

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102824\
 Data File : VY020036.D
 Acq On : 28 Oct 2024 13:06
 Operator : SY/MD
 Sample : P4578-05
 Misc : 7.93g/5.0mL/MSVOA_Y/SOIL/A
 ALS Vial : 9 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 WB-305-BOT

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\82Y1009245.M

Title : SW846 8260

Signal : TIC: VY020036.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.928	31	34	35	rBV	882	905	1.21%	0.197%
2	2.019	48	49	52	rVB2	1245	921	1.23%	0.200%
3	2.068	52	57	58	rBV2	3317	4329	5.77%	0.942%
4	2.220	78	82	84	rBV3	1888	2598	3.46%	0.565%
5	2.397	109	111	114	rBV3	850	863	1.15%	0.188%
6	2.678	155	157	160	rBV3	903	1022	1.36%	0.222%
7	3.074	219	222	225	rVB3	766	1099	1.46%	0.239%
8	3.525	293	296	301	rVB4	756	941	1.25%	0.205%
9	3.714	324	327	330	rVB3	842	991	1.32%	0.216%
10	3.903	356	358	361	rVB2	1326	1246	1.66%	0.271%
11	3.940	361	364	365	rBV	746	942	1.26%	0.205%
12	4.598	469	472	473	rVV	1029	897	1.20%	0.195%
13	4.616	473	475	479	rVB3	929	1140	1.52%	0.248%
14	4.939	526	528	532	rBV3	807	1230	1.64%	0.268%
15	5.549	624	628	630	rBV3	851	1017	1.36%	0.221%
16	5.787	665	667	671	rVB2	658	935	1.25%	0.203%
17	5.915	684	688	691	rBV3	857	1347	1.80%	0.293%
18	6.061	708	712	717	rVB3	713	1195	1.59%	0.260%
19	6.110	717	720	722	rBV2	823	849	1.13%	0.185%
20	6.220	735	738	742	rBV3	751	1113	1.48%	0.242%
21	6.281	744	748	752	rBV3	610	1105	1.47%	0.240%
22	6.732	818	822	825	rVB3	878	1162	1.55%	0.253%
23	6.774	825	829	832	rVB3	721	876	1.17%	0.191%
24	6.841	835	840	842	rBV2	932	1132	1.51%	0.246%
25	7.104	877	883	886	rVB3	844	1376	1.83%	0.299%
26	7.421	932	935	938	rBV3	1299	1599	2.13%	0.348%
27	7.634	962	970	976	rBV2	9967	24198	32.25%	5.263%
28	7.713	976	983	992	rVB2	23114	53617	71.47%	11.662%
29	7.945	1018	1021	1025	rBV3	802	1499	2.00%	0.326%
30	8.055	1032	1039	1041	rBV5	7121	11600	15.46%	2.523%
31	8.183	1056	1060	1061	rVB2	812	875	1.17%	0.190%
32	8.500	1109	1112	1115	rBV3	631	1023	1.36%	0.223%
33	8.616	1125	1131	1139	rVV2	30885	65548	87.37%	14.257%
34	8.670	1139	1140	1143	rVB3	922	845	1.13%	0.184%
35	8.859	1166	1171	1174	rVB2	767	1099	1.46%	0.239%
36	9.268	1235	1238	1244	rVB3	513	845	1.13%	0.184%

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Integration Parameters: RTEINT.P

Integrator: RTE

Smoothing : ON

Sampling : 1

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Stop Thrs : 0

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Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y1009245.M
Title : SW846 8260

