

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
 Data File : VX039316.D
 Acq On : 18 Dec 2023 16:59
 Operator : JC/MD
 Sample : 05807-17 50X
 Misc : 2.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B18

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: VX039316.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	53	rBV	104509	107393	6.77%	1.250%
2	1.666	91	95	111	rVB	68341	102098	6.44%	1.188%
3	2.306	194	200	210	rVB	192251	301796	19.04%	3.513%
4	2.513	229	234	238	rBV	2638	4009	0.25%	0.047%
5	2.794	275	280	284	rBV2	1905	3161	0.20%	0.037%
6	2.946	298	305	312	rVB3	5283	11891	0.75%	0.138%
7	3.099	323	330	335	rBV5	1626	3428	0.22%	0.040%
8	3.434	381	385	388	rVB2	309	503	0.03%	0.006%
9	3.592	410	411	414	rBV3	311	311	0.02%	0.004%
10	3.922	461	465	468	rVB	324	332	0.02%	0.004%
11	3.958	468	471	474	rBV2	196	304	0.02%	0.004%
12	4.092	490	493	496	rBV2	228	249	0.02%	0.003%
13	4.336	531	533	536	rBV3	213	274	0.02%	0.003%
14	4.452	544	552	565	rBV	95353	263994	16.65%	3.073%
15	5.056	637	651	671	rBV	123710	376273	23.73%	4.380%
16	5.385	698	705	706	rBV3	572	987	0.06%	0.011%
17	5.470	715	719	723	rBV3	676	1262	0.08%	0.015%
18	5.543	729	731	732	rBV	464	399	0.03%	0.005%
19	5.623	742	744	747	rVV2	291	354	0.02%	0.004%
20	5.677	751	753	759	rVV4	397	611	0.04%	0.007%
21	5.970	789	801	808	rBV2	315893	955710	60.28%	11.124%
22	6.281	850	852	854	rBV	268	211	0.01%	0.002%
23	6.555	893	897	899	rVV2	176	291	0.02%	0.003%
24	6.763	921	931	947	rBV	243974	585311	36.92%	6.813%
25	7.122	983	990	997	rBB7	1902	4907	0.31%	0.057%
26	7.311	1011	1021	1038	rBV	194956	433598	27.35%	5.047%
27	7.488	1049	1050	1054	rVB	885	666	0.04%	0.008%
28	7.641	1072	1075	1080	rBV2	177	219	0.01%	0.003%
29	7.830	1103	1106	1108	rBV3	201	240	0.02%	0.003%
30	7.945	1123	1125	1126	rBV	365	254	0.02%	0.003%
31	8.043	1139	1141	1145	rBV2	227	321	0.02%	0.004%
32	8.323	1180	1187	1206	rBV	133871	228173	14.39%	2.656%
33	8.524	1217	1220	1223	rVB2	375	374	0.02%	0.004%
34	8.579	1227	1229	1232	rBV	876	504	0.03%	0.006%
35	8.646	1234	1240	1251	rBV	454718	735761	46.41%	8.564%
36	8.951	1285	1290	1301	rBV	97833	149177	9.41%	1.736%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
 Data File : VX039316.D
 Acq On : 18 Dec 2023 16:59
 Operator : JC/MD
 Sample : 05807-17 50X
 Misc : 2.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B18

