

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY120621\
 Data File : VY006961.D
 Acq On : 06 Dec 2021 15:29
 Operator : SY/MD
 Sample : M4887-04
 Misc : 6.31g/10.0mL/MSVOA_Y/SOIL
 ALS Vial : 8 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 EX8A1

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

Min Area: 0 % 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\SFAMYL120321SMA.M
 Title : VOC Analysis

Signal : TIC: VY006961.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	2.247	65	70	78	rVB	31941	52817	1.64%	1.041%
2	2.766	149	155	167	rBV2	17289	43566	1.36%	0.858%
3	3.156	217	219	220	rBV2	573	419	0.01%	0.008%
4	3.241	231	233	241	rVB3	620	908	0.03%	0.018%
5	3.418	260	262	265	rVB	376	318	0.01%	0.006%
6	3.448	265	267	268	rBV2	260	218	0.01%	0.004%
7	3.521	275	279	281	rVB3	267	353	0.01%	0.007%
8	3.558	284	285	287	rVV3	204	186	0.01%	0.004%
9	3.613	290	294	295	rBV2	233	234	0.01%	0.005%
10	3.851	323	333	344	rBV2	29036	86334	2.69%	1.701%
11	4.101	371	374	375	rBV	263	188	0.01%	0.004%
12	4.198	382	390	399	rVB4	1602	5000	0.16%	0.099%
13	4.259	399	400	404	rBV	369	357	0.01%	0.007%
14	4.338	411	413	415	rBV2	166	168	0.01%	0.003%
15	4.405	418	424	426	rBV3	442	753	0.02%	0.015%
16	4.448	430	431	434	rBV	190	193	0.01%	0.004%
17	4.625	458	460	461	rBV	210	144	0.00%	0.003%
18	4.643	461	463	464	rVV2	164	145	0.00%	0.003%
19	4.716	465	475	486	rVV2	8880	26463	0.82%	0.521%
20	5.125	540	542	543	rBV2	163	152	0.00%	0.003%
21	5.137	543	544	547	rVB	386	227	0.01%	0.004%
22	5.168	547	549	551	rBV	198	232	0.01%	0.005%
23	5.222	556	558	559	rVB	250	144	0.00%	0.003%
24	5.375	580	583	584	rBV	242	167	0.01%	0.003%
25	5.424	589	591	594	rVV	180	149	0.00%	0.003%
26	5.497	601	603	606	rVB	242	186	0.01%	0.004%
27	5.686	630	634	636	rBV	288	450	0.01%	0.009%
28	5.734	636	642	643	rBV2	1666	2482	0.08%	0.049%
29	5.844	658	660	661	rBV2	166	150	0.00%	0.003%
30	5.881	664	666	669	rVV2	334	325	0.01%	0.006%
31	5.911	669	671	673	rVV2	238	181	0.01%	0.004%
32	5.936	673	675	678	rVB	275	234	0.01%	0.005%
33	5.978	678	682	683	rBV2	245	298	0.01%	0.006%
34	6.021	687	689	691	rBV	142	134	0.00%	0.003%
35	6.064	694	696	697	rBV	285	232	0.01%	0.005%
36	6.082	697	699	701	rBV	162	153	0.00%	0.003%