37	9.743	1311	1316	1318	rBV2	786	1130	1.51%	0.246%
38	10.109	1367	1376	1384	rBV	41768	75021	100.00%	16.317%
39	10.201	1390	1391	1394	rBV2	1010	1118	1.49%	0.243%
40	10.286	1403	1405	1408	rBV3	1174	1438	1.92%	0.313%
41	10.469	1432	1435	1438	rBV3	1103	1402	1.87%	0.305%
42	10.505	1438	1441	1444	rVV3	1073	1201	1.60%	0.261%
43	10.566	1448	1451	1454	rBV3	834	1020	1.36%	0.222%
44	10.707	1469	1474	1477	rVB3	540	855	1.14%	0.186%
45	10.841	1494	1496	1501	rBV5	599	1085	1.45%	0.236%
46	10.981	1515	1519	1523	rBV2	867	1565	2.09%	0.340%
47	11.103	1537	1539	1541	rBV	1264	1236	1.65%	0.269%
48	11.328	1573	1576	1582	rVB4	942	1478	1.97%	0.321%
49	11.414	1582	1590	1603	rBV2	26774	51414	68.53%	11.182%
50	11.536	1608	1610	1615	rBV	1143	1336	1.78%	0.291%
51	11.603	1615	1621	1622	rBV2	585	960	1.28%	0.209%
52	11.652	1627	1629	1632	rVB3	833	945	1.26%	0.206%
53	11.810	1651	1655	1656	rBV3	1106	971	1.29%	0.211%
54	11.950	1676	1678	1680	rBV2	800	875	1.17%	0.190%
55	12.139	1707	1709	1712	rBV2	644	1031	1.37%	0.224%
56	12.414	1747	1754	1760	rVB4	17594	33588	44.77%	7.305%
57	12.554	1774	1777	1778	rVB2	1213	1004	1.34%	0.218%
58	12.597	1782	1784	1788	rBV4	1827	3252	4.33%	0.707%
59	12.639	1789	1791	1796	rVV5	1433	2828	3.77%	0.615%
60	12.737	1804	1807	1809	rBV4	815	925	1.23%	0.201%
61	12.968	1842	1845	1849	rVB2	1279	1253	1.67%	0.273%
62	12.999	1849	1850	1853	rBV2	1183	1310	1.75%	0.285%
63	13.035	1855	1856	1858	rVV2	932	901	1.20%	0.196%
64	13.090	1862	1865	1867	rBV2	1274	1275	1.70%	0.277%
65	13.261	1889	1893	1894	rBV2	814	1194	1.59%	0.260%
66	13.304	1894	1900	1903	rVV2	1201	2304	3.07%	0.501%
67	13.346	1903	1907	1913	rVV3	7588	13782	18.37%	2.998%
68	13.584	1945	1946	1949	rVB2	1192	869	1.16%	0.189%
69	13.804	1977	1982	1983	rBV4	1630	1870	2.49%	0.407%
70	13.822	1983	1985	1990	rVV5	1584	2696	3.59%	0.586%
71	13.883	1990	1995	2000	rVV2	7051	11591	15.45%	2.521%
72	13.987	2007	2012	2013	rBV4	1095	1699	2.26%	0.370%
73	14.090	2026	2029	2032	rBV3	882	1119	1.49%	0.243%
74	14.200	2044	2047	2048	rBV3	1191	1192	1.59%	0.259%
75	14.255	2052	2056	2059	rVB6	2620	3483	4.64%	0.758%
76	14.450	2084	2088	2090	rBV4	770	1330	1.77%	0.289%

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Integration Parameters: RTEINT.P

