

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060724\
 Data File : VY018533.D
 Acq On : 07 Jun 2024 17:44
 Operator : SY/MD
 Sample : P2756-01
 Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 OR-02-06062024

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\82Y060324S.M

Title : SW846 8260

Signal : TIC: VY018533.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.010	29	31	33	rBV2	878	921	10.98%	0.969%
2	2.089	42	44	45	rBV2	1109	688	8.20%	0.724%
3	2.107	45	47	48	rBV2	1896	1477	17.60%	1.555%
4	2.290	75	77	81	rBV2	1239	1438	17.14%	1.514%
5	2.552	118	120	122	rBV2	849	702	8.37%	0.739%
6	3.101	208	210	211	rBV2	1151	969	11.55%	1.020%
7	3.150	215	218	222	rVB4	900	1225	14.60%	1.289%
8	3.180	222	223	225	rBV	845	694	8.27%	0.730%
9	3.235	231	232	235	rBV2	587	624	7.44%	0.657%
10	3.339	247	249	252	rVB2	734	612	7.29%	0.644%
11	3.406	257	260	263	rBV3	955	1427	17.01%	1.502%
12	3.503	270	276	277	rBV3	680	1234	14.71%	1.299%
13	3.521	277	279	282	rVB2	809	855	10.19%	0.900%
14	3.558	282	285	286	rBV3	615	642	7.65%	0.676%
15	3.649	298	300	306	rVB5	813	1087	12.96%	1.144%
16	3.704	307	309	311	rBV3	704	560	6.67%	0.589%
17	3.820	325	328	331	rBV2	888	1147	13.67%	1.207%
18	3.899	339	341	343	rVB	1052	761	9.07%	0.801%
19	3.960	349	351	354	rBV2	564	709	8.45%	0.746%
20	4.131	378	379	382	rBV3	758	806	9.61%	0.848%
21	4.418	421	426	427	rBV3	917	958	11.42%	1.008%
22	4.503	439	440	446	rVB5	561	835	9.95%	0.879%
23	4.582	451	453	455	rBV3	829	857	10.21%	0.902%
24	4.601	455	456	459	rVB3	1179	804	9.58%	0.846%
25	4.680	465	469	470	rBV3	708	901	10.74%	0.948%
26	5.070	530	533	534	rBV2	757	752	8.96%	0.791%
27	5.222	555	558	560	rVB3	710	704	8.39%	0.741%
28	5.326	572	575	578	rBV2	542	929	11.07%	0.978%
29	5.478	598	600	601	rBV2	903	701	8.36%	0.738%
30	5.789	649	651	654	rVV3	517	547	6.52%	0.576%
31	5.887	666	667	669	rBV	659	553	6.59%	0.582%
32	5.930	672	674	678	rVB4	768	749	8.93%	0.788%
33	6.076	696	698	702	rBV3	588	792	9.44%	0.834%
34	6.393	747	750	752	rBV2	640	644	7.68%	0.678%
35	6.856	825	826	828	rBV2	837	685	8.16%	0.721%
36	7.021	852	853	857	rBV	783	790	9.42%	0.831%

