

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY120421\
 Data File : VY006933.D
 Acq On : 04 Dec 2021 12:08
 Operator : SY/MD
 Sample : M4884-03
 Misc : 3.93g/10.0mL/MSVOA_Y/SOIL
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 EW9H9

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: VY006933.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	66	70	79	rVB	30081	51426	12.43%	1.563%
2	2.771	150	156	171	rVB	20895	50998	12.33%	1.550%
3	3.509	275	277	280	rBV2	422	503	0.12%	0.015%
4	3.570	285	287	290	rVB	335	285	0.07%	0.009%
5	3.710	309	310	311	rBV	379	209	0.05%	0.006%
6	3.857	323	334	344	rBV	44377	121216	29.31%	3.684%
7	4.070	367	369	371	rBV	225	189	0.05%	0.006%
8	4.186	379	388	389	rBV3	1944	3012	0.73%	0.092%
9	4.472	433	435	438	rVV2	246	311	0.08%	0.009%
10	4.546	445	447	449	rBV	184	232	0.06%	0.007%
11	4.600	454	456	458	rBV2	244	238	0.06%	0.007%
12	4.722	463	476	489	rBV	11616	36532	8.83%	1.110%
13	4.930	503	510	512	rBV3	727	1608	0.39%	0.049%
14	5.058	529	531	533	rVB2	289	207	0.05%	0.006%
15	5.161	546	548	552	rBV	278	325	0.08%	0.010%
16	5.289	567	569	572	rBV	204	239	0.06%	0.007%
17	5.527	606	608	611	rVV2	228	260	0.06%	0.008%
18	5.582	614	617	618	rBV2	182	189	0.05%	0.006%
19	5.612	618	622	623	rVV	225	283	0.07%	0.009%
20	5.661	626	630	632	rBB	245	385	0.09%	0.012%
21	5.679	632	633	636	rBB	230	200	0.05%	0.006%
22	5.747	636	644	652	rBV4	1940	5239	1.27%	0.159%
23	5.905	668	670	675	rBV	222	402	0.10%	0.012%
24	6.216	715	721	722	rBV2	236	358	0.09%	0.011%
25	6.368	745	746	749	rBB	263	257	0.06%	0.008%
26	6.399	749	751	753	rBV	181	217	0.05%	0.007%
27	6.515	768	770	773	rBV	292	311	0.08%	0.009%
28	6.588	778	782	783	rBV2	219	223	0.05%	0.007%
29	6.649	789	792	796	rBB	265	374	0.09%	0.011%
30	6.698	796	800	803	rBV	239	334	0.08%	0.010%
31	6.759	806	810	811	rVB	211	228	0.06%	0.007%
32	6.807	815	818	819	rVB	303	242	0.06%	0.007%
33	6.893	819	832	841	rBV	25018	73794	17.84%	2.243%
34	7.277	891	895	897	rBV2	249	339	0.08%	0.010%
35	7.344	905	906	909	rVB	492	345	0.08%	0.010%
36	7.368	909	910	913	rBV2	276	236	0.06%	0.007%

