

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052924\
 Data File : VY018401.D
 Acq On : 29 May 2024 15:52
 Operator : SY/MD
 Sample : P2612-10
 Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/B
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 72-11933

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\82Y052224S.M

Title : SW846 8260

Signal : TIC: VY018401.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.887	173	175	177	rBV2	849	756	2.46%	0.379%
2	3.064	199	204	205	rVB3	661	700	2.28%	0.351%
3	3.113	210	212	216	rVB5	551	644	2.10%	0.323%
4	3.308	242	244	248	rBV4	810	732	2.38%	0.367%
5	3.838	329	331	334	rBV2	727	765	2.49%	0.383%
6	3.899	338	341	343	rBV3	672	927	3.02%	0.464%
7	3.973	350	353	356	rBV3	773	1063	3.46%	0.533%
8	4.320	407	410	412	rBV3	897	1166	3.79%	0.584%
9	4.485	433	437	438	rBV3	600	701	2.28%	0.351%
10	5.045	527	529	532	rVB2	677	734	2.39%	0.368%
11	5.076	532	534	536	rBV2	867	841	2.74%	0.421%
12	5.155	544	547	549	rBV3	1112	852	2.77%	0.427%
13	5.277	561	567	569	rBV5	817	1137	3.70%	0.570%
14	5.369	580	582	585	rVB2	794	666	2.17%	0.334%
15	5.472	597	599	603	rVB3	999	948	3.08%	0.475%
16	5.515	603	606	608	rVB2	792	668	2.17%	0.335%
17	5.558	611	613	617	rVB5	790	960	3.12%	0.481%
18	5.625	621	624	626	rBV2	880	867	2.82%	0.434%
19	5.740	639	643	644	rBV2	953	1067	3.47%	0.535%
20	5.954	676	678	680	rBV3	760	702	2.28%	0.352%
21	6.338	740	741	746	rVB3	600	631	2.05%	0.316%
22	6.381	746	748	750	rBV2	523	654	2.13%	0.328%
23	6.503	765	768	771	rBV2	461	768	2.50%	0.385%
24	6.570	777	779	782	rVB3	741	698	2.27%	0.350%
25	6.856	824	826	828	rBV2	848	643	2.09%	0.322%
26	7.100	865	866	869	rBV2	568	635	2.07%	0.318%
27	7.307	895	900	902	rBV5	868	1410	4.59%	0.706%
28	7.368	905	910	912	rBV2	800	1432	4.66%	0.717%
29	7.545	936	939	942	rVB3	604	801	2.61%	0.401%
30	7.710	961	966	972	rBV4	3289	7256	23.61%	3.635%
31	7.783	972	978	986	rVB4	7937	18295	59.52%	9.165%
32	7.954	1003	1006	1009	rVB2	763	1154	3.75%	0.578%
33	8.008	1009	1015	1016	rBV2	745	1130	3.68%	0.566%
34	8.136	1029	1036	1042	rBV4	3699	8259	26.87%	4.138%
35	8.234	1046	1052	1053	rBV5	762	1089	3.54%	0.546%
36	8.295	1061	1062	1064	rVB	1031	632	2.06%	0.317%

