

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
 Data File : VX042218.D
 Acq On : 05 Jul 2024 18:03
 Operator : JC/MD
 Sample : P3100-17ME
 Misc : 4.21g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D08ME

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\SFAMXML070324WMA.M

Title : VOC Analysis

Signal : TIC: VX042218.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	24	28	40	rVB2	14216	18799	2.82%	0.339%
2	1.374	42	47	48	rBV	15970	20715	3.10%	0.374%
3	1.648	68	92	95	rBV5	17944	70590	10.58%	1.274%
4	2.276	189	195	211	rBV	98871	188552	28.25%	3.403%
5	2.721	262	268	284	rBV	29888	70129	10.51%	1.266%
6	2.940	300	304	320	rVB	5332	13849	2.07%	0.250%
7	3.282	358	360	362	rBV2	85	95	0.01%	0.002%
8	3.410	379	381	385	rVB2	222	202	0.03%	0.004%
9	3.440	385	386	390	rVB	163	186	0.03%	0.003%
10	3.477	390	392	395	rBV2	218	304	0.05%	0.005%
11	3.593	409	411	413	rBV	126	104	0.02%	0.002%
12	3.733	431	434	436	rBV2	136	162	0.02%	0.003%
13	3.861	453	455	457	rBV	123	123	0.02%	0.002%
14	3.891	457	460	462	rVB	151	141	0.02%	0.003%
15	3.916	462	464	469	rBV	128	206	0.03%	0.004%
16	3.965	469	472	473	rBV	190	127	0.02%	0.002%
17	4.093	490	493	495	rBV2	115	137	0.02%	0.002%
18	4.349	533	535	536	rBV	158	98	0.01%	0.002%
19	4.495	551	559	577	rBV	41270	148981	22.32%	2.689%
20	5.056	640	651	667	rBV	79944	247776	37.12%	4.472%
21	5.300	689	691	693	rBV2	172	180	0.03%	0.003%
22	5.397	701	707	716	rVB4	467	1140	0.17%	0.021%
23	5.556	728	733	742	rVB3	515	1442	0.22%	0.026%
24	5.806	773	774	777	rVB	136	90	0.01%	0.002%
25	5.964	789	800	816	rBV2	234129	667464	100.00%	12.046%
26	6.214	837	841	842	rBV2	222	255	0.04%	0.005%
27	6.397	866	871	873	rBV2	349	605	0.09%	0.011%
28	6.537	892	894	897	rBV2	170	209	0.03%	0.004%
29	6.671	914	916	917	rBV	156	129	0.02%	0.002%
30	6.757	921	930	946	rBV	217989	528453	79.17%	9.537%
31	7.123	984	990	994	rVB4	1342	2911	0.44%	0.053%
32	7.238	1000	1009	1012	rBV4	563	1324	0.20%	0.024%
33	7.305	1012	1020	1045	rVV	130125	297914	44.63%	5.376%
34	7.622	1070	1072	1077	rVB2	255	327	0.05%	0.006%
35	7.659	1077	1078	1080	rBV2	140	129	0.02%	0.002%
36	7.720	1086	1088	1089	rBV2	96	92	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
 Data File : VX042218.D
 Acq On : 05 Jul 2024 18:03
 Operator : JC/MD
 Sample : P3100-17ME
 Misc : 4.21g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D08ME

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\SFAMXML070324WMA.M
 Title : VOC Analysis

