

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY120421\
 Data File : VY006951.D
 Acq On : 04 Dec 2021 18:43
 Operator : SY/MD
 Sample : M4884-21
 Misc : 4.89g/10.0mL/MSVOA_Y/SOIL
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 EW9K5

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: VY006951.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	82	rVB	57191	98284	14.34%	2.202%
2	2.772	149	156	170	rVB	34748	81353	11.87%	1.823%
3	3.253	230	235	240	rBV2	571	1295	0.19%	0.029%
4	3.479	270	272	275	rBV2	235	340	0.05%	0.008%
5	3.619	292	295	298	rVB2	239	354	0.05%	0.008%
6	3.643	298	299	301	rBV2	189	199	0.03%	0.004%
7	3.686	304	306	308	rVB	237	163	0.02%	0.004%
8	3.723	308	312	314	rBV	195	276	0.04%	0.006%
9	3.747	314	316	318	rVB	319	237	0.03%	0.005%
10	3.857	321	334	346	rBV	66716	178452	26.03%	3.998%
11	4.040	360	364	366	rBV	301	429	0.06%	0.010%
12	4.131	376	379	380	rBV	242	211	0.03%	0.005%
13	4.192	384	389	399	rVV4	1384	4220	0.62%	0.095%
14	4.265	399	401	404	rVB	300	334	0.05%	0.007%
15	4.320	407	410	411	rBV	239	169	0.02%	0.004%
16	4.363	415	417	420	rBV	175	176	0.03%	0.004%
17	4.412	422	425	429	rBV2	206	218	0.03%	0.005%
18	4.454	429	432	435	rBV	212	240	0.04%	0.005%
19	4.527	440	444	445	rBV	162	210	0.03%	0.005%
20	4.722	463	476	488	rVB3	9001	28182	4.11%	0.631%
21	4.875	500	501	504	rBV	321	292	0.04%	0.007%
22	4.911	504	507	508	rVV	226	198	0.03%	0.004%
23	5.070	527	533	534	rBV2	237	231	0.03%	0.005%
24	5.204	553	555	557	rVV2	300	259	0.04%	0.006%
25	5.247	560	562	564	rVB	242	190	0.03%	0.004%
26	5.265	564	565	566	rBV	323	179	0.03%	0.004%
27	5.308	570	572	575	rVB	248	176	0.03%	0.004%
28	5.570	613	615	618	rVB2	178	220	0.03%	0.005%
29	5.643	624	627	629	rVB3	247	240	0.04%	0.005%
30	5.747	636	644	645	rBV3	1346	2467	0.36%	0.055%
31	5.972	679	681	683	rBV	152	176	0.03%	0.004%
32	6.222	717	722	724	rVV2	196	347	0.05%	0.008%
33	6.265	727	729	731	rBV2	262	259	0.04%	0.006%
34	6.393	748	750	753	rBV2	261	264	0.04%	0.006%
35	6.472	759	763	766	rVB3	246	350	0.05%	0.008%
36	6.497	766	767	770	rBV	184	210	0.03%	0.005%

