

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120921\
 Data File : VX025667.D
 Acq On : 09 Dec 2021 18:20
 Operator : JC/MD
 Sample : M4975-10
 Misc : 6.62g/5mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGKT4

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_X\Method\SFAMXML112221WMA.M
 Title : VOC Analysis

Signal : TIC: VX025667.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	43	46	53	rVB	47688	56689	7.24%	1.348%
2	1.648	88	92	100	rVB	30588	38008	4.85%	0.904%
3	2.282	190	196	206	rBV	89157	147820	18.87%	3.514%
4	2.776	276	277	279	rBV2	645	597	0.08%	0.014%
5	2.947	300	305	313	rBV2	3121	7180	0.92%	0.171%
6	3.154	337	339	342	rBV2	454	631	0.08%	0.015%
7	3.221	348	350	353	rBV	338	388	0.05%	0.009%
8	3.349	369	371	373	rBV2	475	285	0.04%	0.007%
9	3.593	410	411	413	rBV	414	289	0.04%	0.007%
10	3.642	417	419	420	rBV	386	215	0.03%	0.005%
11	4.007	478	479	483	rBV2	223	290	0.04%	0.007%
12	4.379	539	540	543	rBV	386	226	0.03%	0.005%
13	4.428	546	548	549	rBV	404	245	0.03%	0.006%
14	4.489	549	558	582	rBV2	15126	73122	9.34%	1.738%
15	5.062	639	652	670	rBV	47366	163966	20.93%	3.898%
16	5.215	676	677	680	rVB	461	263	0.03%	0.006%
17	5.379	692	704	712	rBV4	4752	14486	1.85%	0.344%
18	5.458	716	717	720	rVB2	450	270	0.03%	0.006%
19	5.489	720	722	724	rBV2	255	252	0.03%	0.006%
20	5.519	725	727	730	rVB2	374	296	0.04%	0.007%
21	5.964	790	800	816	rBV2	139397	405668	51.79%	9.644%
22	6.361	861	865	866	rBV2	1431	1703	0.22%	0.040%
23	6.763	922	931	947	rVB	105904	272441	34.78%	6.477%
24	6.922	955	957	959	rBV	286	238	0.03%	0.006%
25	7.123	983	990	997	rBV2	9156	20763	2.65%	0.494%
26	7.208	1000	1004	1006	rBV3	528	908	0.12%	0.022%
27	7.312	1013	1021	1034	rVB	76674	178174	22.75%	4.236%
28	7.562	1061	1062	1067	rVV2	350	497	0.06%	0.012%
29	7.684	1081	1082	1085	rBV2	276	240	0.03%	0.006%
30	7.885	1114	1115	1119	rBV	250	280	0.04%	0.007%
31	8.062	1142	1144	1147	rBV2	249	306	0.04%	0.007%
32	8.092	1147	1149	1151	rVB2	266	252	0.03%	0.006%
33	8.214	1168	1169	1171	rBV	211	202	0.03%	0.005%
34	8.263	1176	1177	1180	rBV	376	285	0.04%	0.007%
35	8.330	1180	1188	1198	rBV	51751	96039	12.26%	2.283%
36	8.464	1207	1210	1213	rBV	283	277	0.04%	0.007%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
 Title : VOC Analysis

