

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052623\
 Data File : VY013897.D
 Acq On : 26 May 2023 16:47
 Operator : KP/MD
 Sample : 02945-01
 Misc : 5.05g/5.0mL/MSVOA_Y/SOIL
 ALS Vial : 11 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 SB20

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\82Y052323S.M
 Title : SW846 8260

Signal : TIC: VY013897.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.113	46	48	50	rBV2	736	878	3.50%	0.443%
2	2.205	60	63	64	rBV2	1373	1478	5.89%	0.746%
3	2.259	70	72	73	rBV	685	668	2.66%	0.337%
4	2.320	80	82	83	rBV2	678	468	1.86%	0.236%
5	2.583	122	125	129	rVB3	787	1093	4.35%	0.552%
6	2.625	129	132	133	rBV	721	652	2.60%	0.329%
7	2.729	145	149	152	rVB3	326	493	1.96%	0.249%
8	2.802	158	161	165	rBV	816	987	3.93%	0.498%
9	2.954	184	186	190	rBV2	403	510	2.03%	0.258%
10	3.009	192	195	199	rVB2	295	437	1.74%	0.221%
11	3.149	215	218	221	rBV3	324	360	1.43%	0.182%
12	3.308	241	244	246	rBV2	338	401	1.60%	0.202%
13	3.345	249	250	252	rBV	414	378	1.51%	0.191%
14	3.399	257	259	263	rVB2	473	622	2.48%	0.314%
15	3.442	263	266	269	rBV2	583	849	3.38%	0.429%
16	3.674	300	304	307	rBV2	341	572	2.28%	0.289%
17	3.863	333	335	337	rBV3	363	380	1.51%	0.192%
18	3.942	341	348	354	rBV3	966	2879	11.47%	1.454%
19	4.119	375	377	382	rVB3	540	922	3.67%	0.466%
20	4.229	393	395	397	rVB	558	433	1.72%	0.219%
21	4.308	406	408	411	rVB2	323	353	1.41%	0.178%
22	4.710	468	474	482	rVB6	2217	6599	26.28%	3.332%
23	4.972	513	517	518	rVB2	320	355	1.41%	0.179%
24	5.740	639	643	649	rVB2	472	1118	4.45%	0.565%
25	6.027	685	690	691	rBV	310	430	1.71%	0.217%
26	6.112	700	704	707	rVB2	261	419	1.67%	0.212%
27	6.307	731	736	739	rBV2	289	539	2.15%	0.272%
28	6.746	804	808	811	rBV2	313	420	1.67%	0.212%
29	6.807	816	818	819	rBV	450	359	1.43%	0.181%
30	6.850	822	825	827	rVV2	341	398	1.59%	0.201%
31	6.978	841	846	848	rBV3	433	562	2.24%	0.284%
32	7.021	848	853	855	rVV3	363	649	2.58%	0.328%
33	7.057	857	859	864	rVV2	488	658	2.62%	0.332%
34	7.124	867	870	872	rBV2	342	373	1.49%	0.188%
35	7.411	914	917	921	rBV2	256	433	1.72%	0.219%
36	7.496	927	931	933	rBV2	429	554	2.21%	0.280%

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37	7.716	959	967	972	rVV2	4461	9748	38.82%	4.922%
38	7.783	973	978	986	rVB4	5397	12170	48.47%	6.145%
39	7.941	1002	1004	1006	rBV	407	367	1.46%	0.185%
40	8.136	1029	1036	1047	rBV3	5011	11564	46.06%	5.839%

41	8.624	1115	1116	1120	rVB	476	480	1.91%	0.242%
42	8.685	1120	1126	1135	rBV	8056	17270	68.78%	8.720%
43	9.069	1186	1189	1193	rBV2	326	466	1.86%	0.235%
44	9.118	1195	1197	1202	rVB2	301	469	1.87%	0.237%
45	9.344	1230	1234	1236	rBV2	284	442	1.76%	0.223%

46	9.600	1273	1276	1279	rBV2	327	578	2.30%	0.292%
47	9.782	1303	1306	1308	rBV2	460	418	1.66%	0.211%
48	10.179	1364	1371	1379	rBV	13574	25108	100.00%	12.678%
49	10.435	1409	1413	1414	rVB2	312	403	1.61%	0.203%
50	10.642	1442	1447	1450	rBV2	286	546	2.17%	0.276%