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37	6.557	775	777	779	rBV	224	284	0.04%	0.006%
38	6.606	782	785	788	rVB3	229	283	0.04%	0.006%
39	6.716	802	803	805	rBV	261	213	0.03%	0.005%
40	6.783	811	814	815	rBV	260	315	0.05%	0.007%
41	6.887	820	831	841	rBV2	20685	63157	9.21%	1.415%
42	7.478	918	928	943	rVB	89028	217940	31.79%	4.883%
43	7.691	962	963	964	rBV	293	171	0.02%	0.004%
44	7.746	969	972	973	rBV	385	327	0.05%	0.007%
45	8.112	1023	1032	1047	rBV2	180611	534700	78.01%	11.979%
46	8.240	1048	1053	1059	rVB3	2236	4884	0.71%	0.109%
47	8.618	1113	1115	1117	rVB2	253	168	0.02%	0.004%
48	8.691	1119	1127	1136	rBV	156904	311224	45.40%	6.973%
49	8.831	1146	1150	1152	rBV2	205	167	0.02%	0.004%
50	8.941	1159	1168	1179	rVV	351411	685466	100.00%	15.357%
51	9.124	1189	1198	1207	rVV	116998	239771	34.98%	5.372%
52	9.356	1234	1236	1238	rBV2	251	209	0.03%	0.005%
53	9.429	1246	1248	1252	rVB	216	237	0.03%	0.005%
54	9.472	1252	1255	1258	rVB2	347	390	0.06%	0.009%
55	9.502	1258	1260	1263	rBV	303	306	0.04%	0.007%
56	9.581	1272	1273	1275	rVB	306	207	0.03%	0.005%
57	9.606	1275	1277	1278	rBV	236	182	0.03%	0.004%
58	9.667	1284	1287	1288	rVV2	255	199	0.03%	0.004%
59	9.709	1290	1294	1295	rBV2	208	230	0.03%	0.005%
60	9.746	1298	1300	1301	rBV	399	320	0.05%	0.007%
61	9.831	1312	1314	1317	rVV2	291	353	0.05%	0.008%
62	9.892	1317	1324	1332	rVB	69722	123639	18.04%	2.770%
63	10.075	1350	1354	1358	rBV3	678	1321	0.19%	0.030%
64	10.179	1364	1371	1378	rBV	233320	402410	58.71%	9.016%
65	10.246	1378	1382	1388	rVB	5980	9537	1.39%	0.214%
66	10.435	1406	1413	1421	rBV	44980	76937	11.22%	1.724%
67	10.520	1425	1427	1430	rBV3	315	388	0.06%	0.009%
68	10.581	1430	1437	1443	rVV	23268	42204	6.16%	0.946%
69	10.721	1453	1460	1465	rBV	58933	98516	14.37%	2.207%
70	10.788	1465	1471	1482	rVV	81270	128784	18.79%	2.885%
71	10.910	1489	1491	1492	rBV	274	202	0.03%	0.005%
72	10.947	1492	1497	1507	rBV2	16781	29839	4.35%	0.669%
73	11.142	1526	1529	1531	rBV2	373	450	0.07%	0.010%
74	11.191	1535	1537	1539	rBV	204	165	0.02%	0.004%
75	11.246	1544	1546	1547	rBV	270	214	0.03%	0.005%
76	11.270	1549	1550	1552	rVV	458	376	0.05%	0.008%

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77	11.319	1552	1558	1565	rVV	18568	31955	4.66%	0.716%
78	11.380	1566	1568	1570	rVV	315	263	0.04%	0.006%
79	11.490	1579	1586	1596	rVV	209252	327455	47.77%	7.336%
80	11.593	1599	1603	1610	rVB4	661	1050	0.15%	0.024%
81	11.697	1617	1620	1624	rVB3	902	1528	0.22%	0.034%
82	11.916	1654	1656	1657	rVV	286	176	0.03%	0.004%
83	11.965	1660	1664	1665	rBV2	247	231	0.03%	0.005%
84	12.032	1671	1675	1678	rBV4	864	1476	0.22%	0.033%
85	12.252	1708	1711	1715	rBV3	397	511	0.07%	0.011%
86	12.331	1721	1724	1728	rBV4	1405	1632	0.24%	0.037%
87	12.410	1735	1737	1739	rVB3	358	325	0.05%	0.007%
88	12.489	1739	1750	1756	rBV	91516	156373	22.81%	3.503%
89	12.563	1756	1762	1768	rVB	87576	141112	20.59%	3.161%
90	12.630	1770	1773	1776	rBV4	743	943	0.14%	0.021%
91	12.819	1798	1804	1811	rBV	8543	13284	1.94%	0.298%
92	12.940	1822	1824	1825	rBV	324	245	0.04%	0.005%
93	13.069	1842	1845	1850	rVB3	2018	2779	0.41%	0.062%
94	13.184	1859	1864	1870	rVB2	6460	9868	1.44%	0.221%
95	13.282	1876	1880	1885	rVV3	2090	3210	0.47%	0.072%
96	13.422	1897	1903	1909	rBV	118317	183156	26.72%	4.103%
97	13.526	1916	1920	1928	rVB2	7389	11230	1.64%	0.252%
98	13.721	1946	1952	1959	rVB	117526	179517	26.19%	4.022%
99	13.959	1987	1991	1999	rVB2	9661	16813	2.45%	0.377%
100	14.263	2039	2041	2042	rBV2	419	265	0.04%	0.006%