37	7.824	1103	1105	1107	rBV2	149	149	0.02%	0.003%
38	7.891	1115	1116	1119	rBV	149	143	0.02%	0.003%
39	7.915	1119	1120	1123	rVV	109	108	0.02%	0.002%
40	8.128	1153	1155	1156	rBV	114	98	0.01%	0.002%
41	8.165	1160	1161	1164	rBV	139	100	0.01%	0.002%
42	8.189	1164	1165	1169	rBV2	97	143	0.02%	0.003%
43	8.244	1172	1174	1178	rBV	184	178	0.03%	0.003%
44	8.324	1181	1187	1200	rBV	70163	123657	18.53%	2.232%
45	8.513	1216	1218	1219	rBV	214	134	0.02%	0.002%
46	8.580	1228	1229	1233	rBV2	230	252	0.04%	0.005%
47	8.647	1234	1240	1254	rBV	337725	538920	80.74%	9.726%
48	8.952	1285	1290	1303	rBV	51975	80778	12.10%	1.458%
49	9.165	1323	1325	1329	rVB2	118	121	0.02%	0.002%
50	9.275	1338	1343	1349	rBV2	4710	7278	1.09%	0.131%
51	9.397	1357	1363	1382	rBV	162735	342961	51.38%	6.189%
52	9.707	1411	1414	1422	rVB3	1645	2625	0.39%	0.047%
53	10.055	1465	1471	1490	rBV	431000	609598	91.33%	11.001%
54	10.244	1498	1502	1509	rVB	3421	4655	0.70%	0.084%
55	10.311	1509	1513	1517	rVB3	793	1336	0.20%	0.024%
56	10.622	1559	1564	1565	rBV	83	128	0.02%	0.002%
57	10.646	1565	1568	1570	rBV2	404	429	0.06%	0.008%
58	10.768	1587	1588	1590	rBV2	226	191	0.03%	0.003%
59	10.817	1593	1596	1600	rVB2	626	760	0.11%	0.014%
60	10.945	1613	1617	1619	rBV2	2081	2747	0.41%	0.050%
61	11.024	1628	1630	1633	rBV2	181	198	0.03%	0.004%
62	11.091	1638	1641	1646	rBV4	720	1036	0.16%	0.019%
63	11.195	1651	1658	1669	rVV	274958	358211	53.67%	6.465%
64	11.311	1673	1677	1682	rVB	5137	7398	1.11%	0.134%
65	11.488	1703	1706	1710	rVB3	991	1455	0.22%	0.026%
66	11.603	1721	1725	1727	rBV2	134	173	0.03%	0.003%
67	11.701	1736	1741	1743	rBV2	5317	7268	1.09%	0.131%
68	11.731	1743	1746	1749	rVV	9807	14479	2.17%	0.261%
69	11.762	1749	1751	1757	rVB2	8042	10344	1.55%	0.187%
70	11.933	1776	1779	1784	rBV3	372	594	0.09%	0.011%
71	11.975	1784	1786	1789	rBV3	1518	2021	0.30%	0.036%
72	12.024	1789	1794	1804	rVB	461012	575692	86.25%	10.390%
73	12.225	1825	1827	1830	rVB3	530	492	0.07%	0.009%
74	12.323	1837	1843	1856	rBV	368650	492109	73.73%	8.881%
75	12.536	1876	1878	1880	rBV	108	117	0.02%	0.002%
76	12.591	1885	1887	1888	rBV2	240	120	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
 Data File : VX042218.D
 Acq On : 05 Jul 2024 18:03
 Operator : JC/MD
 Sample : P3100-17ME
 Misc : 4.21g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D08ME

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\SFAMXMLM070324WMA.M
 Title : VOC Analysis

77	12.634	1892	1894	1896	rVB	258	177	0.03%	0.003%
78	12.701	1904	1905	1910	rVB	216	260	0.04%	0.005%
79	12.762	1910	1915	1921	rBV2	1507	2248	0.34%	0.041%
80	12.872	1929	1933	1941	rVV2	3407	4861	0.73%	0.088%
81	12.981	1949	1951	1954	rVB2	254	190	0.03%	0.003%
82	13.012	1954	1956	1958	rBV2	103	93	0.01%	0.002%
83	13.079	1965	1967	1968	rBV2	140	102	0.02%	0.002%
84	13.195	1984	1986	1991	rVB2	145	177	0.03%	0.003%
85	13.262	1993	1997	2000	rBV2	289	338	0.05%	0.006%
86	13.402	2016	2020	2028	rVV	5285	7357	1.10%	0.133%
87	13.597	2050	2052	2056	rVB3	370	312	0.05%	0.006%
88	13.688	2063	2067	2072	rBV3	539	841	0.13%	0.015%
89	13.731	2072	2074	2077	rVB	165	117	0.02%	0.002%
90	13.786	2080	2083	2087	rBV	1120	1206	0.18%	0.022%
91	13.890	2098	2100	2105	rVB3	337	407	0.06%	0.007%
92	13.945	2107	2109	2110	rBV	164	133	0.02%	0.002%
93	13.969	2110	2113	2115	rVB2	358	372	0.06%	0.007%
94	14.127	2137	2139	2144	rVB2	307	334	0.05%	0.006%
95	14.207	2150	2152	2155	rBV	266	325	0.05%	0.006%
96	14.432	2183	2189	2195	rBV	9524	12850	1.93%	0.232%
97	14.822	2248	2253	2257	rVB2	19347	24276	3.64%	0.438%
98	15.036	2286	2288	2292	rBV4	701	540	0.08%	0.010%
99	15.920	2429	2433	2436	rBV4	2178	3810	0.57%	0.069%
100	16.188	2472	2477	2483	rVB3	3772	6592	0.99%	0.119%

