

Data Path : Z:\voasrv\HPCHEM1\MSVOA_Y\Data\VY120421\
 Data File : VY006946.D
 Acq On : 04 Dec 2021 16:53
 Operator : SY/MD
 Sample : M4884-16
 Misc : 3.31g/10.0mL/MSVOA_Y/SOIL
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_Y
 ClientSampleId :
 EW9K2

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: VY006946.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	47147	81414	12.21%	2.053%
2	2.711	144	146	148	rBV2	670	627	0.09%	0.016%
3	2.772	148	156	171	rVB	29630	69662	10.45%	1.756%
4	3.022	195	197	201	rVB3	500	535	0.08%	0.013%
5	3.253	233	235	239	rVB3	372	378	0.06%	0.010%
6	3.595	289	291	295	rBV2	363	454	0.07%	0.011%
7	3.851	323	333	344	rBV	52886	145286	21.79%	3.663%
8	3.936	344	347	348	rBV	1287	1404	0.21%	0.035%
9	4.149	379	382	384	rBV2	269	322	0.05%	0.008%
10	4.192	384	389	398	rVB3	1710	4817	0.72%	0.121%
11	4.473	432	435	438	rBV2	219	348	0.05%	0.009%
12	4.564	446	450	451	rBV	282	338	0.05%	0.009%
13	4.716	467	475	485	rBV2	7648	22366	3.36%	0.564%
14	5.210	551	556	557	rBV2	1425	1874	0.28%	0.047%
15	5.375	580	583	586	rBV	404	323	0.05%	0.008%
16	5.539	606	610	614	rVB	264	496	0.07%	0.013%
17	5.655	626	629	633	rBV2	236	354	0.05%	0.009%
18	5.753	635	645	648	rBV3	1669	4602	0.69%	0.116%
19	6.289	729	733	736	rBV	239	317	0.05%	0.008%
20	6.789	812	815	818	rBV3	474	632	0.09%	0.016%
21	6.899	821	833	839	rBV	14637	43809	6.57%	1.105%
22	6.984	839	847	867	rVB	38463	116914	17.54%	2.948%
23	7.167	876	877	881	rVB2	415	337	0.05%	0.008%
24	7.210	881	884	886	rVB2	391	386	0.06%	0.010%
25	7.478	918	928	942	rVB	76163	194672	29.20%	4.909%
26	7.759	972	974	976	rBV	350	381	0.06%	0.010%
27	8.112	1022	1032	1049	rBV2	164351	475754	71.37%	11.996%
28	8.234	1049	1052	1056	rVV3	1053	1538	0.23%	0.039%
29	8.362	1069	1073	1075	rVV2	185	308	0.05%	0.008%
30	8.691	1118	1127	1138	rBV	130222	258559	38.79%	6.519%
31	8.825	1145	1149	1151	rBV3	290	413	0.06%	0.010%
32	8.941	1159	1168	1180	rBV	350896	666621	100.00%	16.809%
33	9.118	1188	1197	1205	rBV	99826	205644	30.85%	5.185%
34	9.264	1218	1221	1226	rBV2	281	466	0.07%	0.012%
35	9.350	1231	1235	1237	rVV	295	363	0.05%	0.009%
36	9.398	1241	1243	1246	rVB2	273	311	0.05%	0.008%