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37	8.435	1081	1085	1087	rBV3	513	775	2.52%	0.388%
38	8.508	1095	1097	1100	rVB3	772	799	2.60%	0.400%
39	8.539	1100	1102	1104	rBV2	621	707	2.30%	0.354%
40	8.691	1116	1127	1136	rBV2	11450	27183	88.44%	13.618%
41	8.880	1155	1158	1159	rBV2	862	687	2.24%	0.344%
42	9.008	1176	1179	1181	rBV3	752	678	2.21%	0.340%
43	9.228	1212	1215	1217	rBV2	749	771	2.51%	0.386%
44	9.252	1217	1219	1221	rBV	603	667	2.17%	0.334%
45	9.368	1236	1238	1241	rBV2	483	657	2.14%	0.329%
46	9.484	1254	1257	1258	rBV2	660	748	2.43%	0.375%
47	9.593	1270	1275	1277	rBV2	644	946	3.08%	0.474%
48	9.721	1294	1296	1298	rBV2	901	752	2.45%	0.377%
49	9.813	1308	1311	1312	rBV2	980	653	2.12%	0.327%
50	10.002	1340	1342	1345	rVB4	829	982	3.19%	0.492%
51	10.038	1345	1348	1349	rBV3	725	678	2.21%	0.340%
52	10.112	1356	1360	1363	rVB5	695	994	3.23%	0.498%
53	10.179	1363	1371	1377	rBV	16206	30736	100.00%	15.398%
54	10.264	1380	1385	1387	rBV4	978	1372	4.46%	0.687%
55	10.691	1453	1455	1458	rVB2	596	706	2.30%	0.354%
56	10.910	1489	1491	1495	rBV	619	807	2.63%	0.404%
57	11.044	1510	1513	1518	rVB3	910	1331	4.33%	0.667%
58	11.105	1520	1523	1524	rVB2	823	697	2.27%	0.349%
59	11.276	1549	1551	1554	rVB2	938	850	2.77%	0.426%
60	11.410	1571	1573	1576	rVB2	947	642	2.09%	0.322%
61	11.489	1579	1586	1595	rBV	13913	24444	79.53%	12.246%
62	11.557	1595	1597	1601	rVB3	867	1219	3.97%	0.611%
63	11.593	1601	1603	1604	rBV3	642	677	2.20%	0.339%
64	11.758	1627	1630	1632	rBV4	873	1084	3.53%	0.543%
65	12.081	1681	1683	1685	rBV2	687	661	2.15%	0.331%
66	12.319	1721	1722	1725	rBV2	899	959	3.12%	0.480%
67	12.404	1733	1736	1738	rBV2	627	639	2.08%	0.320%
68	12.483	1744	1749	1754	rBV6	5668	10158	33.05%	5.089%
69	12.550	1758	1760	1762	rBV	728	679	2.21%	0.340%
70	12.593	1765	1767	1769	rBV	1051	975	3.17%	0.488%
71	12.703	1782	1785	1786	rBV3	800	756	2.46%	0.379%
72	13.166	1859	1861	1863	rBV3	948	756	2.46%	0.379%
73	13.251	1870	1875	1877	rBV	1038	982	3.19%	0.492%
74	13.428	1900	1904	1908	rBV3	4856	7003	22.78%	3.508%
75	13.556	1920	1925	1927	rBV3	1017	1455	4.73%	0.729%
76	14.019	1997	2001	2003	rVB3	619	696	2.26%	0.349%

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77	14.477	2074	2076	2079	rVB2	896	831	2.70%	0.416%
78	14.721	2110	2116	2117	rBV3	1211	1746	5.68%	0.875%
79	14.830	2131	2134	2135	rVB3	782	729	2.37%	0.365%
80	14.873	2139	2141	2145	rVB4	922	1152	3.75%	0.577%
81	14.995	2158	2161	2164	rBV4	531	729	2.37%	0.365%
82	15.178	2189	2191	2194	rVB2	624	789	2.57%	0.395%
83	15.300	2210	2211	2216	rBV4	976	859	2.79%	0.430%
84	15.513	2243	2246	2248	rBV2	568	643	2.09%	0.322%
85	16.080	2337	2339	2342	rBV2	657	789	2.57%	0.395%