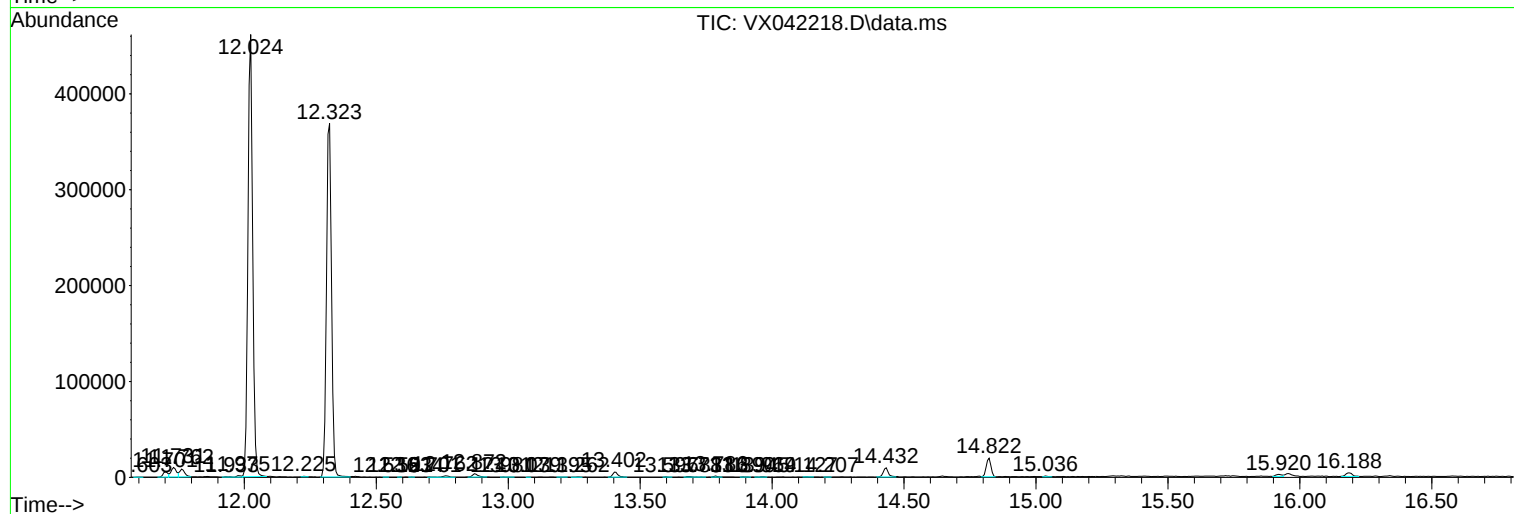
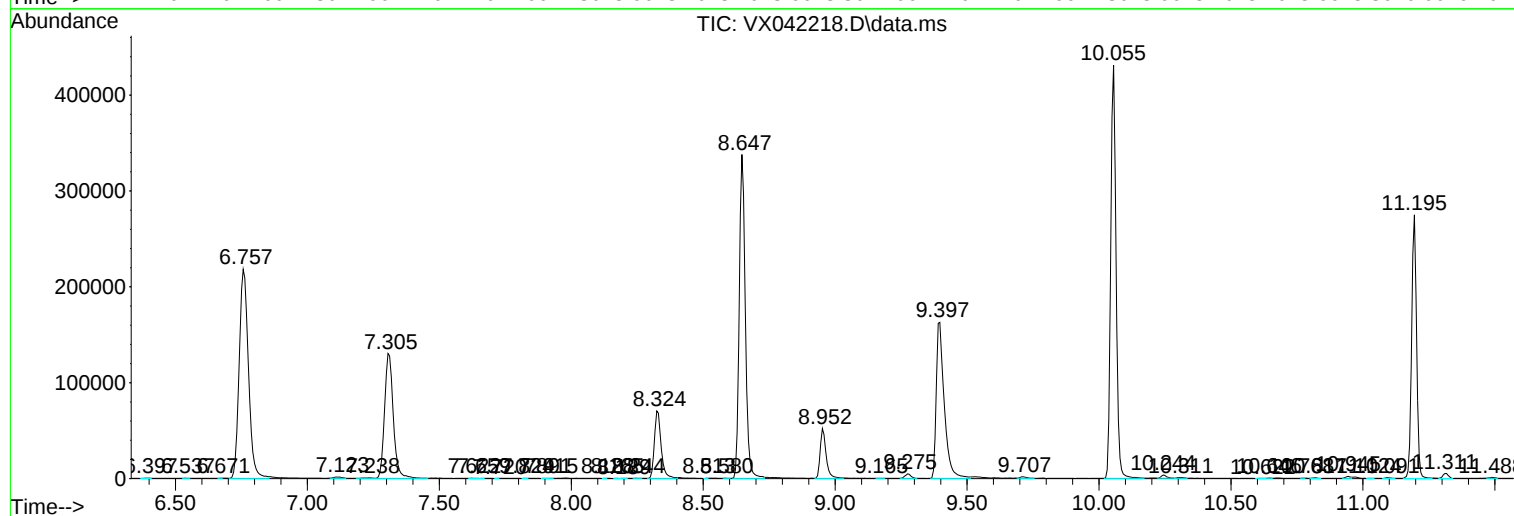
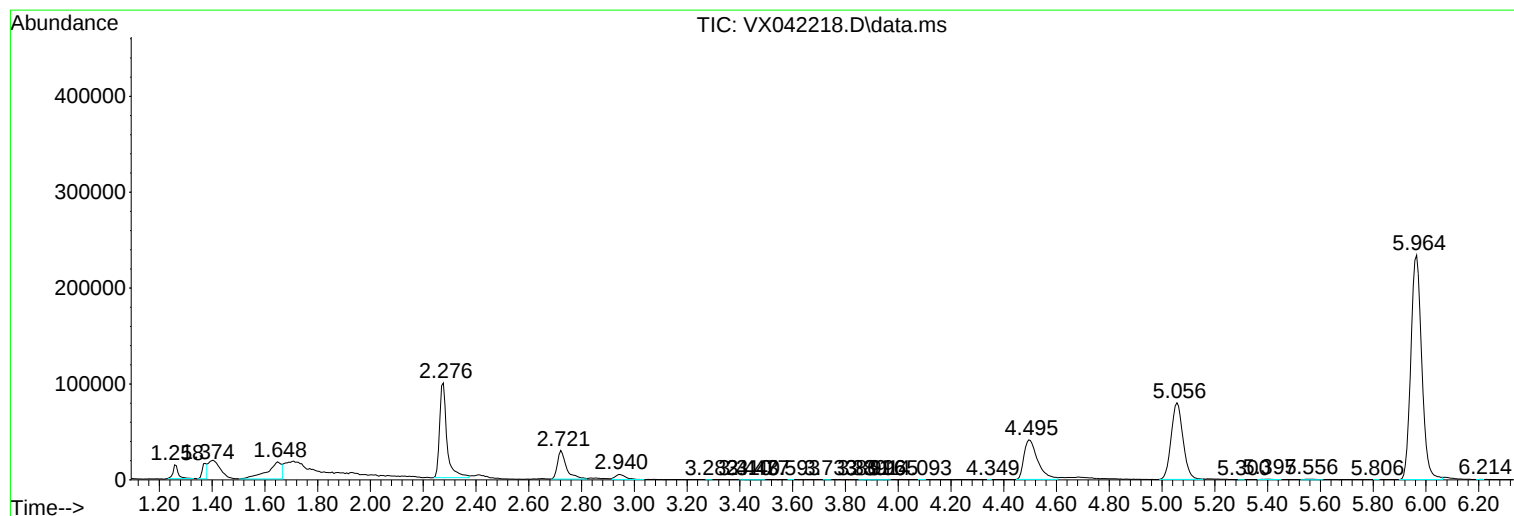
Sum of corrected areas: 5541054

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
Data File : VX042218.D
Acq On : 05 Jul 2024 18:03
Operator : JC/MD
Sample : P3100-17ME
Misc : 4.21g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D08ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
Data File : VX042218.D
Acq On : 05 Jul 2024 18:03
Operator : JC/MD
Sample : P3100-17ME
Misc : 4.21g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D08ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.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\VX070624\
Data File : VX042218.D
Acq On : 05 Jul 2024 18:03
Operator : JC/MD
Sample : P3100-17ME
Misc : 4.21g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D08ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.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