

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120524\
 Data File : VX044158.D
 Acq On : 05 Dec 2024 19:22
 Operator : JC/MD
 Sample : P5066-15 20X
 Misc : 6.65g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28N3

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\SFAMXML120524WMA.M

Title : VOC Analysis

Signal : TIC: VX044158.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	27	rBV3	4401	5429	0.58%	0.081%
2	1.368	43	46	58	rVB	110359	135350	14.54%	2.010%
3	1.642	88	91	105	rVB	94229	157207	16.89%	2.334%
4	2.294	192	198	210	rVB	185768	294834	31.68%	4.377%
5	2.489	227	230	232	rBV2	953	831	0.09%	0.012%
6	2.636	252	254	257	rBV2	433	448	0.05%	0.007%
7	2.745	270	272	274	rBV3	641	675	0.07%	0.010%
8	2.782	274	278	285	rVV5	1310	2873	0.31%	0.043%
9	2.880	291	294	297	rBV3	485	824	0.09%	0.012%
10	3.002	313	314	316	rBV	785	423	0.05%	0.006%
11	3.069	323	325	326	rBV2	672	510	0.05%	0.008%
12	3.123	331	334	336	rBV3	979	1313	0.14%	0.019%
13	3.166	339	341	342	rBV2	696	559	0.06%	0.008%
14	3.276	358	359	362	rVB2	839	543	0.06%	0.008%
15	3.306	362	364	365	rBV	545	555	0.06%	0.008%
16	3.434	379	385	392	rVV5	3773	8414	0.90%	0.125%
17	3.556	403	405	409	rBV4	492	835	0.09%	0.012%
18	3.629	416	417	423	rBV3	559	824	0.09%	0.012%
19	3.672	423	424	427	rBV2	573	644	0.07%	0.010%
20	3.794	442	444	446	rBV2	670	574	0.06%	0.009%
21	3.843	450	452	455	rVV	892	593	0.06%	0.009%
22	3.904	460	462	463	rVB2	912	422	0.05%	0.006%
23	3.922	463	465	468	rBV2	503	444	0.05%	0.007%
24	4.074	487	490	493	rBV3	592	853	0.09%	0.013%
25	4.166	502	505	507	rBV3	508	508	0.05%	0.008%
26	4.227	514	515	519	rVB2	763	386	0.04%	0.006%
27	4.331	530	532	533	rBV	654	539	0.06%	0.008%
28	4.392	541	542	544	rBV	614	493	0.05%	0.007%
29	4.471	546	555	572	rVV	55400	181212	19.47%	2.690%
30	4.751	599	601	602	rVB	778	383	0.04%	0.006%
31	4.910	625	627	630	rBV3	527	489	0.05%	0.007%
32	5.056	639	651	669	rBV	121242	388588	41.76%	5.769%
33	5.275	685	687	690	rVB3	642	728	0.08%	0.011%
34	5.312	690	693	694	rBV2	471	511	0.05%	0.008%
35	5.452	713	716	717	rBV	899	575	0.06%	0.009%
36	5.519	726	727	729	rBV2	624	504	0.05%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120524\
 Data File : VX044158.D
 Acq On : 05 Dec 2024 19:22
 Operator : JC/MD
 Sample : P5066-15 20X
 Misc : 6.65g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28N3

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\SFAMXML120524WMA.M
 Title : VOC Analysis

