

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
 Data File : VX044301.D
 Acq On : 13 Dec 2024 22:49
 Operator : JC/MD
 Sample : P5153-12ME
 Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28P9ME

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: VX044301.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	26	29	32	rVB	7593	8216	0.65%	0.093%
2	1.367	43	46	61	rVB	72571	160779	12.70%	1.828%
3	1.648	89	92	94	rBV	37973	42930	3.39%	0.488%
4	2.282	190	196	208	rBV	216890	352988	27.88%	4.014%
5	2.599	246	248	251	rBV	559	645	0.05%	0.007%
6	2.715	261	267	274	rVV	9708	19681	1.55%	0.224%
7	2.946	299	305	313	rBV5	3027	7408	0.59%	0.084%
8	3.294	360	362	364	rVB	531	393	0.03%	0.004%
9	3.324	364	367	368	rBV2	465	493	0.04%	0.006%
10	3.343	368	370	372	rVB2	587	402	0.03%	0.005%
11	3.416	377	382	390	rVV4	3457	7338	0.58%	0.083%
12	3.702	427	429	434	rVV3	498	801	0.06%	0.009%
13	3.769	439	440	442	rVV2	611	431	0.03%	0.005%
14	3.855	451	454	457	rBV2	601	865	0.07%	0.010%
15	4.086	491	492	495	rVB	826	584	0.05%	0.007%
16	4.117	495	497	500	rBV2	376	514	0.04%	0.006%
17	4.166	503	505	508	rBV3	453	688	0.05%	0.008%
18	4.275	521	523	526	rVB2	581	489	0.04%	0.006%
19	4.318	528	530	532	rBV	615	547	0.04%	0.006%
20	4.361	535	537	540	rBV3	458	463	0.04%	0.005%
21	4.483	549	557	578	rBV	50958	213347	16.85%	2.426%
22	5.050	637	650	668	rBV	161946	523668	41.36%	5.955%
23	5.336	694	697	700	rBV3	486	482	0.04%	0.005%
24	5.373	700	703	705	rVB3	457	510	0.04%	0.006%
25	5.422	710	711	714	rVB	696	428	0.03%	0.005%
26	5.635	743	746	748	rBV2	543	480	0.04%	0.005%
27	5.958	787	799	819	rBV2	433548	1266187	100.00%	14.398%
28	6.239	842	845	848	rBV3	723	877	0.07%	0.010%
29	6.281	848	852	854	rBV3	378	584	0.05%	0.007%
30	6.495	886	887	888	rBV	732	426	0.03%	0.005%
31	6.598	901	904	906	rBV2	909	1130	0.09%	0.013%
32	6.696	918	920	921	rBV2	473	391	0.03%	0.004%
33	6.757	921	930	949	rVV	276449	688104	54.34%	7.825%
34	7.202	1000	1003	1004	rBV3	1246	1274	0.10%	0.014%
35	7.305	1011	1020	1032	rBV	255848	582315	45.99%	6.622%
36	7.476	1045	1048	1049	rBV2	1041	997	0.08%	0.011%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
 Data File : VX044301.D
 Acq On : 13 Dec 2024 22:49
 Operator : JC/MD
 Sample : P5153-12ME
 Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28P9ME

