

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
 Data File : VX044303.D
 Acq On : 13 Dec 2024 23:35
 Operator : JC/MD
 Sample : P5153-09ME
 Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28P7ME

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: VX044303.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	32	rBV3	10697	14476	1.86%	0.263%
2	1.368	43	46	50	rBV	38576	58673	7.55%	1.065%
3	1.587	68	82	83	rBV8	17844	57135	7.35%	1.037%
4	2.276	190	195	211	rVB	119803	200700	25.82%	3.642%
5	2.508	231	233	236	rBV3	373	396	0.05%	0.007%
6	2.758	272	274	275	rBV2	629	536	0.07%	0.010%
7	2.886	292	295	296	rVB	607	513	0.07%	0.009%
8	2.940	296	304	305	rBV5	4048	7175	0.92%	0.130%
9	3.093	327	329	331	rVB3	499	396	0.05%	0.007%
10	3.123	331	334	336	rBV3	663	772	0.10%	0.014%
11	3.422	376	383	390	rVV3	3297	7752	1.00%	0.141%
12	3.550	401	404	405	rBV3	527	469	0.06%	0.009%
13	3.660	420	422	424	rVB2	606	462	0.06%	0.008%
14	3.770	438	440	441	rBV	438	414	0.05%	0.008%
15	3.855	452	454	457	rVB3	642	481	0.06%	0.009%
16	3.989	474	476	479	rVB2	835	626	0.08%	0.011%
17	4.032	482	483	486	rVB2	700	620	0.08%	0.011%
18	4.074	489	490	492	rBV2	727	536	0.07%	0.010%
19	4.349	531	535	536	rVB2	560	642	0.08%	0.012%
20	4.373	536	539	542	rBV3	440	622	0.08%	0.011%
21	4.483	548	557	580	rBV	29060	129889	16.71%	2.357%
22	4.934	630	631	634	rBV3	598	660	0.08%	0.012%
23	5.050	638	650	667	rBV	97811	322362	41.47%	5.850%
24	5.342	696	698	701	rVB2	517	439	0.06%	0.008%
25	5.434	712	713	717	rBV3	479	581	0.07%	0.011%
26	5.775	767	769	771	rVB	641	396	0.05%	0.007%
27	5.800	771	773	776	rBV	790	586	0.08%	0.011%
28	5.830	776	778	779	rBV2	425	416	0.05%	0.008%
29	5.958	789	799	814	rBV2	268190	777255	100.00%	14.106%
30	6.190	835	837	839	rBV2	465	460	0.06%	0.008%
31	6.641	910	911	914	rBV2	497	415	0.05%	0.008%
32	6.757	920	930	947	rBV	201739	488289	62.82%	8.862%
33	7.025	973	974	976	rBV2	497	409	0.05%	0.007%
34	7.098	983	986	987	rBV2	1177	1013	0.13%	0.018%
35	7.117	987	989	991	rVV3	1228	1047	0.13%	0.019%
36	7.202	1001	1003	1004	rBV	710	442	0.06%	0.008%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
 Data File : VX044303.D
 Acq On : 13 Dec 2024 23:35
 Operator : JC/MD
 Sample : P5153-09ME
 Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28P7ME

