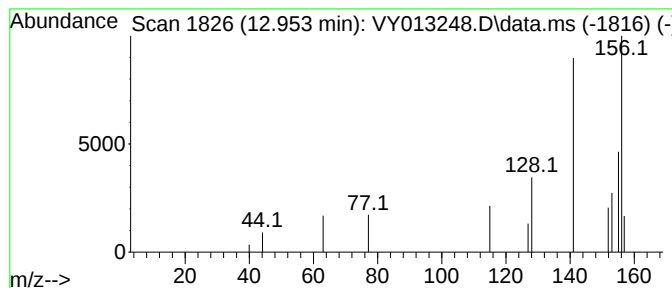
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Naphthalene, 2,7-dimethyl- Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.953	32.40 ug/l	9485	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 2,7-dimethyl-	156	C12H12	000582-16-1	86
2			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	83
3			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	80
4			Naphthalene, 1,5-dimethyl-	156	C12H12	000571-61-9	74
5			Naphthalene, 1,7-dimethyl-	156	C12H12	000575-37-1	72



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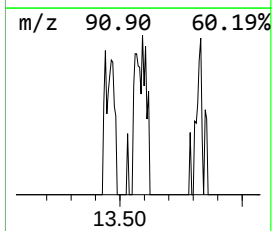
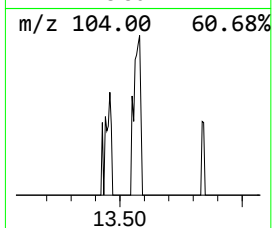
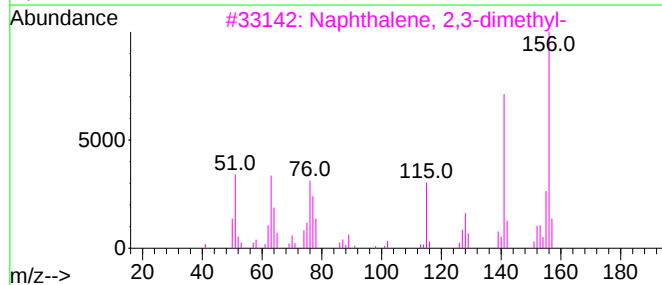
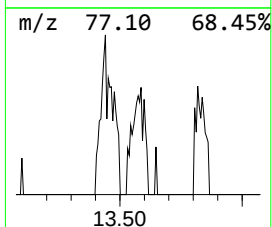
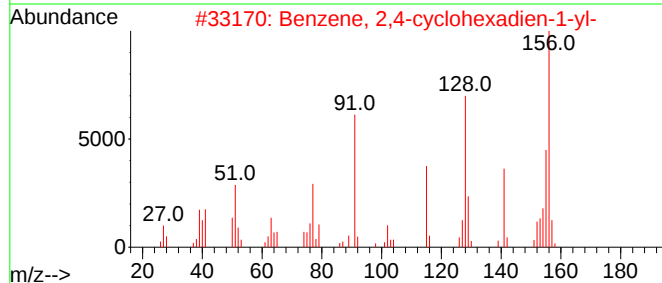
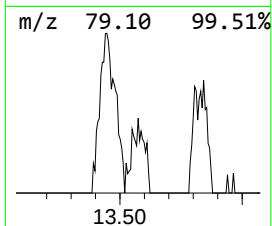
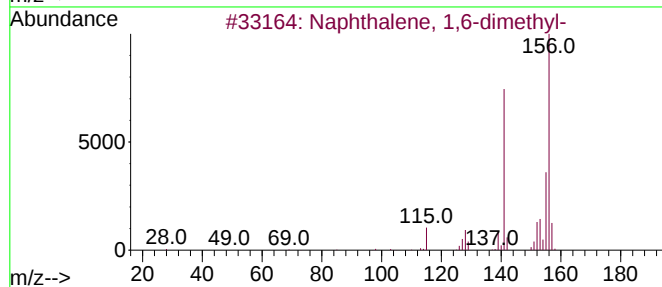
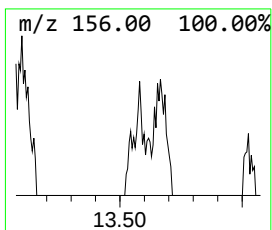
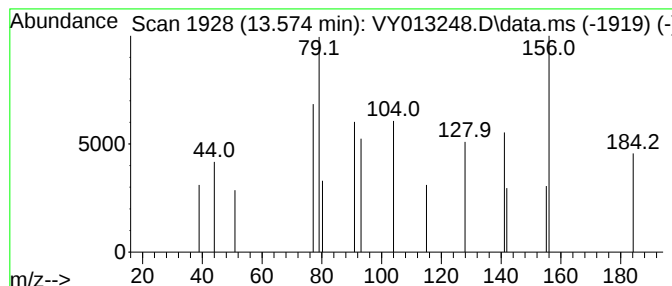
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041123S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown13.574 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.574	17.13 ug/l	5015	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Naphthalene, 1,6-dimethyl-	156	C12H12	000575-43-9	43
2			Benzene, 2,4-cyclohexadien-1-yl-	156	C12H12	021473-05-2	25
3			Naphthalene, 2,3-dimethyl-	156	C12H12	000581-40-8	25
4			Naphthalene, 2,6-dimethyl-	156	C12H12	000581-42-0	22
5			1,4-benzenedicarbonitrile, 2,5-d...	156	C10H8N2	1000404-33-1	22