51	10.673	1450	1452	1456	rVB3	352	509	2.03%	0.257%
52	10.776	1468	1469	1473	rVB	344	357	1.42%	0.180%
53	10.813	1473	1475	1478	rBV2	338	426	1.70%	0.215%
54	10.874	1482	1485	1487	rVB2	498	560	2.23%	0.283%
55	11.002	1503	1506	1509	rBV2	256	414	1.65%	0.209%

56	11.124	1524	1526	1528	rVB	684	511	2.04%	0.258%
57	11.148	1528	1530	1534	rBV2	582	884	3.52%	0.446%
58	11.185	1534	1536	1538	rVB3	510	369	1.47%	0.186%
59	11.233	1541	1544	1545	rBV2	460	497	1.98%	0.251%
60	11.489	1578	1586	1593	rBV2	12173	22424	89.31%	11.323%

61	11.569	1597	1599	1600	rVB2	518	355	1.41%	0.179%
62	11.599	1600	1604	1606	rBV3	360	500	1.99%	0.252%
63	11.624	1606	1608	1611	rBV	419	538	2.14%	0.272%
64	11.800	1634	1637	1641	rVB	365	489	1.95%	0.247%
65	11.855	1641	1646	1650	rVB2	562	839	3.34%	0.424%

66	11.892	1650	1652	1656	rBV2	463	615	2.45%	0.311%
67	11.928	1656	1658	1661	rBV2	386	548	2.18%	0.277%
68	11.995	1667	1669	1670	rBV2	379	408	1.62%	0.206%
69	12.044	1673	1677	1679	rVB2	552	772	3.07%	0.390%
70	12.069	1679	1681	1682	rBV3	664	558	2.22%	0.282%

71	12.148	1693	1694	1696	rBV2	527	362	1.44%	0.183%
72	12.209	1701	1704	1708	rBV4	675	914	3.64%	0.462%
73	12.239	1708	1709	1712	rBV2	572	671	2.67%	0.339%
74	12.276	1714	1715	1717	rBV2	472	393	1.57%	0.198%
75	12.422	1737	1739	1743	rBV5	499	644	2.56%	0.325%

76	12.483	1743	1749	1758	rVB6	8618	16680	66.43%	8.422%
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77	12.593	1764	1767	1768	rBV3	705	586	2.33%	0.296%
78	12.654	1776	1777	1781	rVB4	756	718	2.86%	0.363%
79	12.690	1781	1783	1785	rBV3	572	601	2.39%	0.303%
80	12.715	1785	1787	1789	rVV2	463	387	1.54%	0.195%
81	12.739	1789	1791	1793	rBV2	739	562	2.24%	0.284%
82	12.910	1816	1819	1821	rBV3	491	673	2.68%	0.340%
83	12.947	1823	1825	1826	rBV	677	526	2.09%	0.266%
84	13.184	1859	1864	1866	rBV7	1092	1780	7.09%	0.899%
85	13.270	1876	1878	1880	rBV3	1013	838	3.34%	0.423%
86	13.422	1899	1903	1910	rVB4	9653	15620	62.21%	7.887%
87	13.599	1928	1932	1933	rBV3	1288	1476	5.88%	0.745%
88	13.715	1949	1951	1954	rBV3	620	661	2.63%	0.334%
89	14.202	2029	2031	2034	rBV4	995	1293	5.15%	0.653%
90	14.867	2138	2140	2141	rBV2	717	552	2.20%	0.279%
91	15.099	2174	2178	2179	rBV4	1628	1821	7.25%	0.919%
92	15.312	2211	2213	2215	rVB2	1408	1173	4.67%	0.592%
93	15.556	2248	2253	2255	rBV5	899	1838	7.32%	0.928%
94	15.611	2260	2262	2266	rVB3	1484	1576	6.28%	0.796%
95	15.836	2296	2299	2302	rBV4	767	922	3.67%	0.466%
96	16.184	2354	2356	2357	rVB2	644	451	1.80%	0.228%
97	16.275	2369	2371	2372	rBV2	706	489	1.95%	0.247%
98	16.354	2382	2384	2385	rVB	628	359	1.43%	0.181%
99	16.556	2416	2417	2420	rBV3	540	478	1.90%	0.241%
100	16.708	2441	2442	2445	rVB2	1177	723	2.88%	0.365%