37	8.604	1231	1233	1234	rBV	204	194	0.02%	0.005%
38	8.653	1234	1241	1248	rVV	200655	344996	44.04%	8.201%
39	8.720	1248	1252	1258	rVB2	4035	6576	0.84%	0.156%
40	8.958	1285	1291	1298	rBV	35045	58894	7.52%	1.400%
41	9.177	1326	1327	1329	rBV2	375	295	0.04%	0.007%
42	9.275	1336	1343	1357	rBV	545599	783307	100.00%	18.621%
43	9.397	1357	1363	1373	rBV	95824	161401	20.61%	3.837%
44	9.580	1392	1393	1396	rBV2	259	257	0.03%	0.006%
45	9.628	1399	1401	1404	rBV2	292	319	0.04%	0.008%
46	9.683	1408	1410	1411	rBV2	262	257	0.03%	0.006%
47	9.787	1424	1427	1429	rBV2	273	301	0.04%	0.007%
48	9.976	1456	1458	1460	rVB	333	301	0.04%	0.007%
49	10.006	1460	1463	1465	rBV2	428	527	0.07%	0.013%
50	10.055	1465	1471	1484	rVB	218550	328163	41.89%	7.801%
51	10.195	1492	1494	1499	rVB3	790	1168	0.15%	0.028%
52	10.305	1507	1512	1517	rVB	5769	8023	1.02%	0.191%
53	10.647	1565	1568	1575	rVB2	2974	4150	0.53%	0.099%
54	10.750	1584	1585	1588	rVB	277	202	0.03%	0.005%
55	10.854	1601	1602	1604	rVV2	402	261	0.03%	0.006%
56	10.896	1607	1609	1611	rVB	413	311	0.04%	0.007%
57	10.945	1614	1617	1620	rBV2	603	744	0.09%	0.018%
58	11.116	1642	1645	1650	rVB2	3183	4370	0.56%	0.104%
59	11.195	1653	1658	1666	rVV	145352	185294	23.66%	4.405%
60	11.305	1674	1676	1678	rVB3	691	549	0.07%	0.013%
61	11.384	1686	1689	1691	rVB2	579	617	0.08%	0.015%
62	11.482	1698	1705	1711	rBV3	3184	5230	0.67%	0.124%
63	11.543	1713	1715	1721	rBV	503	705	0.09%	0.017%
64	11.713	1741	1743	1745	rBV2	637	576	0.07%	0.014%
65	11.750	1746	1749	1758	rVB2	3848	5507	0.70%	0.131%
66	11.841	1761	1764	1767	rBV2	720	977	0.12%	0.023%
67	11.933	1776	1779	1784	rBV4	1691	2394	0.31%	0.057%
68	11.976	1784	1786	1789	rVB2	882	532	0.07%	0.013%
69	12.024	1789	1794	1800	rBV	278123	336192	42.92%	7.992%
70	12.152	1812	1815	1823	rVB4	2757	4502	0.57%	0.107%
71	12.323	1835	1843	1850	rBV	249832	309842	39.56%	7.366%
72	12.427	1855	1860	1863	rVB	5796	6676	0.85%	0.159%
73	12.469	1864	1867	1868	rBV2	444	520	0.07%	0.012%
74	12.927	1940	1942	1944	rVB	432	260	0.03%	0.006%
75	12.969	1946	1949	1954	rVB4	635	905	0.12%	0.022%
76	13.055	1959	1963	1965	rVB3	811	1001	0.13%	0.024%

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Stop Thrs : 0

Peak Location: TOP

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
 Title : VOC Analysis

77	13.079	1965	1967	1969	rBV	355	321	0.04%	0.008%
78	13.268	1996	1998	2001	rVB2	973	944	0.12%	0.022%
79	13.463	2028	2030	2034	rVB	362	409	0.05%	0.010%
80	13.591	2049	2051	2054	rBV2	703	747	0.10%	0.018%
81	13.780	2078	2082	2086	rVB	4638	5712	0.73%	0.136%
82	13.865	2093	2096	2097	rBV	298	263	0.03%	0.006%
83	14.036	2122	2124	2127	rBV2	490	323	0.04%	0.008%
84	14.219	2152	2154	2156	rBV	289	229	0.03%	0.005%
85	14.451	2190	2192	2193	rBV	442	297	0.04%	0.007%
86	14.640	2221	2223	2229	rVV4	789	1019	0.13%	0.024%
87	14.707	2232	2234	2235	rBV	328	221	0.03%	0.005%
88	14.823	2251	2253	2255	rBV2	879	859	0.11%	0.020%
89	14.957	2272	2275	2281	rVB4	1878	2235	0.29%	0.053%
90	15.054	2287	2291	2298	rBV5	3658	5998	0.77%	0.143%
91	15.134	2300	2304	2308	rVB4	3097	4223	0.54%	0.100%
92	15.213	2315	2317	2320	rVB2	571	464	0.06%	0.011%
93	15.255	2320	2324	2328	rVB4	2318	3098	0.40%	0.074%
94	15.347	2332	2339	2344	rBV2	59197	90294	11.53%	2.146%
95	15.469	2356	2359	2362	rBV4	1392	1841	0.24%	0.044%
96	15.512	2362	2366	2373	rVB3	4065	6524	0.83%	0.155%
97	15.658	2387	2390	2396	rBV4	1540	2545	0.32%	0.061%
98	15.719	2396	2400	2408	rVV5	4928	10967	1.40%	0.261%
99	15.804	2409	2414	2420	rVB2	9101	14496	1.85%	0.345%
100	16.188	2474	2477	2481	rVB3	1196	1463	0.19%	0.035%