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37	9.606	1274	1277	1279	rBV	261	350	0.05%	0.009%
38	9.746	1296	1300	1304	rBV4	466	637	0.10%	0.016%
39	9.892	1318	1324	1332	rVB	49445	88961	13.35%	2.243%
40	10.069	1347	1353	1357	rBV3	1054	1789	0.27%	0.045%
41	10.112	1357	1360	1364	rVV3	514	717	0.11%	0.018%
42	10.179	1364	1371	1379	rVV	183495	317268	47.59%	8.000%
43	10.240	1379	1381	1388	rVB2	3497	5112	0.77%	0.129%
44	10.435	1404	1413	1420	rBV3	34443	62447	9.37%	1.575%
45	10.581	1430	1437	1442	rVV	24585	45267	6.79%	1.141%
46	10.642	1442	1447	1454	rVV2	18018	30515	4.58%	0.769%
47	10.721	1454	1460	1466	rVV	23447	40000	6.00%	1.009%
48	10.788	1466	1471	1483	rVB	49216	88801	13.32%	2.239%
49	10.947	1491	1497	1505	rBV	15680	28383	4.26%	0.716%
50	11.038	1510	1512	1517	rVB3	942	1280	0.19%	0.032%
51	11.215	1537	1541	1542	rBV2	262	327	0.05%	0.008%
52	11.264	1545	1549	1552	rVV3	450	764	0.11%	0.019%
53	11.319	1552	1558	1567	rVV2	21189	35855	5.38%	0.904%
54	11.404	1570	1572	1575	rVV3	348	388	0.06%	0.010%
55	11.435	1575	1577	1579	rVV3	289	313	0.05%	0.008%
56	11.490	1579	1586	1596	rVV	162887	263294	39.50%	6.639%
57	11.593	1600	1603	1607	rVV3	395	678	0.10%	0.017%
58	11.697	1617	1620	1625	rVB2	1272	1569	0.24%	0.040%
59	11.733	1625	1626	1632	rBV3	191	305	0.05%	0.008%
60	11.819	1638	1640	1641	rBV	424	310	0.05%	0.008%
61	11.959	1658	1663	1664	rBV2	243	335	0.05%	0.008%
62	12.026	1670	1674	1681	rVB2	1102	1757	0.26%	0.044%
63	12.124	1682	1690	1691	rBV3	401	835	0.13%	0.021%
64	12.288	1714	1717	1721	rBV2	317	384	0.06%	0.010%
65	12.331	1721	1724	1726	rBV3	934	1018	0.15%	0.026%
66	12.489	1738	1750	1756	rBV	94552	157428	23.62%	3.969%
67	12.556	1756	1761	1769	rVB	65026	102892	15.43%	2.594%
68	12.630	1769	1773	1778	rBV5	1209	2192	0.33%	0.055%
69	12.733	1787	1790	1791	rBV	516	561	0.08%	0.014%
70	12.764	1793	1795	1798	rVV3	787	845	0.13%	0.021%
71	12.825	1798	1805	1812	rVB3	6319	11226	1.68%	0.283%
72	12.886	1812	1815	1817	rBV3	415	600	0.09%	0.015%
73	13.038	1837	1840	1842	rBV3	749	908	0.14%	0.023%
74	13.062	1842	1844	1850	rVV2	2193	3665	0.55%	0.092%
75	13.123	1850	1854	1858	rVV4	961	1563	0.23%	0.039%
76	13.178	1859	1863	1870	rVB2	8110	12875	1.93%	0.325%

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 Title : VOC Analysis

77	13.282	1876	1880	1886	rVB4	2190	3901	0.59%	0.098%
78	13.422	1897	1903	1909	rBV	102641	157450	23.62%	3.970%
79	13.489	1909	1914	1918	rVV4	2904	5473	0.82%	0.138%
80	13.526	1918	1920	1926	rVB5	1078	1456	0.22%	0.037%
81	13.642	1935	1939	1945	rBV6	1881	2889	0.43%	0.073%
82	13.721	1946	1952	1958	rBV	85409	133838	20.08%	3.375%
83	13.825	1967	1969	1974	rVB3	1045	1246	0.19%	0.031%
84	13.965	1986	1992	2003	rVB	14732	26174	3.93%	0.660%
85	14.081	2009	2011	2012	rBV	501	413	0.06%	0.010%
86	14.184	2024	2028	2029	rVV2	397	596	0.09%	0.015%
87	14.373	2057	2059	2060	rBV	567	312	0.05%	0.008%
88	14.605	2095	2097	2098	rBV	554	455	0.07%	0.011%
89	14.702	2111	2113	2114	rBV2	688	434	0.07%	0.011%
90	14.812	2126	2131	2132	rBV4	789	924	0.14%	0.023%
91	14.940	2148	2152	2155	rBV3	761	1533	0.23%	0.039%
92	15.038	2166	2168	2171	rBV4	517	430	0.06%	0.011%
93	15.093	2176	2177	2181	rBV2	435	542	0.08%	0.014%
94	15.147	2181	2186	2188	rBV2	809	1427	0.21%	0.036%
95	15.172	2188	2190	2193	rBV3	654	664	0.10%	0.017%
96	15.233	2198	2200	2205	rVV5	884	1149	0.17%	0.029%
97	15.318	2209	2214	2218	rVV3	3358	4704	0.71%	0.119%
98	15.507	2244	2245	2247	rBV2	675	651	0.10%	0.016%
99	15.879	2302	2306	2308	rBV4	770	952	0.14%	0.024%
100	15.940	2313	2316	2317	rBV3	1015	919	0.14%	0.023%