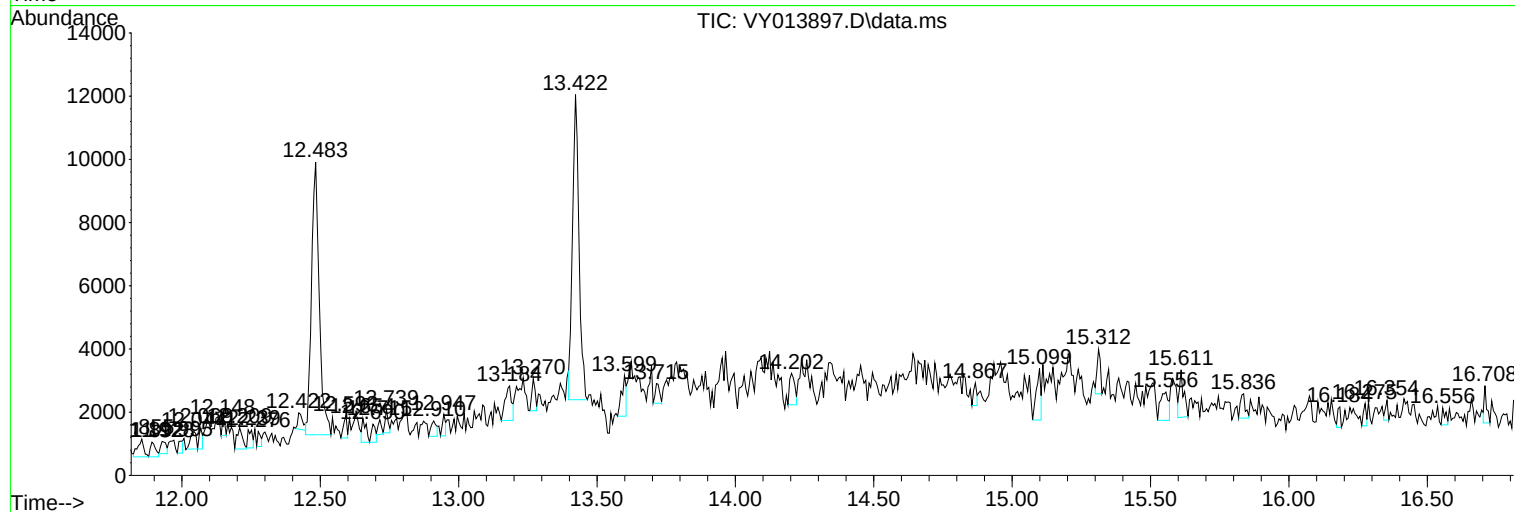
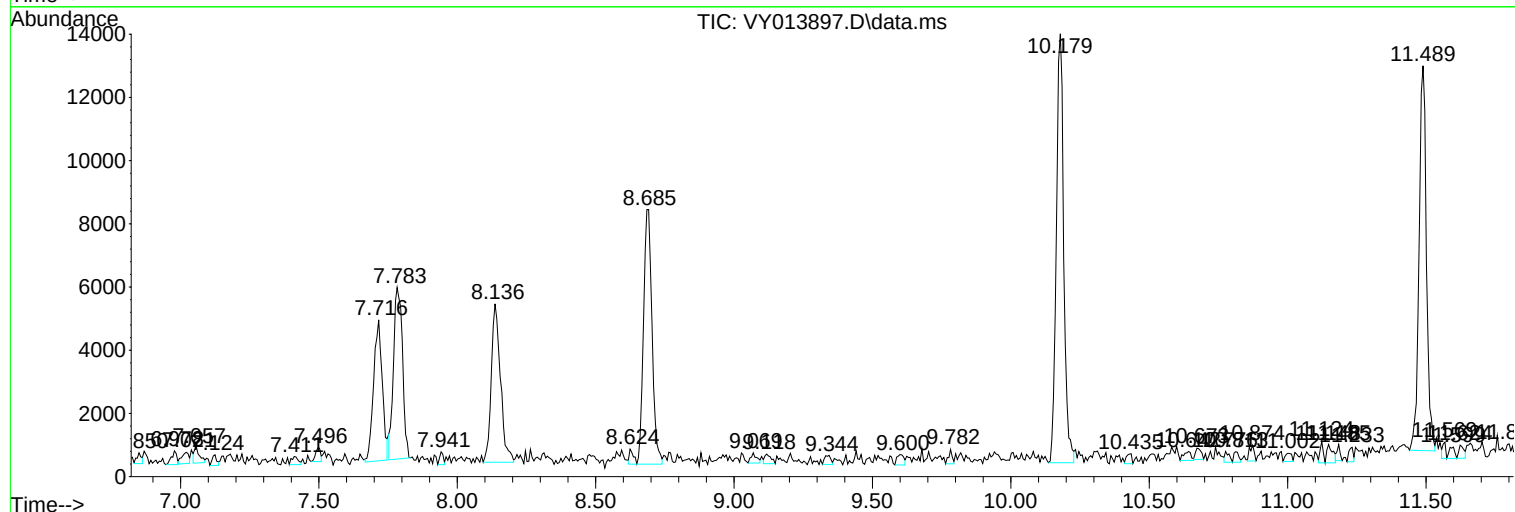
