

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY120421\
 Data File : VY006942.D
 Acq On : 04 Dec 2021 15:26
 Operator : SY/MD
 Sample : M4884-12
 Misc : 4.16g/10.0mL/MSVOA_Y/SOIL
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 EW9J8

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\SFAMLYM120321SMA.M
 Title : VOC Analysis

Signal : TIC: VY006942.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	79	rBV	50407	84176	16.88%	2.032%
2	2.765	148	155	170	rVB	27754	68073	13.65%	1.643%
3	3.235	231	232	234	rBV2	444	290	0.06%	0.007%
4	3.546	282	283	286	rBV2	342	257	0.05%	0.006%
5	3.851	322	333	345	rBV2	63802	184285	36.96%	4.449%
6	4.076	369	370	374	rVB	191	195	0.04%	0.005%
7	4.125	374	378	379	rBV2	266	348	0.07%	0.008%
8	4.198	383	390	400	rVB3	2211	6532	1.31%	0.158%
9	4.326	408	411	412	rBV	244	181	0.04%	0.004%
10	4.338	412	413	416	rBV2	225	248	0.05%	0.006%
11	4.418	424	426	427	rBV	266	203	0.04%	0.005%
12	4.546	444	447	448	rBV	245	218	0.04%	0.005%
13	4.716	465	475	490	rVB2	11047	33814	6.78%	0.816%
14	4.814	490	491	495	rBV	166	183	0.04%	0.004%
15	4.948	512	513	516	rVB	447	268	0.05%	0.006%
16	5.198	552	554	557	rBV	250	347	0.07%	0.008%
17	5.253	561	563	565	rVB	291	223	0.04%	0.005%
18	5.289	565	569	572	rBV	293	453	0.09%	0.011%
19	5.320	572	574	575	rBV	232	182	0.04%	0.004%
20	5.369	579	582	584	rBV2	178	206	0.04%	0.005%
21	5.490	599	602	604	rVB	297	279	0.06%	0.007%
22	5.533	607	609	611	rVV	188	248	0.05%	0.006%
23	5.576	614	616	618	rBV3	232	258	0.05%	0.006%
24	5.740	637	643	652	rBV5	1936	5167	1.04%	0.125%
25	6.015	686	688	691	rVB2	283	300	0.06%	0.007%
26	6.045	691	693	694	rBV2	245	171	0.03%	0.004%
27	6.192	712	717	719	rBV	303	349	0.07%	0.008%
28	6.448	755	759	761	rBV	198	230	0.05%	0.006%
29	6.576	777	780	782	rBV	186	258	0.05%	0.006%
30	6.600	782	784	785	rBV	258	173	0.03%	0.004%
31	6.691	795	799	800	rBV2	349	404	0.08%	0.010%
32	6.887	821	831	841	rBV2	21243	63325	12.70%	1.529%
33	7.484	919	929	940	rVV	82485	211369	42.39%	5.103%
34	7.575	942	944	945	rVB	369	243	0.05%	0.006%
35	7.600	945	948	949	rBV	473	510	0.10%	0.012%
36	7.667	957	959	960	rBV	308	308	0.06%	0.007%

