

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
 Data File : VX042216.D
 Acq On : 05 Jul 2024 17:16
 Operator : JC/MD
 Sample : P3100-15ME
 Misc : 4.14g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D04ME

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: VX042216.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	23	29	39	rVV2	11769	16821	2.50%	0.312%
2	1.367	43	46	66	rVB	29739	79821	11.86%	1.479%
3	1.648	89	92	95	rBV	14627	17801	2.64%	0.330%
4	2.282	190	196	211	rBV	105773	192437	28.58%	3.564%
5	2.721	261	268	274	rBV	17404	34747	5.16%	0.644%
6	2.946	298	305	315	rVB2	4589	11281	1.68%	0.209%
7	3.080	323	327	330	rBV2	148	191	0.03%	0.004%
8	3.233	351	352	355	rVB2	123	96	0.01%	0.002%
9	3.349	368	371	373	rBV2	178	176	0.03%	0.003%
10	3.495	393	395	398	rVV2	96	95	0.01%	0.002%
11	3.580	407	409	412	rBV2	97	118	0.02%	0.002%
12	3.775	437	441	442	rBV2	117	174	0.03%	0.003%
13	3.818	447	448	450	rBV2	120	98	0.01%	0.002%
14	4.038	482	484	487	rVV2	83	97	0.01%	0.002%
15	4.129	498	499	501	rBV	124	106	0.02%	0.002%
16	4.233	515	516	518	rVB	172	113	0.02%	0.002%
17	4.318	528	530	535	rVV2	135	155	0.02%	0.003%
18	4.355	535	536	540	rVB2	219	166	0.02%	0.003%
19	4.489	549	558	578	rBV	42429	145484	21.61%	2.695%
20	5.056	639	651	666	rBV	81175	252949	37.57%	4.685%
21	5.330	694	696	699	rVV2	209	290	0.04%	0.005%
22	5.391	702	706	716	rVV5	943	2333	0.35%	0.043%
23	5.470	716	719	722	rVV	130	139	0.02%	0.003%
24	5.543	727	731	734	rBV3	769	1543	0.23%	0.029%
25	5.690	752	755	756	rBV2	104	102	0.02%	0.002%
26	5.732	761	762	765	rBV	143	171	0.03%	0.003%
27	5.842	779	780	784	rVB2	139	169	0.03%	0.003%
28	5.964	789	800	832	rBV2	231573	673255	100.00%	12.471%
29	6.379	866	868	872	rBV	211	242	0.04%	0.004%
30	6.513	888	890	892	rVB2	177	147	0.02%	0.003%
31	6.555	892	897	901	rBV3	240	476	0.07%	0.009%
32	6.604	904	905	907	rBV	142	122	0.02%	0.002%
33	6.677	913	917	918	rBV2	159	188	0.03%	0.003%
34	6.757	922	930	953	rVV	220668	542488	80.58%	10.048%
35	7.128	984	991	998	rVB5	1546	3895	0.58%	0.072%
36	7.226	1002	1007	1012	rVV4	415	829	0.12%	0.015%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
 Data File : VX042216.D
 Acq On : 05 Jul 2024 17:16
 Operator : JC/MD
 Sample : P3100-15ME
 Misc : 4.14g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D04ME