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Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
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37	6.222	717	722	723	rBV3	197	297	0.01%	0.006%
38	6.295	732	734	737	rVV2	174	167	0.01%	0.003%
39	6.429	754	756	757	rBV	187	125	0.00%	0.002%
40	6.527	770	772	774	rVB	292	244	0.01%	0.005%
41	6.582	779	781	784	rVB2	189	180	0.01%	0.004%
42	6.631	787	789	790	rBV	287	189	0.01%	0.004%
43	6.649	790	792	793	rVB2	210	144	0.00%	0.003%
44	6.679	793	797	798	rBV	151	191	0.01%	0.004%
45	6.893	822	832	839	rBV2	12020	40062	1.25%	0.789%
46	7.472	919	927	942	rVB	43653	114384	3.56%	2.253%
47	7.777	975	977	978	rBV	243	156	0.00%	0.003%
48	7.832	984	986	988	rBV2	240	263	0.01%	0.005%
49	7.899	993	997	1000	rBV2	288	483	0.02%	0.010%
50	7.972	1006	1009	1012	rBV2	372	610	0.02%	0.012%
51	8.112	1023	1032	1047	rVB3	98953	315526	9.82%	6.216%
52	8.234	1047	1052	1059	rVB3	1699	3405	0.11%	0.067%
53	8.313	1063	1065	1067	rBV2	266	246	0.01%	0.005%
54	8.417	1079	1082	1083	rBV	200	217	0.01%	0.004%
55	8.575	1106	1108	1109	rBV	200	125	0.00%	0.002%
56	8.612	1113	1114	1117	rBV2	287	307	0.01%	0.006%
57	8.691	1117	1127	1136	rVB	95418	191548	5.96%	3.774%
58	8.935	1159	1167	1176	rVB	74120	142509	4.44%	2.807%
59	9.039	1181	1184	1185	rBV2	182	185	0.01%	0.004%
60	9.118	1185	1197	1208	rBV	60351	122685	3.82%	2.417%
61	9.252	1218	1219	1220	rBV	208	117	0.00%	0.002%
62	9.270	1220	1222	1225	rVB2	310	286	0.01%	0.006%
63	9.551	1267	1268	1271	rBV2	280	235	0.01%	0.005%
64	9.581	1271	1273	1275	rBV2	186	180	0.01%	0.004%
65	9.886	1317	1323	1330	rVB	29289	50948	1.59%	1.004%
66	10.032	1344	1347	1348	rBV2	239	223	0.01%	0.004%
67	10.075	1348	1354	1359	rVB3	824	1566	0.05%	0.031%
68	10.179	1364	1371	1377	rVV	75116	128382	4.00%	2.529%
69	10.240	1377	1381	1386	rVB2	2887	4173	0.13%	0.082%
70	10.435	1406	1413	1420	rVB	16757	28106	0.87%	0.554%
71	10.575	1429	1436	1444	rVB2	9019	16484	0.51%	0.325%
72	10.715	1451	1459	1466	rBV	1998988	3212914	100.00%	63.295%
73	10.788	1466	1471	1482	rVB3	34081	68664	2.14%	1.353%
74	10.947	1491	1497	1505	rVB	13102	20878	0.65%	0.411%
75	11.252	1546	1547	1552	rBV	205	184	0.01%	0.004%
76	11.313	1552	1557	1567	rBV2	8062	14024	0.44%	0.276%

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77	11.435	1575	1577	1578	rBV2	189	145	0.00%	0.003%
78	11.490	1579	1586	1593	rVV	77852	124383	3.87%	2.450%
79	11.593	1598	1603	1606	rBV4	1082	1387	0.04%	0.027%
80	11.703	1616	1621	1628	rVB4	1220	2285	0.07%	0.045%
81	11.752	1628	1629	1631	rBV	293	212	0.01%	0.004%
82	12.032	1671	1675	1680	rVB3	839	1323	0.04%	0.026%
83	12.313	1719	1721	1723	rVB	206	140	0.00%	0.003%
84	12.331	1723	1724	1726	rBV	293	227	0.01%	0.004%
85	12.386	1731	1733	1735	rBV	313	242	0.01%	0.005%
86	12.489	1741	1750	1756	rBV	37436	61743	1.92%	1.216%
87	12.556	1756	1761	1769	rVB	32909	51941	1.62%	1.023%
88	12.617	1769	1771	1775	rBV4	557	774	0.02%	0.015%
89	12.764	1791	1795	1799	rBV4	2251	3765	0.12%	0.074%
90	12.819	1800	1804	1810	rVB3	4399	7134	0.22%	0.141%
91	12.910	1817	1819	1820	rVB	372	151	0.00%	0.003%
92	13.069	1840	1845	1849	rVB3	1242	1800	0.06%	0.035%
93	13.117	1849	1853	1857	rBV3	987	1336	0.04%	0.026%
94	13.178	1859	1863	1868	rVB3	2811	4722	0.15%	0.093%
95	13.282	1876	1880	1883	rVB4	899	1485	0.05%	0.029%
96	13.422	1898	1903	1909	rBV	33072	51735	1.61%	1.019%
97	13.526	1916	1920	1926	rVB4	4267	6570	0.20%	0.129%
98	13.636	1935	1938	1943	rBV5	1217	1543	0.05%	0.030%
99	13.721	1947	1952	1959	rVB	20568	32015	1.00%	0.631%
100	13.965	1987	1992	2000	rVB2	7398	12759	0.40%	0.251%

