

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
 Data File : VX039320.D
 Acq On : 18 Dec 2023 18:32
 Operator : JC/MD
 Sample : 05835-03 100X
 Misc : 4.69g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B33

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\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039320.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.367	43	46	57	rVB	99346	101021	11.71%	1.451%
2	1.666	91	95	107	rBV	62249	90206	10.45%	1.295%
3	2.306	194	200	210	rBV	174621	273427	31.69%	3.926%
4	2.794	275	280	285	rBV4	1643	2919	0.34%	0.042%
5	2.940	297	304	311	rBV3	4146	9646	1.12%	0.139%
6	3.227	349	351	353	rBV	240	252	0.03%	0.004%
7	3.672	420	424	427	rBV2	228	279	0.03%	0.004%
8	4.269	519	522	523	rVB2	202	193	0.02%	0.003%
9	4.300	523	527	528	rVB	337	281	0.03%	0.004%
10	4.318	528	530	533	rBV2	186	264	0.03%	0.004%
11	4.452	544	552	568	rBV	90890	259565	30.08%	3.727%
12	4.897	623	625	627	rBV2	207	195	0.02%	0.003%
13	4.952	632	634	637	rBV	230	192	0.02%	0.003%
14	5.056	640	651	670	rBV	114081	350186	40.58%	5.028%
15	5.348	696	699	701	rBV2	169	211	0.02%	0.003%
16	5.483	719	721	725	rVB2	329	258	0.03%	0.004%
17	5.562	731	734	737	rVB2	272	346	0.04%	0.005%
18	5.653	746	749	750	rBV2	219	218	0.03%	0.003%
19	5.867	781	784	785	rVB2	226	200	0.02%	0.003%
20	5.970	789	801	820	rBV2	289221	862954	100.00%	12.391%
21	6.482	884	885	887	rBV	265	238	0.03%	0.003%
22	6.549	892	896	898	rBV2	213	302	0.03%	0.004%
23	6.659	910	914	917	rBV2	170	327	0.04%	0.005%
24	6.763	922	931	948	rBV	233068	561351	65.05%	8.061%
25	7.055	977	979	980	rBV2	268	178	0.02%	0.003%
26	7.123	984	990	996	rVB6	1418	3479	0.40%	0.050%
27	7.305	1012	1020	1035	rBV	177598	399648	46.31%	5.739%
28	7.446	1041	1043	1045	rVB2	411	268	0.03%	0.004%
29	7.702	1082	1085	1089	rBV2	258	430	0.05%	0.006%
30	7.799	1100	1101	1104	rVV2	274	277	0.03%	0.004%
31	8.025	1135	1138	1141	rVB	226	244	0.03%	0.004%
32	8.324	1181	1187	1198	rBV	120006	204389	23.68%	2.935%
33	8.586	1228	1230	1231	rVB	484	210	0.02%	0.003%
34	8.647	1234	1240	1258	rBV	411808	667305	77.33%	9.582%
35	8.951	1284	1290	1304	rBV	90219	137638	15.95%	1.976%
36	9.208	1330	1332	1335	rBV3	277	324	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
 Data File : VX039320.D
 Acq On : 18 Dec 2023 18:32
 Operator : JC/MD
 Sample : 05835-03 100X
 Misc : 4.69g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B33