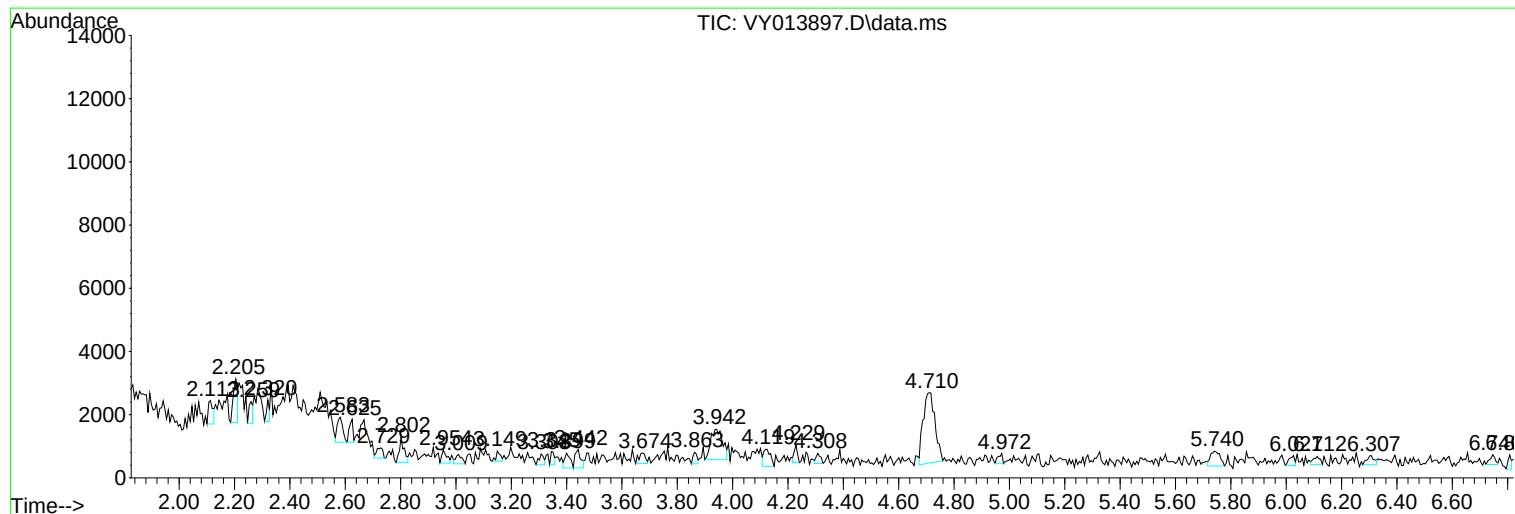
Sum of corrected areas: 198048