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37	7.070	857	861	863	rBV2	681	1076	12.82%	1.133%
38	7.277	892	895	896	rBV2	990	1070	12.75%	1.126%
39	7.405	913	916	918	rVB2	888	822	9.80%	0.865%
40	7.454	921	924	928	rVB4	659	1066	12.71%	1.122%
41	7.570	942	943	946	rVB2	658	570	6.79%	0.600%
42	7.606	948	949	951	rBV2	605	572	6.82%	0.602%
43	7.844	986	988	989	rBV2	964	581	6.92%	0.612%
44	7.960	1005	1007	1009	rBV2	671	620	7.39%	0.653%
45	8.289	1060	1061	1063	rBV2	805	809	9.64%	0.851%
46	8.350	1067	1071	1072	rBV2	790	989	11.79%	1.041%
47	8.514	1095	1098	1101	rBV3	1095	1456	17.35%	1.532%
48	8.551	1103	1104	1106	rBV	811	619	7.38%	0.652%
49	8.618	1112	1115	1118	rBV4	520	554	6.60%	0.583%
50	8.667	1121	1123	1124	rBV2	2042	1584	18.88%	1.667%
51	8.746	1135	1136	1138	rBV2	692	600	7.15%	0.632%
52	8.825	1146	1149	1153	rBV3	549	865	10.31%	0.910%
53	8.862	1153	1155	1159	rVV2	702	776	9.25%	0.817%
54	9.002	1175	1178	1182	rBV5	810	1335	15.91%	1.405%
55	9.197	1206	1210	1212	rBV4	615	973	11.60%	1.024%
56	9.325	1228	1231	1235	rBV6	820	1242	14.80%	1.307%
57	9.417	1245	1246	1249	rVB3	828	803	9.57%	0.845%
58	9.466	1249	1254	1257	rBV3	1068	1791	21.35%	1.885%
59	9.563	1268	1270	1272	rBV3	739	792	9.44%	0.834%
60	9.679	1287	1289	1292	rVB2	1028	974	11.61%	1.025%
61	9.831	1311	1314	1317	rBV3	765	882	10.51%	0.928%
62	9.862	1317	1319	1323	rVB4	892	1166	13.90%	1.227%
63	9.904	1323	1326	1330	rBV4	822	1515	18.06%	1.595%
64	10.173	1366	1370	1378	rVB3	4735	8390	100.00%	8.831%
65	10.276	1385	1387	1389	rVB2	1020	790	9.42%	0.831%
66	10.301	1389	1391	1394	rBV2	511	732	8.72%	0.770%
67	10.471	1417	1419	1424	rVB3	503	586	6.98%	0.617%
68	10.514	1424	1426	1428	rBV4	740	765	9.12%	0.805%
69	11.087	1517	1520	1522	rVB4	851	912	10.87%	0.960%
70	11.441	1575	1578	1579	rBV2	773	900	10.73%	0.947%
71	11.538	1593	1594	1596	rVB2	1216	763	9.09%	0.803%
72	11.691	1617	1619	1622	rBV2	512	671	8.00%	0.706%
73	11.947	1659	1661	1664	rVB3	1008	822	9.80%	0.865%
74	11.989	1664	1668	1670	rBV3	1002	1260	15.02%	1.326%
75	12.087	1682	1684	1685	rBV2	640	592	7.06%	0.623%
76	12.300	1716	1719	1722	rBV3	549	851	10.14%	0.896%

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77	12.374	1730	1731	1733	rVB2	1046	583	6.95%	0.614%
78	12.410	1735	1737	1740	rBV2	686	671	8.00%	0.706%
79	12.477	1744	1748	1755	rBV9	1630	2886	34.40%	3.038%
80	12.678	1778	1781	1784	rVB3	634	703	8.38%	0.740%
81	12.733	1788	1790	1792	rBV2	854	885	10.55%	0.931%
82	12.855	1808	1810	1813	rBV3	578	594	7.08%	0.625%
83	12.953	1824	1826	1830	rBV4	565	712	8.49%	0.749%
84	13.075	1843	1846	1847	rBV2	1039	828	9.87%	0.871%
85	13.306	1882	1884	1887	rBV	553	574	6.84%	0.604%
86	13.666	1941	1943	1946	rBV3	520	629	7.50%	0.662%
87	13.843	1971	1972	1975	rBV3	865	692	8.25%	0.728%
88	13.910	1981	1983	1984	rBV2	805	640	7.63%	0.674%
89	13.953	1988	1990	1993	rVB3	658	680	8.10%	0.716%
90	14.081	2007	2011	2013	rVV2	815	1078	12.85%	1.135%
91	14.154	2019	2023	2026	rVB2	1033	1238	14.76%	1.303%
92	15.123	2180	2182	2185	rBV2	676	704	8.39%	0.741%
93	15.154	2185	2187	2189	rVB2	916	585	6.97%	0.616%
94	15.282	2204	2208	2210	rBV4	792	1065	12.69%	1.121%
95	15.519	2245	2247	2249	rVB3	810	590	7.03%	0.621%
96	15.592	2256	2259	2261	rBV4	642	716	8.53%	0.754%
97	15.720	2278	2280	2282	rBV2	780	931	11.10%	0.980%
98	16.086	2337	2340	2343	rBV5	700	893	10.64%	0.940%
99	16.379	2386	2388	2390	rBV2	483	605	7.21%	0.637%
100	16.604	2423	2425	2427	rBV2	751	613	7.31%	0.645%