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Max Peaks: 100

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
Title : SW846 8260

77	14.486	2092	2094	2096	rVB3	1241	1098	1.46%	0.239%
78	14.541	2099	2103	2105	rBV4	2398	3824	5.10%	0.832%
79	14.602	2111	2113	2117	rVB4	958	1249	1.66%	0.272%
80	14.682	2123	2126	2128	rBV4	1083	1123	1.50%	0.244%
81	14.858	2152	2155	2159	rBV6	971	1382	1.84%	0.301%
82	14.992	2173	2177	2181	rBV4	736	940	1.25%	0.204%
83	15.084	2189	2192	2193	rBV3	637	848	1.13%	0.184%
84	15.322	2229	2231	2232	rBV2	1064	861	1.15%	0.187%
85	15.340	2232	2234	2238	rVV4	1745	1681	2.24%	0.366%
86	15.486	2255	2258	2260	rVB4	901	1194	1.59%	0.260%
87	15.523	2260	2264	2266	rBV4	1040	1671	2.23%	0.363%
88	15.547	2266	2268	2272	rVB4	868	1245	1.66%	0.271%
89	15.681	2289	2290	2295	rVB5	821	891	1.19%	0.194%
90	15.724	2295	2297	2299	rBV2	879	943	1.26%	0.205%
91	15.809	2309	2311	2313	rBV3	788	961	1.28%	0.209%
92	15.864	2318	2320	2322	rBV2	905	852	1.14%	0.185%
93	15.986	2336	2340	2341	rBV2	1434	1265	1.69%	0.275%
94	16.035	2344	2348	2351	rBV5	1351	1919	2.56%	0.417%
95	16.364	2399	2402	2404	rBV3	981	1124	1.50%	0.244%
96	16.547	2426	2432	2434	rVB4	1145	1276	1.70%	0.278%
97	16.596	2436	2440	2443	rBV5	523	886	1.18%	0.193%
98	16.645	2446	2448	2450	rBV	733	858	1.14%	0.187%
99	16.693	2454	2456	2459	rVB3	1049	1113	1.48%	0.242%
100	16.730	2459	2462	2463	rBV2	1078	1046	1.39%	0.228%