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	7.665	1078	1079	1081	rBV2	631	438	0.03%	0.005%
38	7.732	1087	1090	1091	rVB2	663	538	0.04%	0.006%
39	7.750	1091	1093	1095	rVB	584	490	0.04%	0.006%
40	7.994	1131	1133	1137	rVB2	731	758	0.06%	0.009%
41	8.238	1171	1173	1177	rBV4	637	719	0.06%	0.008%
42	8.281	1179	1180	1181	rBV	893	394	0.03%	0.004%
43	8.324	1181	1187	1200	rBV	145283	251794	19.89%	2.863%
44	8.647	1233	1240	1255	rBV	607720	976664	77.13%	11.106%
45	8.951	1284	1290	1300	rBV	97263	161181	12.73%	1.833%
46	9.275	1341	1343	1347	rVB3	448	384	0.03%	0.004%
47	9.390	1357	1362	1377	rBV	262707	482626	38.12%	5.488%
48	9.701	1412	1413	1415	rBV	608	596	0.05%	0.007%
49	9.957	1450	1455	1456	rBV3	658	709	0.06%	0.008%
50	10.049	1465	1470	1487	rBV	555747	810863	64.04%	9.220%
51	10.287	1508	1509	1510	rBV	629	390	0.03%	0.004%
52	10.530	1548	1549	1552	rVB3	537	446	0.04%	0.005%
53	10.604	1560	1561	1564	rVB2	619	490	0.04%	0.006%
54	10.640	1564	1567	1568	rBV3	649	688	0.05%	0.008%
55	10.756	1582	1586	1587	rBV3	544	735	0.06%	0.008%
56	10.805	1592	1594	1597	rBV3	538	786	0.06%	0.009%
57	10.963	1617	1620	1624	rBV4	1907	2458	0.19%	0.028%
58	11.189	1652	1657	1666	rBV	450346	585003	46.20%	6.652%
59	11.439	1694	1698	1699	rBV2	575	600	0.05%	0.007%
60	11.482	1701	1705	1710	rVV5	2552	4425	0.35%	0.050%
61	11.616	1725	1727	1730	rBV3	906	1056	0.08%	0.012%
62	11.640	1730	1731	1733	rVV	539	414	0.03%	0.005%
63	11.707	1737	1742	1746	rVB3	846	1308	0.10%	0.015%
64	11.750	1746	1749	1752	rBV3	409	549	0.04%	0.006%
65	11.853	1765	1766	1768	rVB	850	458	0.04%	0.005%
66	11.975	1785	1786	1788	rVB2	1006	530	0.04%	0.006%
67	12.018	1788	1793	1808	rBV	552812	728294	57.52%	8.282%
68	12.170	1816	1818	1821	rVB4	1001	772	0.06%	0.009%
69	12.225	1825	1827	1829	rVB2	756	494	0.04%	0.006%
70	12.317	1837	1842	1851	rBV	674364	860990	68.00%	9.790%
71	12.420	1857	1859	1864	rVB5	1549	2281	0.18%	0.026%
72	12.585	1883	1886	1887	rVB2	1049	724	0.06%	0.008%
73	12.609	1887	1890	1891	rBV2	678	642	0.05%	0.007%
74	12.670	1899	1900	1903	rBV2	705	831	0.07%	0.009%
75	12.756	1913	1914	1920	rVB4	1030	1380	0.11%	0.016%
76	12.847	1928	1929	1931	rBV2	628	460	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
 Data File : VX044301.D
 Acq On : 13 Dec 2024 22:49
 Operator : JC/MD
 Sample : P5153-12ME
 Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 36 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28P9ME

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

77	12.902	1936	1938	1940	rBV2	745	593	0.05%	0.007%
78	13.201	1984	1987	1988	rBV3	427	403	0.03%	0.005%
79	13.268	1994	1998	2003	rBV5	2378	3291	0.26%	0.037%
80	13.414	2020	2022	2025	rBV4	777	1104	0.09%	0.013%
81	13.609	2050	2054	2055	rBV3	436	537	0.04%	0.006%
82	13.676	2063	2065	2068	rBV3	987	1231	0.10%	0.014%
83	13.755	2076	2078	2081	rBV3	371	506	0.04%	0.006%
84	13.780	2081	2082	2084	rVB2	718	499	0.04%	0.006%
85	13.944	2105	2109	2114	rBV4	749	1145	0.09%	0.013%
86	14.036	2122	2124	2127	rVB3	1917	1778	0.14%	0.020%
87	14.140	2139	2141	2143	rVB3	982	742	0.06%	0.008%
88	14.231	2151	2156	2157	rBV2	648	776	0.06%	0.009%
89	14.371	2174	2179	2180	rBV3	784	1097	0.09%	0.012%
90	14.633	2219	2222	2223	rBV3	474	517	0.04%	0.006%
91	14.755	2239	2242	2246	rVB4	1848	2142	0.17%	0.024%
92	14.816	2250	2252	2255	rVB2	649	399	0.03%	0.005%
93	14.859	2257	2259	2261	rBV2	696	477	0.04%	0.005%
94	14.950	2272	2274	2275	rBV	771	543	0.04%	0.006%
95	15.054	2288	2291	2293	rBV3	489	567	0.04%	0.006%
96	15.170	2308	2310	2313	rBV3	694	628	0.05%	0.007%
97	15.200	2313	2315	2316	rBV2	795	520	0.04%	0.006%
98	15.408	2348	2349	2351	rBV2	631	406	0.03%	0.005%
99	16.304	2494	2496	2497	rVB	818	389	0.03%	0.004%
100	16.718	2562	2564	2566	rBV	787	644	0.05%	0.007%

