

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
 Data File : VX039325.D
 Acq On : 18 Dec 2023 20:50
 Operator : JC/MD
 Sample : 05835-06 100X
 Misc : 5.61g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B43

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: VX039325.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	54	rBV	88088	92569	11.05%	1.368%
2	1.666	91	95	109	rVB	62787	88483	10.56%	1.308%
3	2.306	194	200	209	rBV	170248	266741	31.83%	3.942%
4	2.514	231	234	237	rBV3	533	838	0.10%	0.012%
5	2.788	274	279	285	rVB4	1641	2894	0.35%	0.043%
6	2.947	298	305	317	rVB2	4557	10577	1.26%	0.156%
7	3.075	325	326	328	rBV	343	284	0.03%	0.004%
8	3.233	350	352	355	rVV	285	312	0.04%	0.005%
9	3.312	362	365	367	rBV2	194	282	0.03%	0.004%
10	3.373	373	375	379	rBV2	195	234	0.03%	0.003%
11	3.550	402	404	407	rBV	265	240	0.03%	0.004%
12	3.593	410	411	418	rBV2	152	243	0.03%	0.004%
13	3.757	436	438	441	rBV2	253	324	0.04%	0.005%
14	3.971	469	473	476	rBV	202	289	0.03%	0.004%
15	4.050	484	486	490	rBV2	274	352	0.04%	0.005%
16	4.123	496	498	503	rVB	284	438	0.05%	0.006%
17	4.172	503	506	511	rBV2	251	519	0.06%	0.008%
18	4.379	538	540	543	rBV	249	233	0.03%	0.003%
19	4.452	543	552	564	rBV	89014	248586	29.66%	3.674%
20	4.922	627	629	632	rBV2	205	239	0.03%	0.004%
21	5.056	638	651	668	rBV	104329	336204	40.12%	4.969%
22	5.404	704	708	710	rBV	225	283	0.03%	0.004%
23	5.556	729	733	734	rBV2	324	304	0.04%	0.004%
24	5.629	743	745	747	rVB	340	293	0.03%	0.004%
25	5.666	747	751	753	rBV2	230	414	0.05%	0.006%
26	5.721	758	760	762	rBV2	251	226	0.03%	0.003%
27	5.970	789	801	817	rBV2	276548	838055	100.00%	12.385%
28	6.294	850	854	855	rBV2	211	258	0.03%	0.004%
29	6.355	862	864	865	rBV	288	210	0.03%	0.003%
30	6.476	882	884	887	rBV2	182	226	0.03%	0.003%
31	6.580	898	901	905	rBV2	183	360	0.04%	0.005%
32	6.763	921	931	947	rBV	224707	542199	64.70%	8.013%
33	7.013	969	972	975	rBV2	280	325	0.04%	0.005%
34	7.043	975	977	980	rVV2	216	221	0.03%	0.003%
35	7.117	984	989	997	rVB4	1431	3330	0.40%	0.049%
36	7.306	1012	1020	1036	rBV	174331	388173	46.32%	5.737%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
 Data File : VX039325.D
 Acq On : 18 Dec 2023 20:50
 Operator : JC/MD
 Sample : 05835-06 100X
 Misc : 5.61g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B43

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	7.476	1046	1048	1057	rVB2	651	1482	0.18%	0.022%
38	7.549	1057	1060	1062	rBV2	220	282	0.03%	0.004%
39	7.580	1062	1065	1066	rVB	305	217	0.03%	0.003%
40	7.714	1086	1087	1091	rBV2	214	217	0.03%	0.003%

41	7.946	1123	1125	1128	rBV2	229	325	0.04%	0.005%
42	8.257	1174	1176	1179	rBV2	210	255	0.03%	0.004%
43	8.324	1181	1187	1200	rBV	116398	197611	23.58%	2.920%
44	8.507	1213	1217	1220	rBV2	327	629	0.08%	0.009%
45	8.580	1225	1229	1234	rVB3	574	530	0.06%	0.008%

46	8.647	1234	1240	1259	rBV	405372	651585	77.75%	9.630%
47	8.818	1267	1268	1271	rVB2	324	202	0.02%	0.003%
48	8.952	1285	1290	1304	rVV	83760	130789	15.61%	1.933%
49	9.275	1339	1343	1345	rVB2	529	700	0.08%	0.010%
50	9.384	1355	1361	1375	rBV	391158	570669	68.09%	8.434%