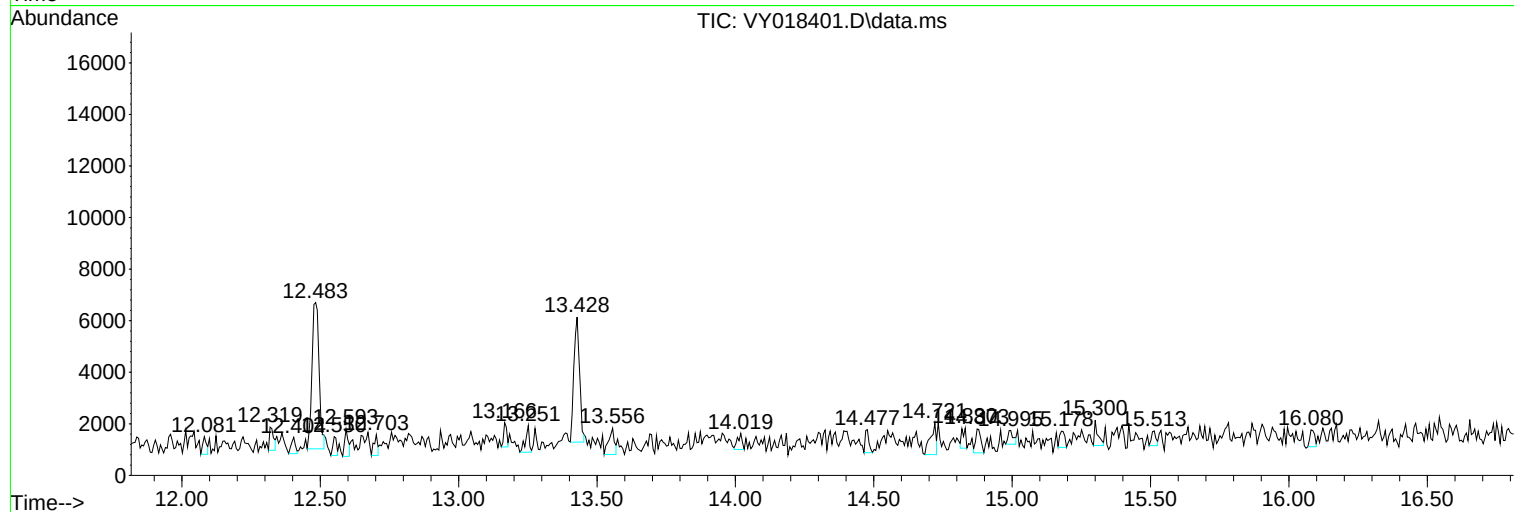
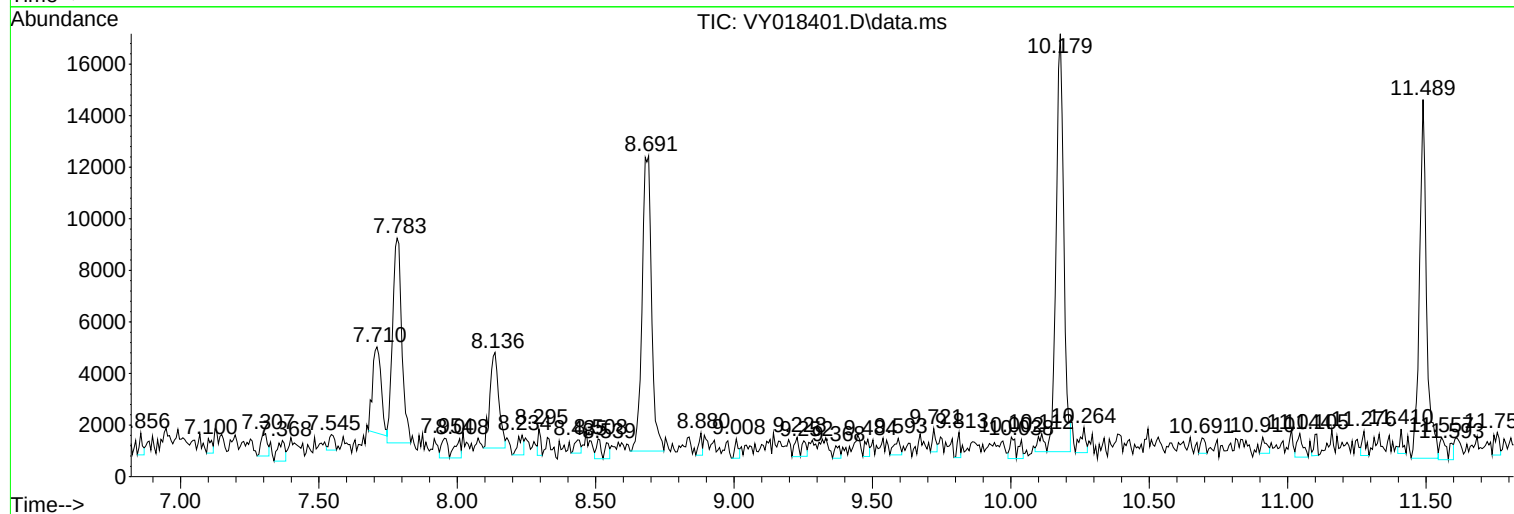
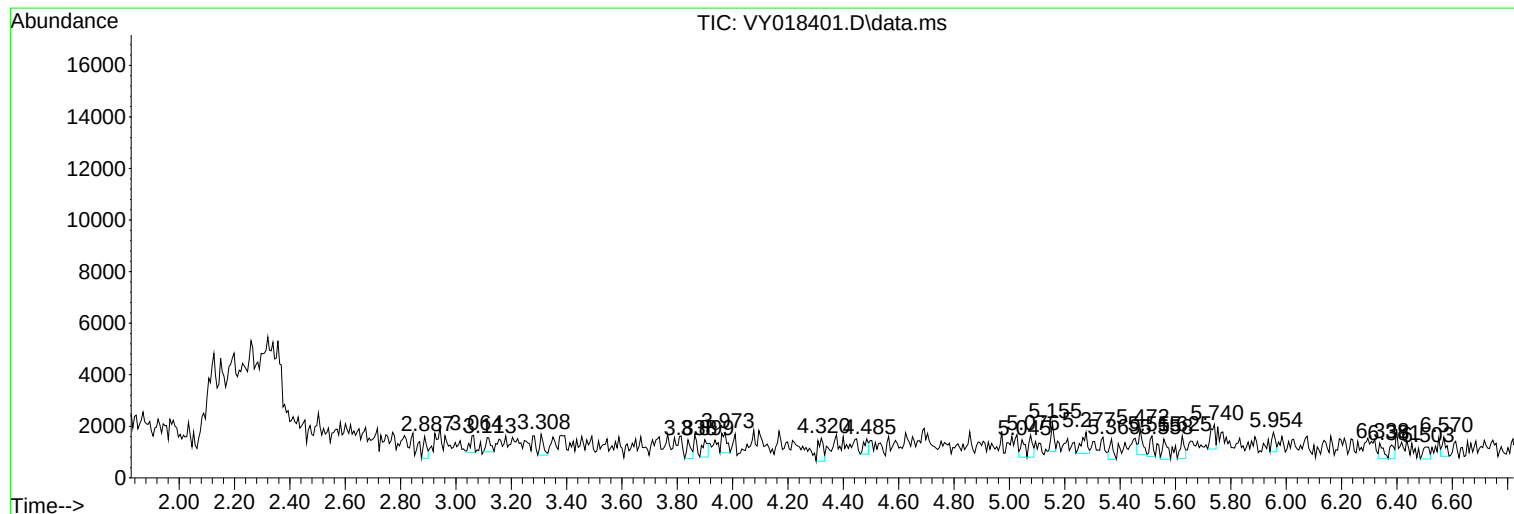
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Instrument :
MSVOA_Y
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052224S.M
Quant Title : SW846 8260