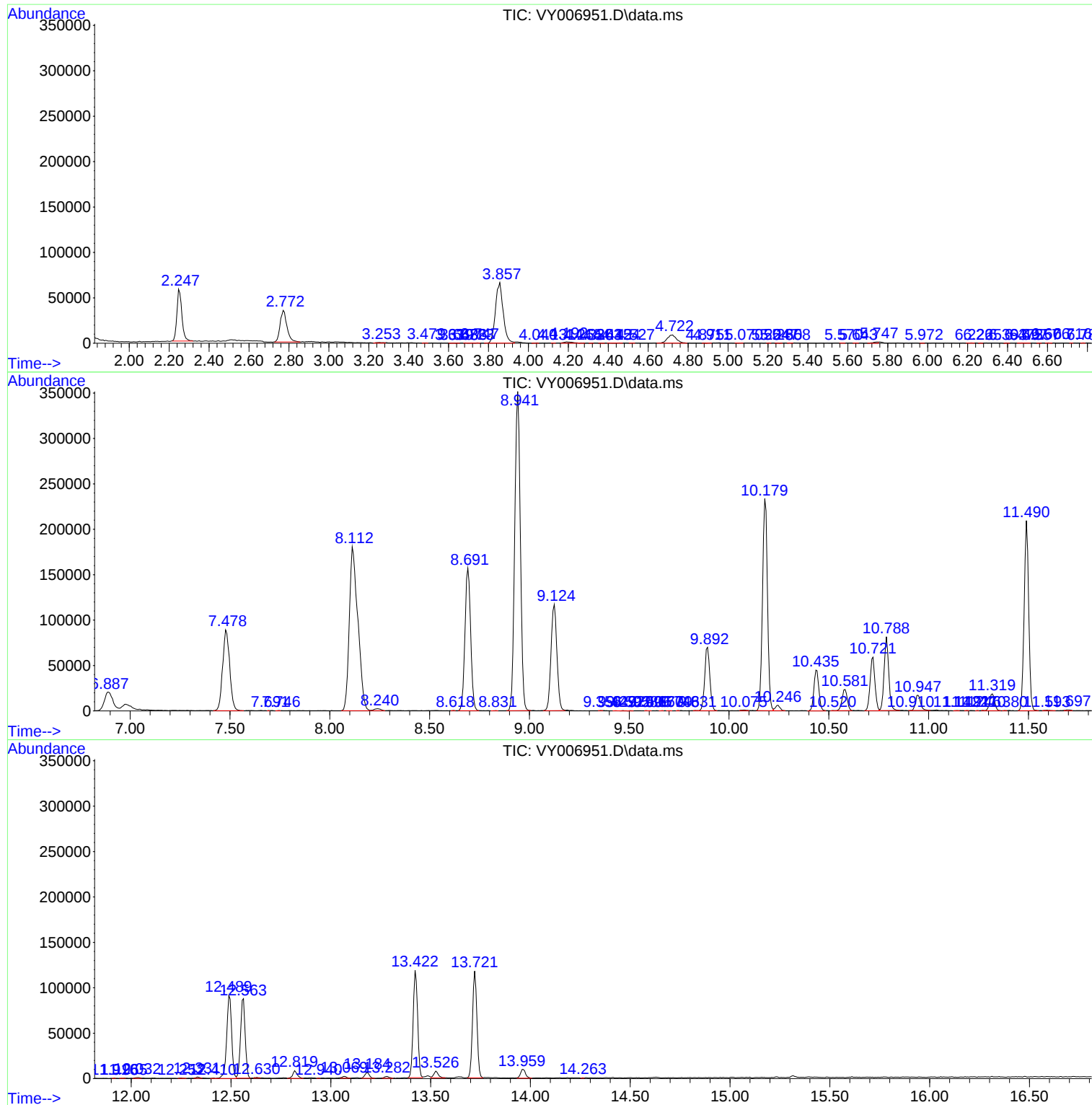
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
Quant Title : VOC Analysis

