

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060724\
 Data File : VY018531.D
 Acq On : 07 Jun 2024 16:54
 Operator : SY/MD
 Sample : P2707-08
 Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 CHA-1

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: VY018531.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.101	42	46	48	rBV4	2118	3173	13.05%	1.748%
2	2.473	104	107	108	rBV3	807	875	3.60%	0.482%
3	2.564	118	122	123	rBV4	718	928	3.82%	0.511%
4	2.912	177	179	182	rVB2	1072	851	3.50%	0.469%
5	2.954	182	186	189	rBV6	1170	2173	8.94%	1.197%
6	3.046	197	201	202	rBV3	717	934	3.84%	0.514%
7	3.204	220	227	228	rBV4	784	1266	5.21%	0.697%
8	3.326	244	247	250	rBV2	1093	1241	5.11%	0.684%
9	3.357	250	252	254	rVV3	917	885	3.64%	0.487%
10	3.418	261	262	265	rVB2	1111	958	3.94%	0.528%
11	3.460	265	269	270	rBV3	972	1209	4.97%	0.666%
12	3.546	279	283	286	rBV5	824	1334	5.49%	0.735%
13	3.692	303	307	312	rBV4	727	1380	5.68%	0.760%
14	4.155	381	383	386	rBV4	491	627	2.58%	0.345%
15	4.308	404	408	409	rBV3	880	797	3.28%	0.439%
16	4.515	438	442	444	rBV4	817	1210	4.98%	0.666%
17	4.667	464	467	468	rBV3	857	840	3.46%	0.463%
18	4.838	491	495	497	rBV2	790	787	3.24%	0.433%
19	4.984	517	519	522	rBV3	615	624	2.57%	0.344%
20	5.265	561	565	566	rBV3	653	899	3.70%	0.495%
21	5.460	594	597	598	rBV2	708	678	2.79%	0.373%
22	5.649	626	628	632	rBV4	992	994	4.09%	0.547%
23	5.789	649	651	655	rVV4	545	634	2.61%	0.349%
24	5.826	655	657	660	rVB	564	662	2.72%	0.365%
25	5.868	660	664	666	rVB4	1143	1588	6.53%	0.875%
26	6.307	735	736	739	rVB3	1083	677	2.79%	0.373%
27	7.033	854	855	859	rVB4	629	622	2.56%	0.343%
28	7.325	901	903	906	rVB2	762	685	2.82%	0.377%
29	7.374	908	911	913	rVV4	716	1069	4.40%	0.589%
30	7.435	917	921	922	rBV2	605	857	3.53%	0.472%
31	7.466	924	926	931	rVB5	720	1211	4.98%	0.667%
32	7.551	938	940	944	rVB2	814	931	3.83%	0.513%
33	7.703	958	965	971	rBV7	3850	10195	41.94%	5.615%
34	7.783	974	978	983	rVB4	4745	9024	37.13%	4.970%
35	7.844	986	988	990	rBV2	664	746	3.07%	0.411%
36	7.917	997	1000	1003	rBV3	711	676	2.78%	0.372%