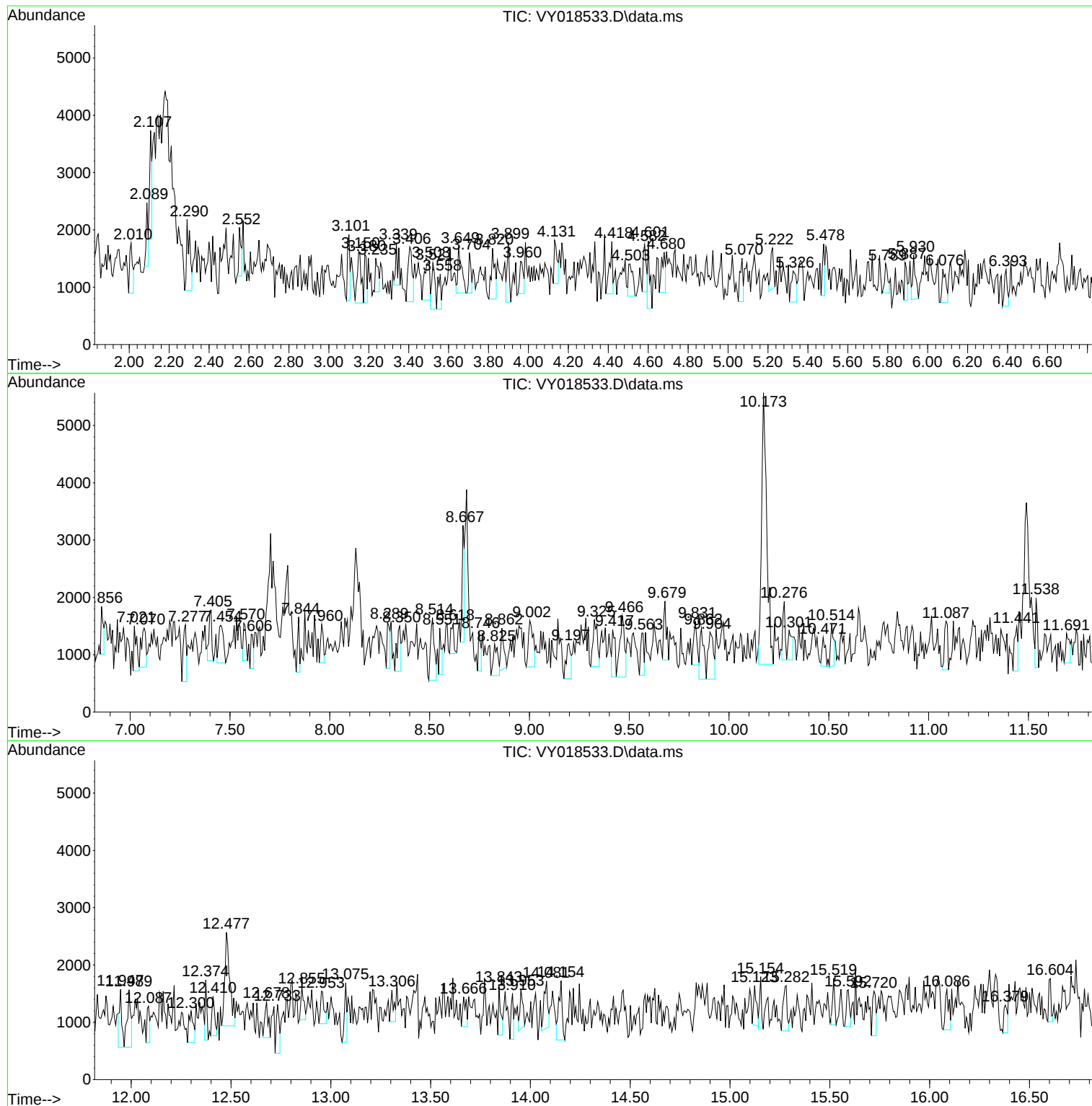
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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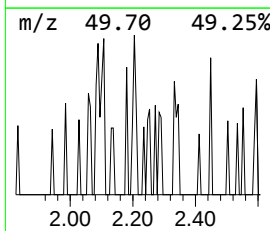
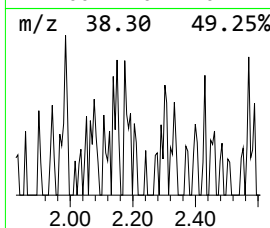
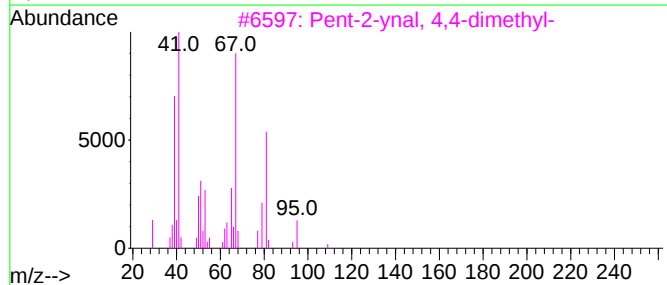
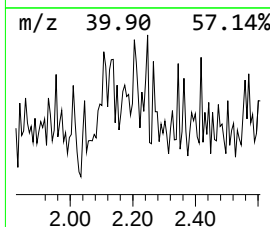
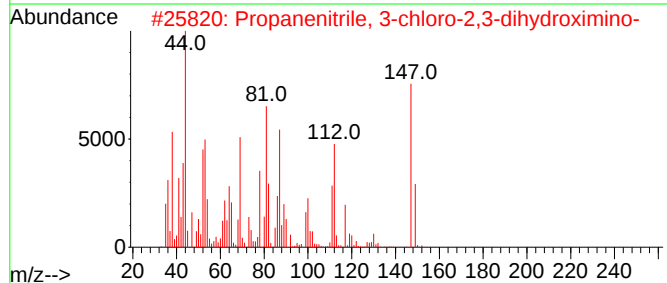
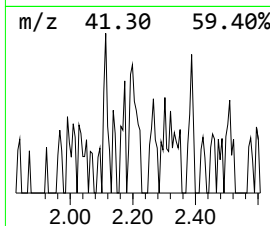
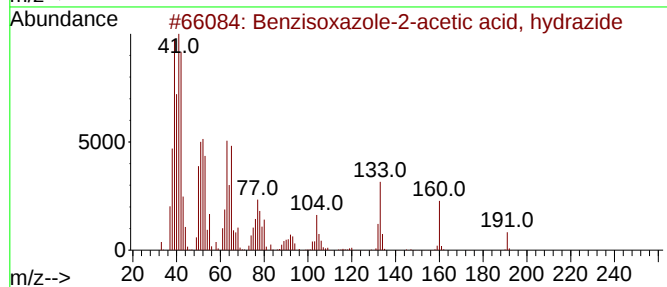
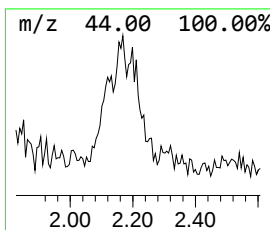
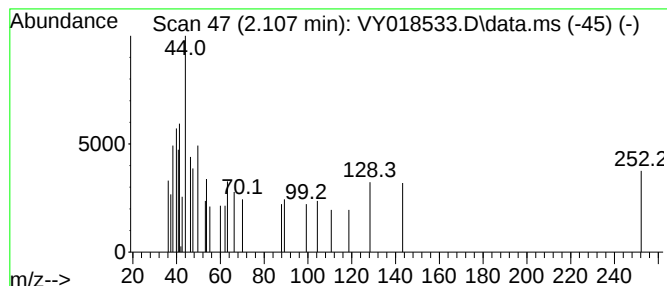
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060324S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown2.107 Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.107	127.11 ug/l	1477	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzisoxazole-2-acetic acid, hyd...	191	C9H9N3O2	055244-10-5	42
2			Propanenitrile, 3-chloro-2,3-dih...	147	C3H2ClN3O2	139912-33-7	32
3			Pent-2-ynal, 4,4-dimethyl-	110	C7H10O	002579-21-7	28
4			Pyridine, 2-amino-3,5-dinitro-	184	C5H4N4O4	003073-30-1	28
5			5-Cyclopropyl-2H-1,2,3,4-tetrazole	110	C4H6N4	027943-07-3	17



