

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121123\
 Data File : VX039140.D
 Acq On : 11 Dec 2023 13:51
 Operator : JC/MD
 Sample : 05646-14DL 2000X
 Misc : 2.54g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AS1DL

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\SFAMXLM120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039140.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	42	46	57	rBV	138347	144801	10.15%	1.422%
2	1.672	91	96	106	rBV	88377	128714	9.02%	1.264%
3	2.306	194	200	211	rVB	243641	380545	26.68%	3.737%
4	2.422	217	219	222	rBV	849	713	0.05%	0.007%
5	3.404	378	380	382	rBV	630	422	0.03%	0.004%
6	4.081	489	491	492	rVB	710	279	0.02%	0.003%
7	4.446	543	551	566	rBV	101870	291010	20.40%	2.858%
8	4.934	629	631	634	rBV2	325	384	0.03%	0.004%
9	5.056	640	651	668	rBV	138899	442551	31.03%	4.346%
10	5.288	687	689	691	rBV2	438	296	0.02%	0.003%
11	5.330	694	696	699	rBV2	490	513	0.04%	0.005%
12	5.970	789	801	822	rBV2	378965	1149436	80.58%	11.287%
13	6.678	915	917	919	rBV	358	280	0.02%	0.003%
14	6.757	921	930	945	rBV	276765	670660	47.02%	6.586%
15	7.117	983	989	993	rBV4	1492	3309	0.23%	0.032%
16	7.171	996	998	999	rBV	429	295	0.02%	0.003%
17	7.214	1003	1005	1006	rBV	875	488	0.03%	0.005%
18	7.306	1012	1020	1038	rBV	232073	516655	36.22%	5.073%
19	7.598	1066	1068	1072	rBV2	442	452	0.03%	0.004%
20	7.635	1072	1074	1075	rBV	393	307	0.02%	0.003%
21	8.013	1133	1136	1138	rBV2	329	349	0.02%	0.003%
22	8.220	1166	1170	1171	rBV	329	485	0.03%	0.005%
23	8.324	1181	1187	1201	rBV	173420	285063	19.98%	2.799%
24	8.647	1233	1240	1251	rBV	579089	909338	63.75%	8.929%
25	8.817	1266	1268	1270	rBV2	469	406	0.03%	0.004%
26	8.866	1274	1276	1277	rBV2	423	318	0.02%	0.003%
27	8.946	1284	1289	1300	rBV	123847	192660	13.51%	1.892%
28	9.336	1351	1353	1355	rBV	339	389	0.03%	0.004%
29	9.384	1355	1361	1375	rBV	452022	672011	47.11%	6.599%
30	9.580	1392	1393	1396	rBV	393	297	0.02%	0.003%
31	9.634	1400	1402	1406	rVB	528	552	0.04%	0.005%
32	9.695	1409	1412	1416	rVV3	1457	1785	0.13%	0.018%
33	9.848	1435	1437	1439	rBV	462	330	0.02%	0.003%
34	9.927	1449	1450	1455	rVB2	491	576	0.04%	0.006%
35	10.055	1465	1471	1488	rVB	574438	895563	62.78%	8.794%
36	10.360	1516	1521	1523	rBV	338	453	0.03%	0.004%

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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
 Title : VOC Analysis

37	10.829	1595	1598	1601	rBV2	366	513	0.04%	0.005%
38	10.970	1620	1621	1624	rBV2	351	436	0.03%	0.004%
39	11.012	1627	1628	1631	rBV	470	396	0.03%	0.004%
40	11.085	1634	1640	1645	rBV3	1242	2332	0.16%	0.023%

41	11.189	1652	1657	1667	rVV	443961	552821	38.76%	5.429%
42	11.366	1685	1686	1690	rVB	346	288	0.02%	0.003%
43	11.549	1715	1716	1720	rVB2	432	332	0.02%	0.003%
44	11.604	1720	1725	1726	rBV	412	452	0.03%	0.004%
45	11.707	1741	1742	1746	rBV2	386	341	0.02%	0.003%