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



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Instrument :
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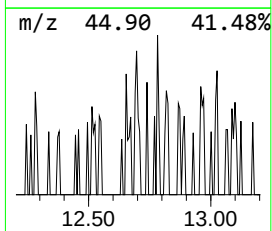
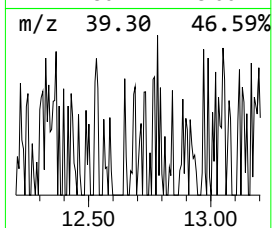
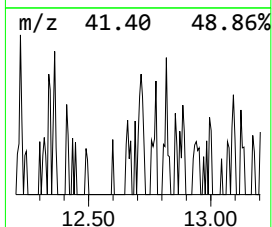
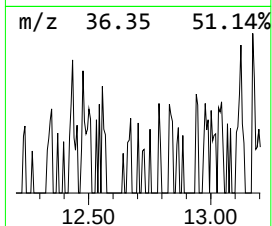
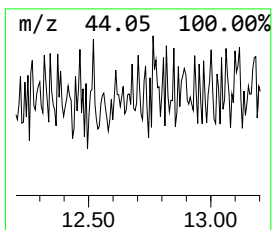
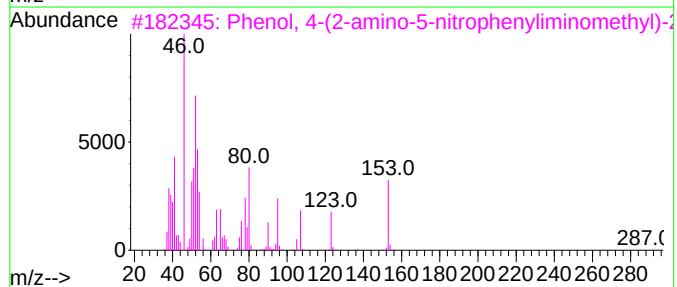
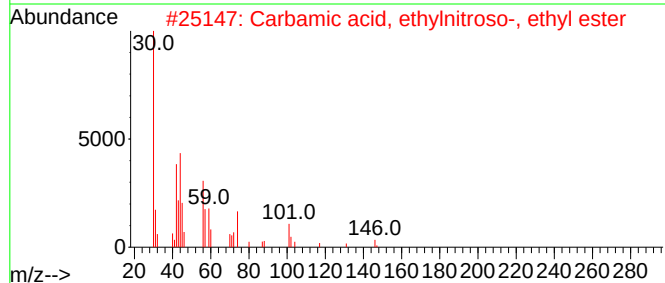
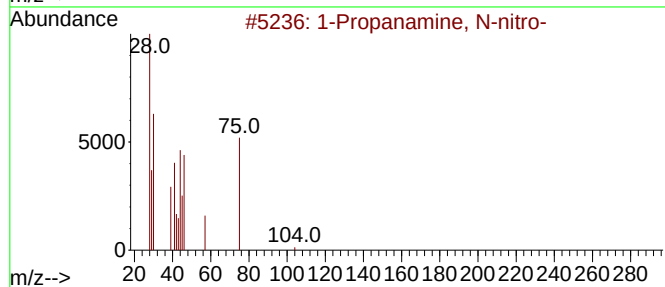
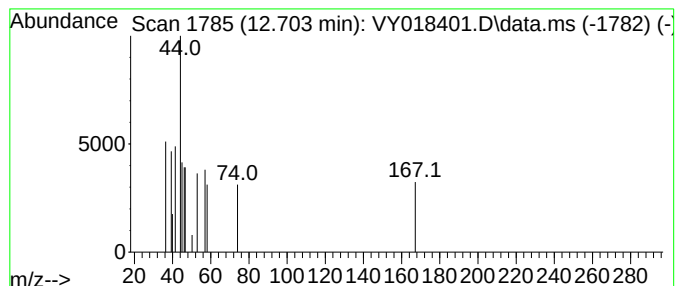
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052224S.M
Quant Title : SW846 8260

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

Peak Number 2 unknown12.703 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.703	5.40 ug/l	756	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanamine, N-nitro-	104	C3H8N2O2	000627-07-6	40
2			Carbamic acid, ethylnitroso-, et...	146	C5H10N2O3	000614-95-9	9
3			Phenol, 4-(2-amino-5-nitrophenyl...	287	C14H13N3O4	306744-56-9	9
4			Hydrazine, methyl-	46	CH6N2	000060-34-4	5
5			Thietane	74	C3H6S	000287-27-4	5