37	5.586	736	738	740	rBV3	586	537	0.06%	0.008%
38	5.964	789	800	818	rBV2	309745	930575	100.00%	13.816%
39	6.245	845	846	849	rVB3	621	462	0.05%	0.007%
40	6.537	892	894	897	rVB2	899	1102	0.12%	0.016%
41	6.562	897	898	900	rBV2	975	751	0.08%	0.011%
42	6.629	906	909	910	rBV	573	360	0.04%	0.005%
43	6.757	921	930	944	rBV	226619	549547	59.05%	8.159%
44	7.111	983	988	995	rBV8	2561	6490	0.70%	0.096%
45	7.306	1011	1020	1034	rBV	194311	427903	45.98%	6.353%
46	7.604	1066	1069	1071	rVB2	594	668	0.07%	0.010%
47	7.623	1071	1072	1073	rBV	616	378	0.04%	0.006%
48	7.732	1087	1090	1091	rBV2	849	881	0.09%	0.013%
49	8.019	1136	1137	1141	rBV3	590	872	0.09%	0.013%
50	8.068	1143	1145	1146	rVB	824	413	0.04%	0.006%
51	8.153	1157	1159	1160	rBV	584	457	0.05%	0.007%
52	8.324	1181	1187	1199	rBV	115994	195158	20.97%	2.898%
53	8.647	1234	1240	1251	rBV	434312	689555	74.10%	10.238%
54	8.909	1281	1283	1284	rBV2	465	463	0.05%	0.007%
55	8.952	1285	1290	1307	rVV	76528	125570	13.49%	1.864%
56	9.067	1307	1309	1312	rVV3	1122	824	0.09%	0.012%
57	9.104	1313	1315	1318	rVB3	730	750	0.08%	0.011%
58	9.281	1342	1344	1345	rVB	747	375	0.04%	0.006%
59	9.311	1347	1349	1350	rVB2	675	370	0.04%	0.005%
60	9.385	1356	1361	1375	rBV	258024	400248	43.01%	5.943%
61	9.781	1424	1426	1429	rBV2	583	632	0.07%	0.009%
62	9.811	1429	1431	1432	rBV	637	367	0.04%	0.005%
63	10.055	1465	1471	1484	rBV	443277	642152	69.01%	9.534%
64	10.238	1499	1501	1503	rBV	662	604	0.06%	0.009%
65	10.275	1506	1507	1510	rBV2	614	636	0.07%	0.009%
66	10.342	1517	1518	1520	rBV	751	399	0.04%	0.006%
67	10.421	1529	1531	1532	rBV	530	404	0.04%	0.006%
68	10.470	1537	1539	1541	rBV3	610	571	0.06%	0.008%
69	10.549	1549	1552	1555	rBV2	542	757	0.08%	0.011%
70	10.628	1563	1565	1568	rBV2	709	893	0.10%	0.013%
71	10.701	1575	1577	1579	rBV2	465	427	0.05%	0.006%
72	10.957	1617	1619	1622	rVB2	626	502	0.05%	0.007%
73	11.128	1645	1647	1650	rBV4	504	579	0.06%	0.009%
74	11.189	1652	1657	1666	rVV	339371	430754	46.29%	6.396%
75	11.366	1685	1686	1688	rBV	1158	799	0.09%	0.012%
76	11.634	1728	1730	1731	rBV2	548	489	0.05%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120524\
 Data File : VX044158.D
 Acq On : 05 Dec 2024 19:22
 Operator : JC/MD
 Sample : P5066-15 20X
 Misc : 6.65g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28N3

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\SFAMXLM120524WMA.M
 Title : VOC Analysis

77	11.671	1735	1736	1738	rBV	818	592	0.06%	0.009%
78	11.756	1748	1750	1753	rBV4	573	631	0.07%	0.009%
79	12.018	1788	1793	1803	rBV	426976	538513	57.87%	7.995%
80	12.195	1820	1822	1823	rVB2	977	580	0.06%	0.009%
81	12.262	1832	1833	1837	rBV3	693	846	0.09%	0.013%
82	12.317	1837	1842	1853	rVV	439824	550739	59.18%	8.177%
83	12.616	1890	1891	1896	rBV3	457	682	0.07%	0.010%
84	12.872	1930	1933	1934	rBV2	641	691	0.07%	0.010%
85	12.908	1937	1939	1941	rBV2	523	444	0.05%	0.007%
86	12.963	1946	1948	1950	rVV	535	351	0.04%	0.005%
87	13.268	1996	1998	2001	rVB3	1093	906	0.10%	0.013%
88	13.292	2001	2002	2006	rVB2	1087	746	0.08%	0.011%
89	13.341	2006	2010	2011	rBV2	642	781	0.08%	0.012%
90	13.695	2066	2068	2071	rBV4	805	784	0.08%	0.012%
91	13.792	2078	2084	2087	rBV6	1342	3047	0.33%	0.045%
92	14.036	2121	2124	2128	rVB6	2764	3352	0.36%	0.050%
93	14.170	2144	2146	2147	rBV2	674	462	0.05%	0.007%
94	14.615	2216	2219	2221	rVB3	3578	3669	0.39%	0.054%
95	14.755	2238	2242	2246	rBV3	5391	7419	0.80%	0.110%
96	15.493	2359	2363	2367	rBV3	4313	6137	0.66%	0.091%
97	16.213	2477	2481	2484	rBV4	1182	2049	0.22%	0.030%
98	16.298	2493	2495	2497	rBV3	1323	1170	0.13%	0.017%
99	16.377	2505	2508	2513	rBV4	2254	2783	0.30%	0.041%
100	16.688	2556	2559	2561	rBV4	920	1318	0.14%	0.020%