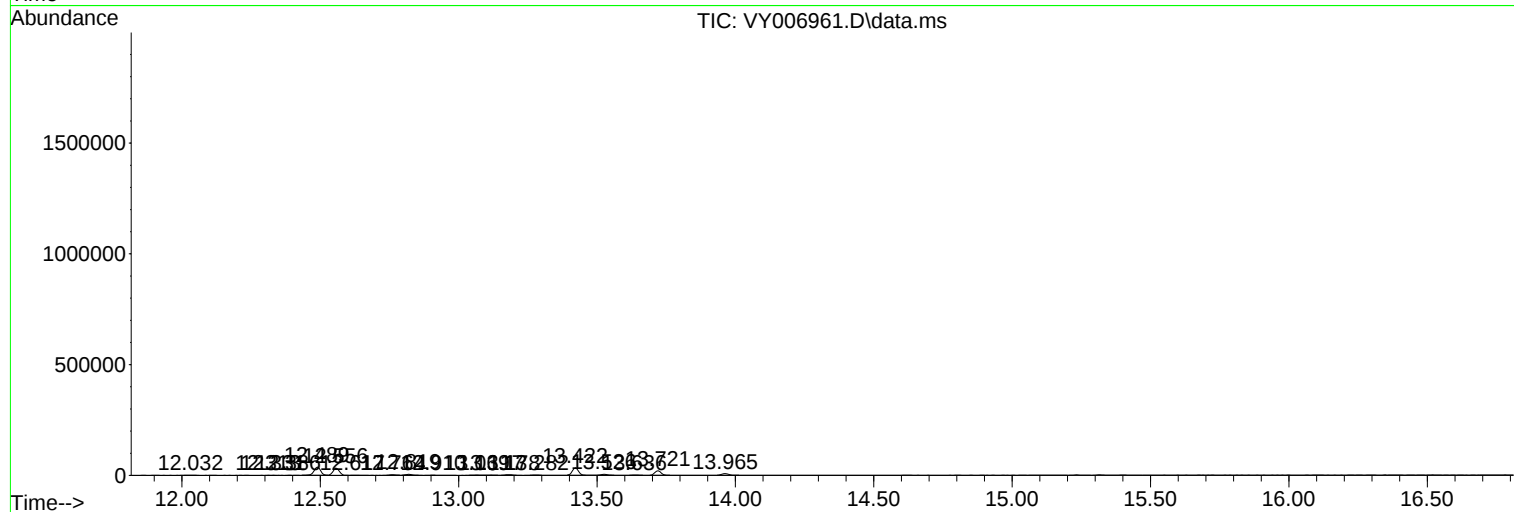
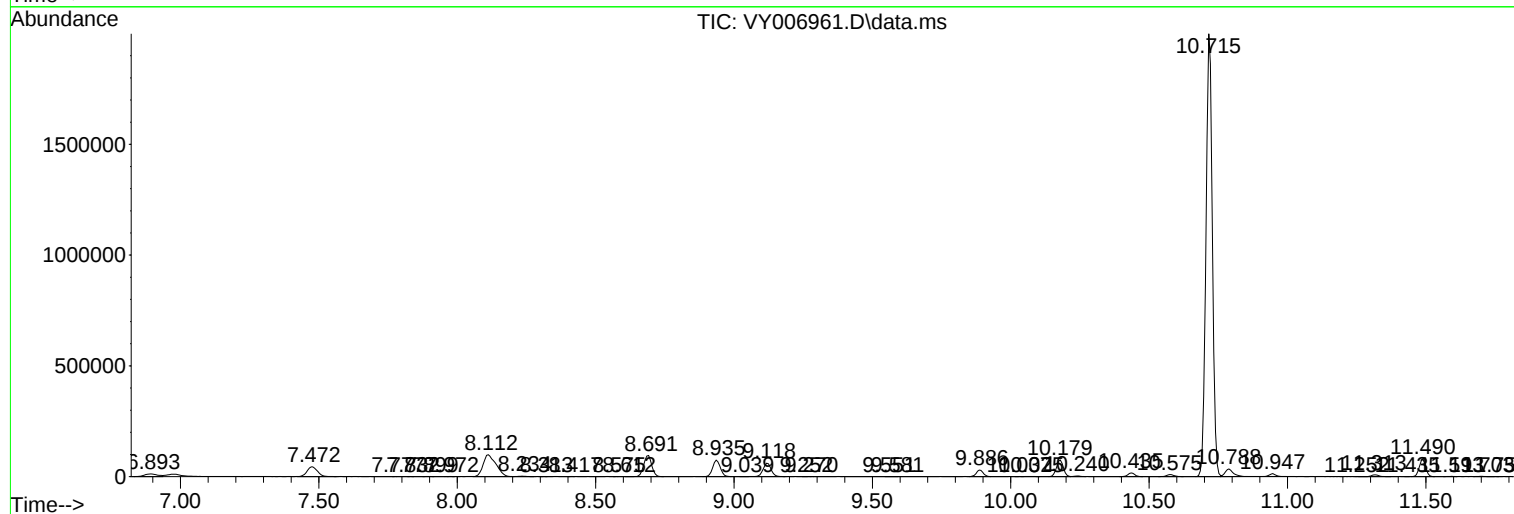