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	7.305	1012	1020	1041	rVV	129465	298714	44.37%	5.533%
38	7.464	1044	1046	1048	rVV2	139	132	0.02%	0.002%
39	7.482	1048	1049	1054	rVB3	342	377	0.06%	0.007%
40	7.671	1077	1080	1083	rBV	118	158	0.02%	0.003%
41	7.775	1096	1097	1099	rVB	274	110	0.02%	0.002%
42	7.958	1124	1127	1128	rBV2	238	206	0.03%	0.004%
43	7.976	1128	1130	1134	rVB2	272	354	0.05%	0.007%
44	8.128	1154	1155	1157	rBV	243	123	0.02%	0.002%
45	8.268	1176	1178	1179	rBV2	109	96	0.01%	0.002%
46	8.323	1181	1187	1202	rVV	70143	126853	18.84%	2.350%
47	8.427	1202	1204	1208	rVV3	364	538	0.08%	0.010%
48	8.482	1211	1213	1214	rBV2	132	97	0.01%	0.002%
49	8.500	1214	1216	1217	rVB	217	122	0.02%	0.002%
50	8.531	1217	1221	1222	rBV2	259	310	0.05%	0.006%
51	8.646	1234	1240	1251	rBV	336263	533014	79.17%	9.873%
52	8.951	1285	1290	1314	rVB	52795	84679	12.58%	1.569%
53	9.122	1316	1318	1319	rVB	208	114	0.02%	0.002%
54	9.232	1335	1336	1338	rBV2	185	162	0.02%	0.003%
55	9.274	1339	1343	1349	rVB2	1906	2799	0.42%	0.052%
56	9.323	1349	1351	1353	rVB	193	122	0.02%	0.002%
57	9.390	1357	1362	1380	rBV	178023	330192	49.04%	6.116%
58	9.713	1411	1415	1420	rBV2	1285	1841	0.27%	0.034%
59	9.799	1428	1429	1433	rBV	175	173	0.03%	0.003%
60	9.860	1436	1439	1443	rBV2	221	239	0.04%	0.004%
61	9.921	1447	1449	1452	rVB2	190	154	0.02%	0.003%
62	9.951	1452	1454	1456	rBV	156	99	0.01%	0.002%
63	10.055	1465	1471	1492	rBV	452745	619005	91.94%	11.466%
64	10.195	1492	1494	1495	rVV3	450	354	0.05%	0.007%
65	10.244	1498	1502	1510	rVV2	2598	3580	0.53%	0.066%
66	10.311	1510	1513	1517	rVB3	679	908	0.13%	0.017%
67	10.646	1566	1568	1569	rBV2	246	183	0.03%	0.003%
68	10.780	1589	1590	1594	rVB2	169	135	0.02%	0.003%
69	10.933	1613	1615	1618	rBV2	130	140	0.02%	0.003%
70	10.969	1618	1621	1628	rVB3	1395	2153	0.32%	0.040%
71	11.091	1638	1641	1647	rVB2	1170	1601	0.24%	0.030%
72	11.195	1652	1658	1669	rBV	260402	349834	51.96%	6.480%
73	11.311	1675	1677	1683	rVB2	1082	1255	0.19%	0.023%
74	11.463	1698	1702	1705	rBV3	239	337	0.05%	0.006%
75	11.554	1715	1717	1722	rVB2	157	212	0.03%	0.004%
76	11.713	1742	1743	1746	rVB	200	123	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
 Data File : VX042216.D
 Acq On : 05 Jul 2024 17:16
 Operator : JC/MD
 Sample : P3100-15ME
 Misc : 4.14g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 22 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D04ME

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

77	11.756	1746	1750	1754	rBB4	307	515	0.08%	0.010%
78	11.804	1754	1758	1760	rBV2	151	201	0.03%	0.004%
79	12.024	1789	1794	1809	rVB	468989	570007	84.66%	10.558%
80	12.231	1825	1828	1830	rBV3	473	571	0.08%	0.011%
81	12.323	1837	1843	1853	rBV	350631	474933	70.54%	8.797%
82	12.725	1907	1909	1912	rBV2	204	184	0.03%	0.003%
83	12.762	1912	1915	1920	rVB3	364	598	0.09%	0.011%
84	12.816	1923	1924	1926	rVV	165	109	0.02%	0.002%
85	12.871	1929	1933	1944	rVV2	2585	4399	0.65%	0.081%
86	12.944	1944	1945	1948	rVB	206	129	0.02%	0.002%
87	13.121	1973	1974	1978	rVV	230	209	0.03%	0.004%
88	13.408	2017	2021	2024	rBV3	772	1121	0.17%	0.021%
89	13.487	2031	2034	2036	rBV2	137	120	0.02%	0.002%
90	13.597	2049	2052	2055	rVB4	376	479	0.07%	0.009%
91	13.633	2055	2058	2059	rBV	98	101	0.02%	0.002%
92	13.688	2064	2067	2071	rBV2	531	675	0.10%	0.013%
93	13.743	2074	2076	2077	rVB2	207	114	0.02%	0.002%
94	13.786	2077	2083	2088	rBV3	722	1425	0.21%	0.026%
95	13.963	2110	2112	2116	rBV3	396	530	0.08%	0.010%
96	14.030	2121	2123	2124	rBV2	164	106	0.02%	0.002%
97	14.091	2131	2133	2135	rBV	122	99	0.01%	0.002%
98	14.432	2186	2189	2190	rBV3	606	643	0.10%	0.012%
99	14.682	2229	2230	2233	rBV2	317	333	0.05%	0.006%
100	14.828	2252	2254	2255	rBV2	296	209	0.03%	0.004%

