

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
 Data File : VX030647.D
 Acq On : 16 Aug 2022 12:04
 Operator : JC/MD
 Sample : N4168-06
 Misc : 5.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EX9B5

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\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030647.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	55	rVB	92675	133188	12.02%	1.426%
2	1.660	90	94	100	rBV	39871	63225	5.71%	0.677%
3	2.191	180	181	182	rBV	1273	622	0.06%	0.007%
4	2.276	189	195	207	rBV	234776	377884	34.11%	4.047%
5	2.593	245	247	249	rBV2	511	510	0.05%	0.005%
6	2.660	256	258	261	rBV2	606	672	0.06%	0.007%
7	2.770	273	276	277	rBV3	4214	3930	0.35%	0.042%
8	2.831	283	286	295	rVB4	5425	11454	1.03%	0.123%
9	2.947	297	305	312	rBV2	15723	42611	3.85%	0.456%
10	3.166	339	341	342	rBV	631	540	0.05%	0.006%
11	3.422	377	383	386	rVV5	876	1784	0.16%	0.019%
12	3.837	447	451	454	rBV2	387	536	0.05%	0.006%
13	3.977	472	474	475	rBV	587	473	0.04%	0.005%
14	4.160	501	504	508	rBV2	658	711	0.06%	0.008%
15	4.349	532	535	538	rVB	746	686	0.06%	0.007%
16	4.391	538	542	546	rBV2	300	473	0.04%	0.005%
17	4.501	549	560	583	rBV2	48729	234430	21.16%	2.511%
18	5.062	640	652	668	rVV	140504	444896	40.15%	4.765%
19	5.349	698	699	702	rBV2	828	789	0.07%	0.008%
20	5.373	702	703	706	rBV3	792	1015	0.09%	0.011%
21	5.800	770	773	774	rBV2	802	1031	0.09%	0.011%
22	5.964	789	800	815	rBV2	395656	1107982	100.00%	11.867%
23	6.233	839	844	845	rBV2	473	579	0.05%	0.006%
24	6.373	860	867	868	rBV4	1687	2527	0.23%	0.027%
25	6.550	893	896	898	rVV2	610	548	0.05%	0.006%
26	6.763	921	931	950	rVV	391030	938396	84.69%	10.050%
27	7.013	970	972	979	rVB2	540	1015	0.09%	0.011%
28	7.110	979	988	999	rBV5	11632	34636	3.13%	0.371%
29	7.220	1001	1006	1012	rVV2	2619	5737	0.52%	0.061%
30	7.312	1012	1021	1038	rVB	224099	501229	45.24%	5.368%
31	7.470	1045	1047	1049	rBV	648	532	0.05%	0.006%
32	7.623	1070	1072	1074	rVB2	544	431	0.04%	0.005%
33	7.720	1080	1088	1093	rBV4	2082	4380	0.40%	0.047%
34	7.848	1107	1109	1111	rBV2	459	488	0.04%	0.005%
35	7.970	1119	1129	1137	rBV6	2819	8864	0.80%	0.095%
36	8.147	1156	1158	1163	rVB4	1056	1239	0.11%	0.013%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
 Data File : VX030647.D
 Acq On : 16 Aug 2022 12:04
 Operator : JC/MD
 Sample : N4168-06
 Misc : 5.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EX9B5

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\SFAMXML080422WMA.M
 Title : VOC Analysis