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052323S.M
Quant Title : SW846 8260

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



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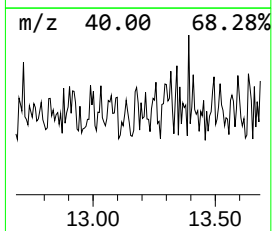
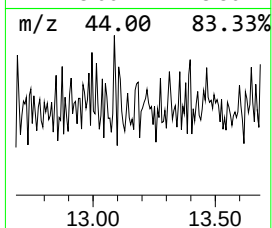
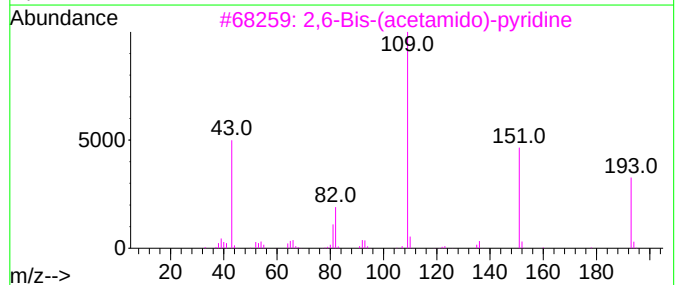
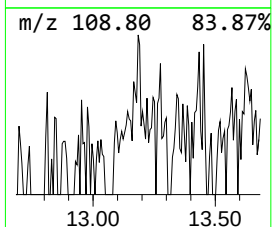
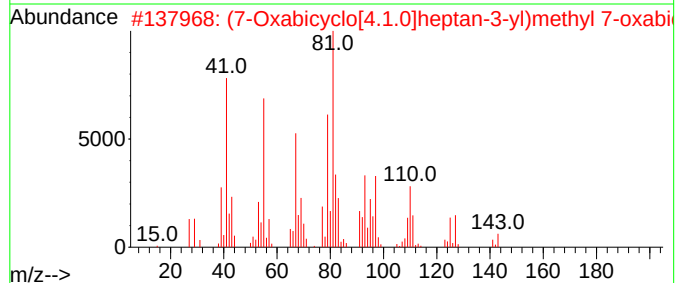
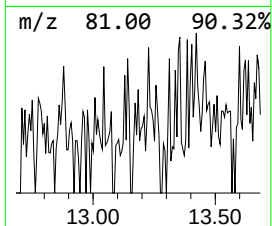
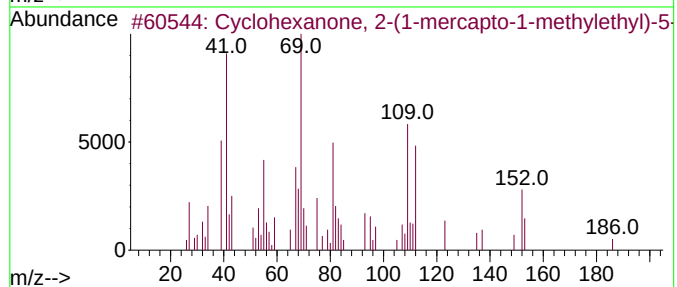
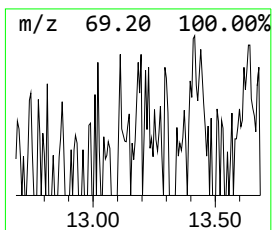
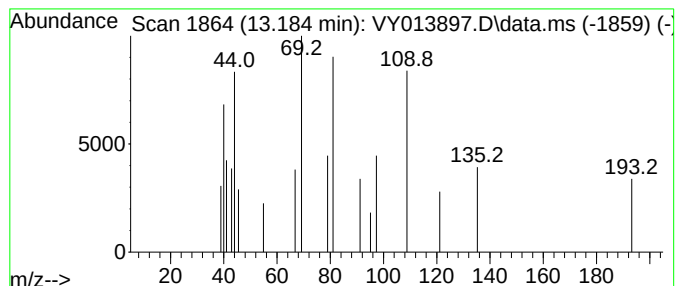
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052323S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown13.184 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.184	5.70 ug/l	1780	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Cyclohexanone, 2-(1-mercapto-1-methyl-ethyl)-5-	186	C10H18OS	033281-91-3	12
2			(7-Oxabicyclo[4.1.0]heptan-3-yl)methyl 7-oxabicyclo[4.1.0]heptan-3-yl	252	C14H20O4	1000473-40-7	10
3			2,6-Bis-(acetamido)-pyridine	193	C9H11N3O2	005441-02-1	9
4			(1-Bromo-pentyl)-cyclopropane	190	C8H15Br	088106-30-3	9
5			Cyclohexanol, 3-(aminomethyl)-3,...	171	C10H21NO	015647-11-7	9