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041123\
Data File : VY013248.D
Acq On : 11 Apr 2023 17:23
Operator : KP/MD
Sample : 02257-01
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
ELI-SOLID-0407

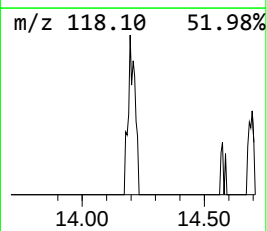
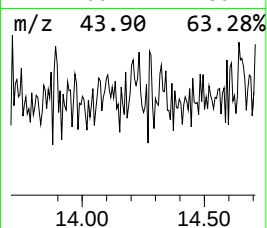
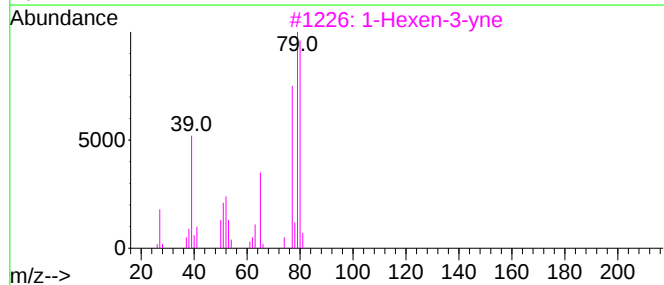
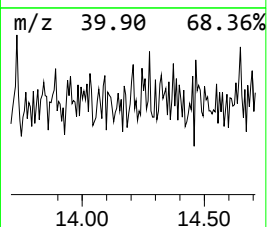
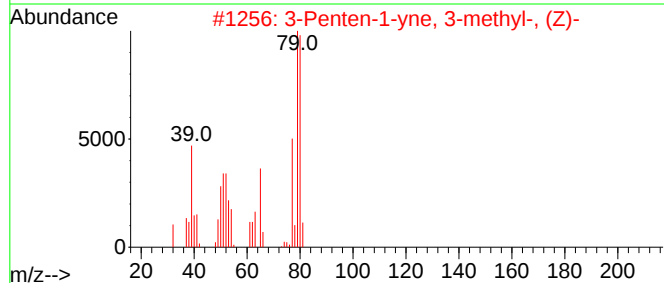
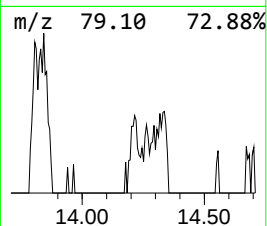
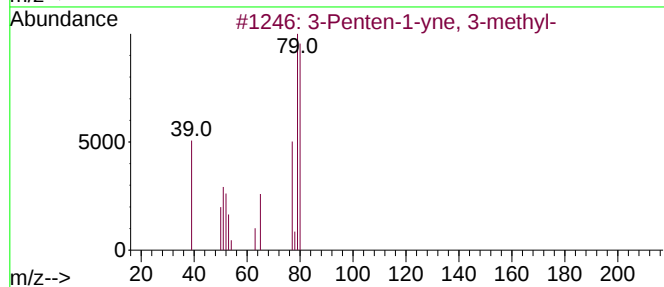
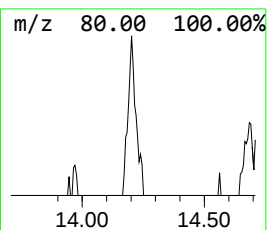
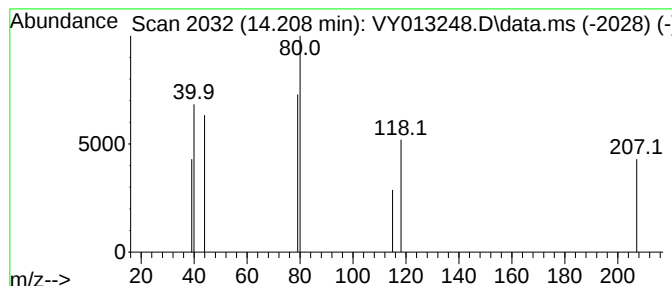
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Quant Title : SW846 8260