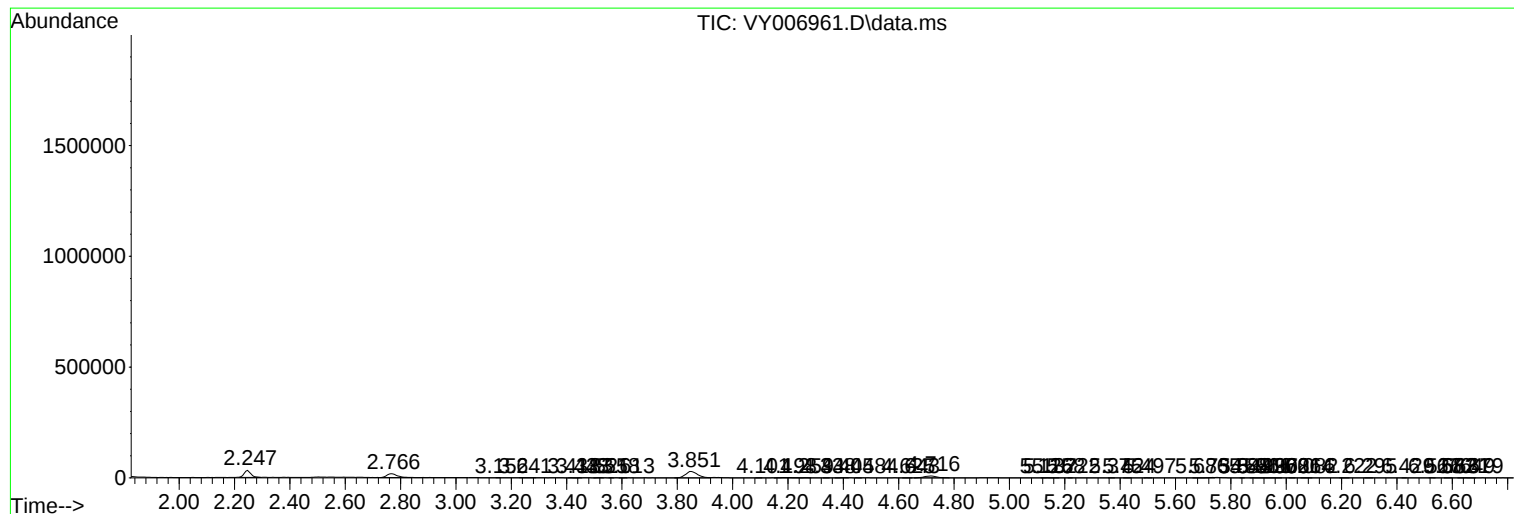
Sum of corrected areas: 5076089