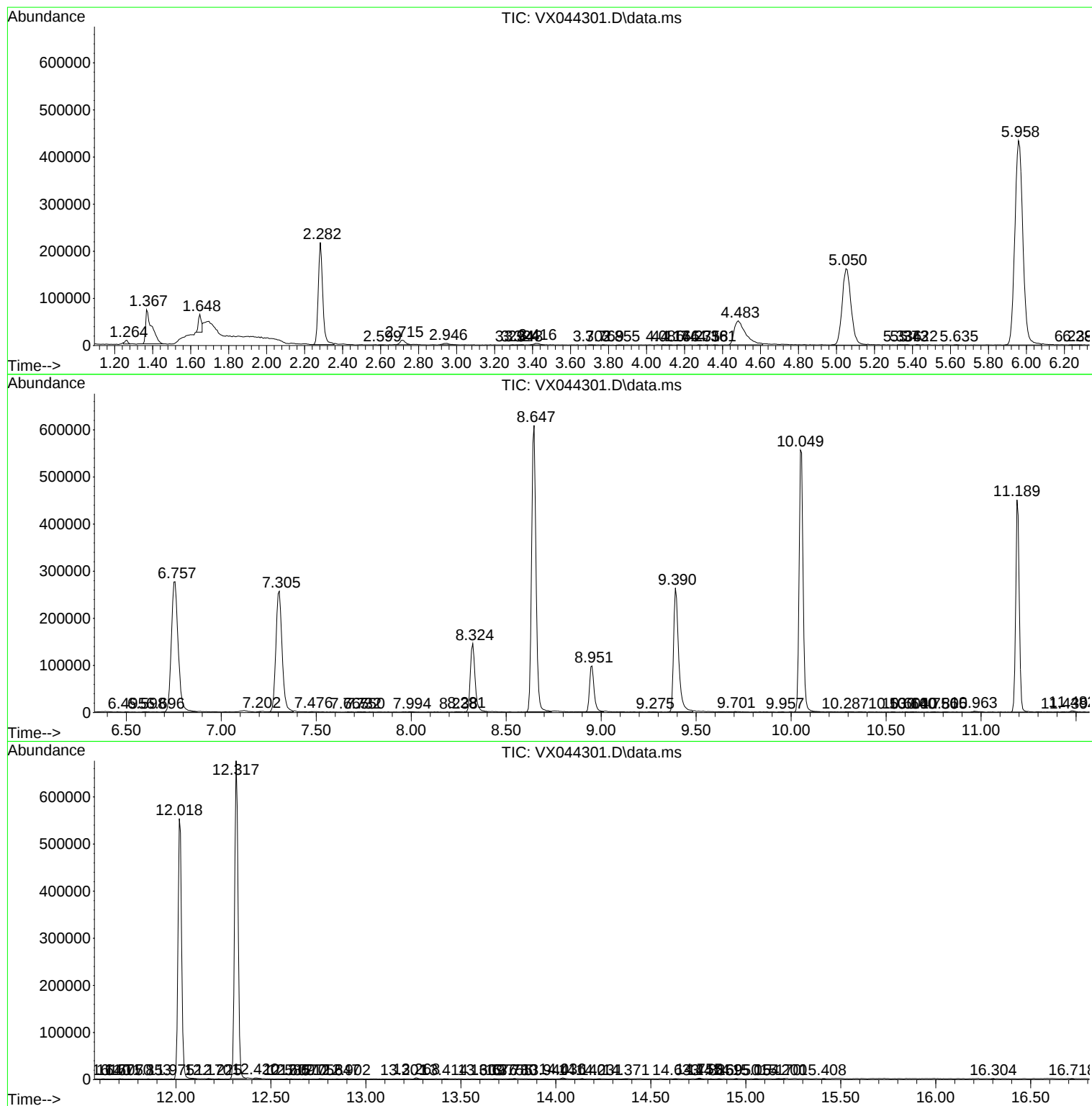
Sum of corrected areas: 8794147

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
Data File : VX044301.D
Acq On : 13 Dec 2024 22:49
Operator : JC/MD
Sample : P5153-12ME
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28P9ME

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\VX121324\
Data File : VX044301.D
Acq On : 13 Dec 2024 22:49
Operator : JC/MD
Sample : P5153-12ME
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28P9ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120524WMA.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\VX121324\
Data File : VX044301.D
Acq On : 13 Dec 2024 22:49
Operator : JC/MD
Sample : P5153-12ME
Misc : 6.52g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 36 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28P9ME

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