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Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
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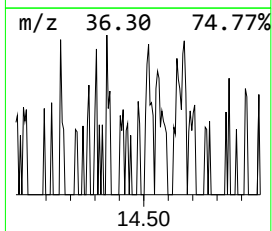
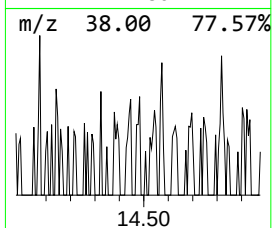
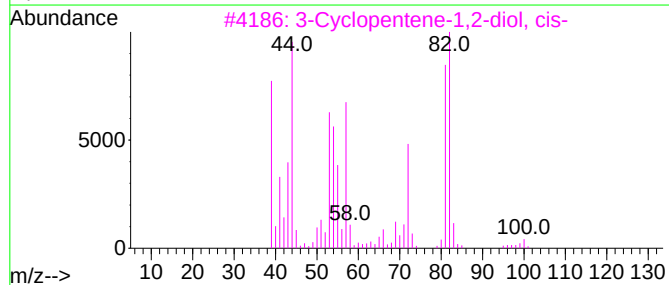
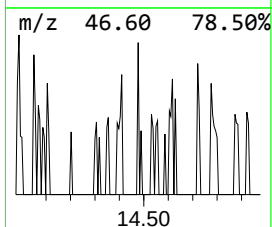
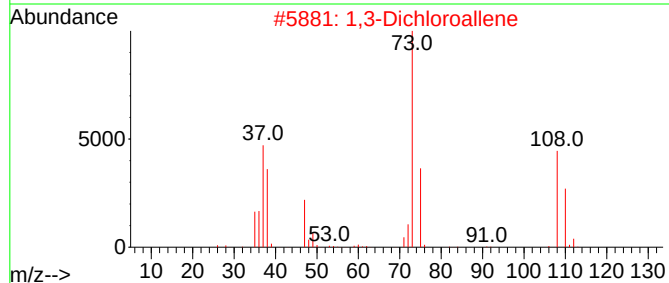
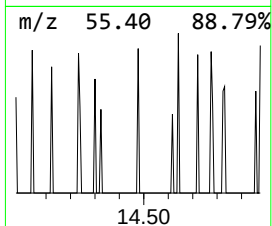
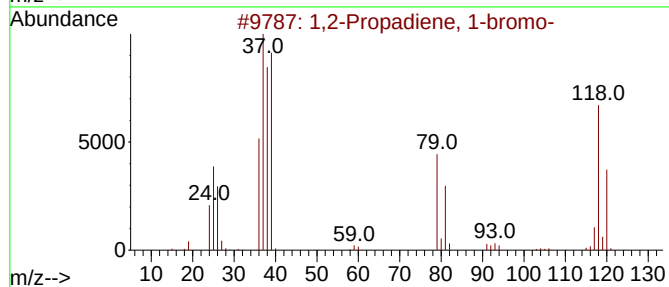
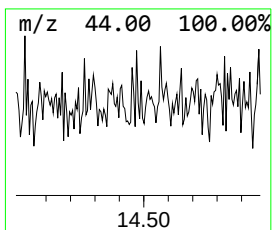
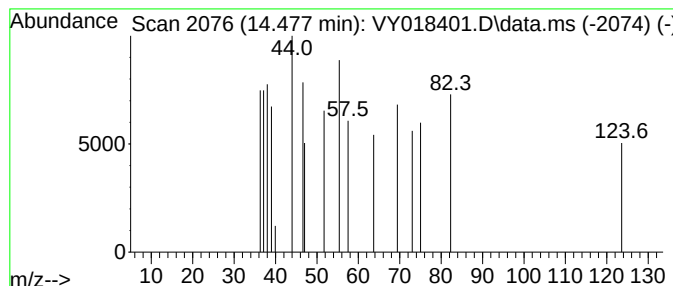
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052224S.M
Quant Title : SW846 8260

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

Peak Number 5 unknown14.477 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.477	5.93 ug/l	831	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1,2-Propadiene, 1-bromo-	118	C3H3Br	010024-18-7	23
2			1,3-Dichloroallene	108	C3H2Cl2	083682-32-0	23
3			3-Cyclopentene-1,2-diol, cis-	100	C5H8O2	000694-29-1	9
4			Tetrazolo[1,5-b]pyridazine	121	C4H3N5	000274-89-5	9
5			1,3-Butadiene, 1,1,2-trifluoro-	108	C4H3F3	000565-65-1	9