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ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
EX8A1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
Quant Title : VOC Analysis

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



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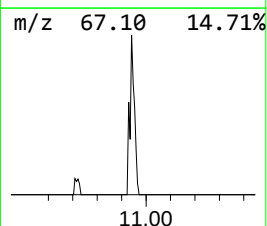
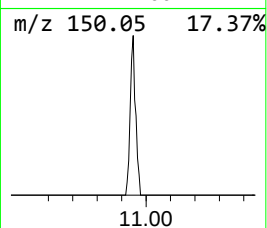
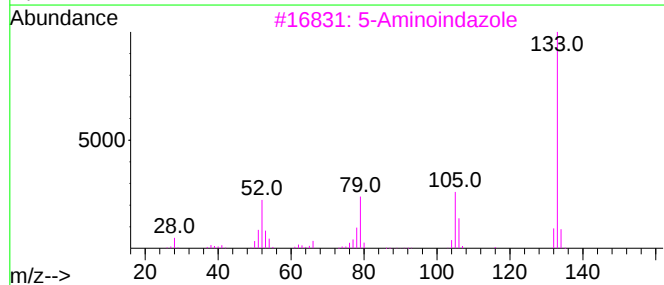
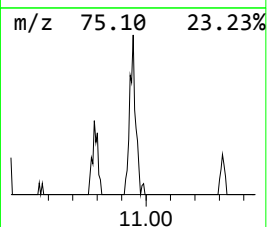
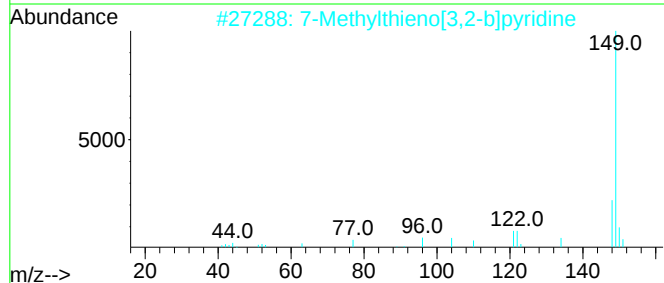
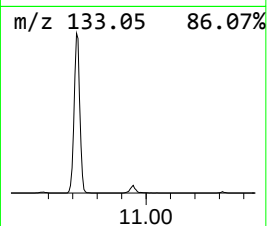
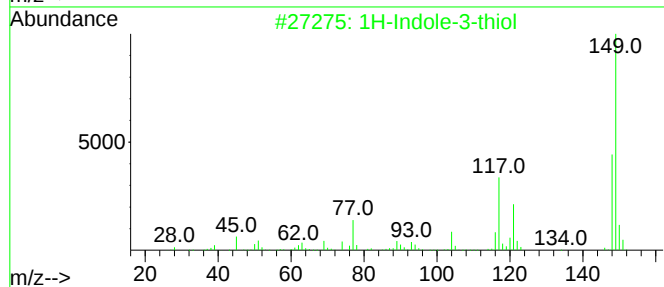
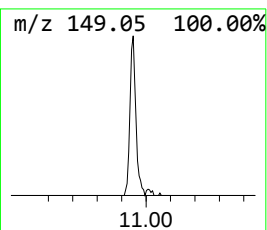
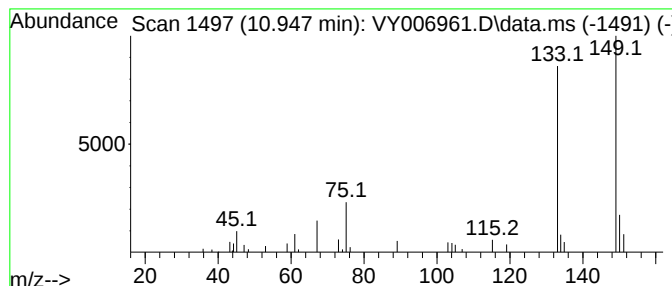
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYLM120321SMA.M
Quant Title : VOC Analysis

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

Peak Number 4 unknown-01 Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	4.20 ug/L	20878	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1H-Indole-3-thiol	149	C8H7NS	000480-94-4	35
2			7-Methylthieno[3,2-b]pyridine	149	C8H7NS	013362-83-9	35
3			5-Aminoindazole	133	C7H7N3	019335-11-6	27
4			Acetylthiosemicarbazide	133	C3H7N3OS	002302-88-7	27
5			(Tert.-butyldimethylsilyl)oxyurea	190	C7H18N2O2Si	1000453-67-1	23