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CHA-1

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Integrator: RTE

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37	7.972	1007	1009	1011	rBV2	820	624	2.57%	0.344%
38	8.039	1019	1020	1024	rVB3	813	737	3.03%	0.406%
39	8.136	1026	1036	1042	rBV3	4627	11431	47.03%	6.296%
40	8.484	1092	1093	1100	rVB4	943	1398	5.75%	0.770%
41	8.551	1100	1104	1105	rBV3	924	1126	4.63%	0.620%
42	8.685	1120	1126	1133	rVV3	6782	13399	55.13%	7.380%
43	8.904	1160	1162	1164	rBV2	791	687	2.83%	0.378%
44	9.093	1191	1193	1196	rBV3	661	837	3.44%	0.461%
45	9.289	1220	1225	1227	rBV2	657	896	3.69%	0.494%
46	9.471	1253	1255	1259	rBV4	637	736	3.03%	0.405%
47	9.801	1308	1309	1312	rBV3	828	767	3.16%	0.422%
48	9.929	1328	1330	1333	rVB	1260	1159	4.77%	0.638%
49	9.953	1333	1334	1337	rBV	1089	1028	4.23%	0.566%
50	10.014	1342	1344	1346	rVB	741	617	2.54%	0.340%
51	10.044	1346	1349	1351	rBV3	1005	1231	5.06%	0.678%
52	10.099	1354	1358	1359	rVB3	515	644	2.65%	0.355%
53	10.172	1363	1370	1378	rBV2	12515	24306	100.00%	13.387%
54	10.294	1388	1390	1391	rBV	730	667	2.74%	0.367%
55	10.709	1455	1458	1461	rBV3	920	1129	4.64%	0.622%
56	10.782	1469	1470	1473	rVB	979	729	3.00%	0.402%
57	10.916	1487	1492	1493	rBV3	581	851	3.50%	0.469%
58	11.063	1514	1516	1519	rBV3	724	630	2.59%	0.347%
59	11.209	1538	1540	1542	rVB2	921	780	3.21%	0.430%
60	11.227	1542	1543	1546	rBV	871	1037	4.27%	0.571%
61	11.392	1568	1570	1574	rBV3	1011	1182	4.86%	0.651%
62	11.434	1576	1577	1580	rVV3	758	777	3.20%	0.428%
63	11.489	1580	1586	1591	rVV3	7234	13756	56.60%	7.577%
64	11.532	1591	1593	1595	rVB	966	877	3.61%	0.483%
65	11.648	1610	1612	1614	rBV	645	789	3.25%	0.435%
66	11.697	1617	1620	1621	rVV3	823	909	3.74%	0.501%
67	11.739	1625	1627	1629	rVB2	815	702	2.89%	0.387%
68	11.886	1648	1651	1653	rVB2	855	811	3.34%	0.447%
69	11.934	1656	1659	1662	rVB3	707	702	2.89%	0.387%
70	11.983	1662	1667	1670	rBV5	713	1008	4.15%	0.555%
71	12.081	1681	1683	1687	rBV3	532	733	3.02%	0.404%
72	12.337	1721	1725	1727	rBV4	542	686	2.82%	0.378%
73	12.483	1745	1749	1755	rVB6	5078	8813	36.26%	4.854%
74	12.581	1762	1765	1769	rVB3	1092	1225	5.04%	0.675%
75	12.776	1793	1797	1798	rBV	608	759	3.12%	0.418%
76	12.849	1807	1809	1811	rBV2	707	714	2.94%	0.393%

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77	12.910	1814	1819	1821	rBV4	843	1219	5.02%	0.671%
78	13.032	1835	1839	1842	rBV4	938	1361	5.60%	0.750%
79	13.251	1870	1875	1876	rVB3	631	831	3.42%	0.458%
80	13.294	1880	1882	1885	rVB2	847	724	2.98%	0.399%
81	13.324	1885	1887	1889	rBV2	667	738	3.04%	0.406%
82	13.422	1899	1903	1909	rBV4	3276	5198	21.39%	2.863%
83	13.471	1909	1911	1913	rVB	872	687	2.83%	0.378%
84	13.507	1913	1917	1919	rBV4	631	910	3.74%	0.501%
85	13.526	1919	1920	1924	rVB2	665	677	2.79%	0.373%
86	13.708	1948	1950	1951	rBV2	1066	626	2.58%	0.345%
87	13.794	1962	1964	1967	rBV	958	1200	4.94%	0.661%
88	14.190	2027	2029	2032	rVB	937	1107	4.55%	0.610%
89	14.245	2032	2038	2040	rVB2	827	1152	4.74%	0.635%
90	14.269	2040	2042	2044	rBV2	1009	947	3.90%	0.522%
91	14.373	2057	2059	2062	rBV2	558	701	2.88%	0.386%
92	14.617	2095	2099	2100	rBV2	746	766	3.15%	0.422%
93	14.885	2140	2143	2145	rBV3	746	882	3.63%	0.486%
94	15.306	2211	2212	2215	rBV2	1082	1038	4.27%	0.572%
95	15.513	2243	2246	2249	rBV3	860	945	3.89%	0.520%
96	15.629	2262	2265	2267	rVB3	630	859	3.53%	0.473%
97	15.653	2267	2269	2271	rBV2	1038	755	3.11%	0.416%
98	15.702	2274	2277	2279	rBV4	575	617	2.54%	0.340%
99	15.842	2298	2300	2302	rBV2	709	713	2.93%	0.393%
100	15.903	2307	2310	2312	rBV3	847	777	3.20%	0.428%