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	9.152	1319	1323	1325	rBV	327	451	0.03%	0.005%
38	9.274	1339	1343	1347	rBV4	2164	2850	0.18%	0.033%
39	9.384	1355	1361	1377	rBV	435402	620871	39.16%	7.227%
40	9.616	1396	1399	1402	rBV	463	546	0.03%	0.006%
41	9.701	1410	1413	1419	rVB4	749	1081	0.07%	0.013%
42	9.774	1422	1425	1428	rVB	277	365	0.02%	0.004%
43	9.854	1434	1438	1439	rBV2	326	266	0.02%	0.003%
44	10.055	1465	1471	1488	rBV2	531549	910118	57.40%	10.593%
45	10.195	1491	1494	1502	rVB2	2077	3487	0.22%	0.041%
46	10.280	1504	1508	1509	rBV2	408	517	0.03%	0.006%
47	10.311	1509	1513	1519	rVB2	2070	3154	0.20%	0.037%
48	10.433	1531	1533	1537	rVB2	241	259	0.02%	0.003%
49	10.469	1537	1539	1543	rBV	217	308	0.02%	0.004%
50	10.652	1563	1569	1578	rVB7	1882	5033	0.32%	0.059%
51	10.750	1584	1585	1589	rVB	307	251	0.02%	0.003%
52	10.896	1605	1609	1611	rBV2	329	425	0.03%	0.005%
53	10.963	1616	1620	1626	rVB2	2620	3705	0.23%	0.043%
54	11.012	1626	1628	1630	rBV2	232	227	0.01%	0.003%
55	11.036	1630	1632	1634	rBV	251	226	0.01%	0.003%
56	11.091	1637	1641	1646	rVB3	794	1197	0.08%	0.014%
57	11.189	1652	1657	1664	rBV	358918	468727	29.56%	5.456%
58	11.280	1670	1672	1673	rBV	209	222	0.01%	0.003%
59	11.365	1683	1686	1690	rVV3	2315	2972	0.19%	0.035%
60	11.457	1696	1701	1710	rBV3	2839	4363	0.28%	0.051%
61	11.628	1728	1729	1733	rBV2	197	211	0.01%	0.002%
62	11.707	1736	1742	1744	rBV2	201	261	0.02%	0.003%
63	11.756	1744	1750	1755	rBV2	2818	3645	0.23%	0.042%
64	11.811	1758	1759	1762	rBV2	182	225	0.01%	0.003%
65	11.969	1780	1785	1788	rBV2	3186	4156	0.26%	0.048%
66	12.036	1788	1796	1806	rVV2	738327	1585470	100.00%	18.454%
67	12.176	1816	1819	1822	rVB3	402	406	0.03%	0.005%
68	12.317	1837	1842	1852	rBV	492620	649698	40.98%	7.562%
69	12.505	1870	1873	1874	rBV2	288	319	0.02%	0.004%
70	12.548	1879	1880	1884	rVB	227	215	0.01%	0.003%
71	12.579	1884	1885	1888	rBV2	331	305	0.02%	0.004%
72	12.762	1912	1915	1918	rVV	668	777	0.05%	0.009%
73	12.871	1931	1933	1936	rVB2	234	255	0.02%	0.003%
74	12.914	1938	1940	1942	rBV	376	240	0.02%	0.003%
75	12.944	1942	1945	1948	rVB3	378	480	0.03%	0.006%
76	13.036	1959	1960	1963	rVB2	249	238	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
 Data File : VX039316.D
 Acq On : 18 Dec 2023 16:59
 Operator : JC/MD
 Sample : 05807-17 50X
 Misc : 2.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 20 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0B18

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	13.115	1969	1973	1977	rVV2	4006	5083	0.32%	0.059%
78	13.499	2033	2036	2038	rBV	206	212	0.01%	0.002%
79	13.591	2047	2051	2058	rVB3	4794	7065	0.45%	0.082%
80	13.780	2078	2082	2089	rVB2	7451	9957	0.63%	0.116%
81	13.871	2095	2097	2099	rBV	327	310	0.02%	0.004%
82	13.963	2108	2112	2118	rVB2	5291	6682	0.42%	0.078%
83	14.030	2121	2123	2126	rBV2	189	243	0.02%	0.003%
84	14.133	2135	2140	2144	rBV2	1388	2096	0.13%	0.024%
85	14.353	2174	2176	2179	rVV2	248	223	0.01%	0.003%
86	14.603	2216	2217	2220	rBV	319	360	0.02%	0.004%
87	14.676	2226	2229	2231	rBV2	346	331	0.02%	0.004%
88	14.700	2231	2233	2234	rBV2	307	233	0.01%	0.003%
89	14.828	2253	2254	2257	rVV2	298	219	0.01%	0.003%
90	14.877	2259	2262	2263	rBV	278	318	0.02%	0.004%
91	15.011	2283	2284	2288	rVB	509	361	0.02%	0.004%
92	15.060	2291	2292	2296	rBV3	315	403	0.03%	0.005%
93	15.164	2305	2309	2310	rBV	325	464	0.03%	0.005%
94	15.389	2344	2346	2351	rVB4	847	984	0.06%	0.011%
95	15.670	2391	2392	2397	rVB2	474	502	0.03%	0.006%
96	15.731	2400	2402	2403	rBV	318	254	0.02%	0.003%
97	15.828	2416	2418	2422	rBV3	407	604	0.04%	0.007%
98	16.297	2494	2495	2497	rBV2	326	210	0.01%	0.002%
99	16.474	2522	2524	2525	rBV2	338	296	0.02%	0.003%
100	16.730	2565	2566	2568	rBV2	337	222	0.01%	0.003%