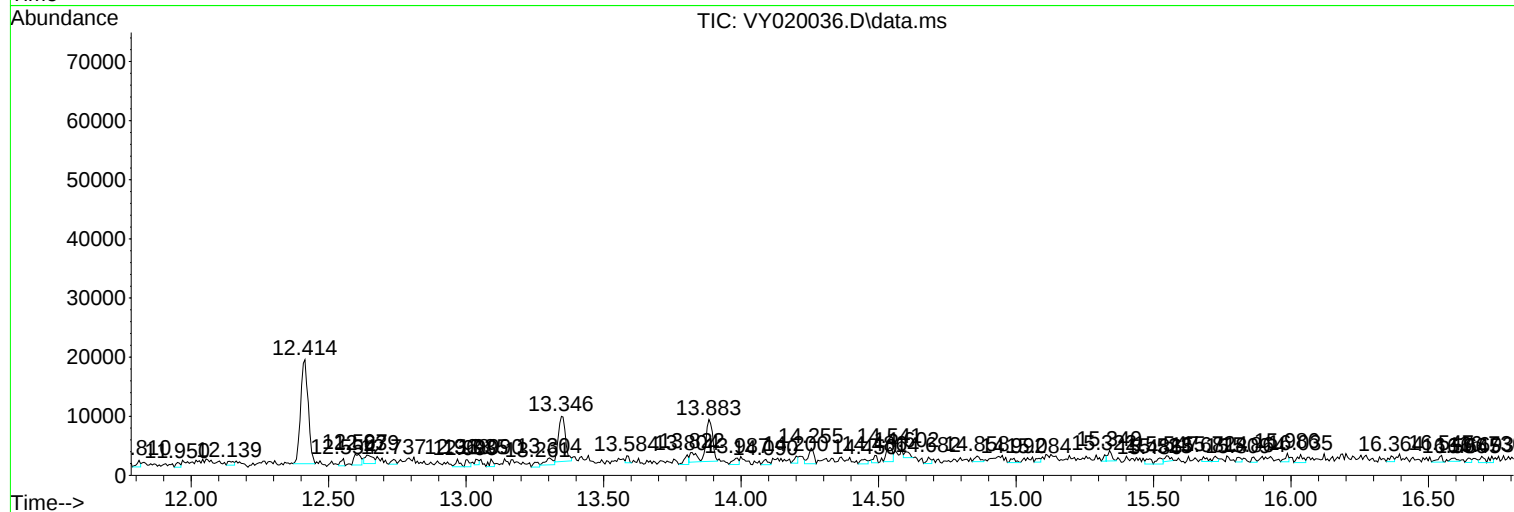
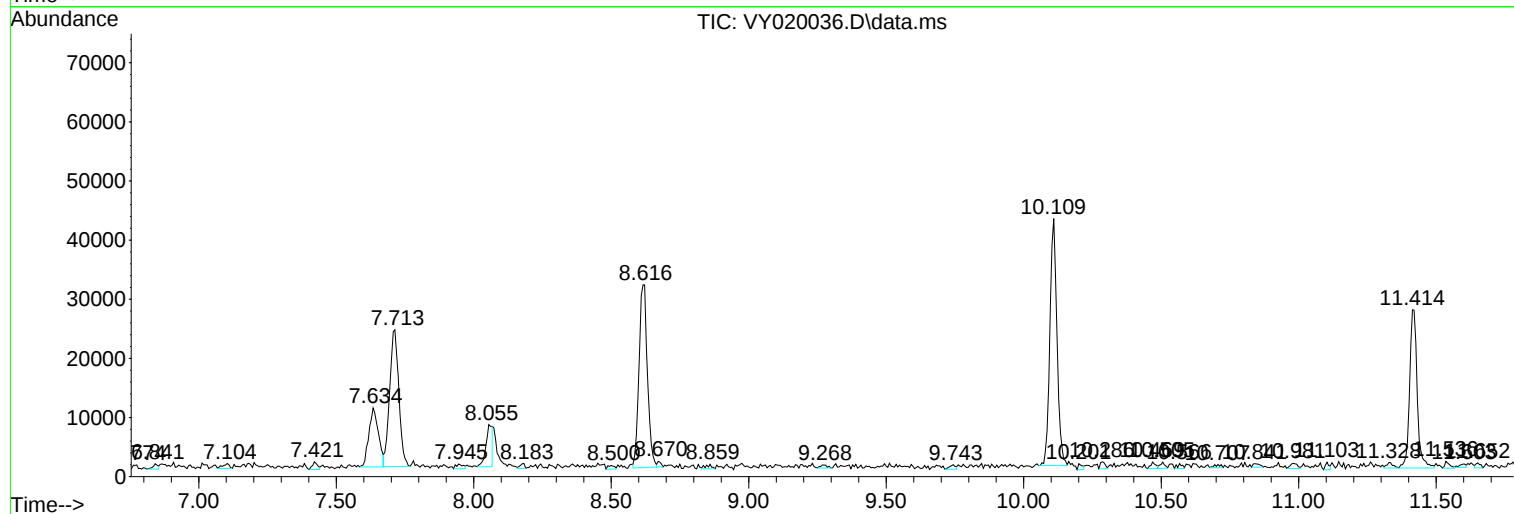