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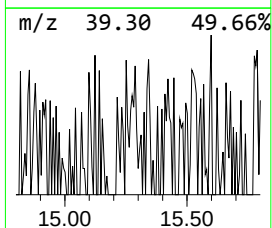
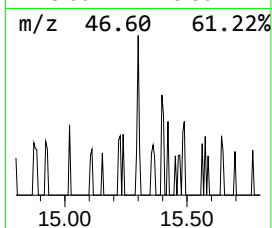
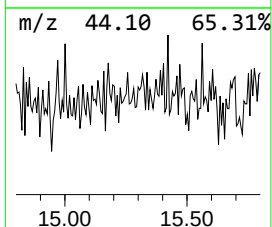
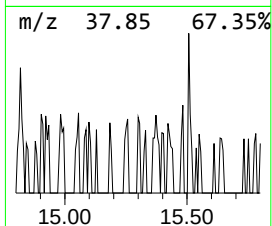
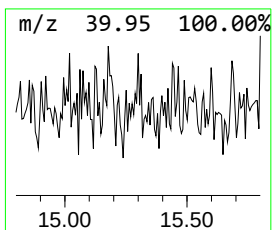
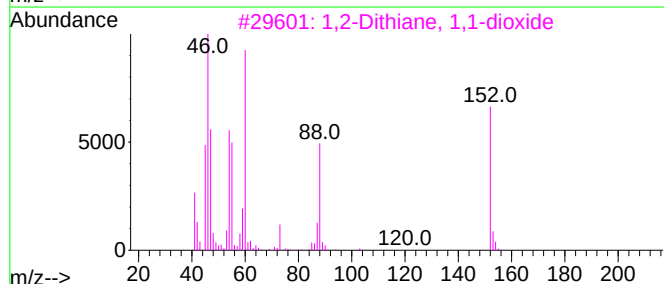
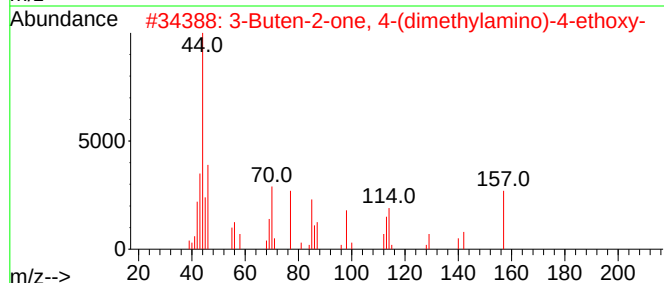
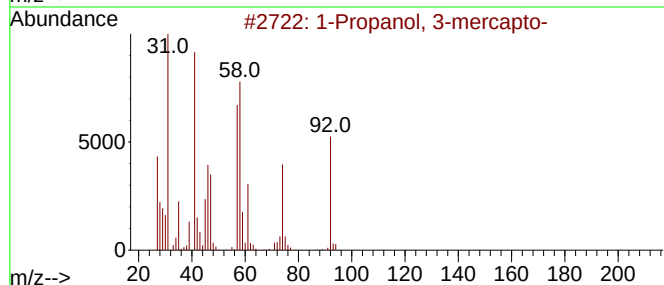
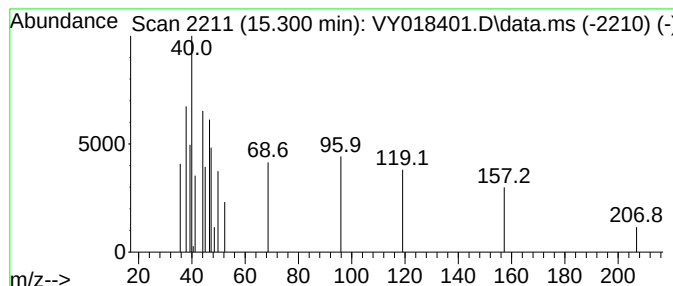
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052224S.M
Quant Title : SW846 8260

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

Peak Number 9 unknown15.300 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.300	6.13 ug/l	859	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Propanol, 3-mercapto-	92	C3H8OS	019721-22-3	12
2			3-Buten-2-one, 4-(dimethylamino)...	157	C8H15NO2	049582-71-0	9
3			1,2-Dithiane, 1,1-dioxide	152	C4H8O2S2	018321-15-8	9
4			Cystine	240	C6H12N2O4S2	000056-89-3	4
5			[1,2,5]-Oxadiazolo[3,4-b]pyrazin...	190	C4Cl2N4O	153493-48-2	4