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37	7.484	920	929	941	rVB	68583	168739	40.80%	5.128%
38	7.636	951	954	955	rBV	272	278	0.07%	0.008%
39	7.667	957	959	961	rVV	356	366	0.09%	0.011%
40	7.691	961	963	965	rVV	313	285	0.07%	0.009%
41	7.746	969	972	973	rBV	228	270	0.07%	0.008%
42	7.777	975	977	982	rVB	240	352	0.09%	0.011%
43	7.825	982	985	987	rBV	216	229	0.06%	0.007%
44	8.118	1022	1033	1047	rBV3	131444	413598	100.00%	12.569%
45	8.234	1047	1052	1060	rVB2	4403	9097	2.20%	0.276%
46	8.533	1098	1101	1109	rVV4	264	455	0.11%	0.014%
47	8.691	1118	1127	1138	rBV	172881	335951	81.23%	10.209%
48	8.935	1161	1167	1172	rVB5	1128	2443	0.59%	0.074%
49	8.996	1173	1177	1180	rBB5	207	294	0.07%	0.009%
50	9.124	1184	1198	1209	rBV	91607	182502	44.13%	5.546%
51	9.203	1209	1211	1215	rBV3	319	390	0.09%	0.012%
52	9.313	1228	1229	1232	rVB	260	201	0.05%	0.006%
53	9.343	1232	1234	1236	rBV	288	196	0.05%	0.006%
54	9.368	1236	1238	1240	rBV2	328	310	0.07%	0.009%
55	9.410	1244	1245	1248	rBV2	201	192	0.05%	0.006%
56	9.447	1250	1251	1254	rVB	328	264	0.06%	0.008%
57	9.502	1254	1260	1261	rBV2	958	1064	0.26%	0.032%
58	9.545	1266	1267	1272	rVB2	341	417	0.10%	0.013%
59	9.697	1286	1292	1295	rVB2	354	631	0.15%	0.019%
60	9.746	1295	1300	1303	rBV2	412	557	0.13%	0.017%
61	9.776	1303	1305	1309	rBV2	288	335	0.08%	0.010%
62	9.831	1312	1314	1317	rBV	235	209	0.05%	0.006%
63	9.892	1317	1324	1334	rBV	50469	86812	20.99%	2.638%
64	9.971	1335	1337	1343	rVB4	702	881	0.21%	0.027%
65	10.075	1349	1354	1358	rBV3	997	1682	0.41%	0.051%
66	10.179	1363	1371	1378	rVV	146550	248764	60.15%	7.560%
67	10.246	1378	1382	1388	rVB	6973	11262	2.72%	0.342%
68	10.386	1404	1405	1407	rBV	325	261	0.06%	0.008%
69	10.441	1407	1414	1424	rVB	32667	54988	13.30%	1.671%
70	10.581	1428	1437	1445	rBV	33130	60153	14.54%	1.828%
71	10.788	1463	1471	1478	rBV	82341	133790	32.35%	4.066%
72	10.886	1485	1487	1488	rBV	297	191	0.05%	0.006%
73	10.947	1491	1497	1507	rBV2	19498	35444	8.57%	1.077%
74	11.136	1525	1528	1529	rBV	352	459	0.11%	0.014%
75	11.209	1538	1540	1543	rBV2	341	442	0.11%	0.013%
76	11.319	1551	1558	1565	rVB2	25401	42765	10.34%	1.300%

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77	11.489	1580	1586	1596	rVB	211709	342386	82.78%	10.405%
78	11.556	1596	1597	1598	rVV	548	247	0.06%	0.008%
79	11.593	1601	1603	1607	rVB4	1076	1148	0.28%	0.035%
80	11.697	1616	1620	1627	rVB	1660	2628	0.64%	0.080%
81	11.812	1637	1639	1642	rBV2	214	233	0.06%	0.007%
82	12.032	1672	1675	1682	rVB4	1278	2215	0.54%	0.067%
83	12.154	1692	1695	1698	rBV	285	353	0.09%	0.011%
84	12.184	1698	1700	1702	rBV3	281	295	0.07%	0.009%
85	12.282	1714	1716	1717	rBV2	285	181	0.04%	0.006%
86	12.331	1721	1724	1732	rBV4	1141	1520	0.37%	0.046%
87	12.489	1741	1750	1756	rBV	129682	218147	52.74%	6.629%
88	12.562	1756	1762	1769	rVB	81787	132106	31.94%	4.015%
89	12.617	1769	1771	1773	rBV2	504	518	0.13%	0.016%
90	12.825	1798	1805	1811	rBV	9891	15969	3.86%	0.485%
91	12.910	1817	1819	1821	rVB3	552	445	0.11%	0.014%
92	13.032	1837	1839	1840	rBV2	652	478	0.12%	0.015%
93	13.068	1842	1845	1848	rVV3	1450	2141	0.52%	0.065%
94	13.117	1851	1853	1855	rVV	915	963	0.23%	0.029%
95	13.184	1859	1864	1871	rVB3	10479	17352	4.20%	0.527%
96	13.288	1877	1881	1885	rVB4	1655	2587	0.63%	0.079%
97	13.422	1897	1903	1910	rBV	145053	224777	54.35%	6.831%
98	13.532	1917	1921	1927	rVB4	2555	3975	0.96%	0.121%
99	13.721	1946	1952	1960	rVB	86162	134584	32.54%	4.090%
100	13.965	1987	1992	1997	rVB2	21705	36067	8.72%	1.096%