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

37	9.269	1341	1342	1344	rBV2	474	445	0.05%	0.006%
38	9.384	1355	1361	1375	rBV	412552	591791	68.58%	8.498%
39	9.695	1409	1412	1417	rVB3	901	1389	0.16%	0.020%
40	9.921	1447	1449	1453	rBV2	176	191	0.02%	0.003%
41	10.055	1465	1471	1482	rBV	496637	688097	79.74%	9.881%
42	10.195	1492	1494	1497	rBV	827	746	0.09%	0.011%
43	10.311	1509	1513	1520	rVB3	610	1175	0.14%	0.017%
44	10.427	1531	1532	1535	rVB	366	238	0.03%	0.003%
45	10.470	1535	1539	1542	rBV2	229	436	0.05%	0.006%
46	10.652	1565	1569	1572	rBV2	641	820	0.10%	0.012%
47	10.963	1617	1620	1624	rVV2	667	763	0.09%	0.011%
48	11.091	1639	1641	1645	rVB2	412	427	0.05%	0.006%
49	11.189	1652	1657	1664	rBV	341211	446882	51.79%	6.417%
50	11.354	1683	1684	1688	rVB2	282	240	0.03%	0.003%
51	11.451	1698	1700	1707	rVB2	546	894	0.10%	0.013%
52	11.506	1707	1709	1711	rBV	236	256	0.03%	0.004%
53	11.756	1746	1750	1754	rVB3	606	788	0.09%	0.011%
54	11.914	1771	1776	1778	rBV	263	363	0.04%	0.005%
55	11.939	1778	1780	1782	rBV2	286	275	0.03%	0.004%
56	11.969	1782	1785	1788	rVB3	618	690	0.08%	0.010%
57	12.024	1788	1794	1803	rBV	531754	688421	79.77%	9.885%
58	12.201	1821	1823	1825	rVB	247	176	0.02%	0.003%
59	12.244	1827	1830	1831	rVB	255	177	0.02%	0.003%
60	12.317	1837	1842	1853	rBV	444950	594188	68.86%	8.532%
61	12.457	1863	1865	1867	rVB	418	249	0.03%	0.004%
62	12.494	1869	1871	1874	rVB	321	283	0.03%	0.004%
63	12.707	1901	1906	1907	rVB2	229	258	0.03%	0.004%
64	12.750	1911	1913	1914	rBV	463	460	0.05%	0.007%
65	12.768	1914	1916	1920	rVV	835	737	0.09%	0.011%
66	12.829	1924	1926	1928	rVB2	204	177	0.02%	0.003%
67	12.847	1928	1929	1932	rBV2	185	205	0.02%	0.003%
68	13.067	1962	1965	1967	rBV2	238	310	0.04%	0.004%
69	13.115	1971	1973	1976	rBV2	569	665	0.08%	0.010%
70	13.158	1979	1980	1982	rBV	250	219	0.03%	0.003%
71	13.243	1992	1994	1998	rVB2	162	245	0.03%	0.004%
72	13.329	2006	2008	2011	rBV2	224	228	0.03%	0.003%
73	13.371	2011	2015	2017	rBV2	172	202	0.02%	0.003%
74	13.402	2017	2020	2023	rVB2	205	294	0.03%	0.004%
75	13.438	2023	2026	2028	rBV	354	294	0.03%	0.004%
76	13.597	2048	2052	2056	rBV4	778	1113	0.13%	0.016%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
 Data File : VX039320.D
 Acq On : 18 Dec 2023 18:32
 Operator : JC/MD
 Sample : 05835-03 100X
 Misc : 4.69g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B33

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\SFAMXML120523WMA.M
 Title : VOC Analysis

77	13.743	2074	2076	2078	rBV2	228	201	0.02%	0.003%
78	13.786	2078	2083	2085	rBV3	454	700	0.08%	0.010%
79	13.963	2110	2112	2116	rBV	344	399	0.05%	0.006%
80	14.060	2126	2128	2133	rVB2	206	240	0.03%	0.003%
81	14.127	2135	2139	2143	rBV	1370	1787	0.21%	0.026%
82	14.322	2169	2171	2177	rVB3	183	191	0.02%	0.003%
83	14.365	2177	2178	2181	rBV	259	204	0.02%	0.003%
84	14.396	2181	2183	2187	rVB2	151	189	0.02%	0.003%
85	14.579	2211	2213	2215	rVB	354	203	0.02%	0.003%
86	14.627	2218	2221	2223	rBV2	168	226	0.03%	0.003%
87	14.658	2223	2226	2227	rBV2	263	270	0.03%	0.004%
88	14.761	2239	2243	2245	rBV2	394	427	0.05%	0.006%
89	14.804	2247	2250	2253	rBV3	370	468	0.05%	0.007%
90	14.859	2256	2259	2260	rVV2	233	237	0.03%	0.003%
91	14.908	2264	2267	2268	rVB2	244	201	0.02%	0.003%
92	14.999	2278	2282	2285	rVB2	233	371	0.04%	0.005%
93	15.133	2301	2304	2306	rBV2	397	456	0.05%	0.007%
94	15.548	2370	2372	2373	rBV	290	195	0.02%	0.003%
95	15.682	2392	2394	2396	rBV	245	206	0.02%	0.003%
96	16.103	2461	2463	2468	rVB2	470	561	0.07%	0.008%
97	16.145	2468	2470	2471	rBV2	261	204	0.02%	0.003%
98	16.511	2528	2530	2533	rBV	473	399	0.05%	0.006%
99	16.578	2539	2541	2545	rVB2	341	343	0.04%	0.005%
100	16.645	2551	2552	2554	rVB	373	188	0.02%	0.003%