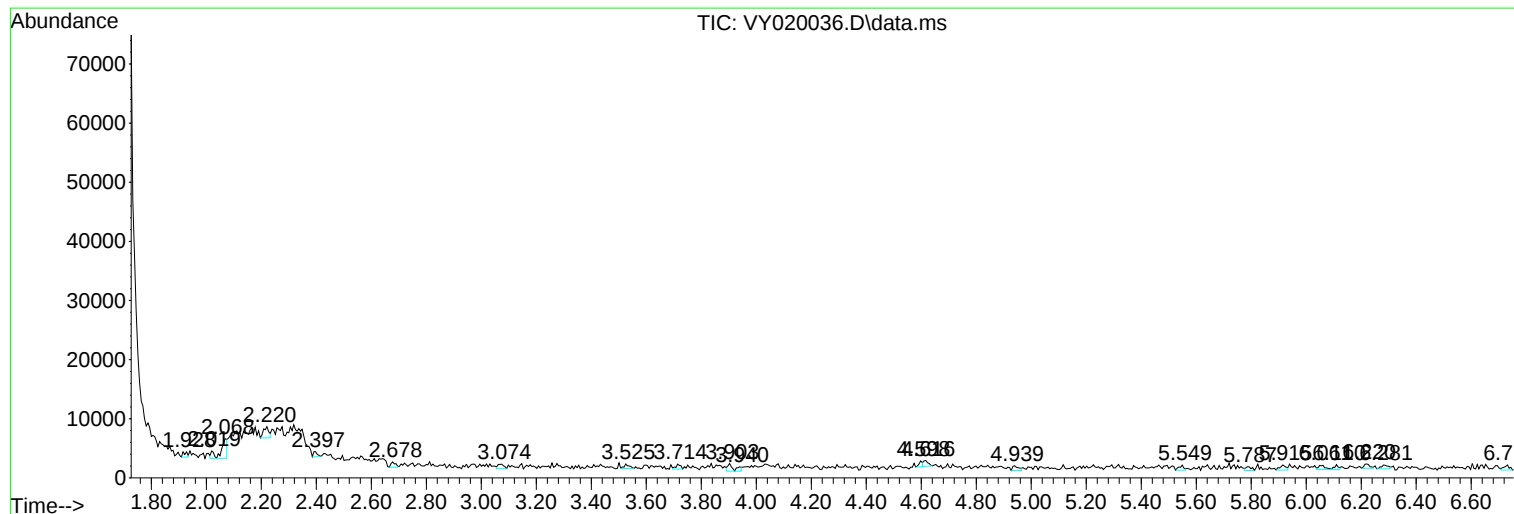
Sum of corrected areas: 459775