46	11.774	1752	1753	1755	rBV	400	364	0.03%	0.004%
47	11.969	1780	1785	1788	rBV	15332	19398	1.36%	0.190%
48	12.024	1788	1794	1809	rVB2	670262	1426416	100.00%	14.007%
49	12.189	1818	1821	1822	rBV2	358	299	0.02%	0.003%
50	12.317	1837	1842	1857	rVB2	642653	891868	62.53%	8.758%

51	12.603	1887	1889	1894	rVB2	403	613	0.04%	0.006%
52	12.640	1894	1895	1897	rBV	342	337	0.02%	0.003%
53	12.701	1904	1905	1908	rVV	453	315	0.02%	0.003%
54	12.744	1911	1912	1915	rBV	475	381	0.03%	0.004%
55	12.792	1919	1920	1924	rVV2	292	386	0.03%	0.004%

56	12.847	1926	1929	1930	rVV2	368	279	0.02%	0.003%
57	12.878	1932	1934	1937	rVB2	408	313	0.02%	0.003%
58	12.914	1937	1940	1942	rBV2	358	433	0.03%	0.004%
59	13.024	1955	1958	1959	rBV	387	346	0.02%	0.003%
60	13.061	1960	1964	1971	rVB4	2787	4960	0.35%	0.049%

61	13.109	1971	1972	1974	rBV	527	435	0.03%	0.004%
62	13.158	1978	1980	1982	rVB	433	408	0.03%	0.004%
63	13.231	1990	1992	1995	rBV	754	815	0.06%	0.008%
64	13.396	2017	2019	2020	rVB	605	334	0.02%	0.003%
65	13.414	2020	2022	2024	rVB2	418	296	0.02%	0.003%

66	13.585	2045	2050	2061	rBV	336686	429543	30.11%	4.218%
67	13.786	2079	2083	2085	rBV3	467	777	0.05%	0.008%
68	13.957	2106	2111	2117	rBV	93053	120900	8.48%	1.187%
69	14.042	2124	2125	2128	rBV2	429	456	0.03%	0.004%
70	14.091	2132	2133	2136	rBV	406	335	0.02%	0.003%

71	14.176	2144	2147	2150	rBV2	509	654	0.05%	0.006%
72	14.207	2150	2152	2155	rBV2	420	486	0.03%	0.005%
73	14.329	2171	2172	2174	rBV	538	413	0.03%	0.004%
74	14.353	2174	2176	2177	rVV2	479	386	0.03%	0.004%
75	14.371	2177	2179	2182	rVB	440	355	0.02%	0.003%

76	14.414	2182	2186	2188	rBV2	530	693	0.05%	0.007%
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Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
 Title : VOC Analysis

77	14.469	2193	2195	2197	rVV2	372	361	0.03%	0.004%
78	14.518	2200	2203	2205	rBV2	267	301	0.02%	0.003%
79	14.597	2214	2216	2217	rBV	393	284	0.02%	0.003%
80	14.640	2221	2223	2224	rVB	471	335	0.02%	0.003%
81	14.658	2224	2226	2228	rBV2	486	560	0.04%	0.005%
82	14.701	2230	2233	2236	rVB2	638	812	0.06%	0.008%
83	14.725	2236	2237	2240	rBV2	353	402	0.03%	0.004%
84	14.786	2243	2247	2251	rVV5	2524	3371	0.24%	0.033%
85	15.024	2283	2286	2289	rBV3	384	455	0.03%	0.004%
86	15.091	2295	2297	2298	rBV	641	357	0.03%	0.004%
87	15.164	2307	2309	2310	rBV	408	295	0.02%	0.003%
88	15.249	2318	2323	2329	rVB4	12119	17010	1.19%	0.167%
89	15.438	2352	2354	2355	rBV2	536	388	0.03%	0.004%
90	15.469	2358	2359	2360	rVV	626	271	0.02%	0.003%
91	15.487	2360	2362	2366	rVB	616	451	0.03%	0.004%
92	15.530	2366	2369	2373	rBV3	356	635	0.04%	0.006%
93	15.585	2377	2378	2381	rBV	445	276	0.02%	0.003%
94	15.853	2421	2422	2424	rVB	393	279	0.02%	0.003%
95	16.091	2458	2461	2462	rBV3	405	346	0.02%	0.003%
96	16.213	2478	2481	2482	rBV2	360	431	0.03%	0.004%
97	16.347	2500	2503	2504	rBV2	495	471	0.03%	0.005%
98	16.572	2538	2540	2541	rBV	292	281	0.02%	0.003%
99	16.590	2541	2543	2545	rVV2	566	424	0.03%	0.004%
100	16.700	2559	2561	2563	rBV2	381	288	0.02%	0.003%