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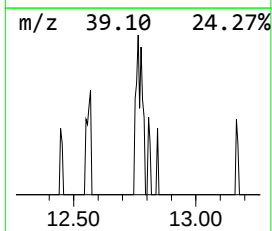
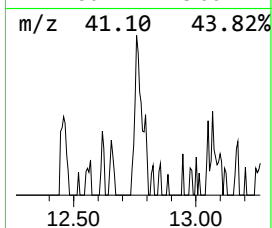
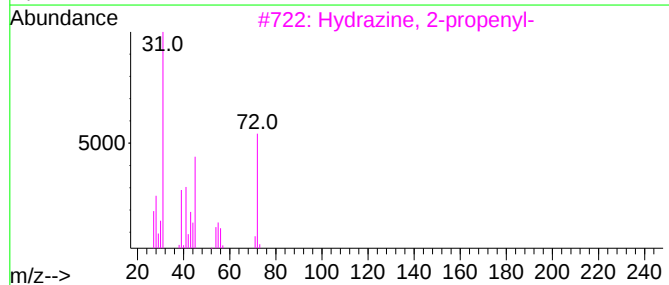
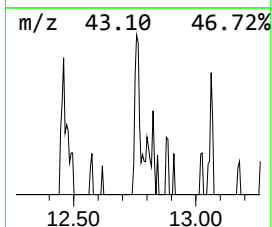
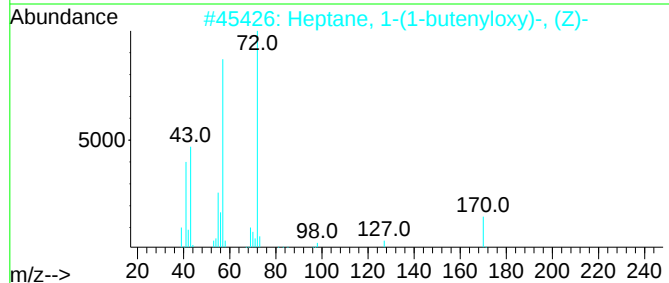
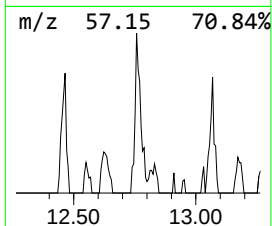
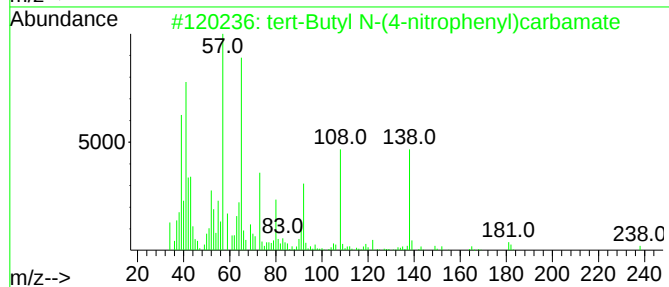
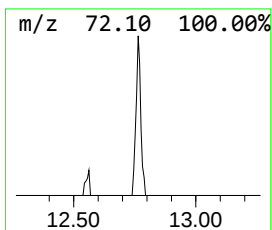
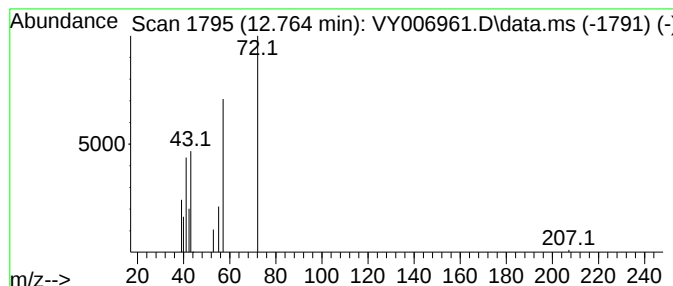
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYLEM120321SMA.M
Quant Title : VOC Analysis

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

Peak Number 7 unknown-02 Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.764	1.82 ug/L	3765	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			tert-Butyl N-(4-nitrophenyl)carb...	238	C11H14N2O4	018437-63-3	9
2			Heptane, 1-(1-butenyloxy)-, (Z)-	170	C11H22O	056052-79-0	9
3			Hydrazine, 2-propenyl-	72	C3H8N2	007422-78-8	5
4			2-Buten-1-ol	72	C4H8O	006117-91-5	5
5			1-Propene, 3-methoxy-	72	C4H8O	000627-40-7	4