37	8.324	1181	1187	1202	rVV	139959	243151	21.95%	2.604%
38	8.647	1234	1240	1247	rBV	543570	883658	79.75%	9.464%
39	8.720	1247	1252	1265	rVB	74432	125092	11.29%	1.340%
40	8.854	1273	1274	1275	rBV	782	484	0.04%	0.005%
41	8.909	1278	1283	1285	rVV4	3460	5741	0.52%	0.061%
42	8.952	1285	1290	1302	rVV	102967	160195	14.46%	1.716%
43	9.055	1306	1307	1310	rVB2	578	461	0.04%	0.005%
44	9.250	1336	1339	1341	rBV2	429	500	0.05%	0.005%
45	9.281	1341	1344	1350	rVB4	868	1821	0.16%	0.020%
46	9.403	1357	1364	1377	rBV	217798	499364	45.07%	5.348%
47	9.537	1383	1386	1391	rBV3	2236	2869	0.26%	0.031%
48	9.720	1412	1416	1425	rBV5	2792	4969	0.45%	0.053%
49	9.854	1434	1438	1442	rBV4	1789	2940	0.27%	0.031%
50	9.903	1444	1446	1450	rVB2	892	933	0.08%	0.010%
51	9.958	1453	1455	1460	rBV3	368	551	0.05%	0.006%
52	10.055	1465	1471	1485	rBV	811496	1080766	97.54%	11.575%
53	10.305	1507	1512	1518	rVV6	2686	4774	0.43%	0.051%
54	10.470	1536	1539	1545	rBV2	395	734	0.07%	0.008%
55	10.592	1555	1559	1560	rBV	411	440	0.04%	0.005%
56	10.653	1564	1569	1577	rVB4	4915	8938	0.81%	0.096%
57	10.714	1577	1579	1581	rBV3	649	586	0.05%	0.006%
58	10.842	1598	1600	1603	rVB	445	478	0.04%	0.005%
59	10.866	1603	1604	1606	rBV	652	475	0.04%	0.005%
60	10.951	1612	1618	1619	rBV3	1187	1901	0.17%	0.020%
61	11.201	1653	1659	1667	rBV	349248	474782	42.85%	5.085%
62	11.262	1667	1669	1670	rVV	903	491	0.04%	0.005%
63	11.311	1672	1677	1682	rVB3	2397	3826	0.35%	0.041%
64	11.378	1685	1688	1689	rBV2	506	467	0.04%	0.005%
65	11.488	1701	1706	1713	rVB4	2569	4623	0.42%	0.050%
66	11.567	1717	1719	1722	rBV	400	528	0.05%	0.006%
67	11.719	1741	1744	1746	rBV	399	632	0.06%	0.007%
68	11.756	1746	1750	1753	rVV4	1010	1228	0.11%	0.013%
69	11.860	1764	1767	1769	rBV	468	550	0.05%	0.006%
70	11.890	1769	1772	1774	rVV2	635	620	0.06%	0.007%
71	11.933	1777	1779	1782	rBV3	835	818	0.07%	0.009%
72	11.975	1782	1786	1788	rVB4	1661	2260	0.20%	0.024%
73	12.024	1788	1794	1807	rBV	817828	1031382	93.09%	11.046%
74	12.232	1823	1828	1831	rBV4	6255	10209	0.92%	0.109%
75	12.323	1838	1843	1851	rVB	616547	754306	68.08%	8.079%
76	12.427	1857	1860	1863	rBV4	2347	2429	0.22%	0.026%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
 Data File : VX030647.D
 Acq On : 16 Aug 2022 12:04
 Operator : JC/MD
 Sample : N4168-06
 Misc : 5.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 7 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 EX9B5

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\SFAMXMLM080422WMA.M
 Title : VOC Analysis

77	12.463	1864	1866	1872	rVB4	1850	2088	0.19%	0.022%
78	12.768	1912	1916	1921	rVB2	5188	7155	0.65%	0.077%
79	12.859	1927	1931	1935	rBV3	5320	7080	0.64%	0.076%
80	12.908	1938	1939	1942	rVB2	903	888	0.08%	0.010%
81	12.951	1944	1946	1948	rVB	775	462	0.04%	0.005%
82	13.103	1966	1971	1978	rBV	15386	18986	1.71%	0.203%
83	13.268	1995	1998	2001	rBV3	1829	2442	0.22%	0.026%
84	13.390	2014	2018	2023	rBV3	750	1588	0.14%	0.017%
85	13.463	2028	2030	2031	rBV2	567	458	0.04%	0.005%
86	13.597	2049	2052	2053	rBV2	683	586	0.05%	0.006%
87	13.695	2064	2068	2071	rBV4	1521	2343	0.21%	0.025%
88	13.756	2075	2078	2080	rVV3	1652	1984	0.18%	0.021%
89	13.798	2081	2085	2091	rVB3	9223	12613	1.14%	0.135%
90	13.902	2099	2102	2103	rBV2	747	734	0.07%	0.008%
91	13.926	2103	2106	2109	rVV4	1510	2221	0.20%	0.024%
92	14.042	2121	2125	2129	rVB3	1885	2531	0.23%	0.027%
93	14.134	2136	2140	2143	rVB	6879	8228	0.74%	0.088%
94	14.262	2156	2161	2164	rVB4	2422	3348	0.30%	0.036%
95	14.493	2197	2199	2203	rVB4	1065	1296	0.12%	0.014%
96	14.609	2216	2218	2223	rVB4	1087	1431	0.13%	0.015%
97	14.646	2223	2224	2229	rBV3	1021	1164	0.11%	0.012%
98	14.829	2252	2254	2257	rBV2	981	1000	0.09%	0.011%
99	15.389	2343	2346	2352	rVB2	2871	4701	0.42%	0.050%
100	16.517	2529	2531	2532	rBV2	953	566	0.05%	0.006%