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
Quant Title : SW846 8260

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



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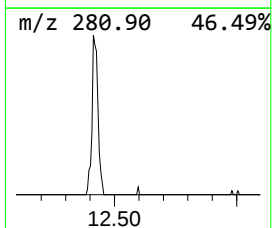
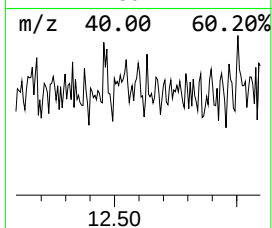
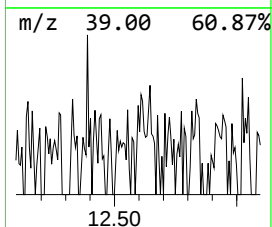
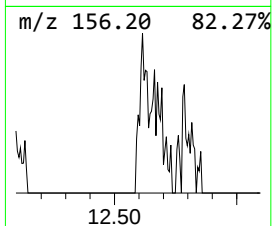
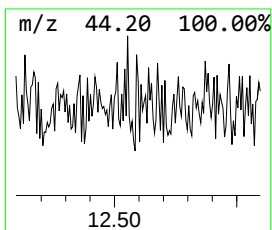
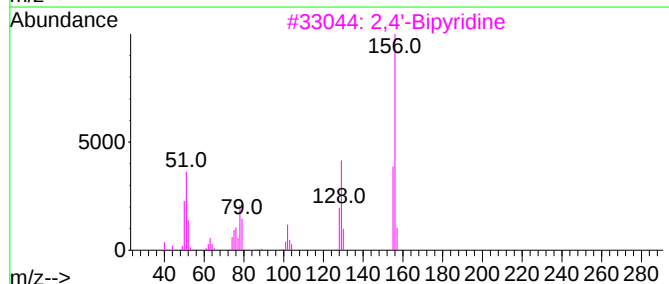
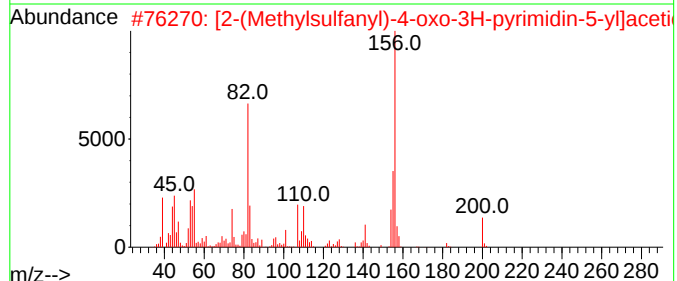
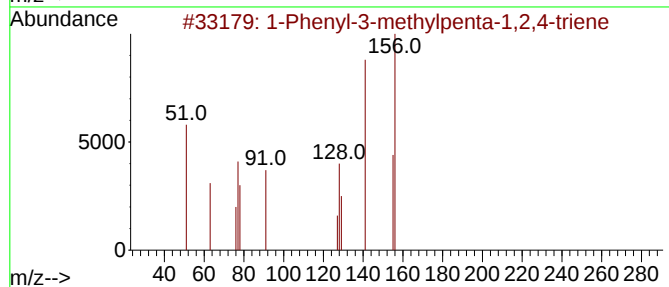
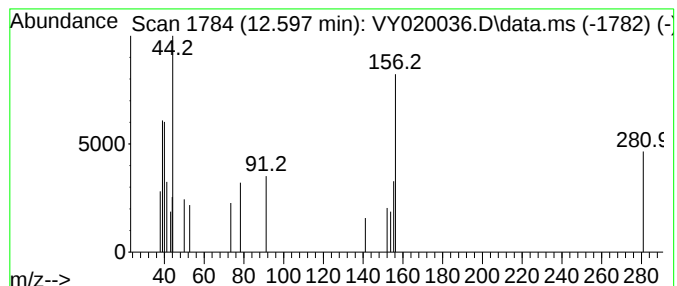
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
Quant Title : SW846 8260