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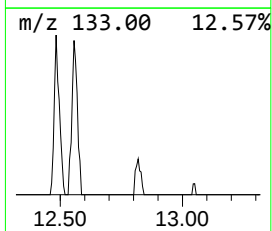
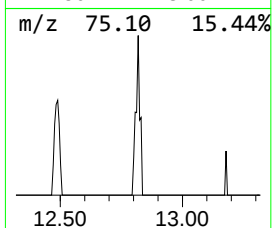
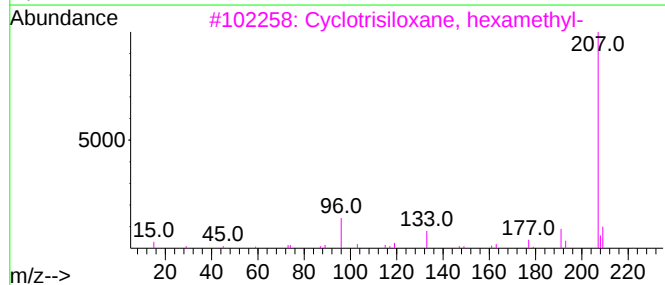
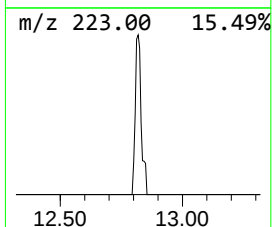
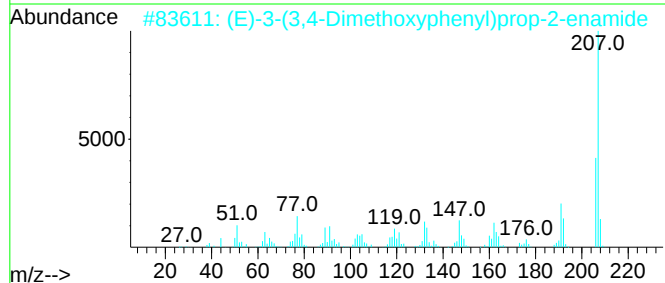
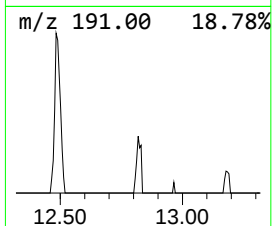
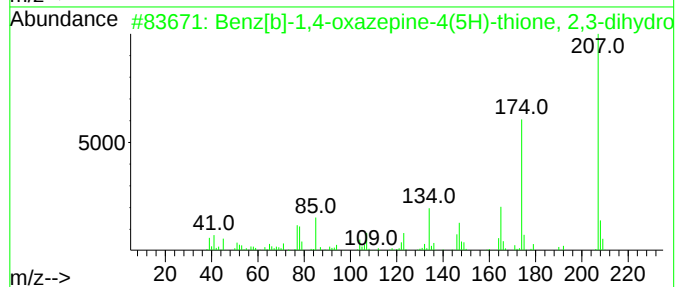
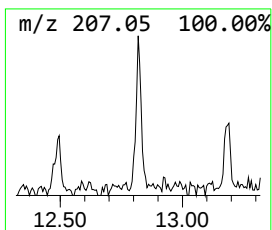
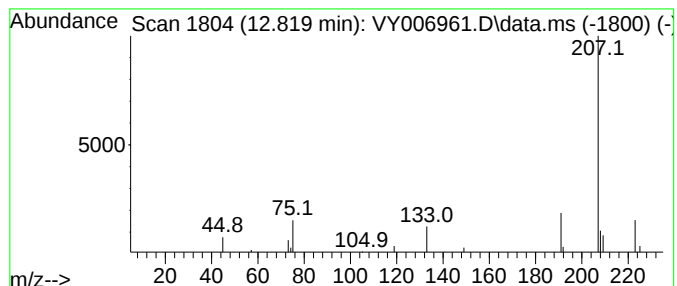
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYLEM120321SMA.M
Quant Title : VOC Analysis

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

Peak Number 8 Benz[b]-1,4-oxazepine-4(5H)... Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.819	3.45 ug/L	7134	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Benz[b]-1,4-oxazepine-4(5H)-thio...	207	C11H13NOS	1000258-63-4	50
2			(E)-3-(3,4-Dimethoxyphenyl)prop...	207	C11H13NO3	130973-10-3	45
3			Cyclotrisiloxane, hexamethyl-	222	C6H18O3Si3	000541-05-9	38
4			N-Methyl-1-adamantaneacetamide	207	C13H21NO	031897-93-5	33
5			[1,2,4]Triazolo[3,4-b][1,3]benzo...	207	C8H5N3S2	006957-85-3	9



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY120621\
Data File : VY006961.D
Acq On : 06 Dec 2021 15:29
Operator : SY/MD
Sample : M4887-04
Misc : 6.31g/10.0mL/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
EX8A1