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

37	7.305	1011	1020	1041	rVV	161835	362302	46.61%	6.575%
38	7.476	1045	1048	1049	rBV2	586	574	0.07%	0.010%
39	7.494	1049	1051	1052	rVB2	787	455	0.06%	0.008%
40	7.525	1052	1056	1060	rBV2	886	1302	0.17%	0.024%
41	8.214	1166	1169	1170	rBV2	698	512	0.07%	0.009%
42	8.324	1180	1187	1198	rBV	83702	148879	19.15%	2.702%
43	8.482	1210	1213	1215	rBV3	553	604	0.08%	0.011%
44	8.592	1229	1231	1232	rBV	547	421	0.05%	0.008%
45	8.647	1234	1240	1250	rVV	354091	568712	73.17%	10.321%
46	8.909	1281	1283	1285	rBV3	512	613	0.08%	0.011%
47	8.952	1285	1290	1300	rVV2	59621	96644	12.43%	1.754%
48	9.128	1317	1319	1321	rBV3	498	460	0.06%	0.008%
49	9.153	1321	1323	1324	rVB2	703	452	0.06%	0.008%
50	9.397	1357	1363	1382	rBV	146202	292123	37.58%	5.302%
51	9.604	1396	1397	1404	rVB7	994	1268	0.16%	0.023%
52	9.677	1406	1409	1411	rBV3	683	1132	0.15%	0.021%
53	9.708	1411	1414	1418	rVB4	1969	2939	0.38%	0.053%
54	9.842	1433	1436	1440	rVB2	645	1015	0.13%	0.018%
55	9.896	1443	1445	1448	rBV2	692	609	0.08%	0.011%
56	10.055	1465	1471	1483	rBV	389147	571967	73.59%	10.380%
57	10.305	1510	1512	1514	rBV2	771	589	0.08%	0.011%
58	10.610	1561	1562	1564	rVB2	716	474	0.06%	0.009%
59	10.640	1564	1567	1571	rBV3	544	931	0.12%	0.017%
60	10.756	1584	1586	1589	rBV3	514	715	0.09%	0.013%
61	10.787	1589	1591	1595	rVV3	668	805	0.10%	0.015%
62	10.817	1595	1596	1600	rVB2	573	574	0.07%	0.010%
63	10.860	1600	1603	1606	rBV2	1033	1222	0.16%	0.022%
64	10.890	1606	1608	1611	rVB3	710	821	0.11%	0.015%
65	10.951	1616	1618	1621	rVB3	508	516	0.07%	0.009%
66	10.982	1621	1623	1628	rBV3	592	633	0.08%	0.011%
67	11.024	1628	1630	1632	rBV2	404	433	0.06%	0.008%
68	11.189	1652	1657	1667	rVB	269618	353575	45.49%	6.417%
69	11.311	1676	1677	1680	rBV2	404	428	0.06%	0.008%
70	11.482	1703	1705	1710	rVB4	1250	1422	0.18%	0.026%
71	11.713	1738	1743	1746	rBV5	890	1191	0.15%	0.022%
72	11.756	1749	1750	1753	rBV	602	458	0.06%	0.008%
73	11.860	1765	1767	1770	rBV2	619	580	0.07%	0.011%
74	11.945	1778	1781	1783	rBV3	597	645	0.08%	0.012%
75	12.018	1788	1793	1807	rBV	353493	481828	61.99%	8.744%
76	12.238	1825	1829	1831	rBV2	621	759	0.10%	0.014%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
 Data File : VX044303.D
 Acq On : 13 Dec 2024 23:35
 Operator : JC/MD
 Sample : P5153-09ME
 Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28P7ME

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	12.317	1837	1842	1852	rBV	381117	490161	63.06%	8.896%
78	12.420	1856	1859	1864	rVB6	1512	2596	0.33%	0.047%
79	12.561	1880	1882	1884	rBV3	545	453	0.06%	0.008%
80	12.640	1893	1895	1898	rBV2	491	478	0.06%	0.009%
81	12.811	1921	1923	1926	rBV2	554	785	0.10%	0.014%
82	12.945	1943	1945	1947	rBV3	579	546	0.07%	0.010%
83	13.036	1958	1960	1962	rVB	701	574	0.07%	0.010%
84	13.128	1973	1975	1978	rVB2	479	397	0.05%	0.007%
85	13.268	1993	1998	2001	rBV3	3665	4888	0.63%	0.089%
86	13.384	2014	2017	2021	rVB4	1965	2424	0.31%	0.044%
87	13.524	2038	2040	2043	rVB4	941	914	0.12%	0.017%
88	13.664	2060	2063	2064	rBV	628	711	0.09%	0.013%
89	13.774	2077	2081	2083	rBV3	1018	1802	0.23%	0.033%
90	13.835	2089	2091	2096	rVB4	2322	2766	0.36%	0.050%
91	14.036	2121	2124	2129	rVB4	4849	5143	0.66%	0.093%
92	14.134	2139	2140	2145	rVB3	1619	1456	0.19%	0.026%
93	14.353	2174	2176	2177	rBV2	990	704	0.09%	0.013%
94	14.499	2198	2200	2205	rBV6	1238	1936	0.25%	0.035%
95	14.749	2239	2241	2245	rVB3	4215	4479	0.58%	0.081%
96	15.487	2359	2362	2366	rBV4	2680	3592	0.46%	0.065%
97	15.810	2412	2415	2419	rBV6	931	1563	0.20%	0.028%
98	15.987	2443	2444	2446	rBV2	1075	865	0.11%	0.016%
99	16.487	2524	2526	2527	rBV2	740	595	0.08%	0.011%
100	16.779	2571	2574	2575	rBV2	674	635	0.08%	0.012%