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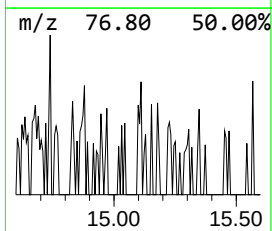
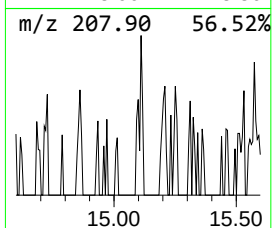
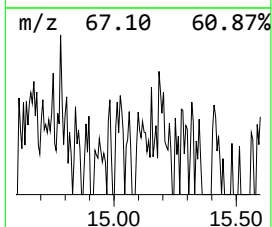
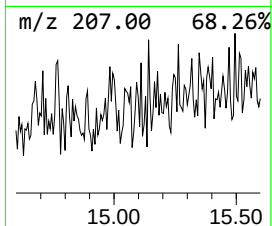
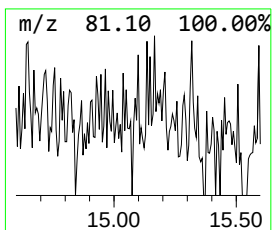
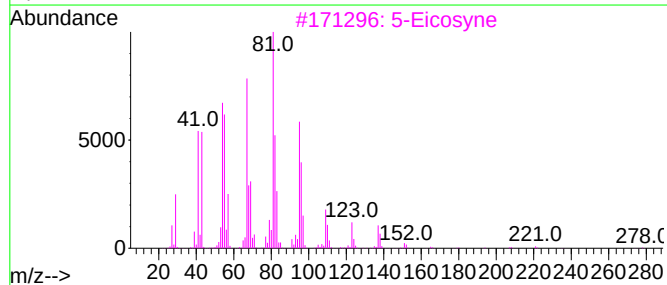
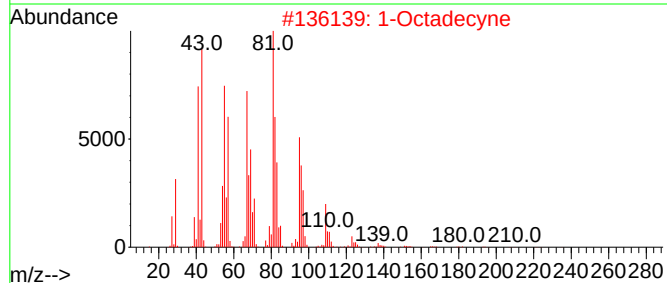
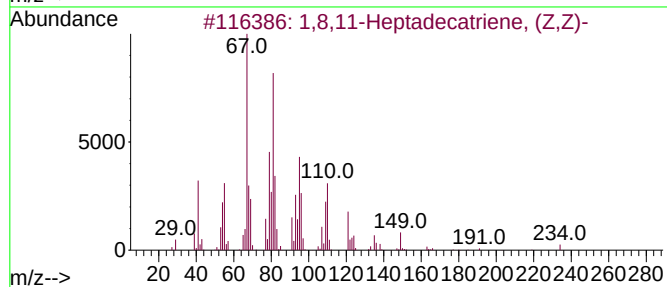
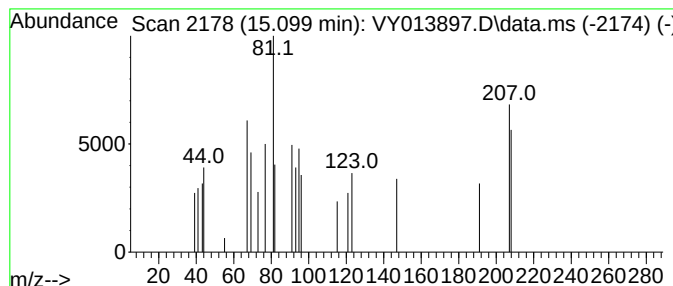
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052323S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown15.099 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.099	5.83 ug/l	1821	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,8,11-Heptadecatriene, (Z,Z)-	234	C17H30	056134-03-3	43
2			1-Octadecyne	250	C18H34	000629-89-0	38
3			5-Eicosyne	278	C20H38	074685-31-7	38
4			9-Methylbicyclo[3.3.1]nonane	138	C10H18	025107-01-1	38
5			1-Pentadecyne	208	C15H28	000765-13-9	32