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



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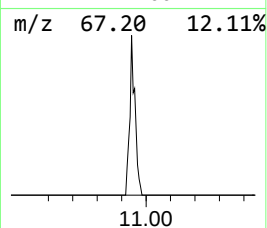
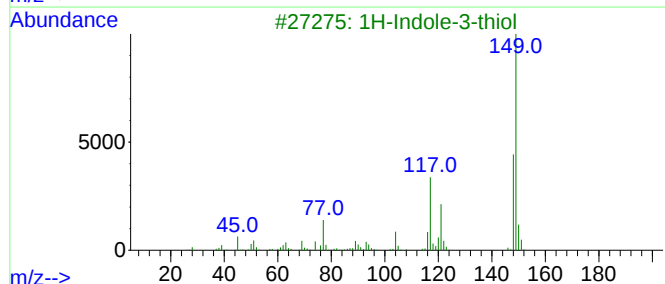
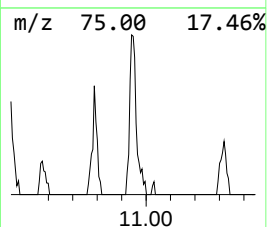
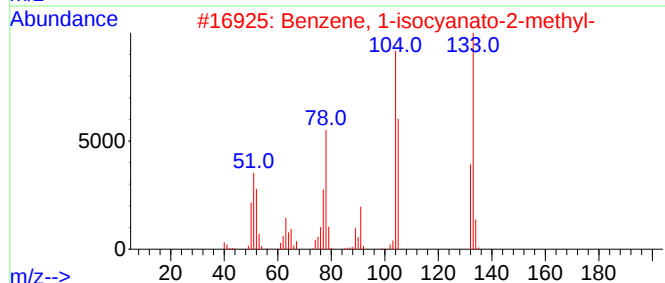
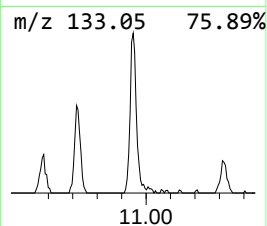
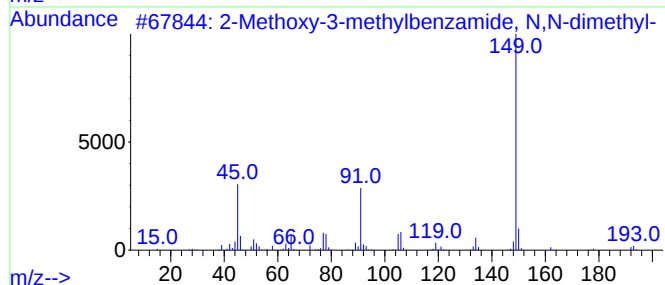
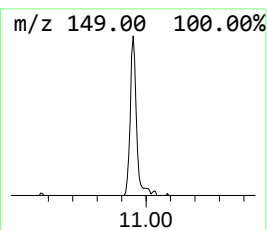
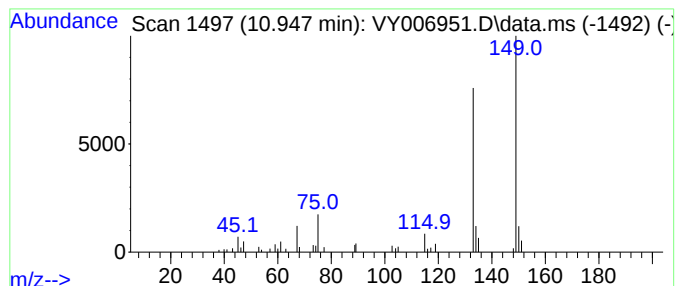
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
Quant Title : VOC Analysis

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

Peak Number 4 unknown-01 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	2.28 ug/L	29839	Chlorobenzene-d5	11.490

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	2-Methoxy-3-methylbenzamide, N,N...	193	C11H15NO2	1369798-01-5	32		
2	Benzene, 1-isocyanato-2-methyl-	133	C8H7NO	000614-68-6	25		
3	1H-Indole-3-thiol	149	C8H7NS	000480-94-4	25		
4	1,2,4-Triazole, 3,5-dithioxo-	133	C2H3N3S2	005650-03-3	25		
5	m-Tolyl isothiocyanate	149	C8H7NS	000621-30-7	25		