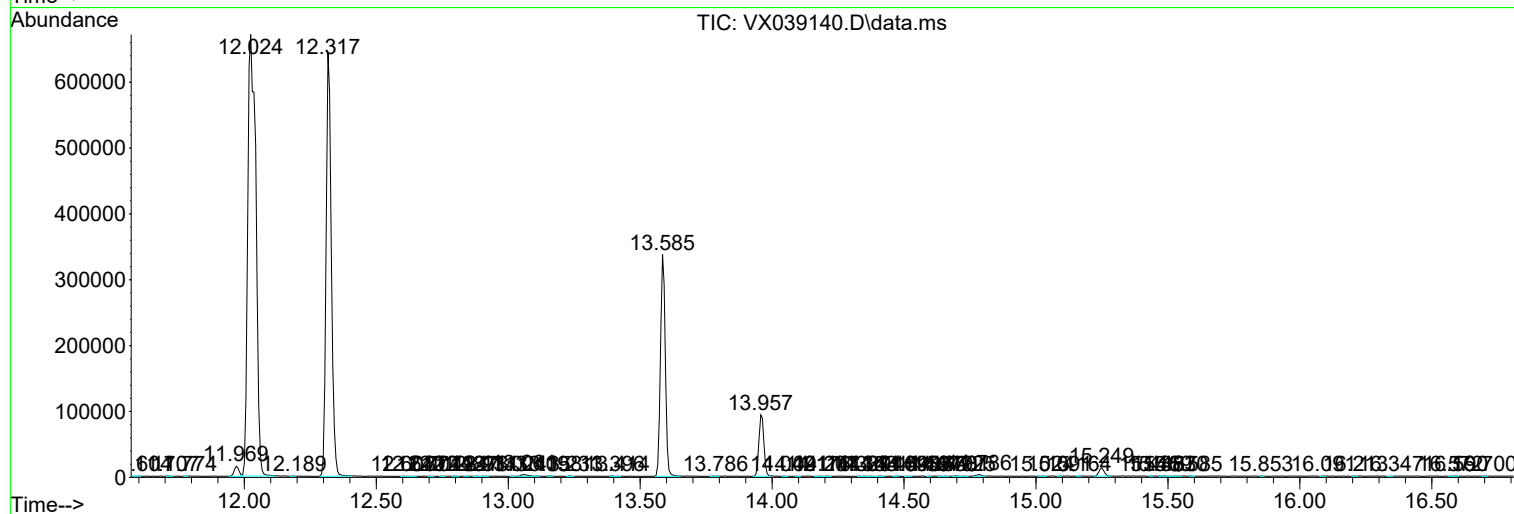
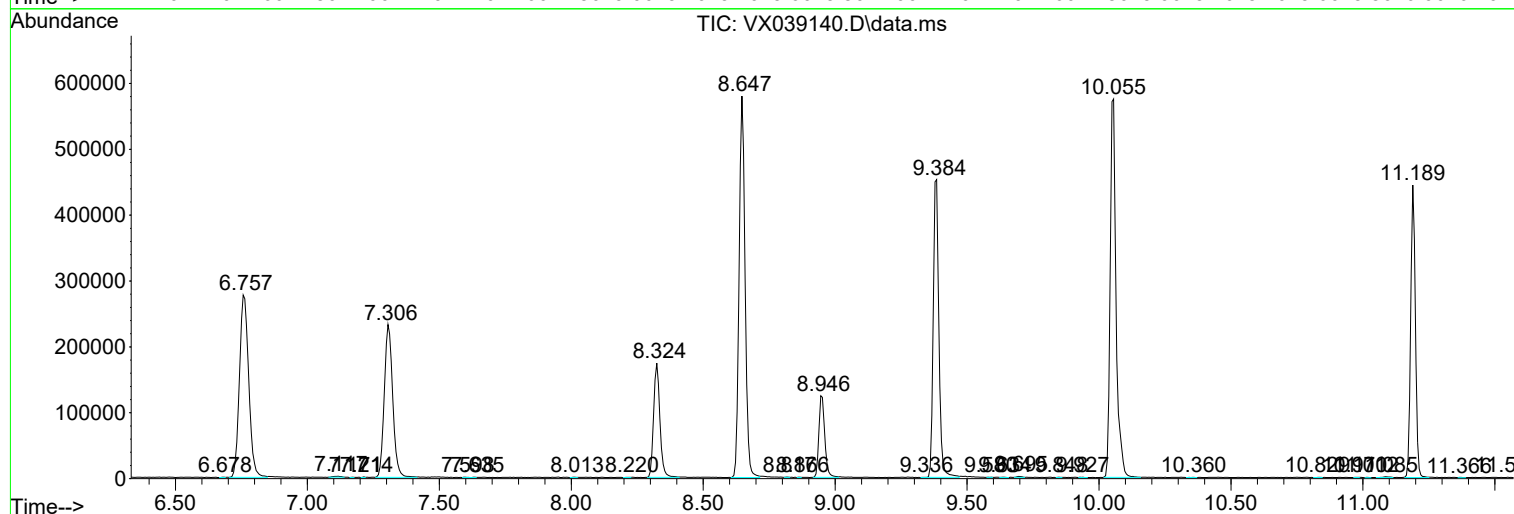
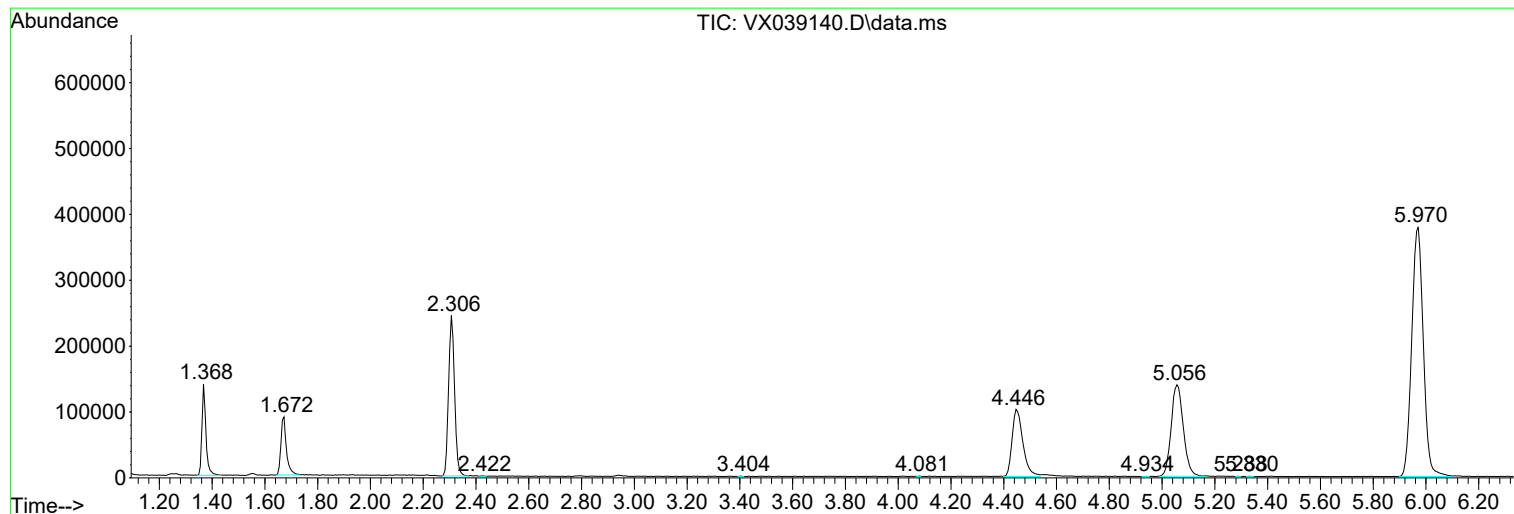
Sum of corrected areas: 10183674

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.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\SFAMXML120523WMA.M
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No Library Search Compounds Detected

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TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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