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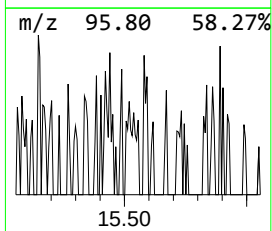
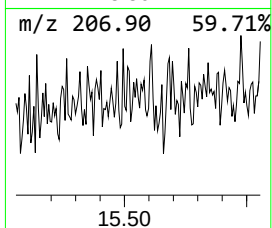
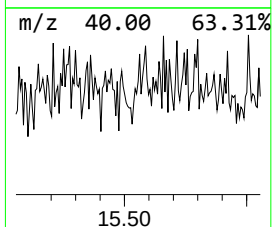
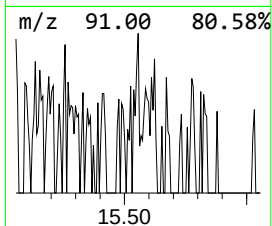
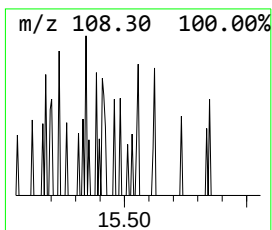
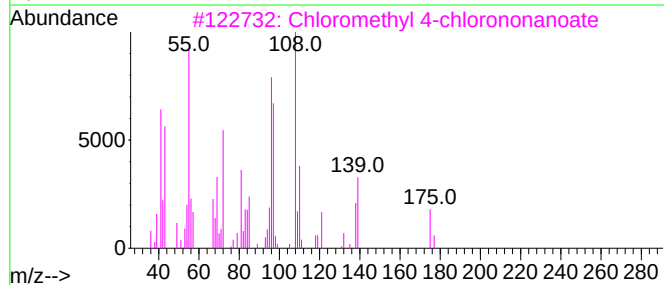
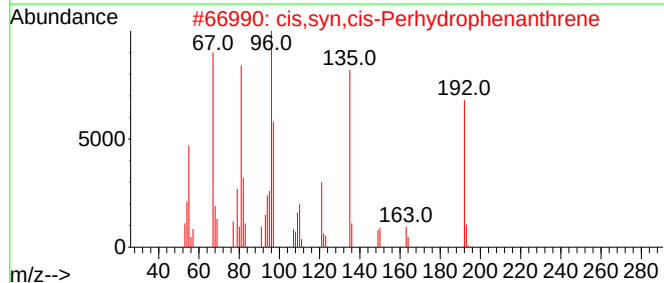
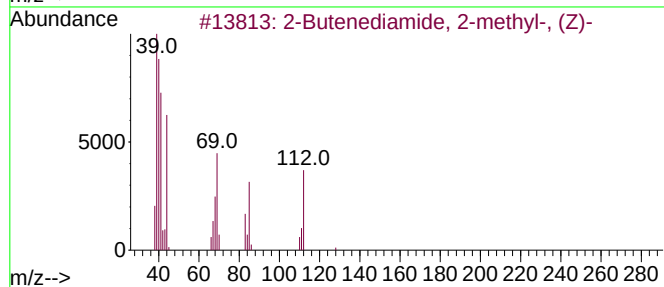
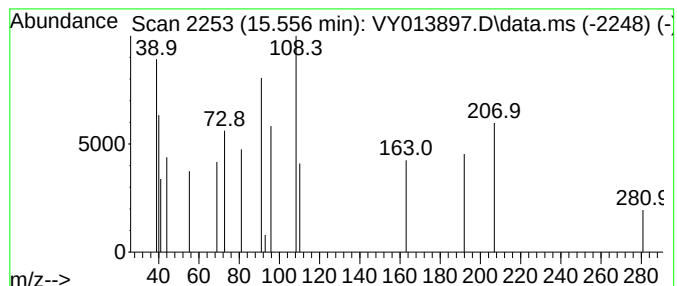
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052323S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown15.556 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.556	5.88 ug/l	1838	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Butenediamide, 2-methyl-, (Z)-	128	C5H8N2O2	041138-17-4	23		
2	cis,syn,cis-Perhydrophenanthrene	192	C14H24	026634-41-3	10		
3	Chloromethyl 4-chlorononanoate	240	C10H18Cl2O2	080418-73-1	9		
4	2-Ethylacridine	207	C15H13N	055751-83-2	7		
5	1,3-Butadiene, 1,1,2-trifluoro-	108	C4H3F3	000565-65-1	5		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052623\
Data File : VY013897.D
Acq On : 26 May 2023 16:47
Operator : KP/MD
Sample : 02945-01
Misc : 5.05g/5.0mL/MSVOA_Y/soil
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB20