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

Peak Number 1 unknown12.597 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.597	11.80 ug/l	3252	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Phenyl-3-methylpenta-1,2,4-triene	156	C12H12	093247-38-2	37
2			[2-(Methylsulfanyl)-4-oxo-3H-pyr...	200	C7H8N2O3S	1000435-23-0	10
3			2,4'-Bipyridine	156	C10H8N2	000581-47-5	9
4			Benzene, 1,3-cyclohexadien-1-yl-	156	C12H12	015619-32-6	9
5			Benzyl alcohol, 4-methoxy-6-fluoro-	156	C8H9FO2	000405-09-4	9



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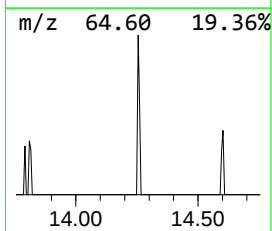
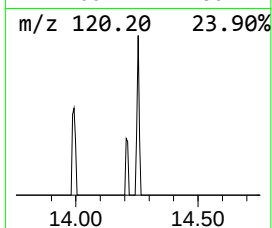
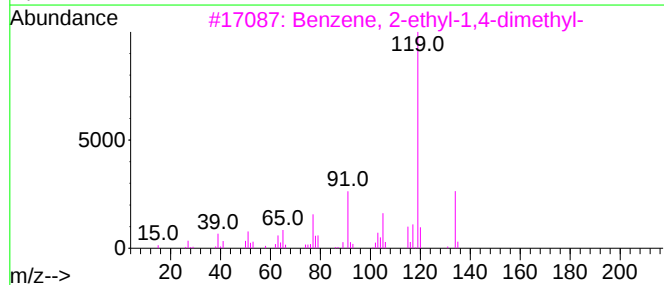
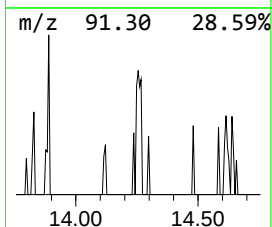
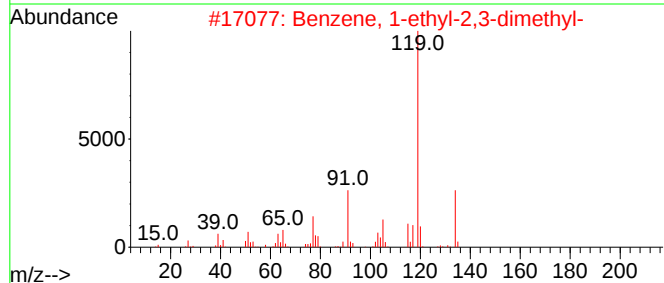
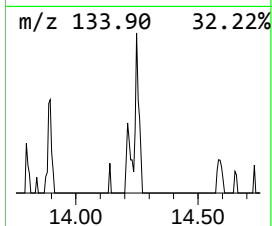
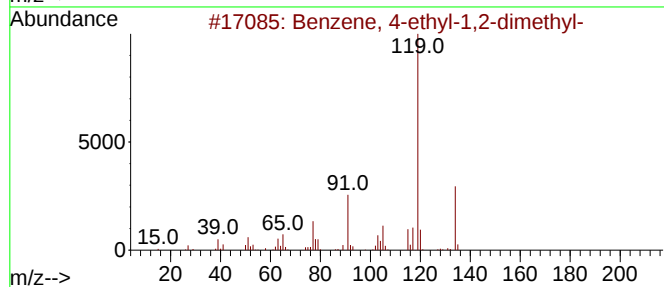
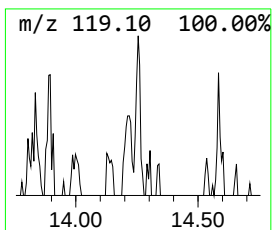
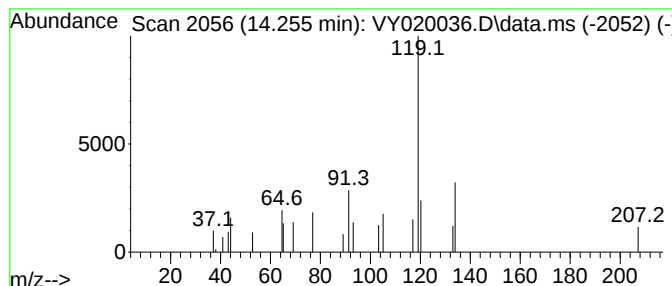
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
Quant Title : SW846 8260

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

Peak Number 7 unknown14.255 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.255	12.64 ug/l	3483	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benzene, 4-ethyl-1,2-dimethyl-	134	C10H14	000934-80-5	49
2			Benzene, 1-ethyl-2,3-dimethyl-	134	C10H14	000933-98-2	49
3			Benzene, 2-ethyl-1,4-dimethyl-	134	C10H14	001758-88-9	49
4			Benzene, 1-ethyl-3,5-dimethyl-	134	C10H14	000934-74-7	47
5			Benzene, 1-ethyl-2,4-dimethyl-	134	C10H14	000874-41-9	46