51	9.695	1410	1412	1419	rVB2	1121	1446	0.17%	0.021%
52	9.836	1433	1435	1439	rVB3	316	432	0.05%	0.006%
53	10.055	1465	1471	1487	rBV	470277	672563	80.25%	9.940%
54	10.311	1510	1513	1517	rVV2	521	703	0.08%	0.010%
55	10.421	1528	1531	1533	rVB2	240	274	0.03%	0.004%

56	10.500	1541	1544	1547	rVB2	158	225	0.03%	0.003%
57	10.640	1564	1567	1568	rBV2	503	537	0.06%	0.008%
58	10.659	1568	1570	1571	rVB2	410	234	0.03%	0.003%
59	10.896	1605	1609	1612	rVB	253	294	0.04%	0.004%
60	10.939	1612	1616	1617	rBV	166	240	0.03%	0.004%

61	10.970	1617	1621	1624	rVB2	519	769	0.09%	0.011%
62	11.085	1638	1640	1646	rVB4	583	765	0.09%	0.011%
63	11.134	1646	1648	1652	rBV2	168	206	0.02%	0.003%
64	11.189	1652	1657	1670	rBV	351636	436459	52.08%	6.450%
65	11.311	1676	1677	1682	rBV2	303	453	0.05%	0.007%

66	11.463	1694	1702	1703	rBV3	602	958	0.11%	0.014%
67	11.756	1748	1750	1753	rVB3	660	766	0.09%	0.011%
68	11.975	1782	1786	1788	rBV3	690	1038	0.12%	0.015%
69	12.018	1788	1793	1806	rVV	501937	668957	79.82%	9.886%
70	12.238	1828	1829	1832	rVB	304	222	0.03%	0.003%

71	12.317	1837	1842	1853	rBV	449119	584978	69.80%	8.645%
72	12.640	1893	1895	1898	rBV	210	211	0.03%	0.003%
73	12.738	1906	1911	1913	rBV2	292	575	0.07%	0.008%
74	12.762	1913	1915	1918	rVB2	655	875	0.10%	0.013%
75	12.792	1918	1920	1924	rBV2	195	209	0.02%	0.003%

76	13.018	1955	1957	1960	rVV	196	206	0.02%	0.003%
----	--------	------	------	------	-----	-----	-----	-------	--------

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
 Data File : VX039325.D
 Acq On : 18 Dec 2023 20:50
 Operator : JC/MD
 Sample : 05835-06 100X
 Misc : 5.61g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 30 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B43

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

77	13.116	1971	1973	1979	rVB4	415	516	0.06%	0.008%
78	13.176	1979	1983	1984	rBV2	228	251	0.03%	0.004%
79	13.280	1996	2000	2003	rBV2	226	307	0.04%	0.005%
80	13.353	2009	2012	2013	rVB2	264	207	0.02%	0.003%
81	13.591	2049	2051	2056	rVV2	772	894	0.11%	0.013%
82	13.786	2078	2083	2085	rBV3	762	895	0.11%	0.013%
83	13.963	2109	2112	2114	rBV2	524	608	0.07%	0.009%
84	14.128	2133	2139	2145	rVV2	1503	2122	0.25%	0.031%
85	14.365	2174	2178	2179	rBV2	262	247	0.03%	0.004%
86	14.457	2190	2193	2195	rBV2	228	210	0.03%	0.003%
87	14.603	2215	2217	2220	rBV	293	271	0.03%	0.004%
88	14.634	2220	2222	2225	rVV2	189	223	0.03%	0.003%
89	14.701	2232	2233	2235	rBV	316	240	0.03%	0.004%
90	14.737	2238	2239	2242	rVB2	364	292	0.03%	0.004%
91	14.768	2242	2244	2247	rVB2	250	246	0.03%	0.004%
92	14.816	2250	2252	2254	rBV2	248	272	0.03%	0.004%
93	15.249	2320	2323	2324	rBV2	239	247	0.03%	0.004%
94	15.371	2342	2343	2344	rBV	322	233	0.03%	0.003%
95	15.450	2353	2356	2361	rBV3	434	595	0.07%	0.009%
96	15.518	2365	2367	2369	rBV	332	272	0.03%	0.004%
97	15.591	2378	2379	2381	rBV	303	263	0.03%	0.004%
98	15.755	2403	2406	2407	rBV	336	307	0.04%	0.005%
99	15.914	2430	2432	2436	rBV2	622	602	0.07%	0.009%
100	16.054	2453	2455	2462	rVB2	229	312	0.04%	0.005%