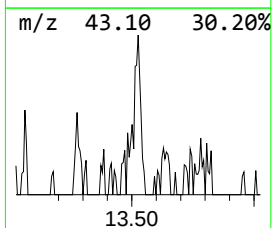
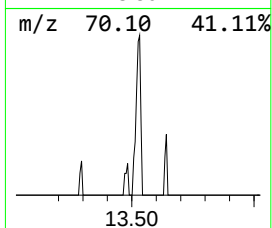
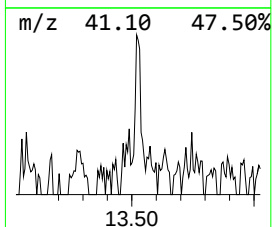
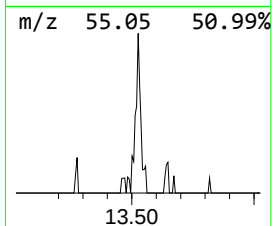
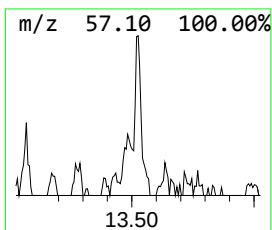
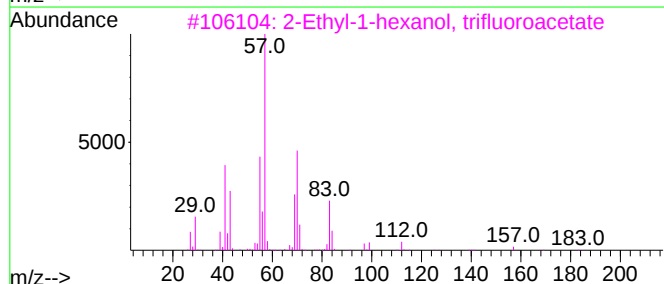
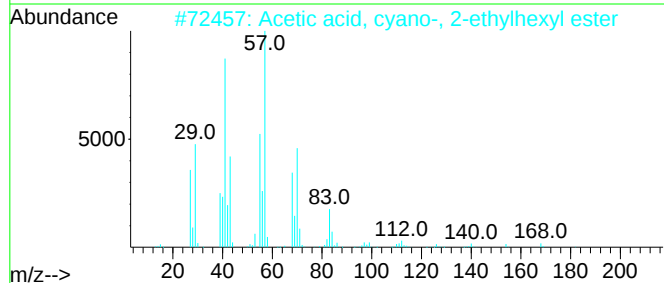
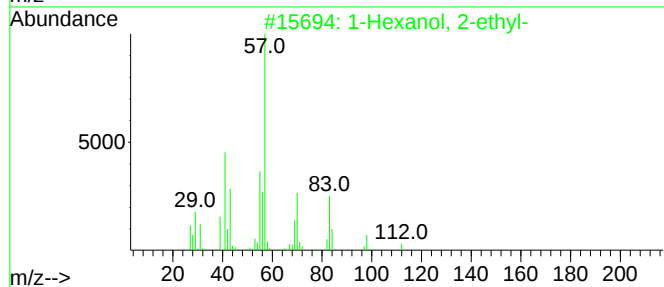
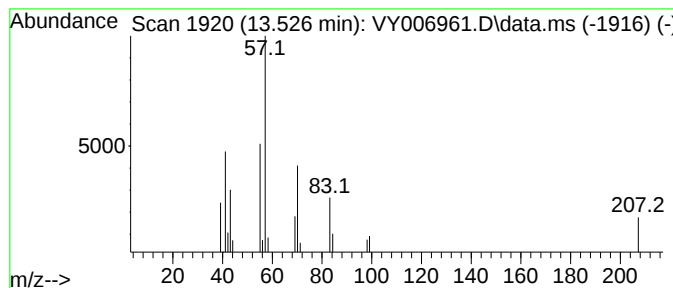
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Quant Title : VOC Analysis

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

Peak Number 10 1-Hexanol, 2-ethyl- Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.526	3.17 ug/L	6570	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	59
2			Acetic acid, cyano-, 2-ethylhexy...	197	C11H19NO2	013361-34-7	59
3			2-Ethyl-1-hexanol, trifluoroacetate	226	C10H17F3O2	053800-08-1	59
4			2-Ethyl-1-hexanol, pentafluoropr...	276	C11H17F5O2	959012-82-9	56
5			Pentadecafluorooctanoic acid, 2-...	526	C16H17F15O2	1000406-80-9	50



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY120621\
Data File : VY006961.D
Acq On : 06 Dec 2021 15:29
Operator : SY/MD
Sample : M4887-04
Misc : 6.31g/10.0mL/MSVOA_Y/SOIL
ALS Vial : 8 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
EX8A1

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	10.947	4.2	ug/L	20878	2	11.490	124383	25.0
unknown-02	12.764	1.8	ug/L	3765	3	13.422	51735	25.0
Benz[b]-1,4-oxa...	12.819	3.5	ug/L	7134	3	13.422	51735	25.0
1-Hexanol, 2-et...	13.526	3.2	ug/L	6570	3	13.422	51735	25.0