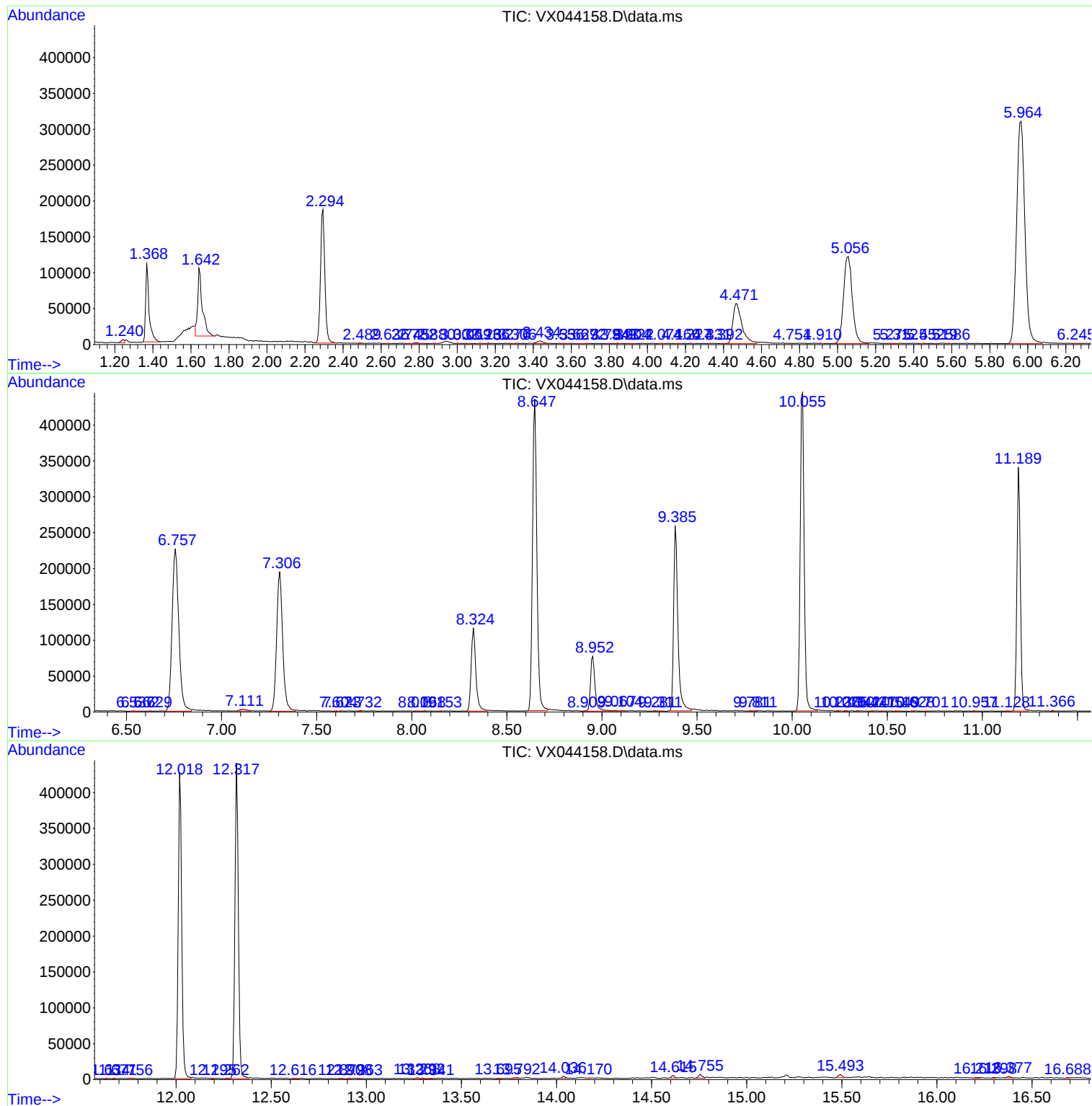
Sum of corrected areas: 6735259

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120524\
Data File : VX044158.D
Acq On : 05 Dec 2024 19:22
Operator : JC/MD
Sample : P5066-15 20X
Misc : 6.65g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28N3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120524WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120524\
Data File : VX044158.D
Acq On : 05 Dec 2024 19:22
Operator : JC/MD
Sample : P5066-15 20X
Misc : 6.65g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28N3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120524WMA.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\VX120524\
Data File : VX044158.D
Acq On : 05 Dec 2024 19:22
Operator : JC/MD
Sample : P5066-15 20X
Misc : 6.65g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28N3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120524WMA.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