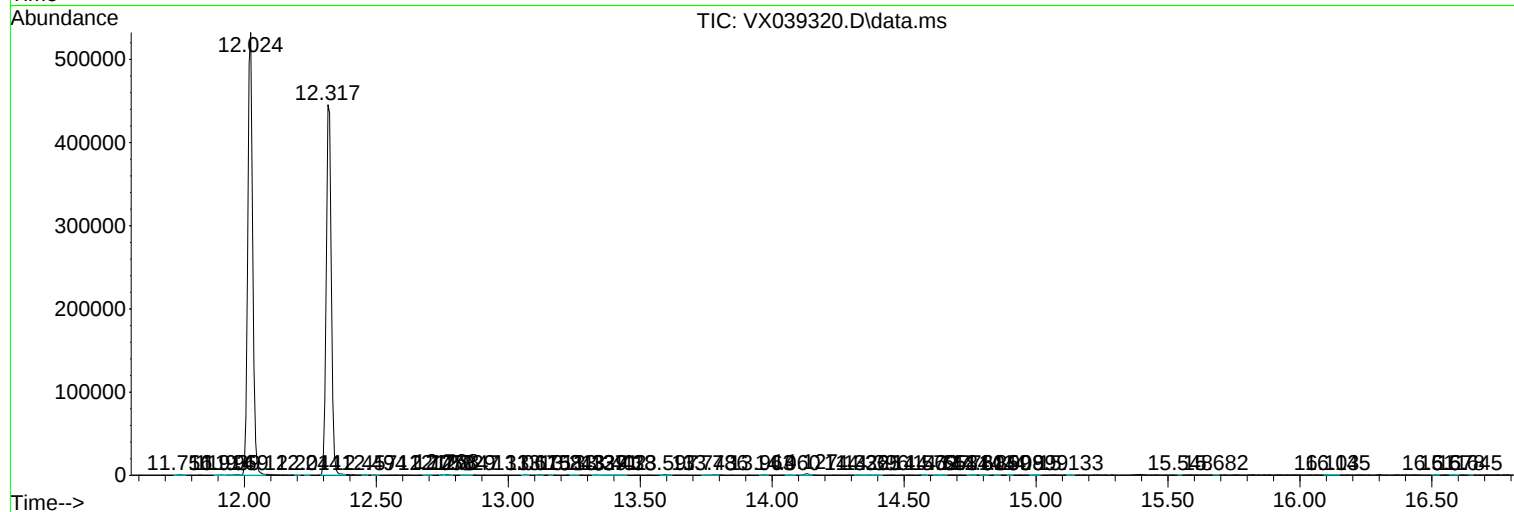
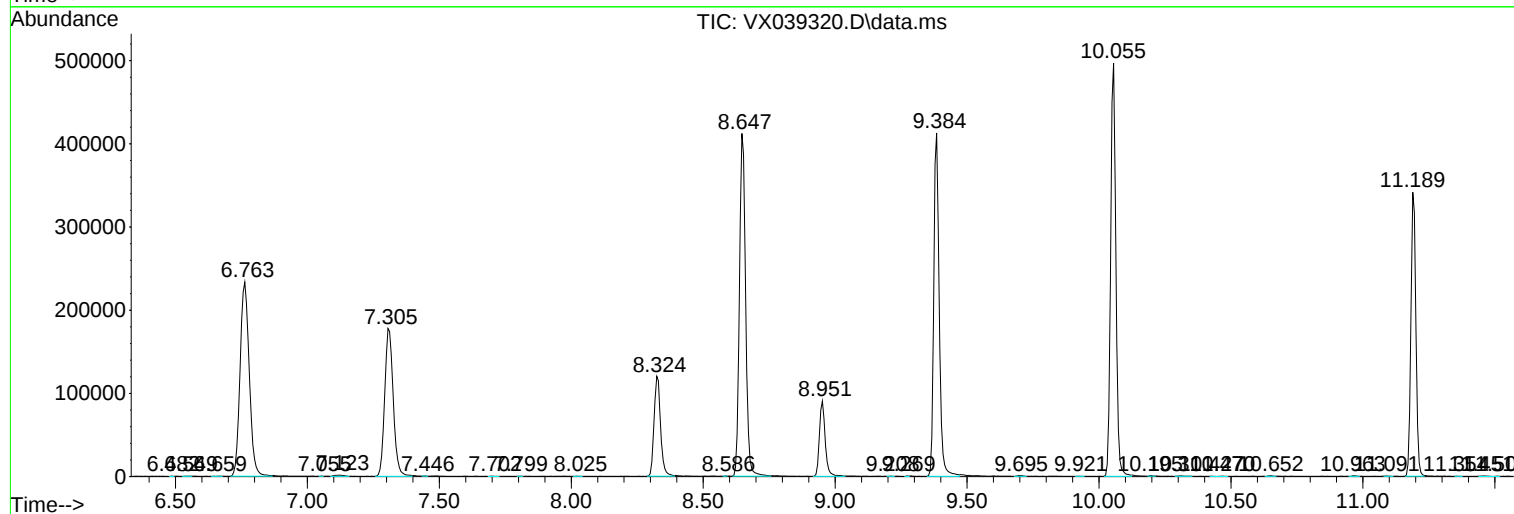
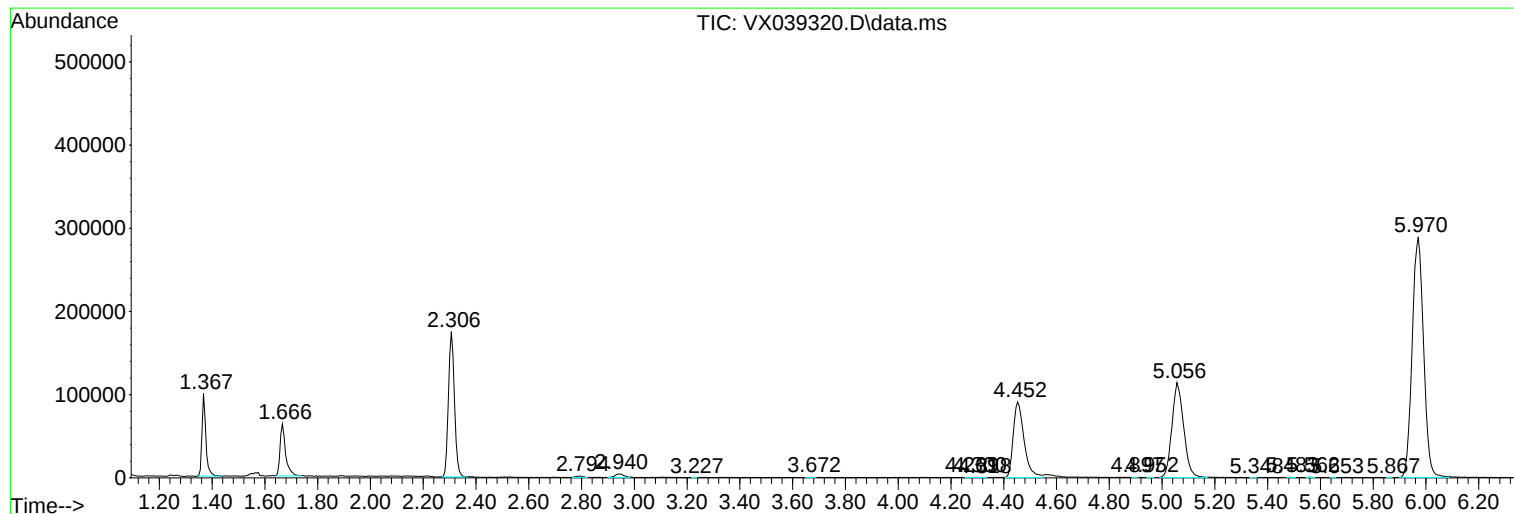
Sum of corrected areas: 6964094

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
Data File : VX039320.D
Acq On : 18 Dec 2023 18:32
Operator : JC/MD
Sample : 05835-03 100X
Misc : 4.69g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B33

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
Data File : VX039320.D
Acq On : 18 Dec 2023 18:32
Operator : JC/MD
Sample : 05835-03 100X
Misc : 4.69g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B33

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

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
Data File : VX039320.D
Acq On : 18 Dec 2023 18:32
Operator : JC/MD
Sample : 05835-03 100X
Misc : 4.69g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B33

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

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