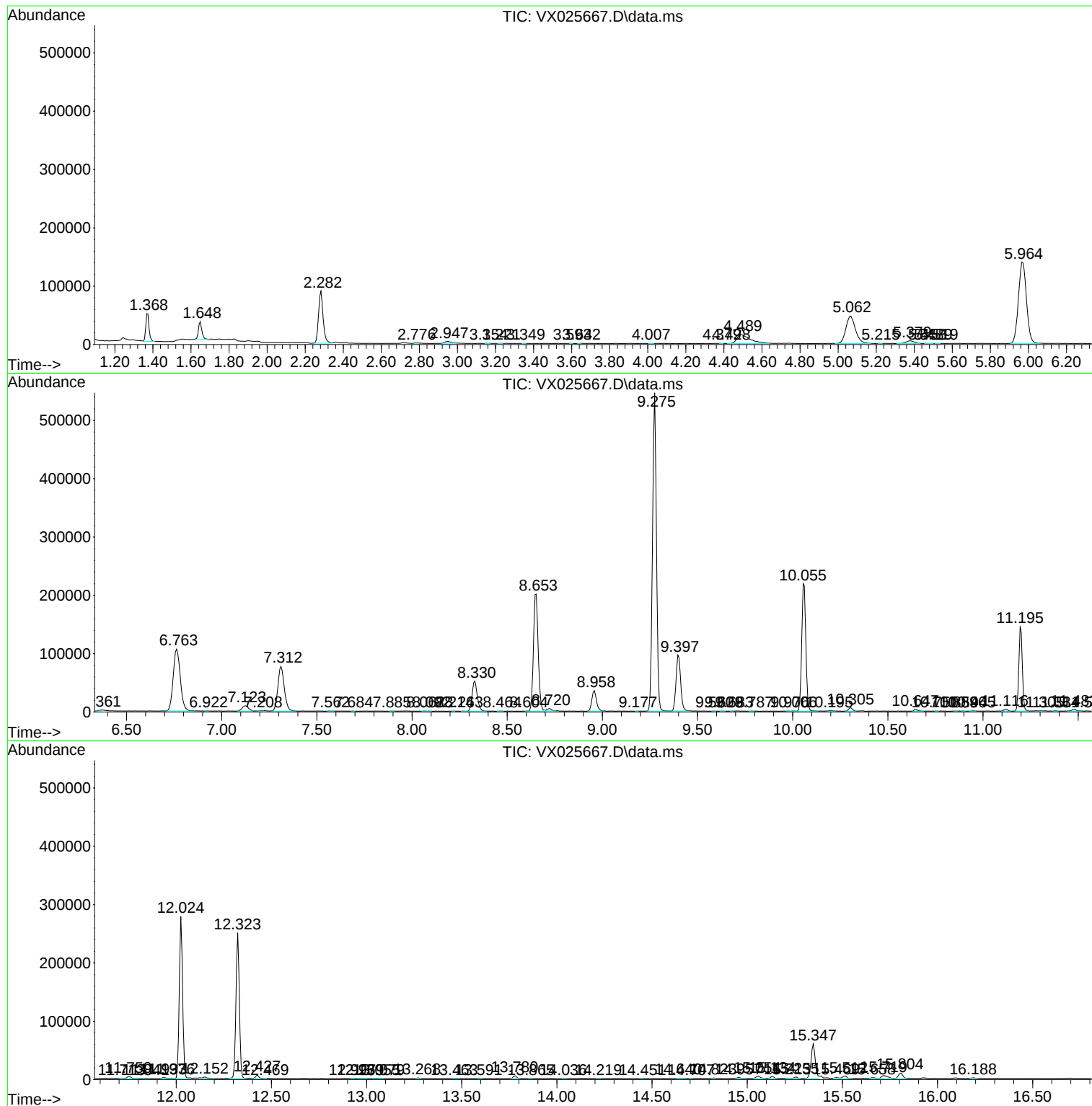
Sum of corrected areas: 4206579

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Instrument :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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