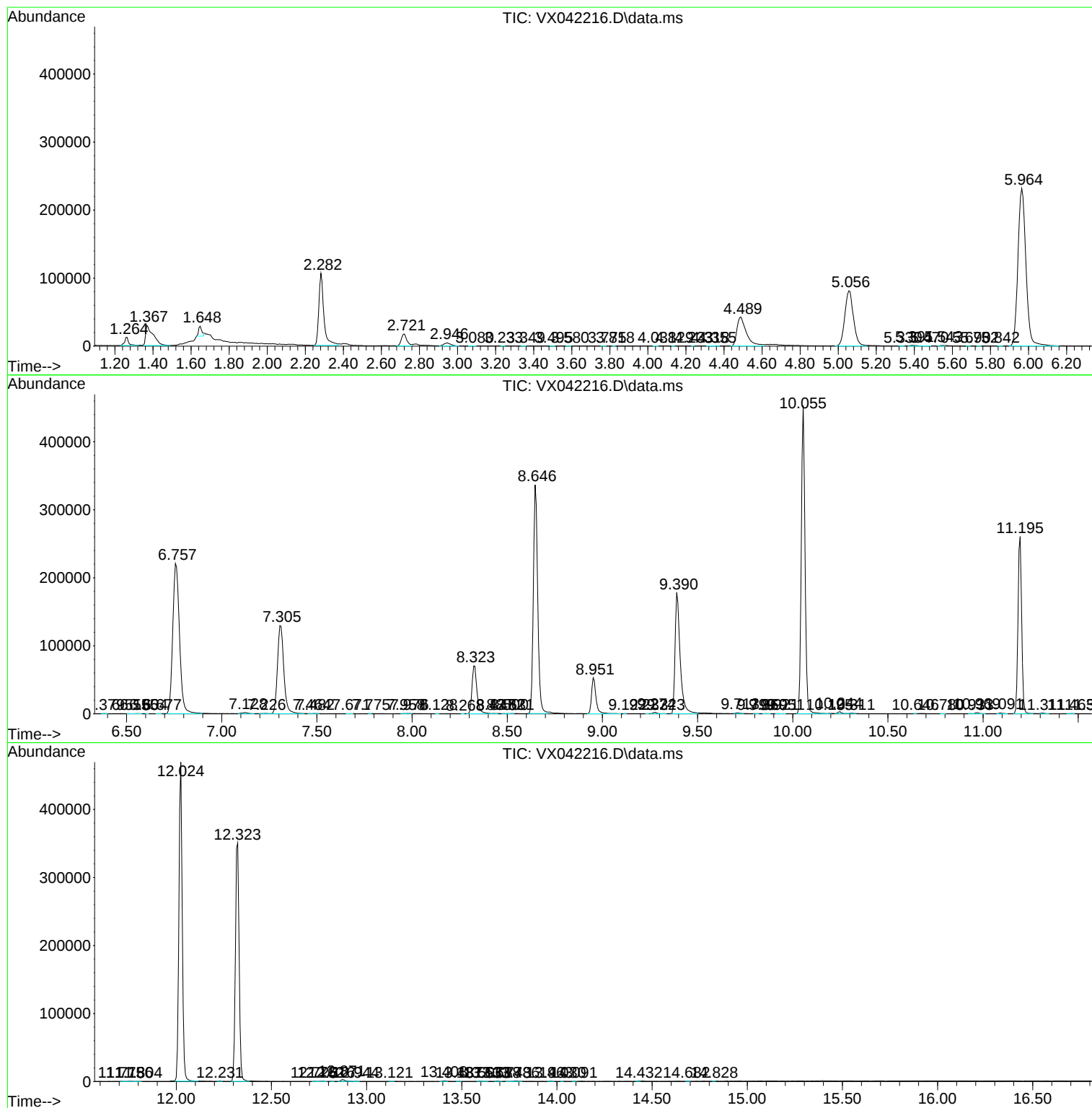
Sum of corrected areas: 5398723

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
Data File : VX042216.D
Acq On : 05 Jul 2024 17:16
Operator : JC/MD
Sample : P3100-15ME
Misc : 4.14g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D04ME

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

TIC Library :
TIC Integration Parameters: LSCINT.P



Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
Data File : VX042216.D
Acq On : 05 Jul 2024 17:16
Operator : JC/MD
Sample : P3100-15ME
Misc : 4.14g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D04ME

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

TIC Library :
TIC Integration Parameters: LSCINT.P

No Library Search Compounds Detected

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070624\
Data File : VX042216.D
Acq On : 05 Jul 2024 17:16
Operator : JC/MD
Sample : P3100-15ME
Misc : 4.14g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 22 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D04ME

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

TIC Library :
TIC Integration Parameters: LSCINT.P

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