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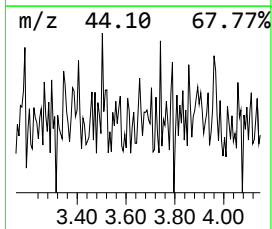
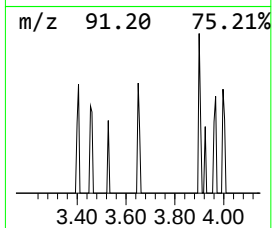
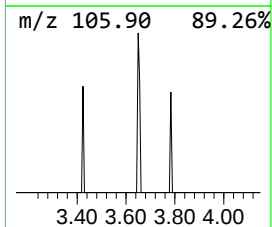
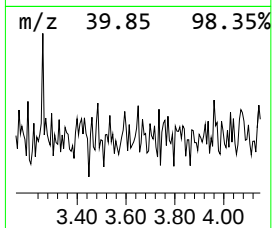
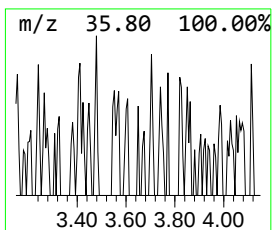
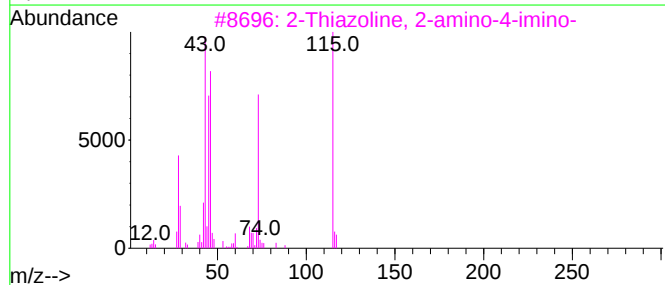
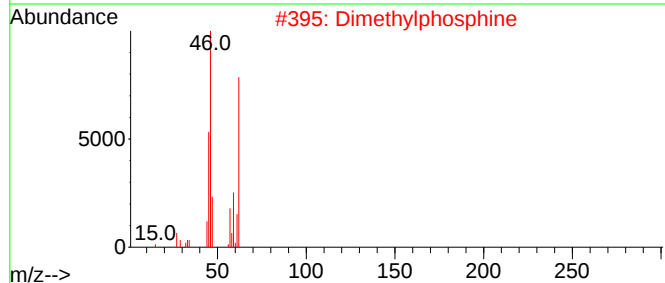
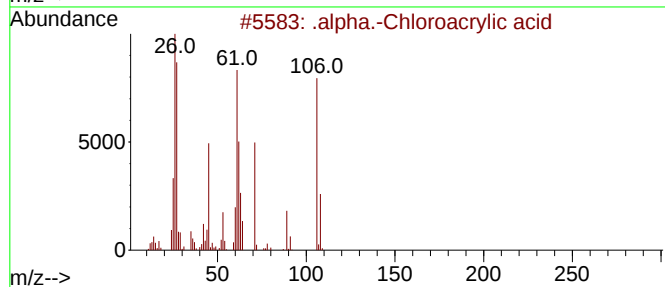
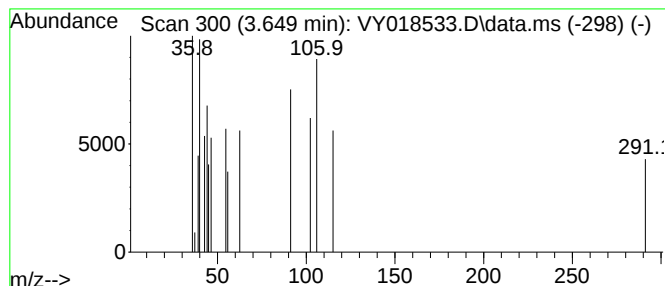
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060324S.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