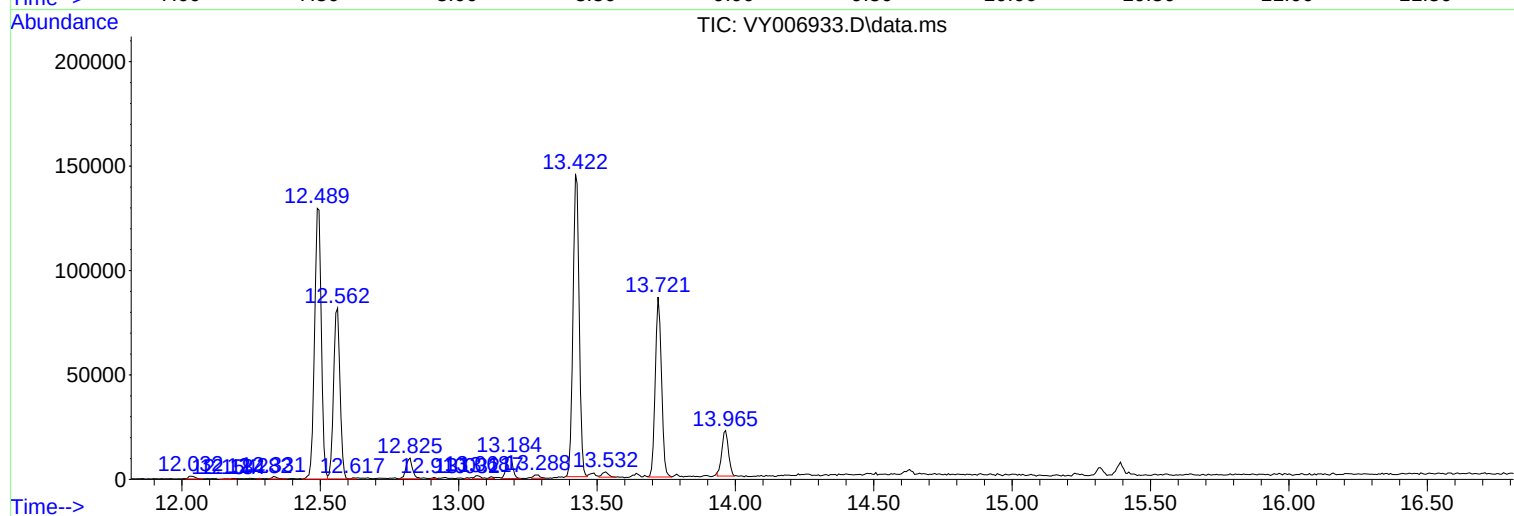
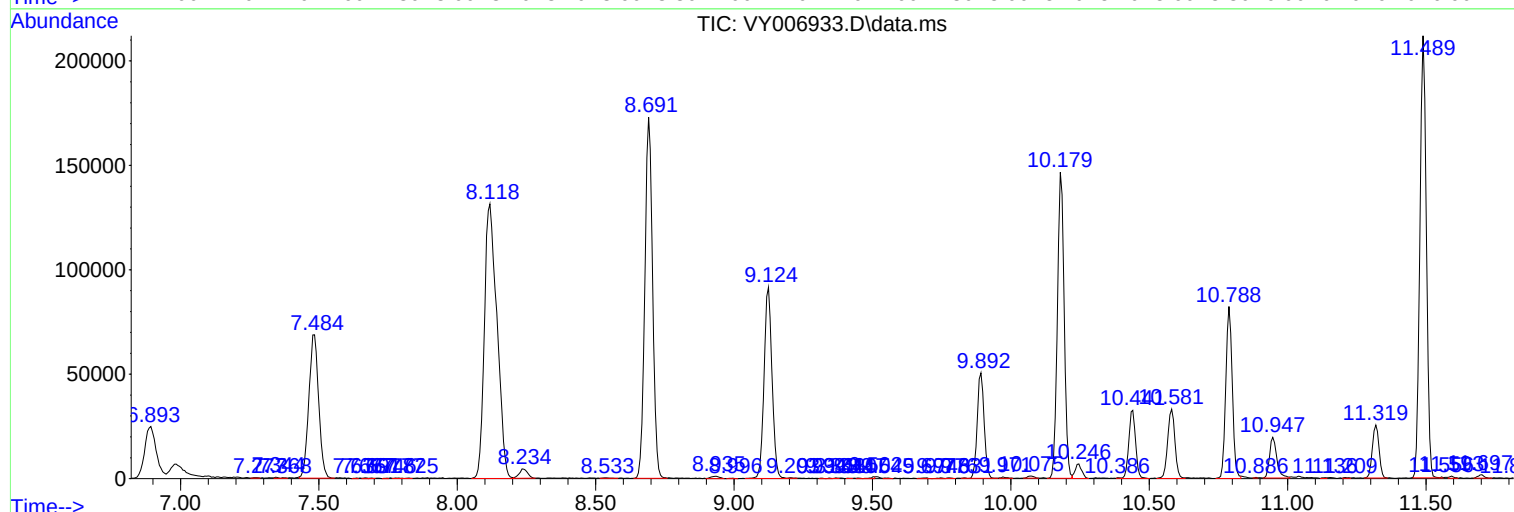
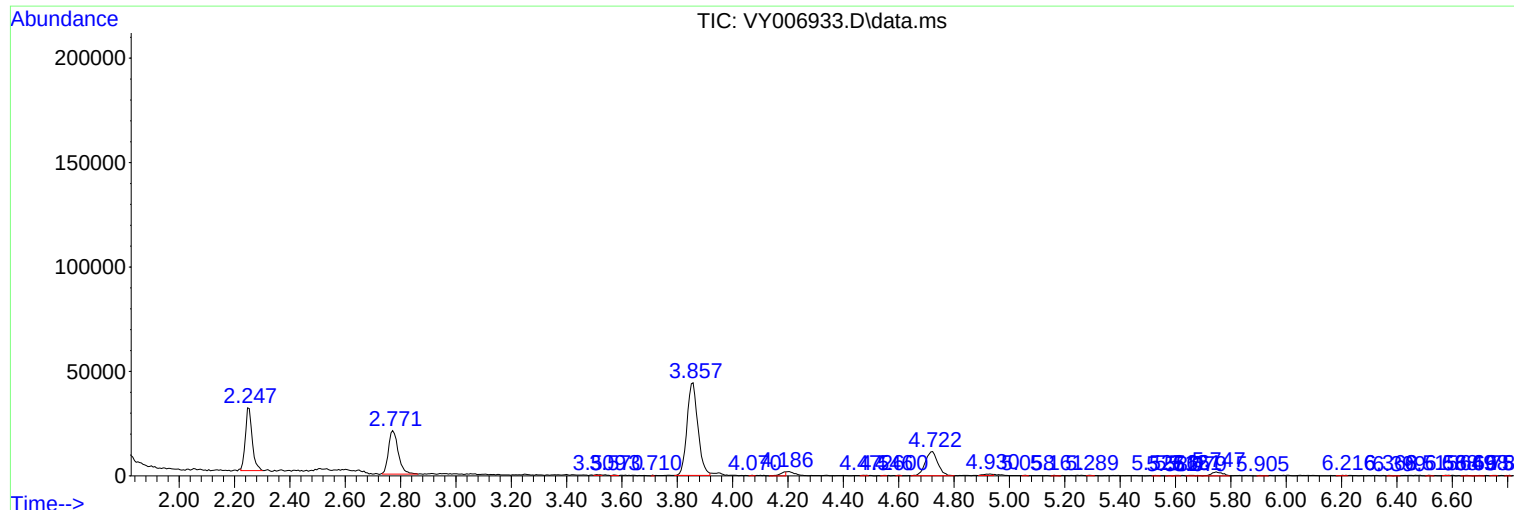
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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
Quant Title : VOC Analysis