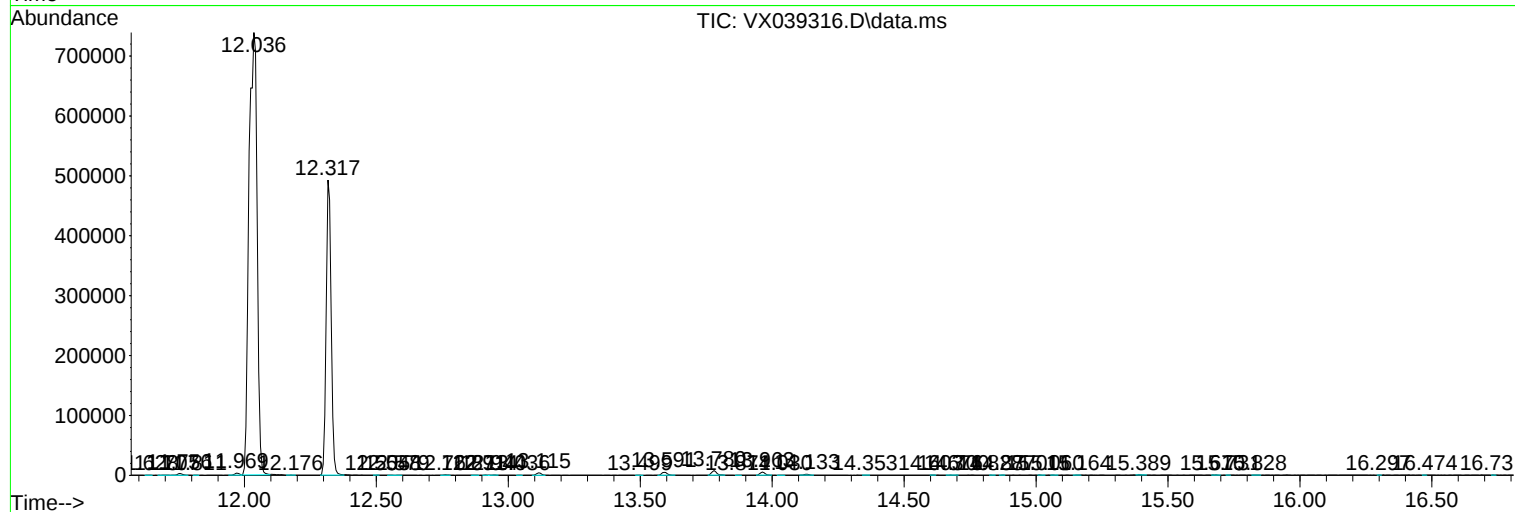
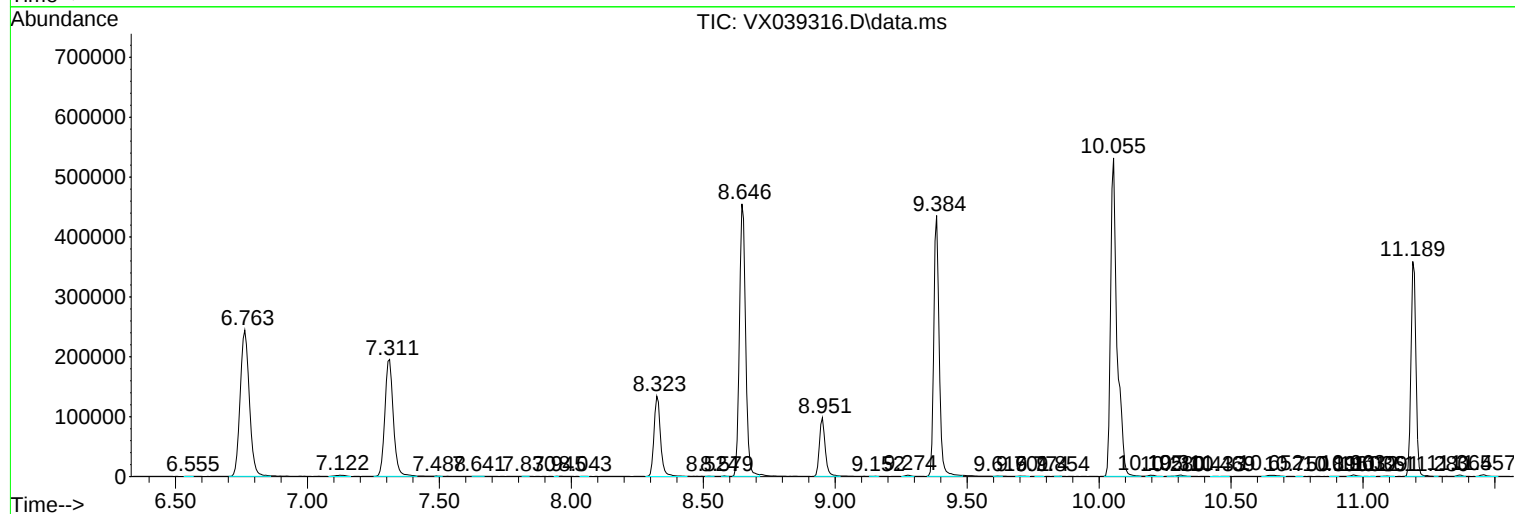
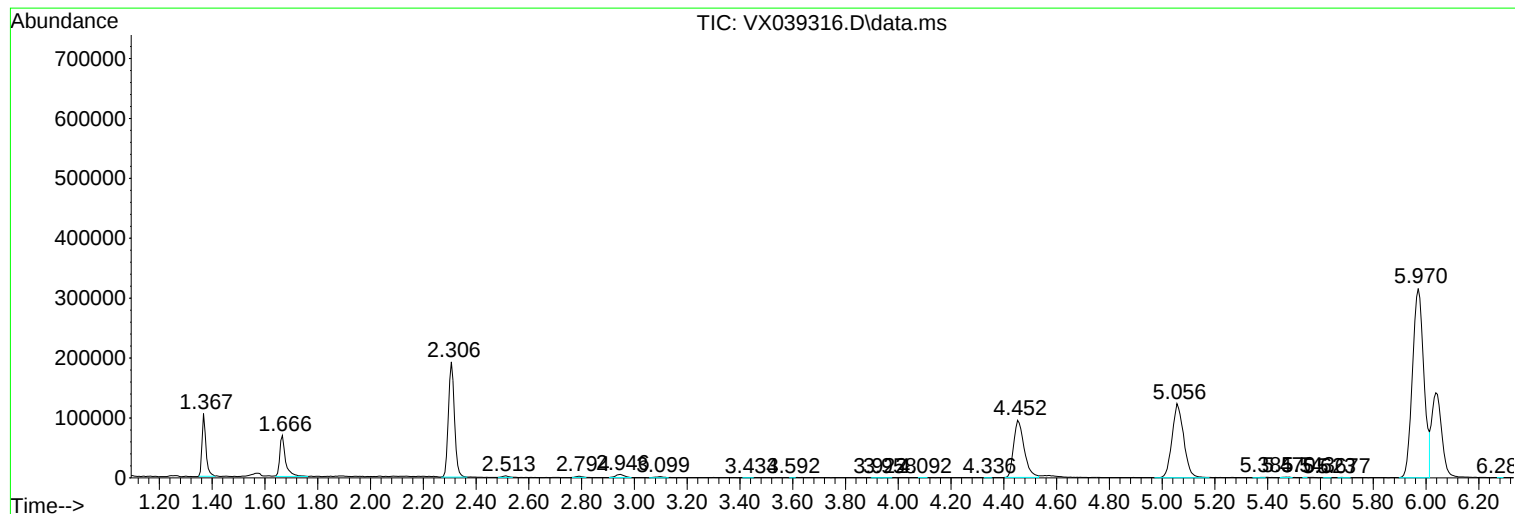
Sum of corrected areas: 8591500

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121823\
Data File : VX039316.D
Acq On : 18 Dec 2023 16:59
Operator : JC/MD
Sample : 05807-17 50X
Misc : 2.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B18

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.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 : VX039316.D
Acq On : 18 Dec 2023 16:59
Operator : JC/MD
Sample : 05807-17 50X
Misc : 2.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B18

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 : VX039316.D
Acq On : 18 Dec 2023 16:59
Operator : JC/MD
Sample : 05807-17 50X
Misc : 2.88g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 20 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0B18

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