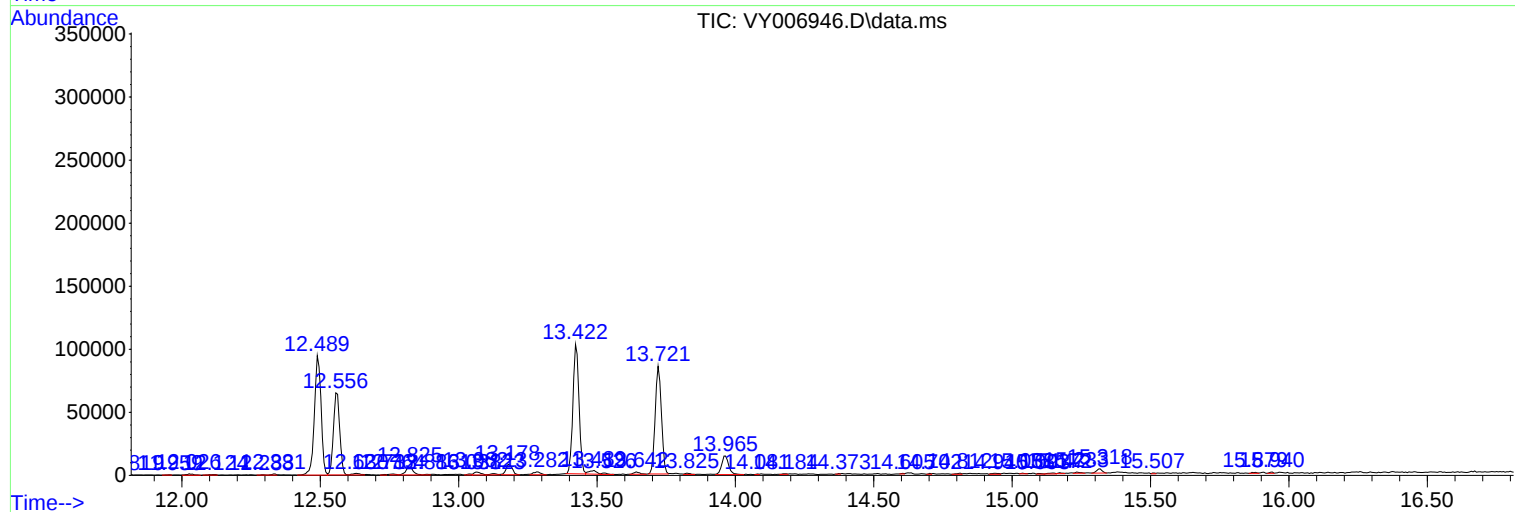
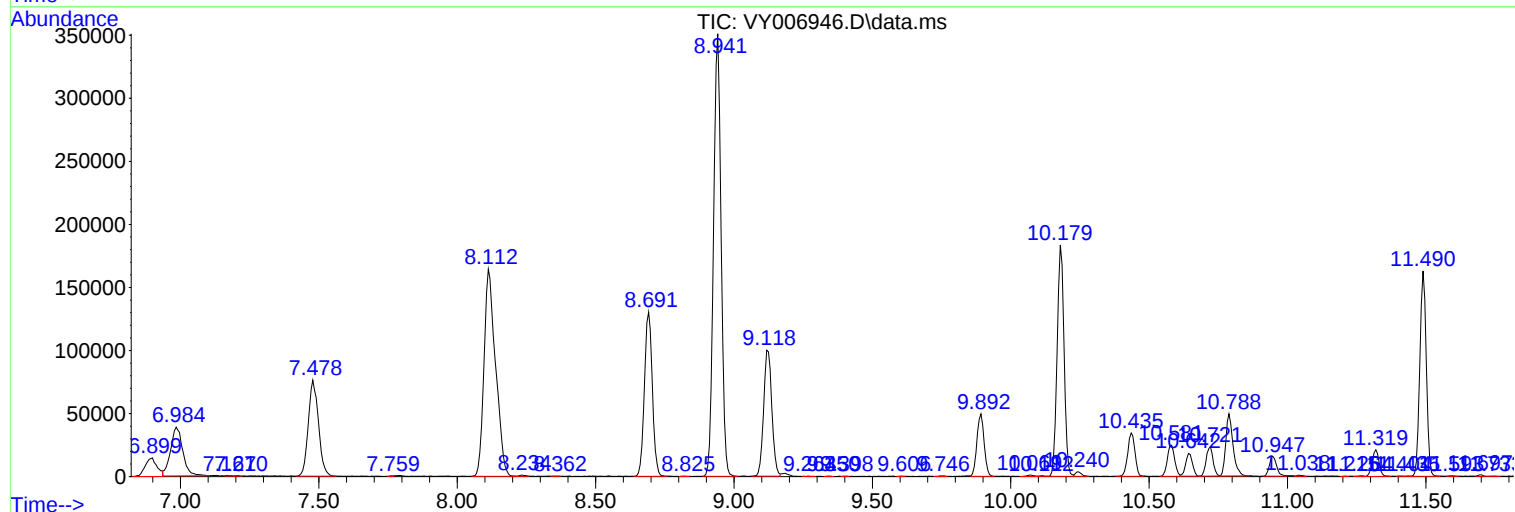