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

Peak Number 6 3-Penten-1-yne, 3-methyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.208	6.00 ug/l	1757	1,4-Dichlorobenzene-d4	13.428

Hit#	of 5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Penten-1-yne, 3-methyl-	80	C6H8	001574-33-0	59
2		3-Penten-1-yne, 3-methyl-, (Z)-	80	C6H8	014272-81-2	45
3		1-Hexen-3-yne	80	C6H8	013721-54-5	45
4		1,3,5-Hexatriene, (E)-	80	C6H8	000821-07-8	9
5		4,7-Methano-1H-indene, octahydro...	148	C11H16	068284-23-1	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041123\
Data File : VY013248.D
Acq On : 11 Apr 2023 17:23
Operator : KP/MD
Sample : 02257-01
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
ELI-SOLID-0407

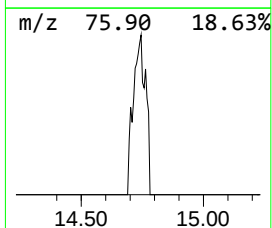
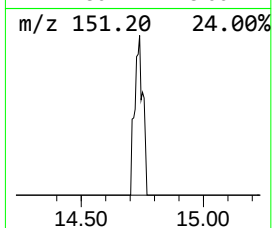
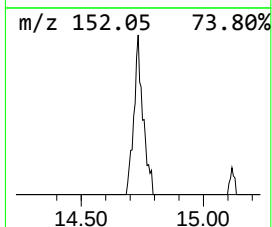
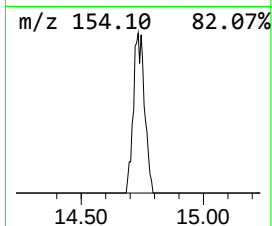
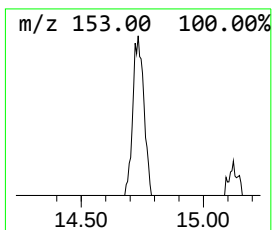
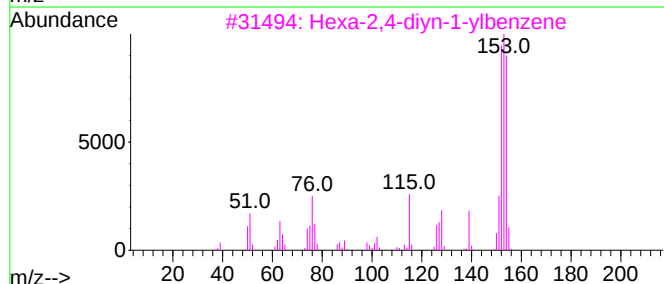
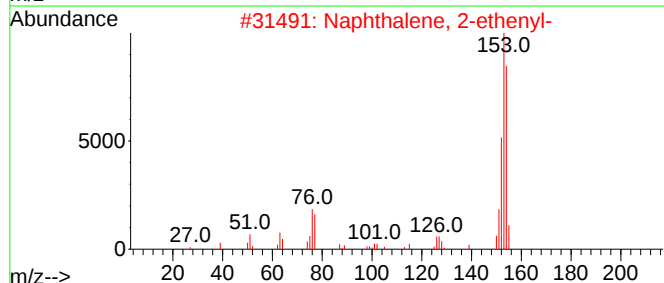
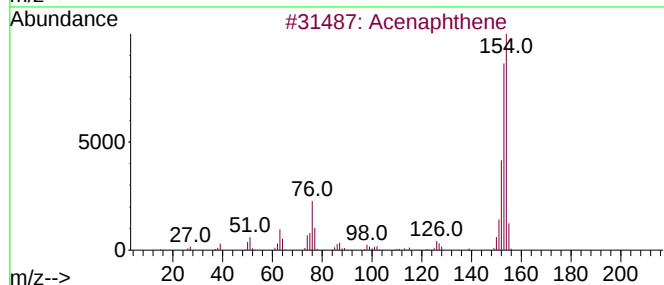
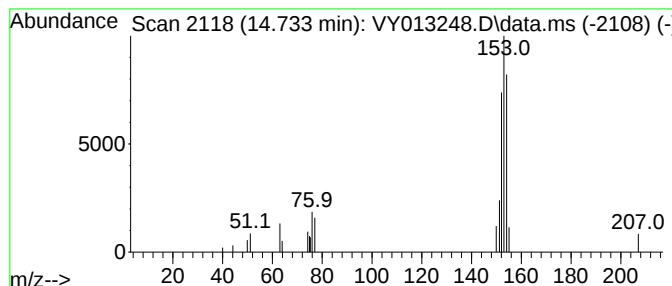
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041123S.M