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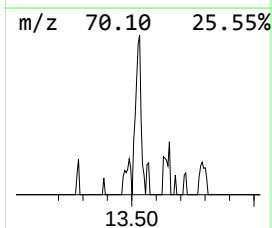
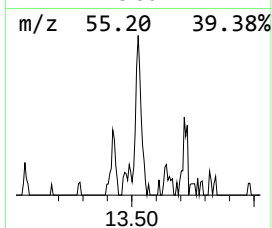
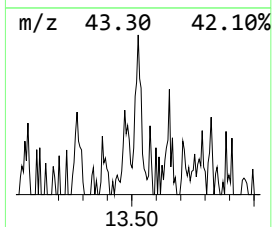
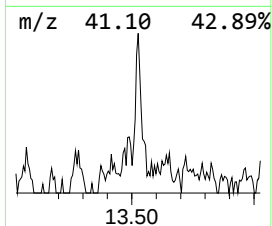
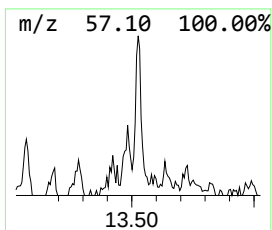
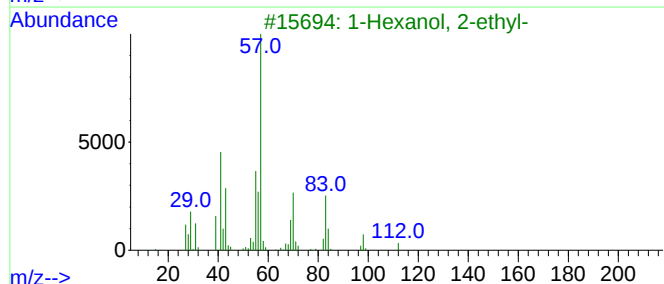
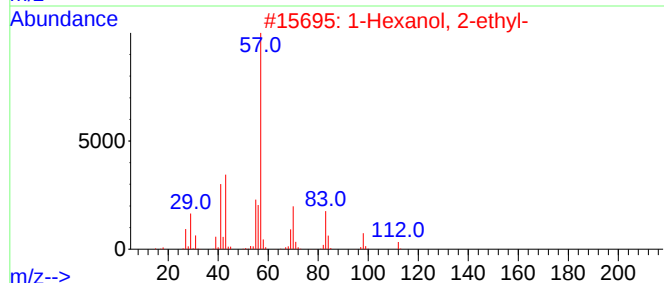
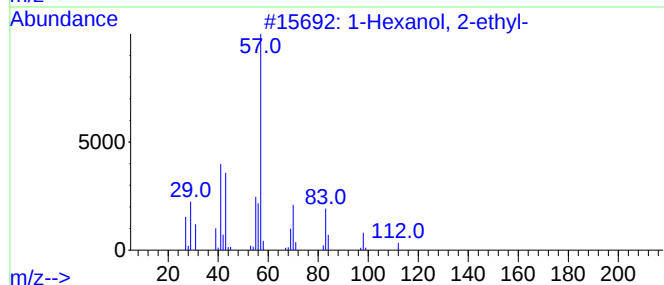
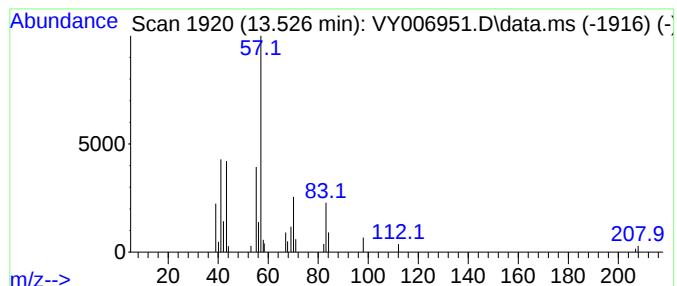
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
Quant Title : VOC Analysis

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

Peak Number 9 1-Hexanol, 2-ethyl- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.526	1.53 ug/L	11230	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	64
2			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	47
3			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	45
4			1-Pentanol, 2-ethyl-4-methyl-	130	C8H18O	000106-67-2	45
5			1-Hexanol, 2-ethyl-	130	C8H18O	000104-76-7	42