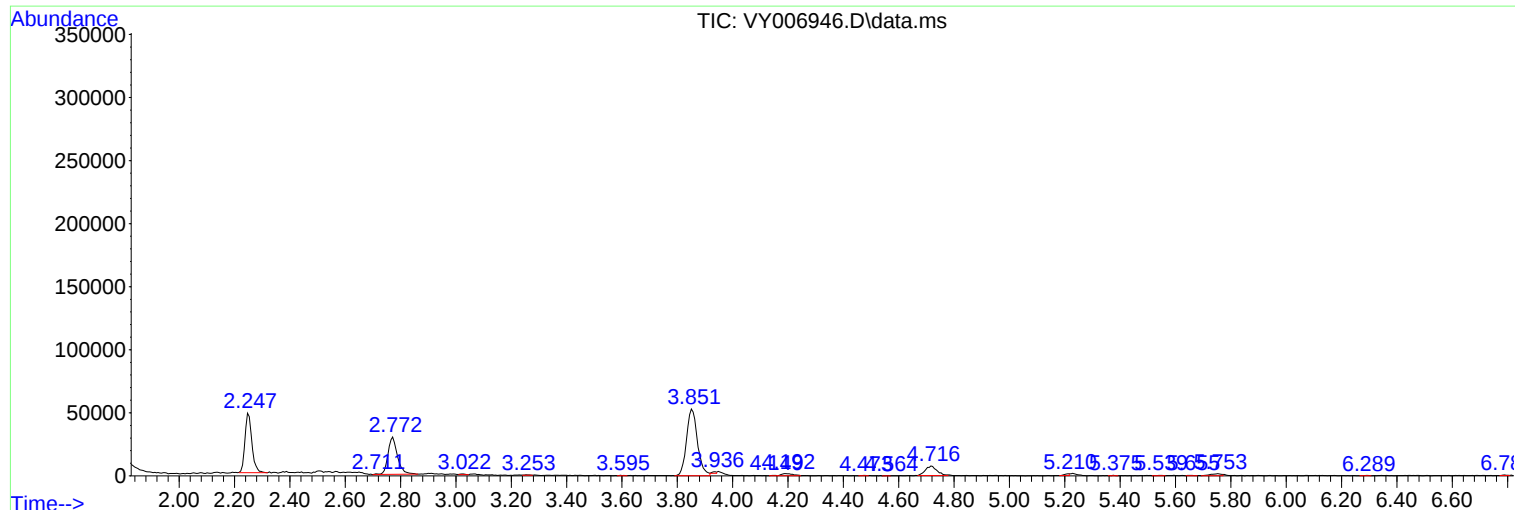
Sum of corrected areas: 3965971