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



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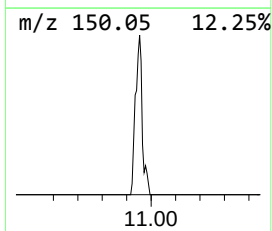
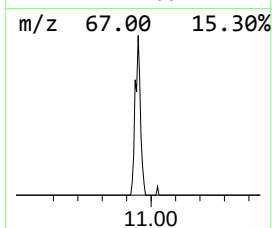
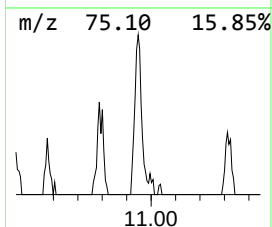
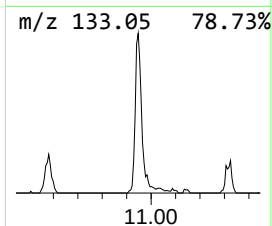
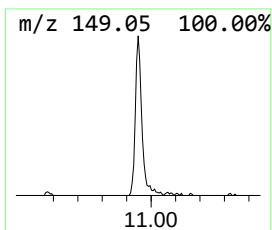
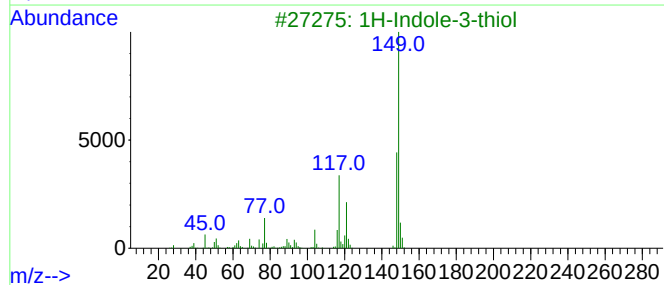
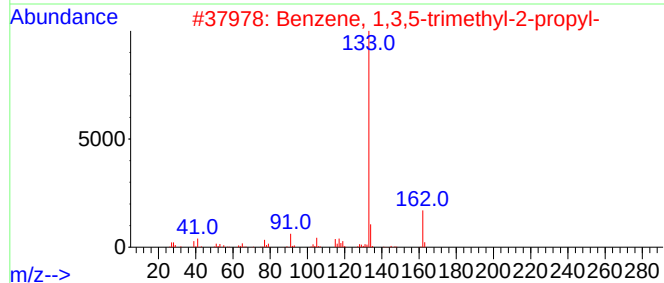
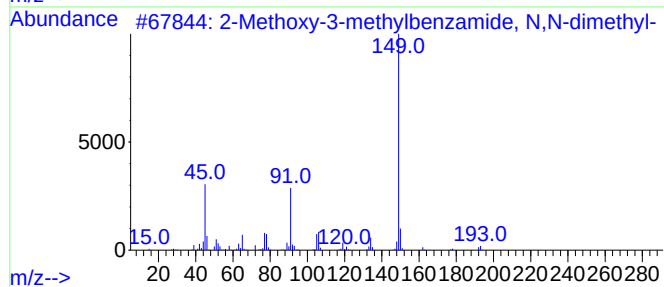
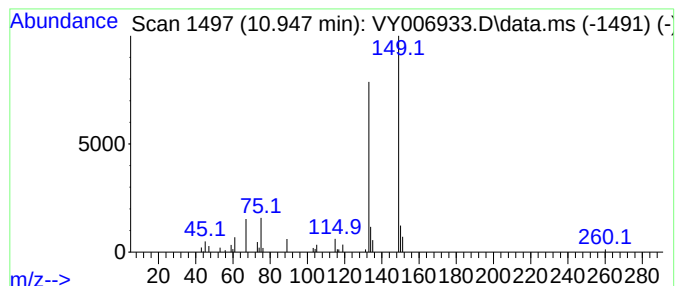
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYLM120321SMA.M
Quant Title : VOC Analysis

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	2.59 ug/L	35444	Chlorobenzene-d5	11.489

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			2-Methoxy-3-methylbenzamide, N,N...	193	C11H15NO2	1369798-01-5	37
2			Benzene, 1,3,5-trimethyl-2-propyl-	162	C12H18	004810-04-2	35
3			1H-Indole-3-thiol	149	C8H7NS	000480-94-4	32
4			4-Ethylbenzoic acid, 3-methylbut...	218	C14H18O2	1000292-54-1	32
5			1,1,3,3-Tetramethyl-1,3-bis[(2Z)...	302	C14H30O3Si2	1000352-70-7	25