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 Title : VOC Analysis

37	7.728	967	969	971	rBV	351	345	0.07%	0.008%
38	7.850	987	989	991	rBV2	375	251	0.05%	0.006%
39	8.002	1011	1014	1016	rBV2	236	262	0.05%	0.006%
40	8.112	1022	1032	1046	rBV2	164596	498600	100.00%	12.037%
41	8.240	1048	1053	1058	rVB3	704	1242	0.25%	0.030%
42	8.295	1060	1062	1065	rBV	221	230	0.05%	0.006%
43	8.325	1065	1067	1069	rBV	238	243	0.05%	0.006%
44	8.520	1097	1099	1103	rBV3	323	344	0.07%	0.008%
45	8.575	1105	1108	1109	rBV2	210	196	0.04%	0.005%
46	8.691	1118	1127	1136	rBV	199964	390092	78.24%	9.417%
47	8.807	1145	1146	1149	rVB2	310	184	0.04%	0.004%
48	8.941	1160	1168	1179	rVV2	66293	131561	26.39%	3.176%
49	9.118	1188	1197	1207	rBV	116228	232955	46.72%	5.624%
50	9.228	1214	1215	1217	rBV	243	171	0.03%	0.004%
51	9.295	1224	1226	1229	rVB2	307	265	0.05%	0.006%
52	9.350	1231	1235	1239	rVB3	392	601	0.12%	0.015%
53	9.429	1245	1248	1250	rBV	255	295	0.06%	0.007%
54	9.447	1250	1251	1253	rBV	227	172	0.03%	0.004%
55	9.471	1253	1255	1256	rBV	264	197	0.04%	0.005%
56	9.532	1262	1265	1267	rBV	287	307	0.06%	0.007%
57	9.636	1281	1282	1287	rVB	272	225	0.05%	0.005%
58	9.715	1293	1295	1297	rBV2	184	229	0.05%	0.006%
59	9.746	1297	1300	1306	rVB2	654	1155	0.23%	0.028%
60	9.795	1306	1308	1310	rBV2	268	296	0.06%	0.007%
61	9.892	1317	1324	1335	rVB	64186	113073	22.68%	2.730%
62	9.965	1335	1336	1337	rBV	265	180	0.04%	0.004%
63	10.032	1343	1347	1348	rBV	234	268	0.05%	0.006%
64	10.069	1350	1353	1363	rVB4	1379	2216	0.44%	0.053%
65	10.179	1363	1371	1378	rBV	210537	351150	70.43%	8.477%
66	10.246	1378	1382	1388	rVB3	4510	7251	1.45%	0.175%
67	10.374	1401	1403	1405	rBV2	318	331	0.07%	0.008%
68	10.435	1407	1413	1423	rVB	42614	70674	14.17%	1.706%
69	10.502	1423	1424	1425	rBV	292	180	0.04%	0.004%
70	10.581	1430	1437	1446	rVB	26914	48846	9.80%	1.179%
71	10.715	1454	1459	1465	rVV3	7856	14032	2.81%	0.339%
72	10.788	1465	1471	1482	rVV	77224	125355	25.14%	3.026%
73	10.947	1491	1497	1507	rBV	14486	26920	5.40%	0.650%
74	11.136	1526	1528	1530	rBV	272	298	0.06%	0.007%
75	11.276	1549	1551	1552	rBV	429	377	0.08%	0.009%
76	11.319	1552	1558	1564	rVV	25427	40945	8.21%	0.988%

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77	11.398	1568	1571	1574	rVV2	367	444	0.09%	0.011%
78	11.489	1578	1586	1598	rVV	291800	465787	93.42%	11.245%
79	11.599	1598	1604	1610	rVB4	540	1162	0.23%	0.028%
80	11.697	1618	1620	1625	rVB	1213	1128	0.23%	0.027%
81	11.739	1625	1627	1632	rVB3	388	434	0.09%	0.010%
82	11.788	1632	1635	1637	rBV2	245	265	0.05%	0.006%
83	11.965	1662	1664	1667	rBV2	255	306	0.06%	0.007%
84	12.331	1720	1724	1728	rBV4	1419	1914	0.38%	0.046%
85	12.489	1741	1750	1756	rBV	108974	181702	36.44%	4.386%
86	12.556	1756	1761	1768	rVB	82129	136186	27.31%	3.288%
87	12.733	1788	1790	1791	rBV	425	338	0.07%	0.008%
88	12.818	1798	1804	1811	rBV2	8417	15388	3.09%	0.371%
89	12.959	1823	1827	1829	rBV3	770	981	0.20%	0.024%
90	12.983	1829	1831	1832	rBV2	395	222	0.04%	0.005%
91	13.068	1840	1845	1850	rVB3	2308	3997	0.80%	0.096%
92	13.184	1859	1864	1870	rVB2	9852	14812	2.97%	0.358%
93	13.282	1875	1880	1886	rVB4	2744	4700	0.94%	0.113%
94	13.355	1889	1892	1893	rBV2	451	445	0.09%	0.011%
95	13.422	1897	1903	1909	rBV	233267	355967	71.39%	8.593%
96	13.641	1935	1939	1942	rBV3	2238	2676	0.54%	0.065%
97	13.721	1946	1952	1960	rVB	121582	190841	38.28%	4.607%
98	13.965	1986	1992	2000	rVB2	16133	28352	5.69%	0.684%
99	14.135	2018	2020	2021	rBV2	540	506	0.10%	0.012%
100	15.318	2210	2214	2218	rVB	4903	7002	1.40%	0.169%