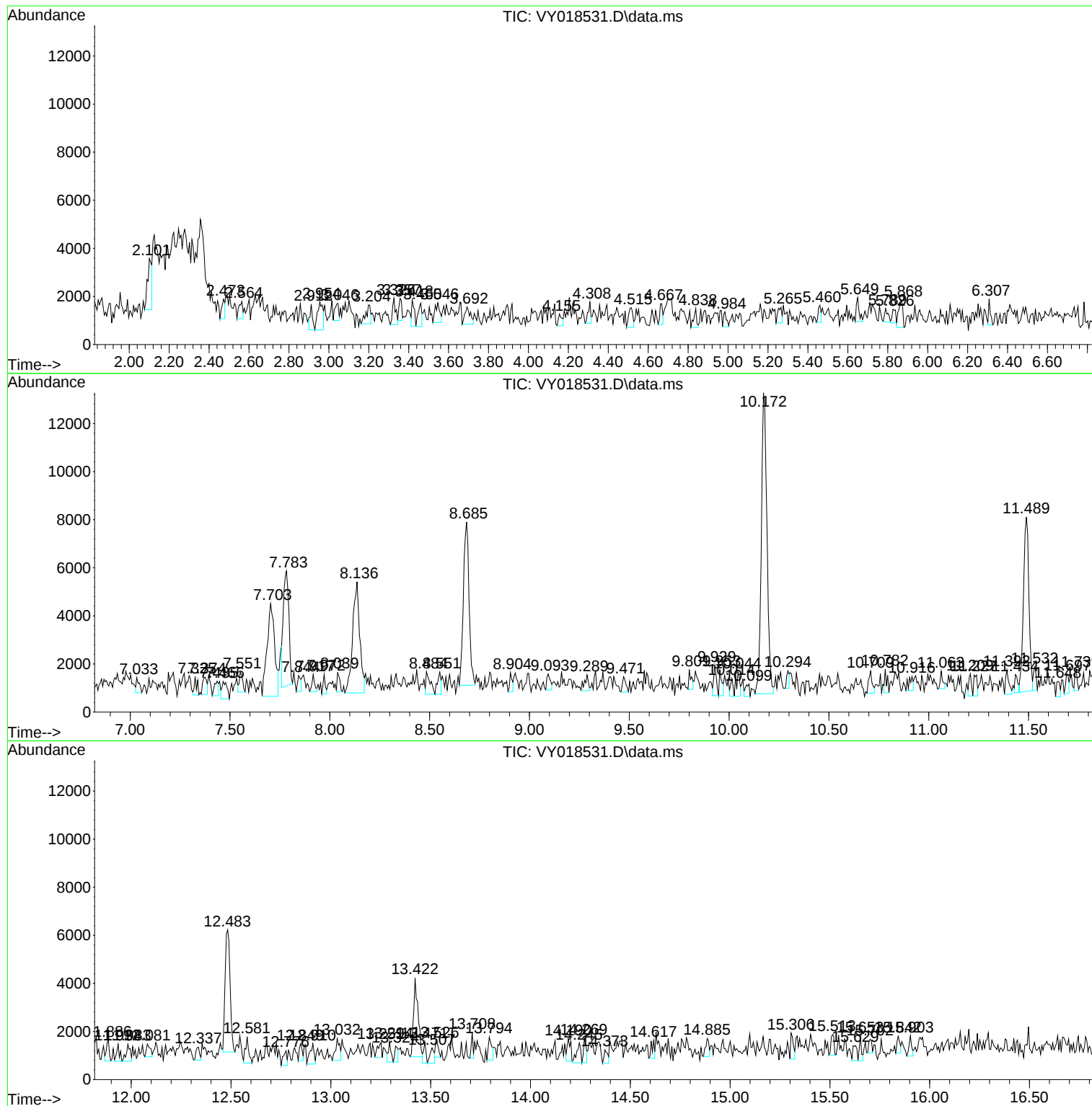
Sum of corrected areas: 181559

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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



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Instrument :
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CHA-1