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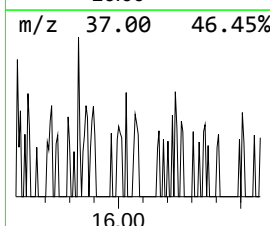
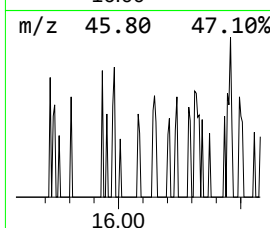
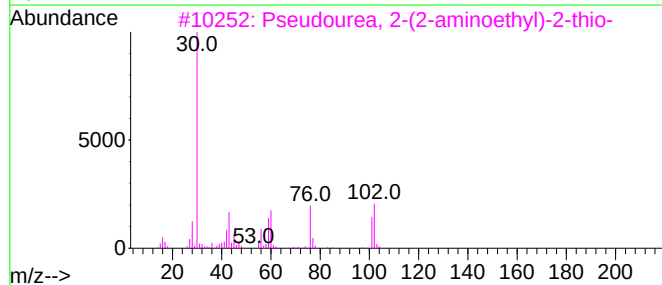
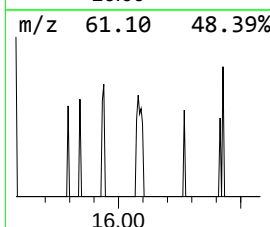
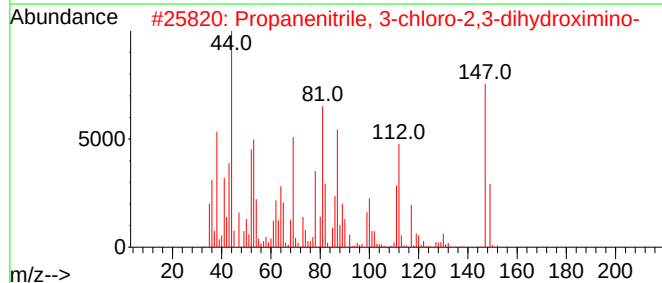
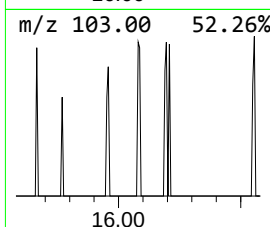
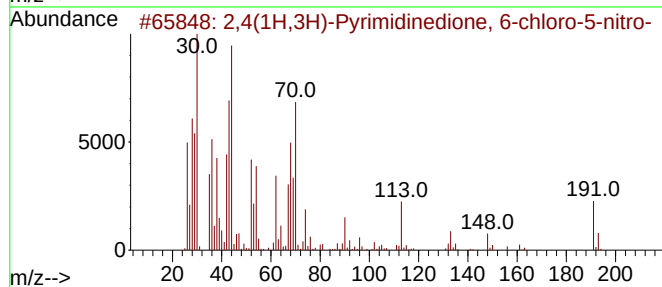
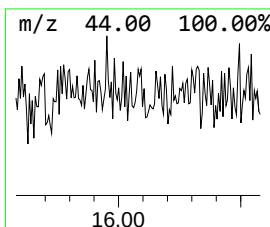
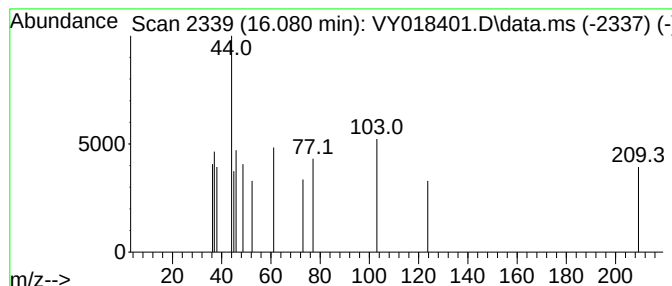
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052224S.M
Quant Title : SW846 8260

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

Peak Number 10 unknown16.080 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
16.080	5.63 ug/l	789	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2,4(1H,3H)-Pyrimidinedione, 6-ch...	191	C4H2ClN3O4	006630-30-4	25		
2	Propanenitrile, 3-chloro-2,3-dih...	147	C3H2ClN3O2	139912-33-7	9		
3	Pseudourea, 2-(2-aminoethyl)-2-t...	119	C3H9N3S	000151-16-6	4		
4	Pyridine-3-carboxamide, 1,2-dihy...	182	C8H10N2O5	079927-21-2	4		
5	3,4-Furandiyl, tetrahydro-, cis-	104	C4H8O3	004358-64-9	4		



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY052924\
Data File : VY018401.D
Acq On : 29 May 2024 15:52
Operator : SY/MD
Sample : P2612-10
Misc : 5.08g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
72-11933

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y052224S.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
unknown12.703	12.703	5.4	ug/l	756	4	13.422	7003	50.0
unknown14.477	14.477	5.9	ug/l	831	4	13.422	7003	50.0
unknown15.300	15.300	6.1	ug/l	859	4	13.422	7003	50.0
unknown16.080	16.080	5.6	ug/l	789	4	13.422	7003	50.0