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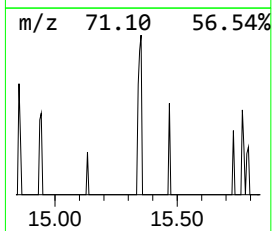
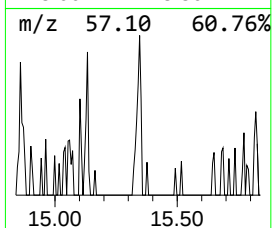
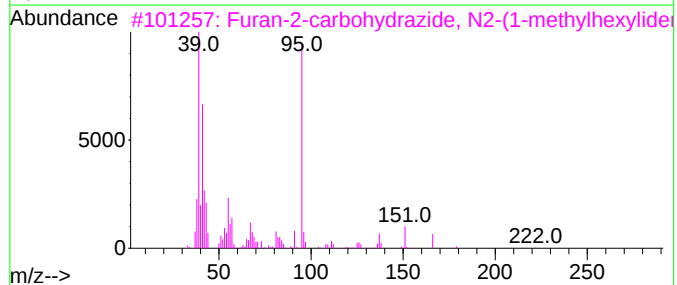
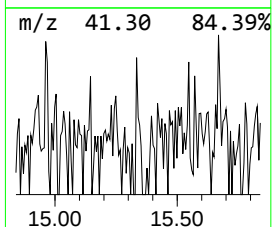
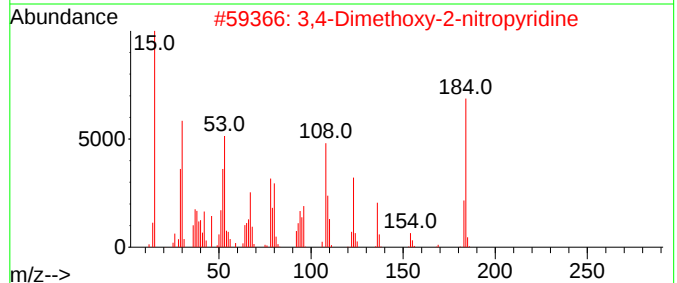
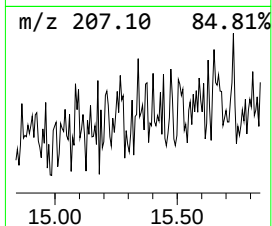
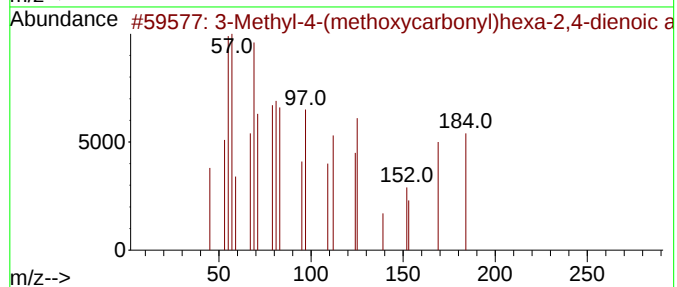
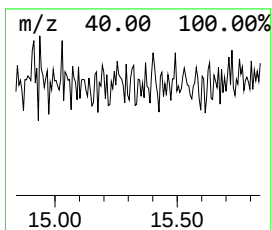
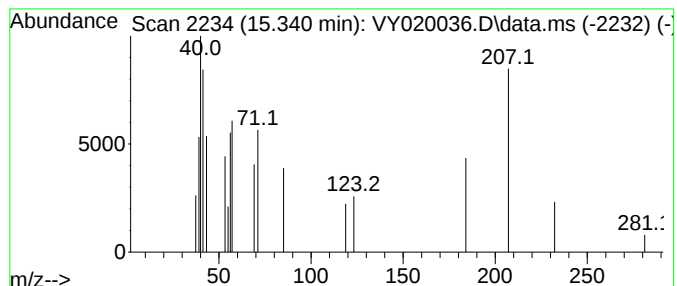
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.M
Quant Title : SW846 8260

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

Peak Number 9 unknown15.340 Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.340	6.10 ug/l	1681	1,4-Dichlorobenzene-d4	13.346

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Methyl-4-(methoxycarbonyl)hexa...	184	C9H12O4	1010104-10-8	35
2			3,4-Dimethoxy-2-nitropyridine	184	C7H8N2O4	1000444-76-6	25
3			Furan-2-carbohydrazide, N2-(1-me...	222	C12H18N2O2	1000263-13-0	23
4			Acetamide, 2-(thiophen-2-yl)-N-m...	281	C16H27NOS	1000421-20-6	11
5			Parthenolide	248	C15H20O3	020554-84-1	10



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY102824\
Data File : VY020036.D
Acq On : 28 Oct 2024 13:06
Operator : SY/MD
Sample : P4578-05
Misc : 7.93g/5.0mL/MSVOA_Y/SOIL/A
ALS Vial : 9 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
WB-305-BOT

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\82Y100924S.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
unknown12.597	12.597	11.8	ug/l	3252	4	13.346	13782	50.0
unknown14.255	14.255	12.6	ug/l	3483	4	13.346	13782	50.0
unknown15.340	15.340	6.1	ug/l	1681	4	13.346	13782	50.0