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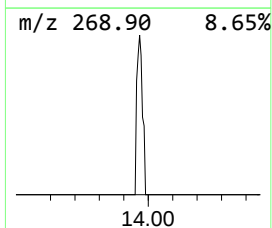
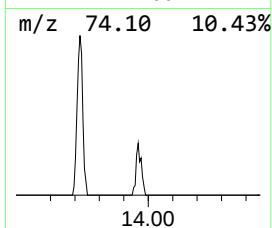
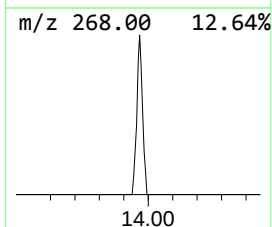
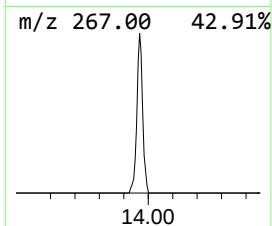
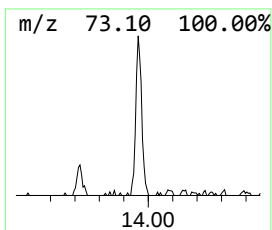
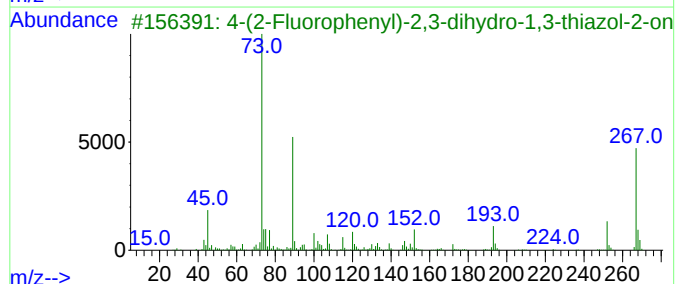
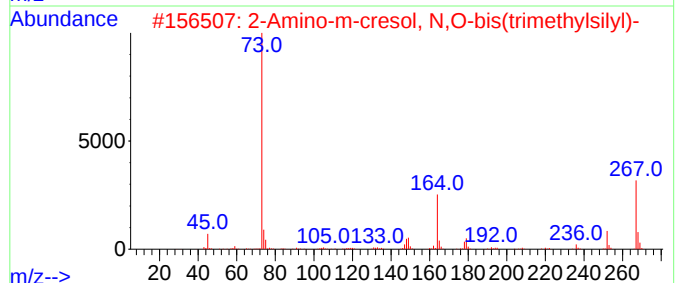
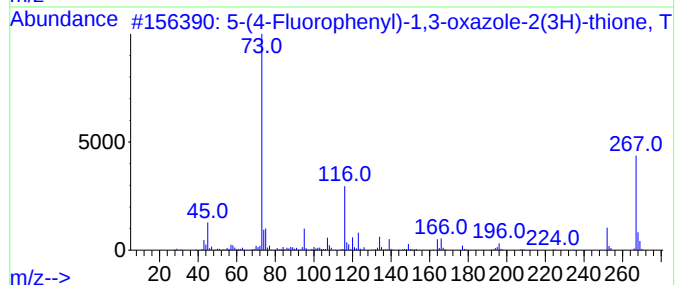
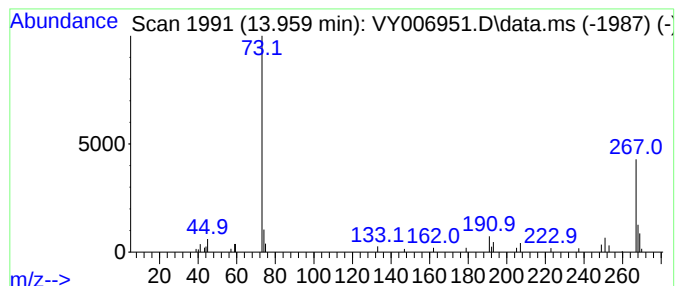
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
Quant Title : VOC Analysis

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

Peak Number 10 5-(4-Fluorophenyl)-1,3-oxaz... Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.959	2.29 ug/L	16813	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-(4-Fluorophenyl)-1,3-oxazole-2...	267	C12H14FNOSSi	1000497-07-6	59
2			2-Amino-m-cresol, N,O-bis(trimet...	267	C13H25NOSi2	1000449-77-1	45
3			4-(2-Fluorophenyl)-2,3-dihydro-1...	267	C12H14FNOSSi	1000504-37-6	45
4			Salicylic acid, 2TMS derivative	282	C13H22O3Si2	003789-85-3	39
5			Salicylic acid, 2TMS derivative	282	C13H22O3Si2	003789-85-3	39



Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY120421\
Data File : VY006951.D
Acq On : 04 Dec 2021 18:43
Operator : SY/MD
Sample : M4884-21
Misc : 4.89g/10.0mL/MSVOA_Y/SOIL
ALS Vial : 25 Sample Multiplier: 1

Instrument :
MSVOA_Y
ClientSampleId :
EW9K5

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	2.3	ug/L	29839	2	11.490	327455	25.0
1-Hexanol, 2-et...	13.526	1.5	ug/L	11230	3	13.422	183156	25.0
5-(4-Fluorophen...	13.959	2.3	ug/L	16813	3	13.422	183156	25.0