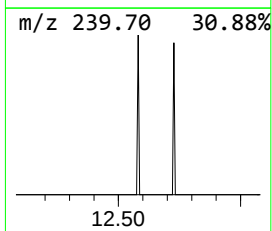
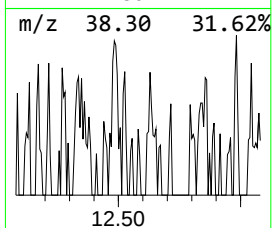
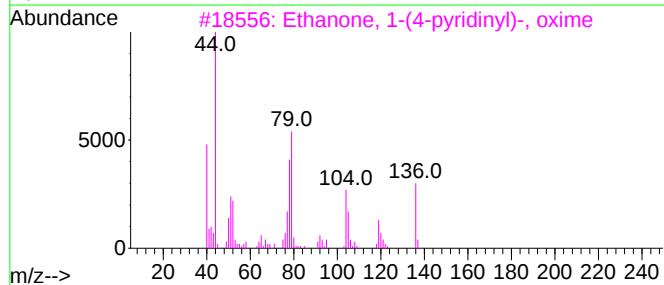
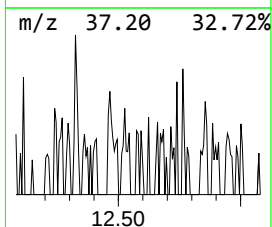
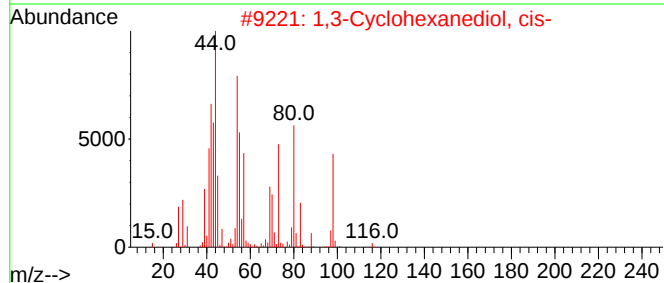
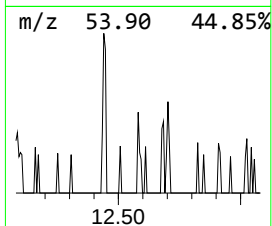
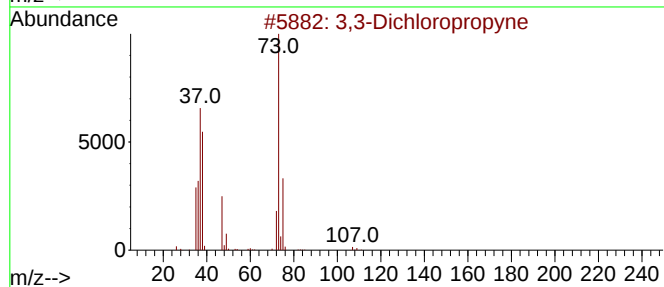
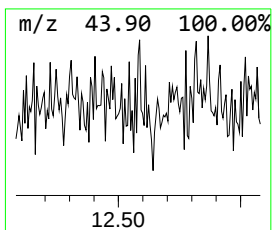
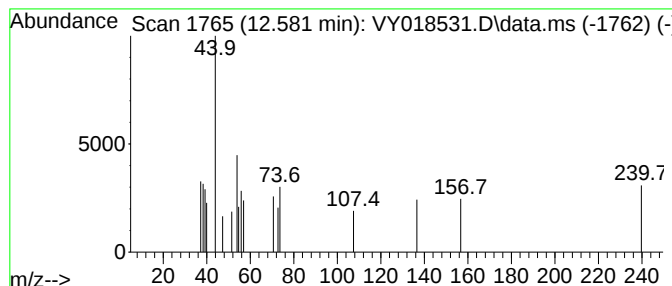
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060324S.M
Quant Title : SW846 8260

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

Peak Number 3 unknown12.581 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.581	11.78 ug/l	1225	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3,3-Dichloropropyne	108	C3H2Cl2	025523-14-2	17
2			1,3-Cyclohexanediol, cis-	116	C6H12O2	000823-18-7	10
3			Ethanone, 1-(4-pyridinyl)-, oxime	136	C7H8N2O	001194-99-6	9
4			3,3'-Iminobispropylamine	131	C6H17N3	000056-18-8	9
5			1,3-Dichloroallene	108	C3H2Cl2	083682-32-0	9