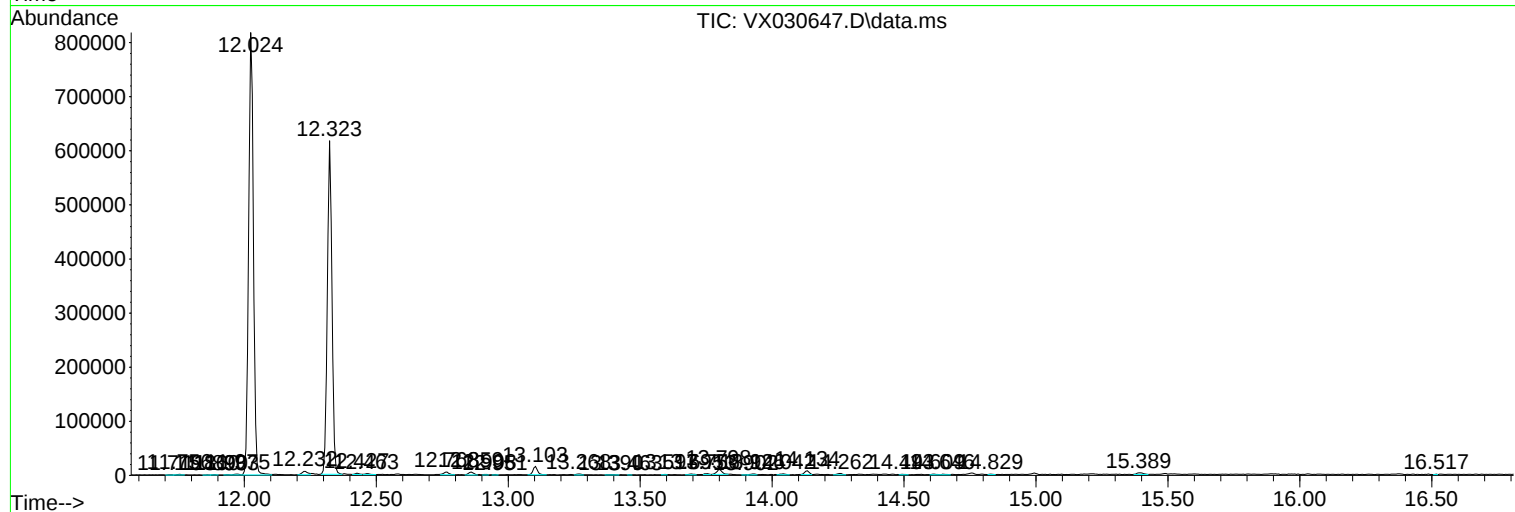
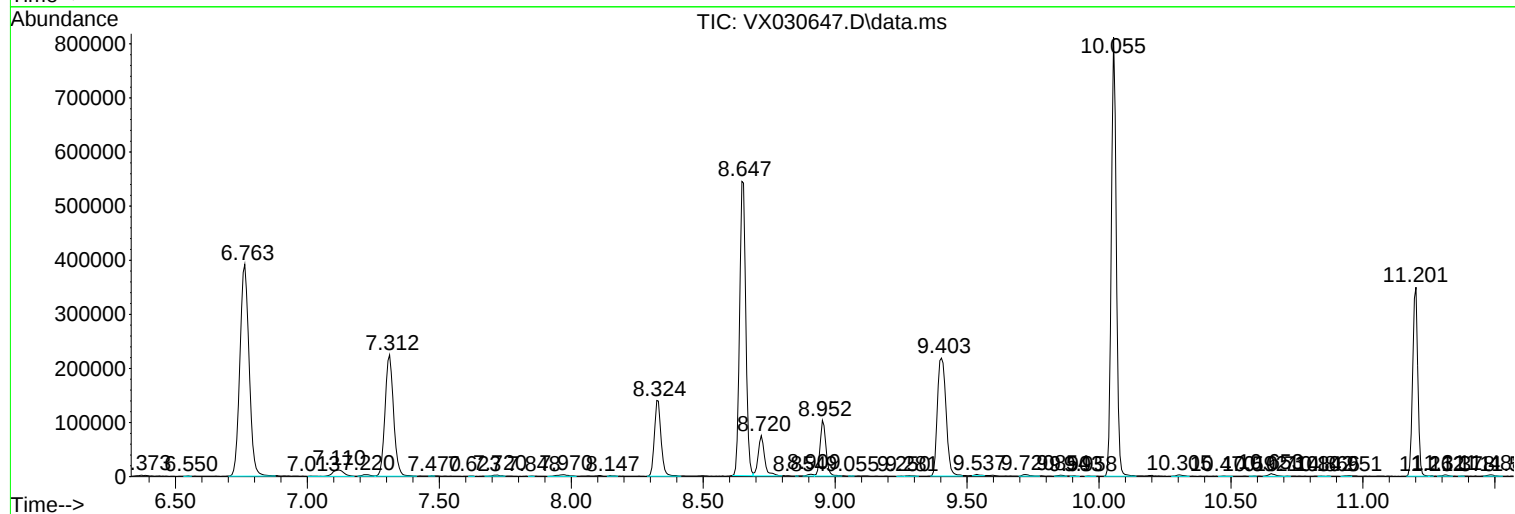
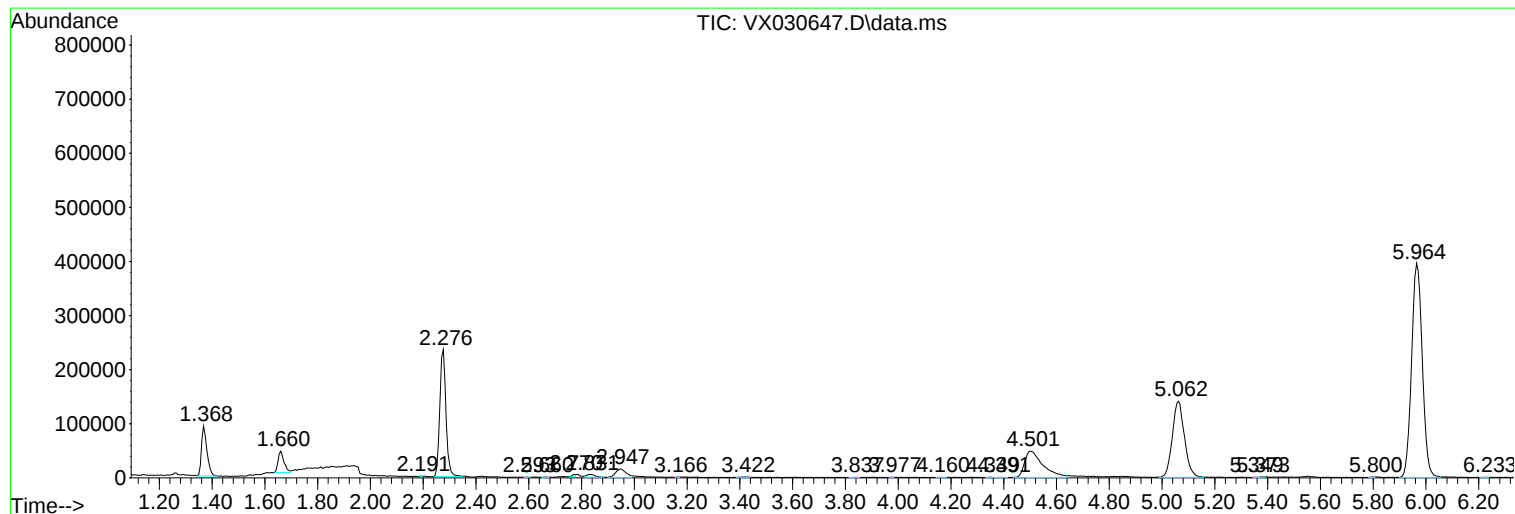
Sum of corrected areas: 9336908

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
Data File : VX030647.D
Acq On : 16 Aug 2022 12:04
Operator : JC/MD
Sample : N4168-06
Misc : 5.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EX9B5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
Data File : VX030647.D
Acq On : 16 Aug 2022 12:04
Operator : JC/MD
Sample : N4168-06
Misc : 5.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EX9B5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXMLM080422WMA.M
Quant Title : VOC Analysis

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

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081622\
Data File : VX030647.D
Acq On : 16 Aug 2022 12:04
Operator : JC/MD
Sample : N4168-06
Misc : 5.55g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 7 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
EX9B5

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

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