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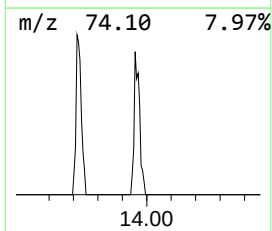
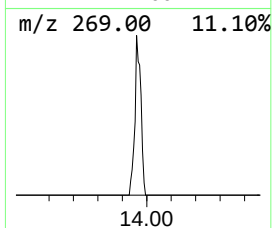
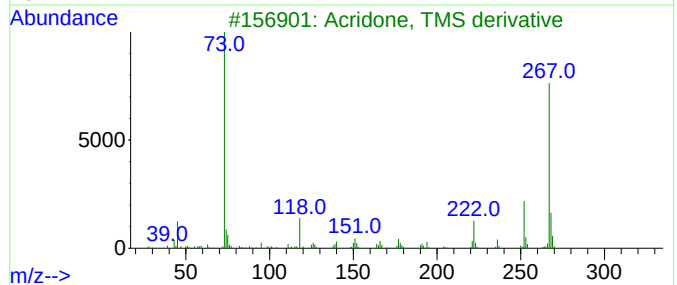
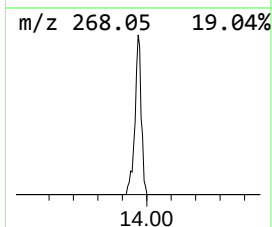
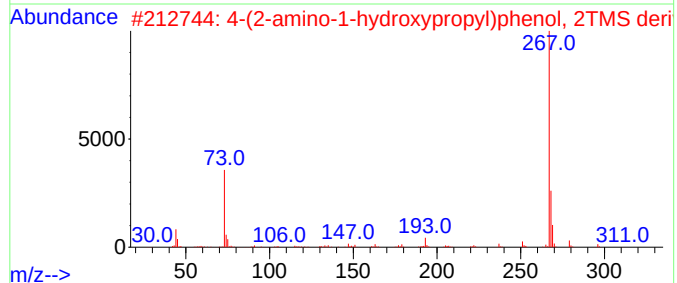
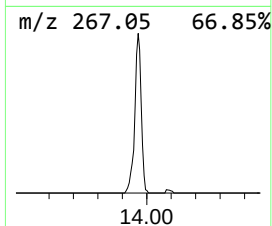
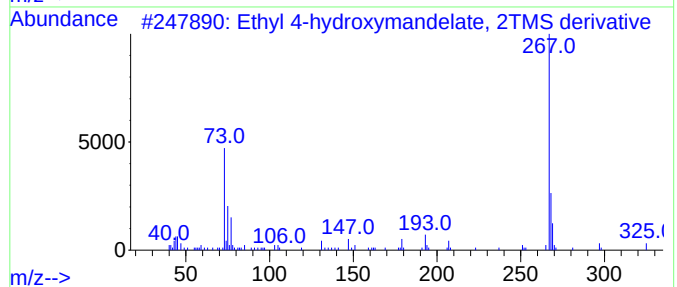
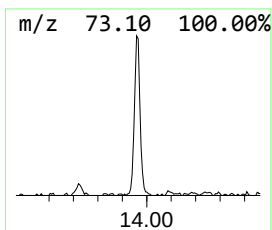
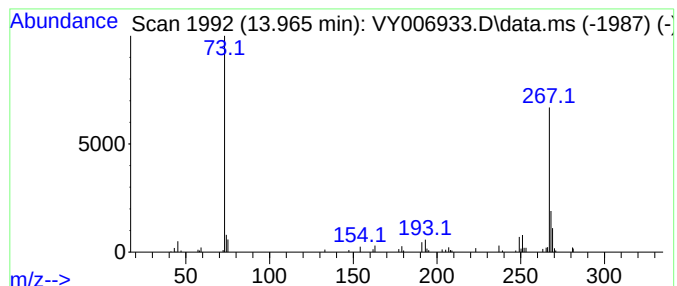
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYL120321SMA.M
Quant Title : VOC Analysis

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

Peak Number 9 Ethyl 4-hydroxymandelate, 2... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.964	4.01 ug/L	36067	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethyl 4-hydroxymandelate, 2TMS d...	340	C16H28O4Si2	1010071-53-3	72
2			4-(2-amino-1-hydroxypropyl)pheno...	311	C15H29NO2Si2	1000478-98-6	64
3			Acridone, TMS derivative	267	C16H17NOSi	1000478-16-0	64
4			4-(2-Acetylamino-1-(trimethylsil...	339	C16H29NO3Si2	1000373-43-5	59
5			Bamethan, 2TMS derivative	353	C18H35NO2Si2	040629-66-1	59



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	10.947	2.6	ug/L	35444	2	11.489	342386	25.0
Ethyl 4-hydroxy...	13.964	4.0	ug/L	36067	3	13.422	224777	25.0