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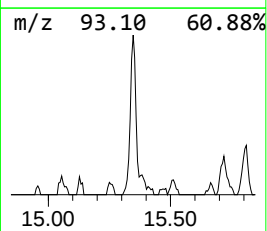
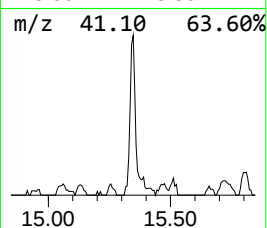
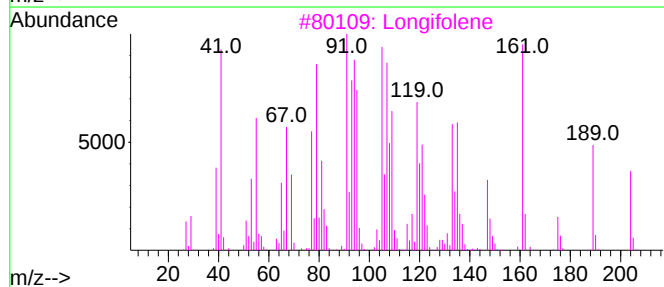
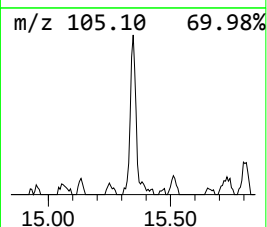
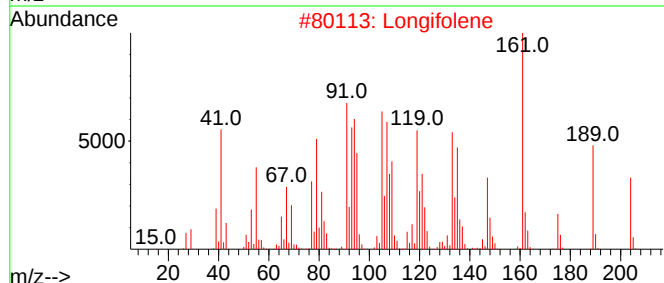
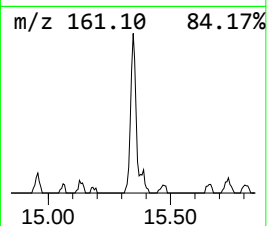
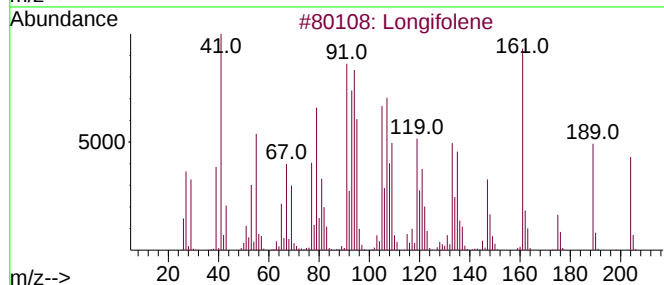
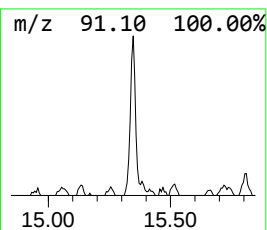
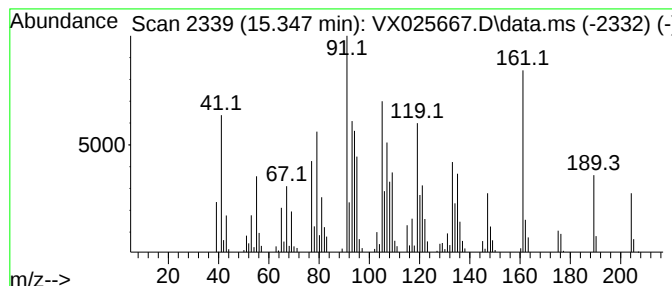
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM112221WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Longifolene Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.347	13.43 ug/L	90294	1,4-Dichlorobenzene-d4	12.024

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Longifolene	204	C15H24	000475-20-7	99
2			Longifolene	204	C15H24	000475-20-7	99
3			Longifolene	204	C15H24	000475-20-7	99
4			Longifolene	204	C15H24	000475-20-7	99
5			Longifolene	204	C15H24	000475-20-7	99



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Longifolene	15.347	13.4	ug/L	90294	3	12.024	336192	50.0