Quant Title : SW846 8260

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

Peak Number 7 Acenaphthene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.733	42.53 ug/l	12453	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Acenaphthene	154	C12H10	000083-32-9	52
2			Naphthalene, 2-ethenyl-	154	C12H10	000827-54-3	49
3			Hexa-2,4-diyne-1-ylbenzene	154	C12H10	000520-74-1	47
4			1,4-Ethenonaphthalene, 1,4-dihydro-	154	C12H10	007322-47-6	43
5			N-(4-Chlorobenzylidene)methylamine	153	C8H8ClN	1010433-53-3	38



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY041123\
Data File : VY013248.D
Acq On : 11 Apr 2023 17:23
Operator : KP/MD
Sample : 02257-01
Misc : 5.07g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
ELI-SOLID-0407

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y041123S.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
Bicyclo[2.2.2]o...	12.038	48.6	ug/l	9294	3	11.489	9553	50.0
Naphthalene, 2,...	12.953	32.4	ug/l	9485	4	13.428	14639	50.0
unknown13.574	13.574	17.1	ug/l	5015	4	13.428	14639	50.0
3-Penten-1-yne,...	14.208	6.0	ug/l	1757	4	13.428	14639	50.0
Acenaphthene	14.733	42.5	ug/l	12453	4	13.428	14639	50.0