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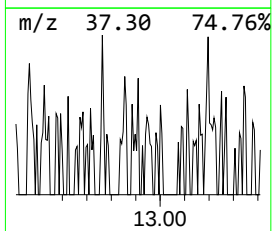
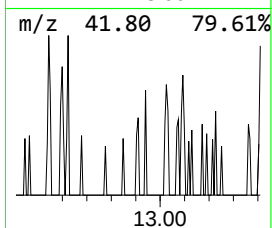
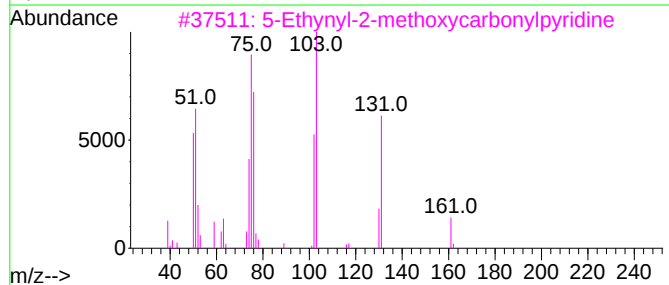
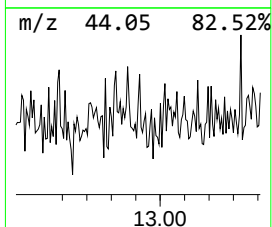
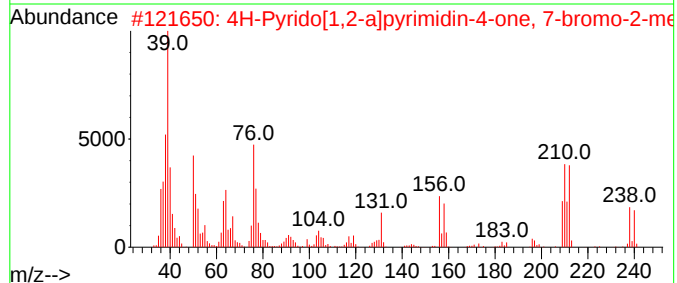
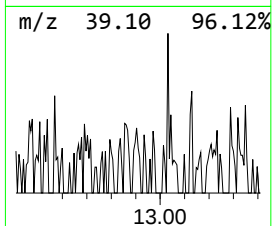
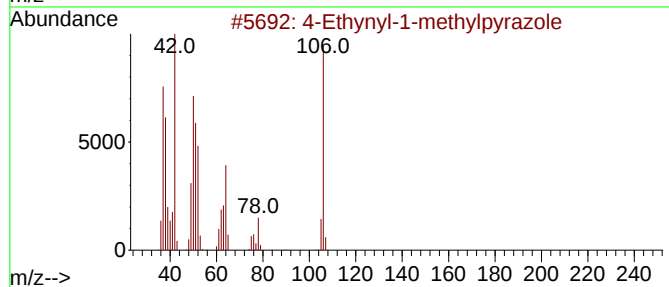
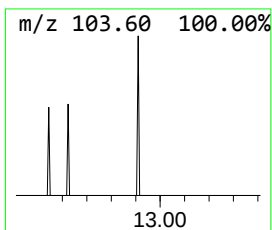
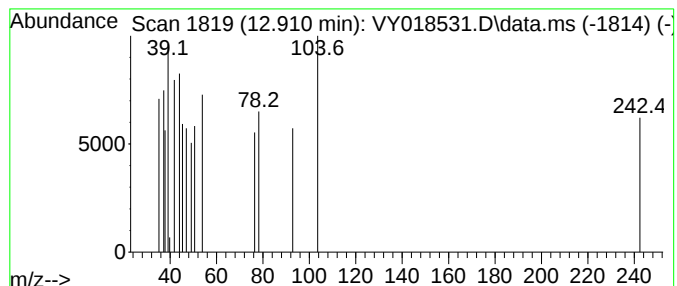
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060324S.M
Quant Title : SW846 8260

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

Peak Number 4 unknown12.910 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.910	11.73 ug/l	1219	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			4-Ethynyl-1-methylpyrazole	106	C6H6N2	039806-89-8	37
2			4H-Pyrido[1,2-a]pyrimidin-4-one,...	238	C9H7BrN2O	064500-11-4	32
3			5-Ethynyl-2-methoxycarbonylpyridine	161	C9H7N02	017880-61-4	9
4			2(3H)-Benzoxazolone, 6-chloro-	169	C7H4ClN02	019932-84-4	9
5			2H-Pyran-5-carboxylic acid, 2-oxo-	140	C6H4O4	000500-05-0	9