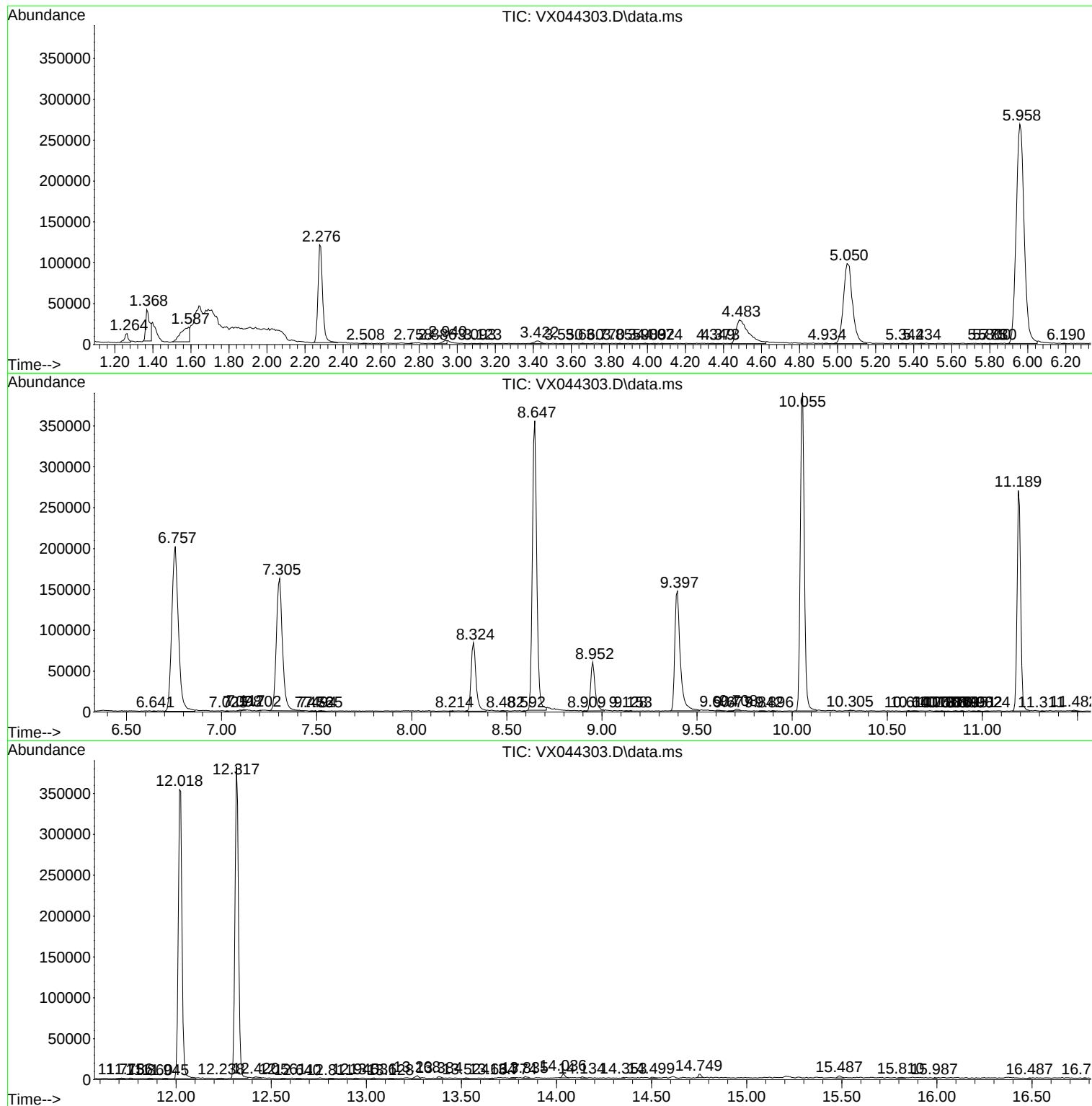
Sum of corrected areas: 5510100

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
Data File : VX044303.D
Acq On : 13 Dec 2024 23:35
Operator : JC/MD
Sample : P5153-09ME
Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28P7ME

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121324\
Data File : VX044303.D
Acq On : 13 Dec 2024 23:35
Operator : JC/MD
Sample : P5153-09ME
Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28P7ME

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\VX121324\
Data File : VX044303.D
Acq On : 13 Dec 2024 23:35
Operator : JC/MD
Sample : P5153-09ME
Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28P7ME

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