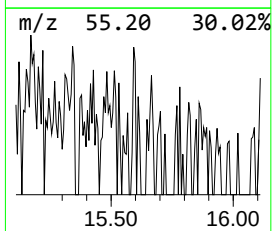
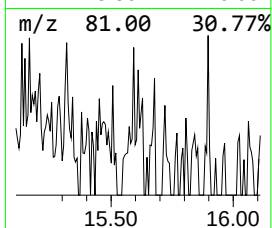
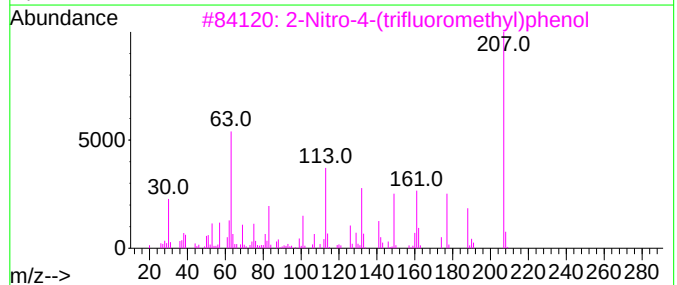
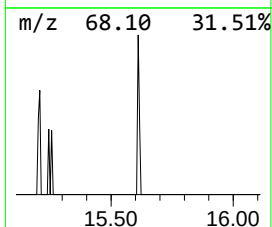
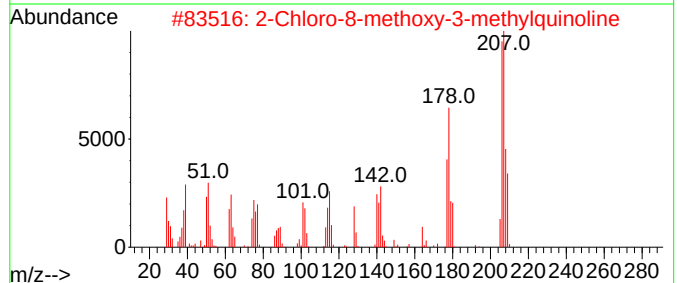
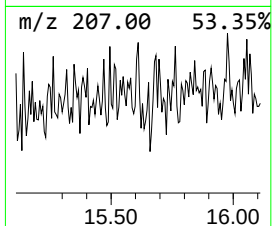
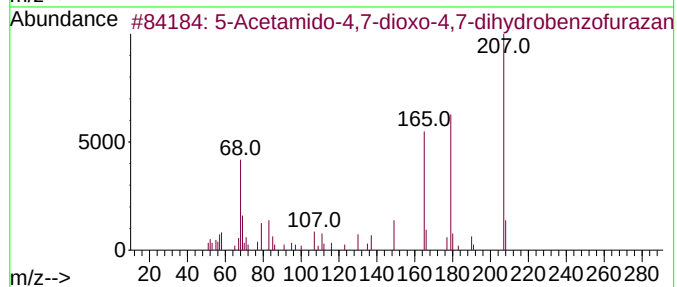
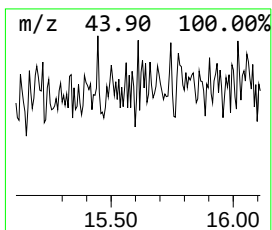
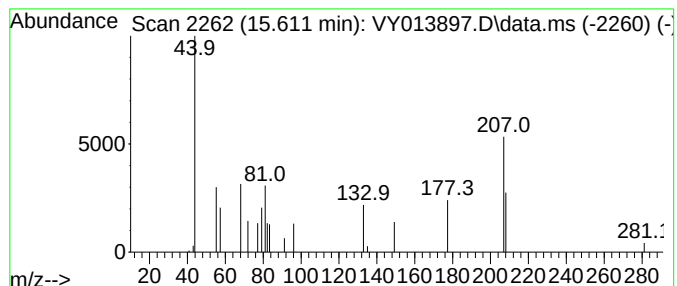
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Quant Title : SW846 8260

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

Peak Number 5 unknown15.611 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.611	5.04 ug/l	1576	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Acetamido-4,7-dioxo-4,7-dihydr...	207	C8H5N3O4	153136-27-7	16
2			2-Chloro-8-methoxy-3-methylquino...	207	C11H10ClNO	132118-31-1	12
3			2-Nitro-4-(trifluoromethyl)phenol	207	C7H4F3NO3	000400-99-7	9
4			2,3-Dihydroxy-6-nitroquinoxaline	207	C8H5N3O4	002379-56-8	9
5			5-Nitro-3-(trifluoromethyl)pyrid...	207	C6H4F3N3O2	1121056-94-7	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052623\
Data File : VY013897.D
Acq On : 26 May 2023 16:47
Operator : KP/MD
Sample : 02945-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL
ALS Vial : 11 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
SB20

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052323S.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
unknown13.184	13.184	5.7	ug/l	1780	4	13.428	15620	50.0
unknown15.099	15.099	5.8	ug/l	1821	4	13.428	15620	50.0
unknown15.556	15.556	5.9	ug/l	1838	4	13.428	15620	50.0
unknown15.611	15.611	5.0	ug/l	1576	4	13.428	15620	50.0