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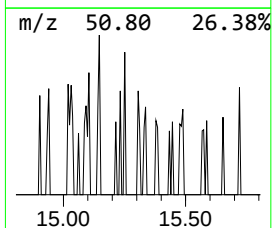
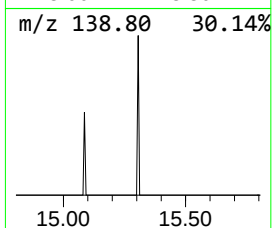
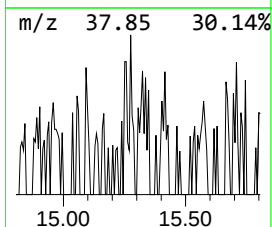
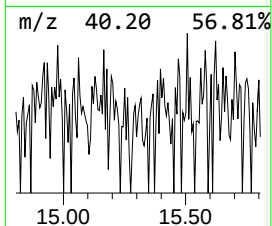
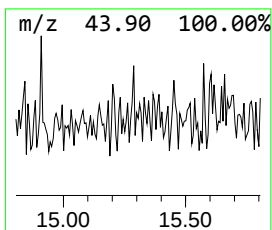
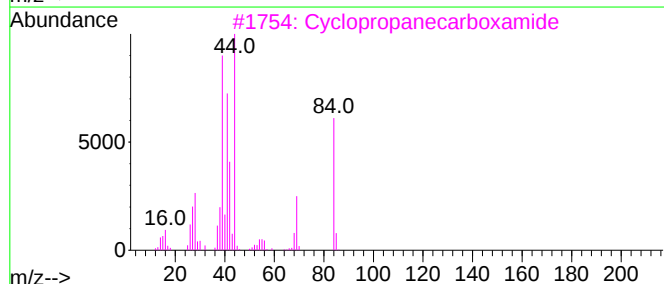
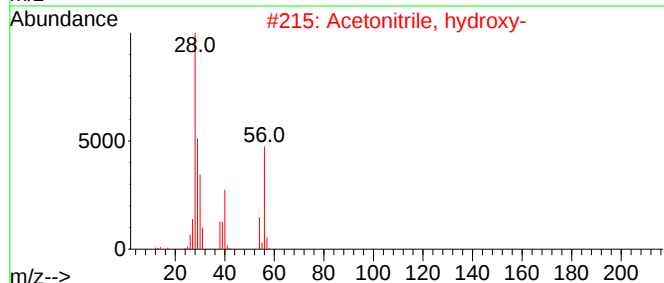
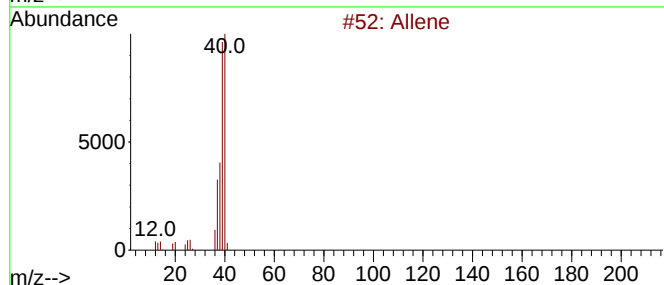
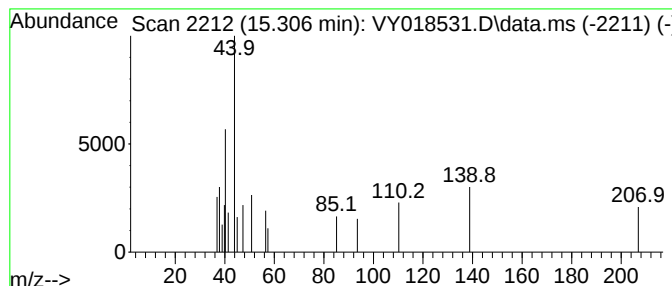
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y060324S.M
Quant Title : SW846 8260

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

Peak Number 10 unknown15.306 Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.306	9.98 ug/l	1038	1,4-Dichlorobenzene-d4	13.428

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Allene	40	C3H4	000463-49-0	12
2			Acetonitrile, hydroxy-	57	C2H3NO	000107-16-4	9
3			Cyclopropanecarboxamide	85	C4H7NO	006228-73-5	9
4			Propanal, 2,2-dimethyl-, oxime	101	C5H11NO	000637-91-2	9
5			1-Tetradecanamine	213	C14H31N	002016-42-4	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY060724\
Data File : VY018531.D
Acq On : 07 Jun 2024 16:54
Operator : SY/MD
Sample : P2707-08
Misc : 5.03g/5.0mL/MSVOA_Y/SOIL/B
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
CHA-1

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
unknown12.581	12.581	11.8	ug/l	1225	4	13.428	5198	50.0
unknown12.910	12.910	11.7	ug/l	1219	4	13.428	5198	50.0
unknown15.306	15.306	10.0	ug/l	1038	4	13.428	5198	50.0