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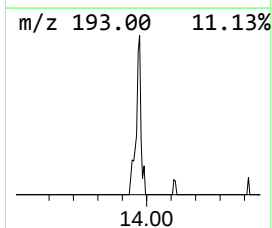
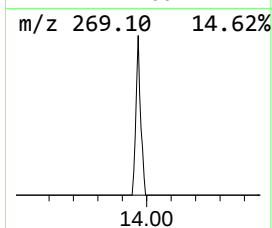
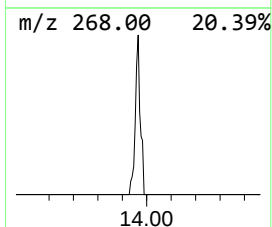
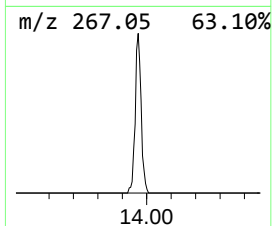
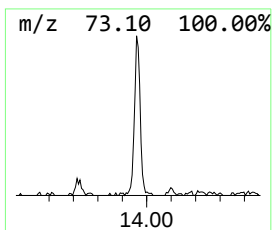
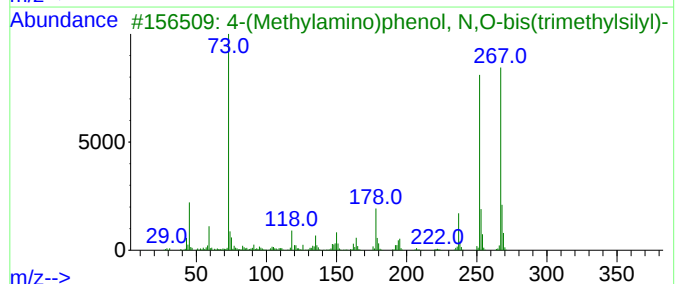
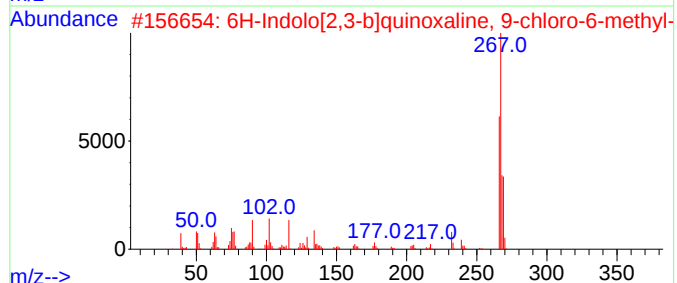
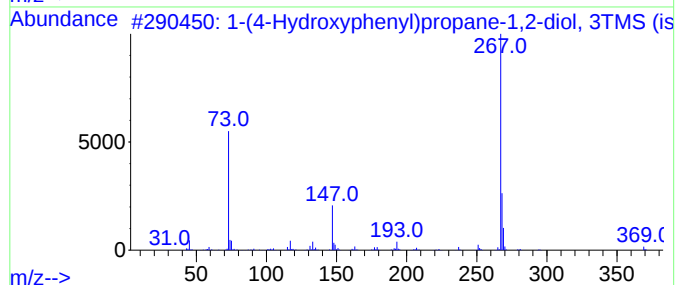
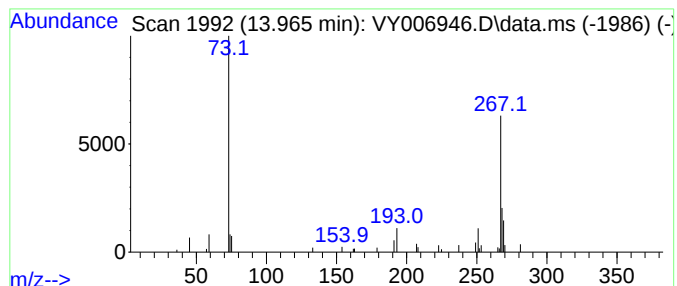
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_Y\methods\SFAMYLM120321SMA.M
Quant Title : VOC Analysis

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

Peak Number 9 1-(4-Hydroxyphenyl)propane-... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.965	4.16 ug/L	26174	1,4-Dichlorobenzene-d4	13.422

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			1-(4-Hydroxyphenyl)propane-1,2-d...	384	C18H36O3Si3	1000495-85-7	53
2			6H-Indolo[2,3-b]quinoxaline, 9-c...	267	C15H10ClN3	1000319-29-1	43
3			4-(Methylamino)phenol, N,O-bis(t...	267	C13H25NOSi2	1000471-13-0	42
4			Butanamide, 2,2,3,3,4,4,4-heptaf...	493	C18H26F7NO3Si2	055471-01-7	42
5			3-Hydroxymandelic acid, ethyl es...	340	C16H28O4Si2	1000071-88-9	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
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