Sum of corrected areas: 6766478

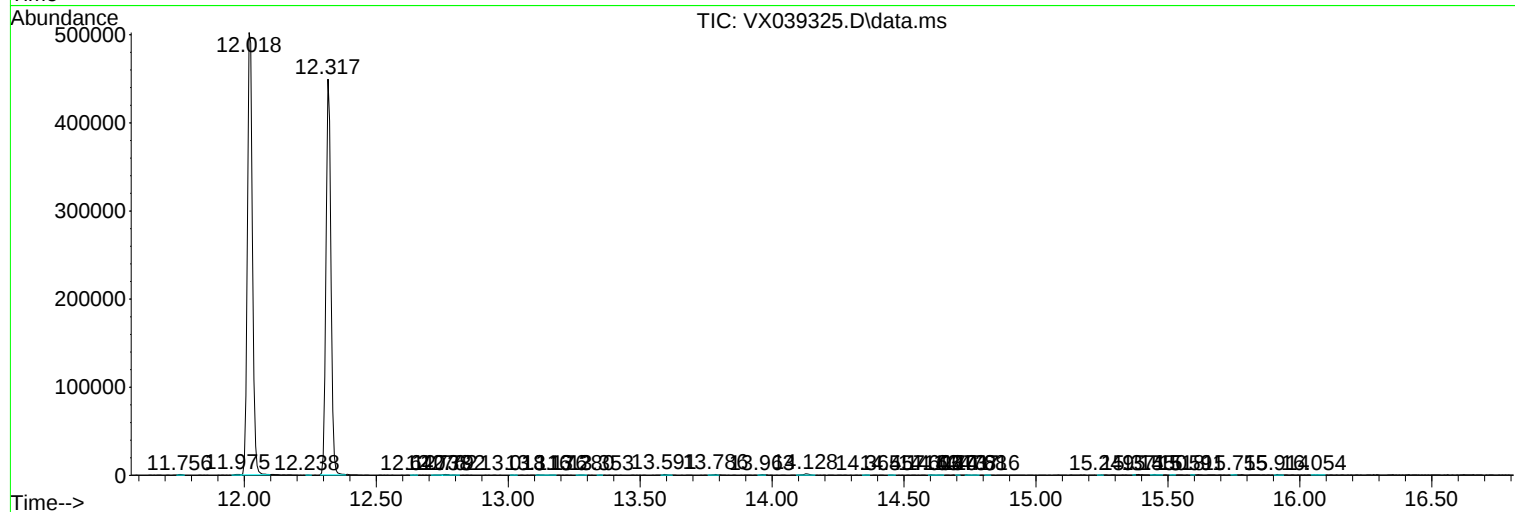
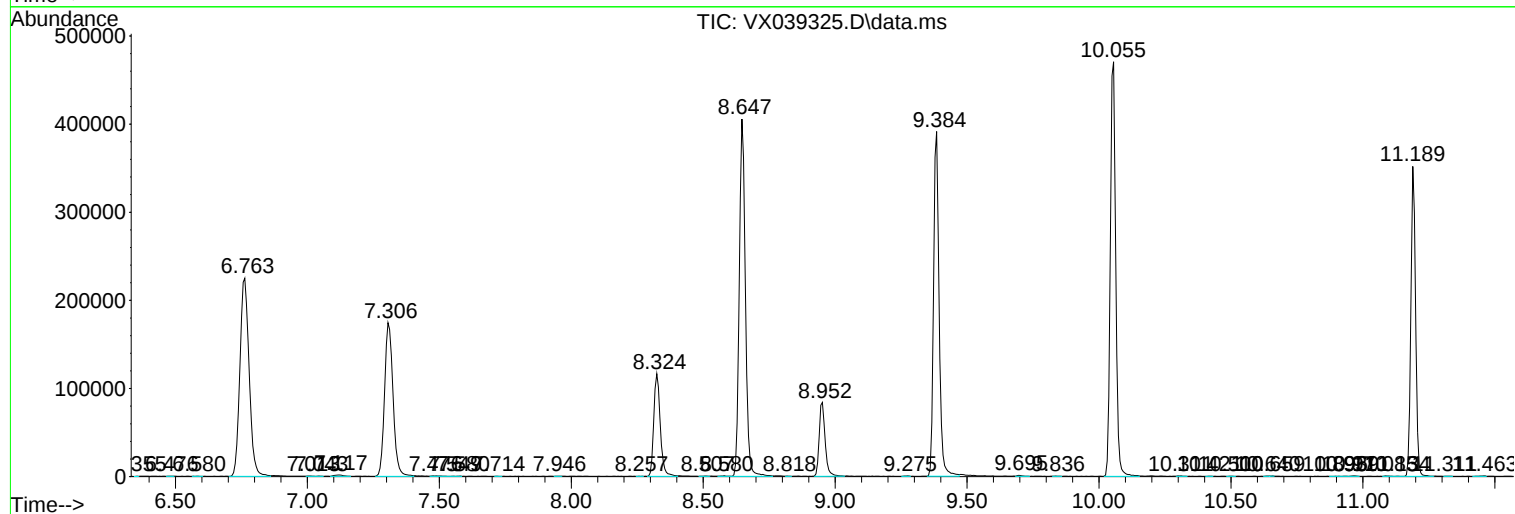
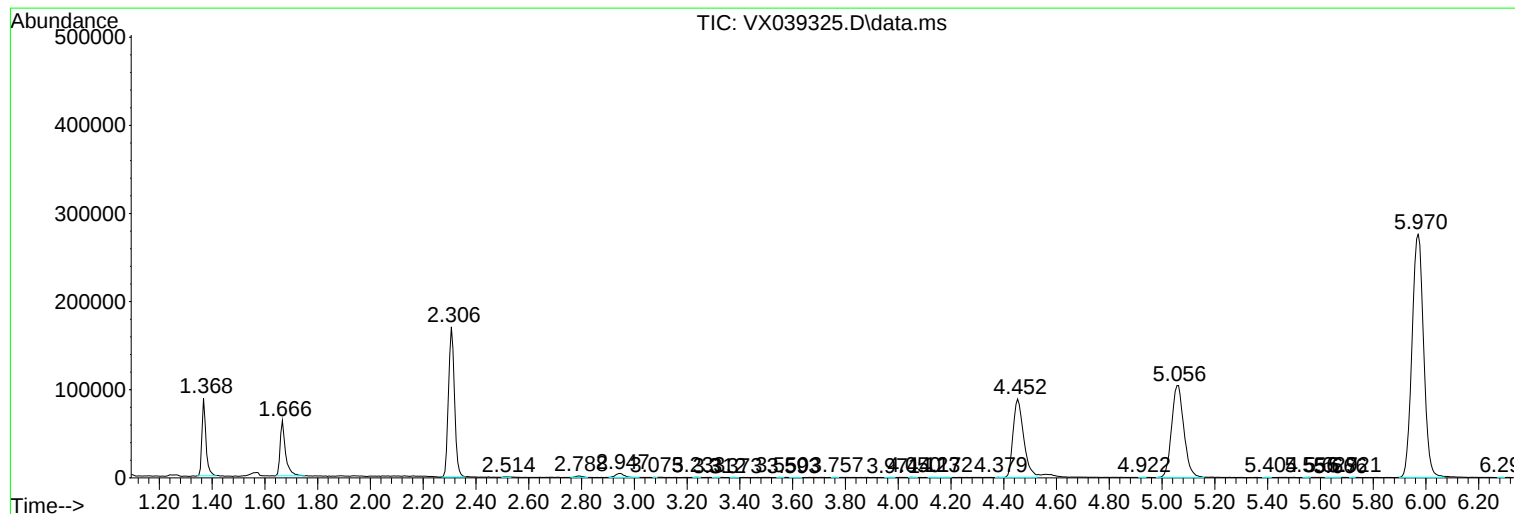
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
Data File : VX039325.D
Acq On : 18 Dec 2023 20:50
Operator : JC/MD
Sample : 05835-06 100X
Misc : 5.61g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B43

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 : VX039325.D
Acq On : 18 Dec 2023 20:50
Operator : JC/MD
Sample : 05835-06 100X
Misc : 5.61g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B43

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 : VX039325.D
Acq On : 18 Dec 2023 20:50
Operator : JC/MD
Sample : 05835-06 100X
Misc : 5.61g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 30 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B43

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	#	RT	Resp	Conc
------------------	----	---------	-------	----------	---	----	------	------