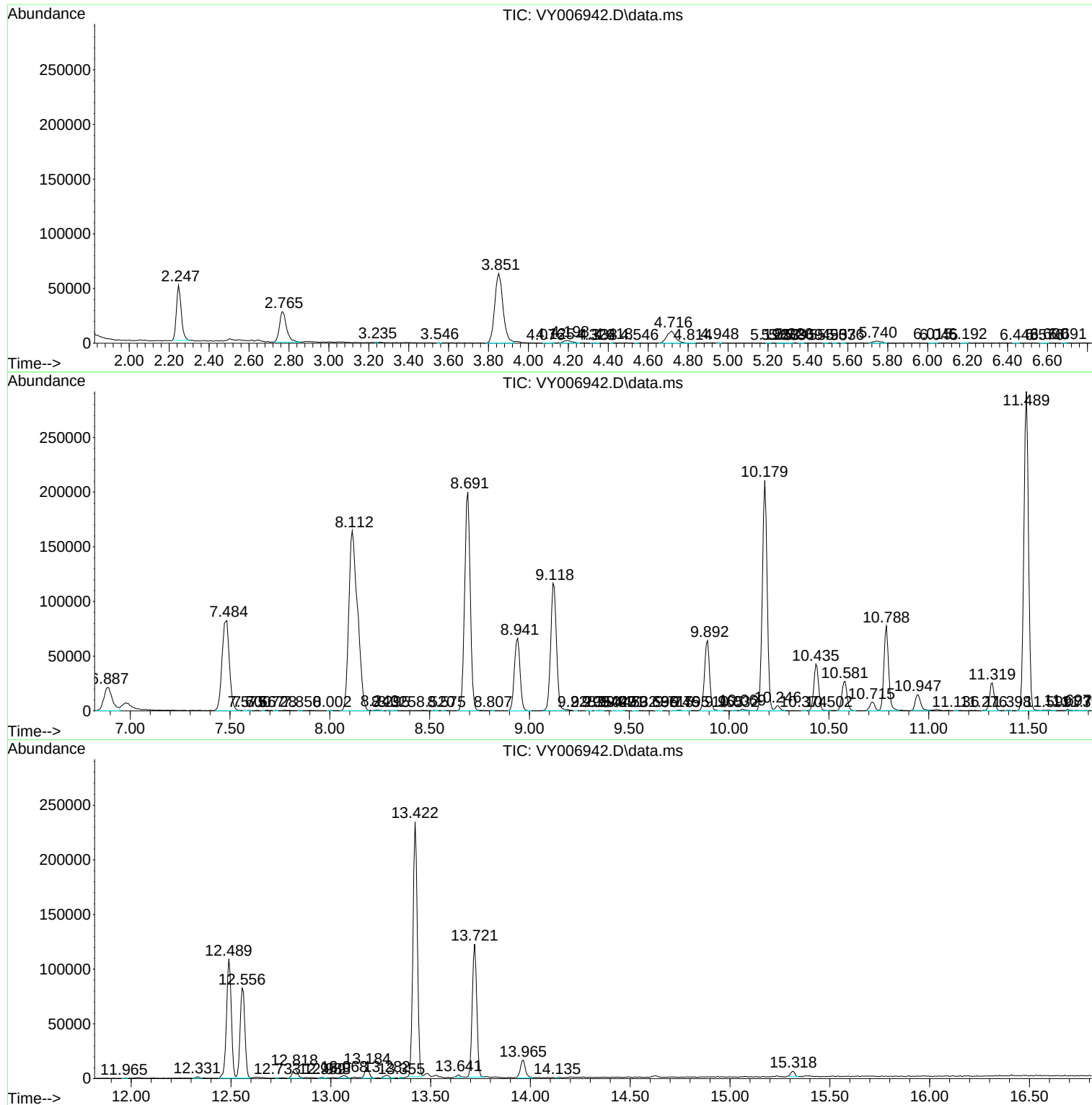
Sum of corrected areas: 4142343

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P



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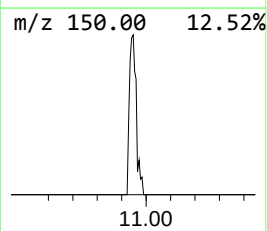
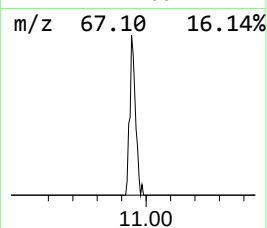
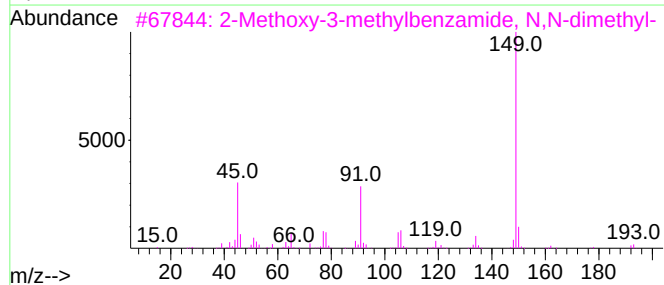
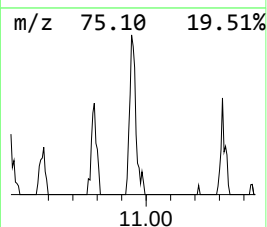
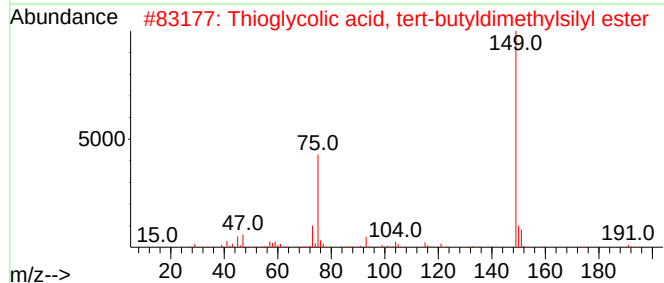
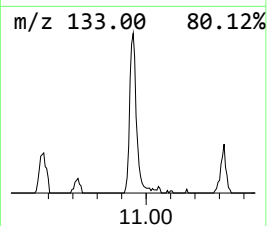
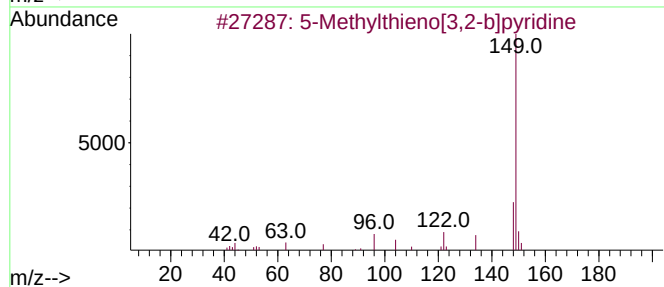
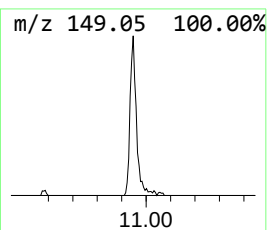
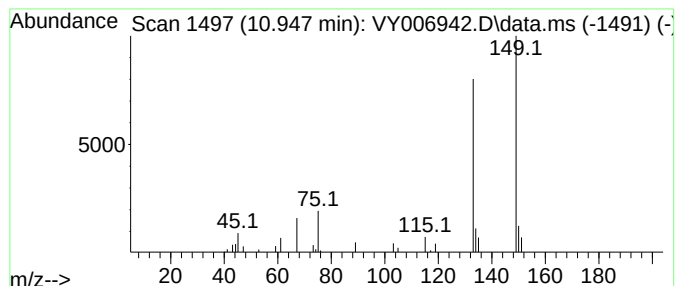
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
Quant Title : VOC Analysis

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

Peak Number 4 unknown-01 Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
10.947	1.44 ug/L	26920	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			5-Methylthieno[3,2-b]pyridine	149	C8H7NS	001759-29-1	35
2			Thioglycolic acid, tert-butyldim...	206	C8H18O2SSi	1000476-01-2	32
3			2-Methoxy-3-methylbenzamide, N,N...	193	C11H15NO2	1369798-01-5	32
4			Silane, diethoxydimethyl-	148	C6H16O2Si	000078-62-6	25
5			1H-Indole-3-thiol	149	C8H7NS	000480-94-4	25