Peak Number 6 unknown3.649 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
3.649	93.55 ug/l	1087	Pentafluorobenzene	7.783

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	.	alpha.-Chloroacrylic acid	106	C3H3ClO2	000598-79-8	25	
2		Dimethylphosphine	62	C2H7P	000676-59-5	16	
3		2-Thiazoline, 2-amino-4-imino-	115	C3H5N3S	026246-29-7	11	
4		Urethane	89	C3H7NO2	000051-79-6	9	
5		[1,3]Dithian-2-one	134	C4H6OS2	035345-24-5	9	



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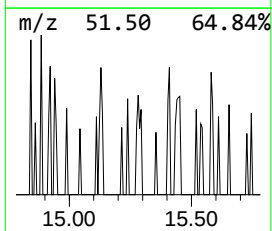
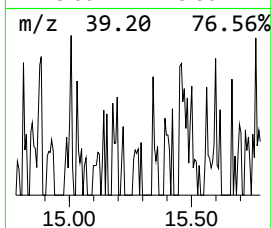
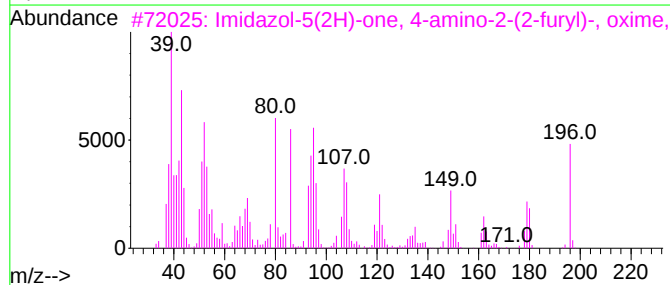
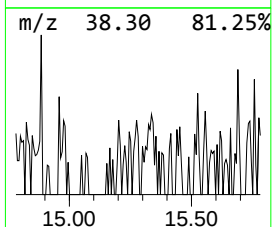
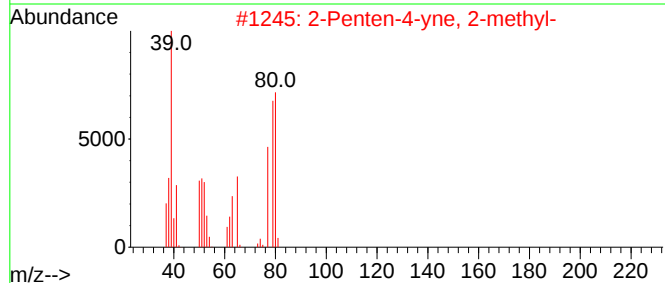
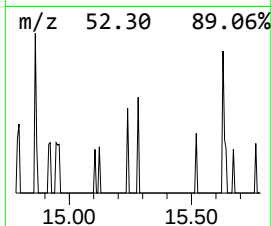
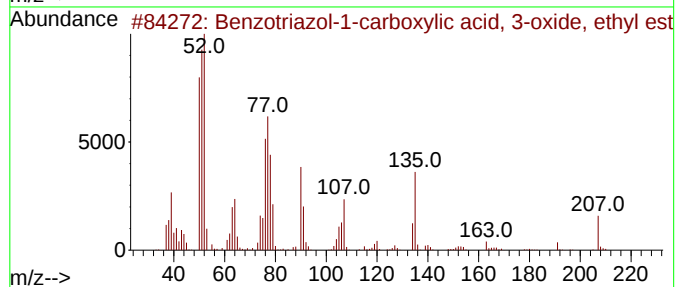
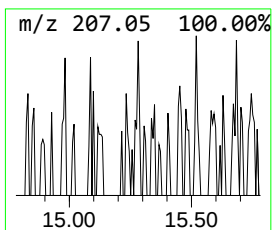
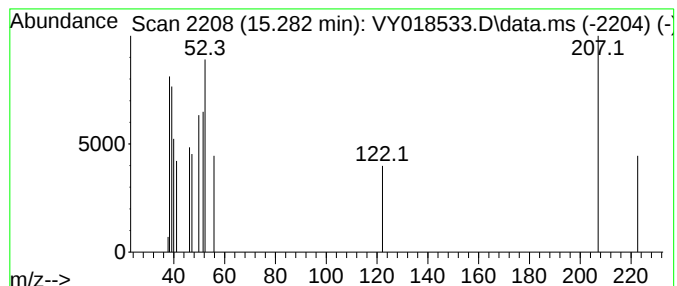
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Quant Title : SW846 8260

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

Peak Number 10 unknown15.281 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.281	92.77 ug/l	1065	1,4-Dichlorobenzene-d4	13.416

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzotriazol-1-carboxylic acid, ...	207	C9H9N3O3	211808-98-9	27
2			2-Penten-4-yne, 2-methyl-	80	C6H8	001595-53-5	25
3			Imidazol-5(2H)-one, 4-amino-2-(2...	196	C7H8N4O3	318259-17-5	9
4			N-Methyl-7-azabicyclo(2,2,1)hept...	109	C7H11N	055590-26-6	9
5			Phenol, 3-(4H-1,2,4-triazol-4-yl)-	161	C8H7N3O	1000410-77-9	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060724\
Data File : VY018533.D
Acq On : 07 Jun 2024 17:44
Operator : SY/MD
Sample : P2756-01
Misc : 5.05g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
OR-02-06062024

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060324S.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
unknown2.107	2.107	127.1	ug/l	1477	1	7.783	581	50.0
unknown3.150	3.150	105.4	ug/l	1225	1	7.783	581	50.0
unknown3.649	3.649	93.5	ug/l	1087	1	7.783	581	50.0
unknown15.281	15.281	92.8	ug/l	1065	4	13.416	574	50.0