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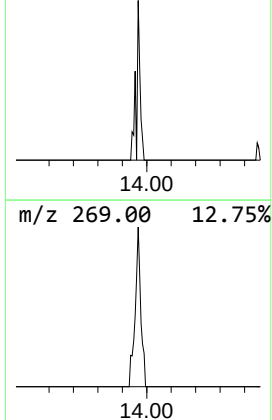
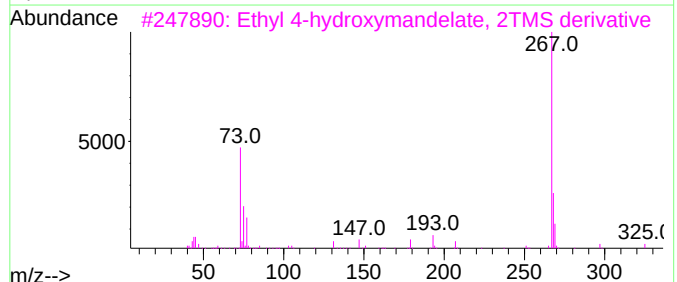
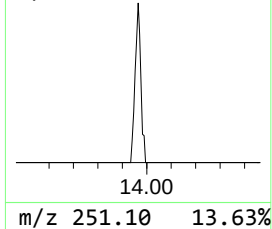
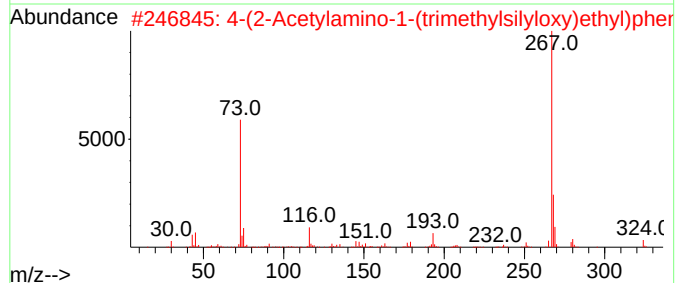
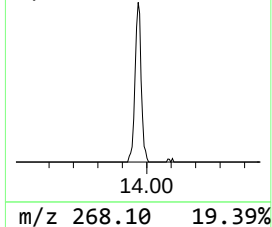
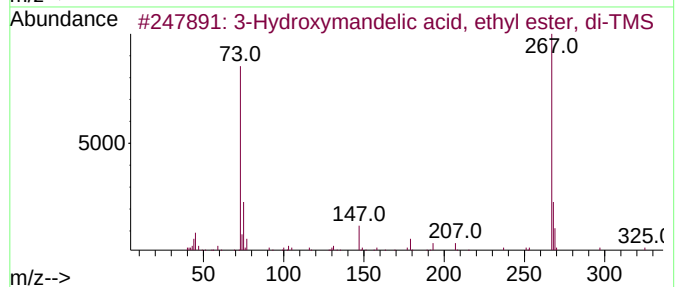
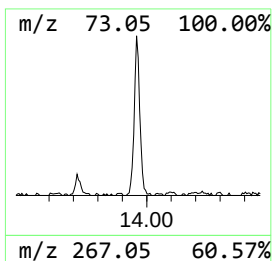
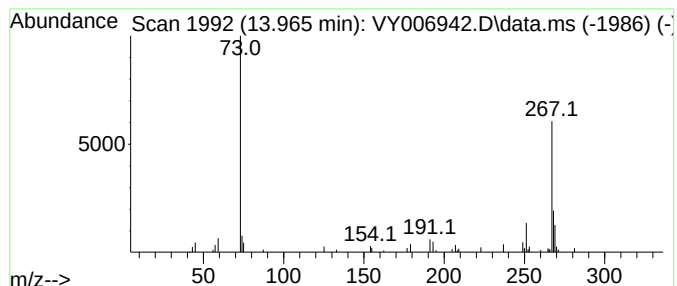
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYLEM120321SMA.M
Quant Title : VOC Analysis

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

Peak Number 7 unknown-02 Concentration Rank 6

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	1.99 ug/L	28352	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			3-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-88-9	64
2			4-(2-Acetylamino-1-(trimethylsil...	339	C16H29NO3Si2	1000373-43-5	50
3			Ethyl 4-hydroxymandelate, 2TMS d...	340	C16H28O4Si2	1010071-53-3	50
4			4-(2-amino-1-hydroxypropyl)pheno...	311	C15H29NO2Si2	1000478-98-6	45
5			Bamethan, 2TMS derivative	353	C18H35NO2Si2	040629-66-1	45



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	10.947	1.4	ug/L	26920	2	11.489	465787	25.0
unknown-02	13.965	2.0	ug/L	28352	3	13.422	355967	25.0