

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120524\
 Data File : VX044148.D
 Acq On : 05 Dec 2024 15:30
 Operator : JC/MD
 Sample : P5066-03 100X
 Misc : 6.19g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28M2

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: VX044148.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	rBV	4008	4265	0.42%	0.058%
2	1.368	42	46	60	rBV	123359	148508	14.70%	2.019%
3	1.642	88	91	102	rVB	98432	149145	14.76%	2.027%
4	2.294	192	198	211	rVB	205755	320227	31.70%	4.353%
5	2.703	263	265	267	rBV2	625	522	0.05%	0.007%
6	2.941	297	304	312	rBV5	2934	7549	0.75%	0.103%
7	3.020	316	317	319	rBV	777	659	0.07%	0.009%
8	3.075	324	326	329	rBV3	810	1186	0.12%	0.016%
9	3.105	329	331	334	rVB3	560	535	0.05%	0.007%
10	3.300	361	363	366	rBV2	591	467	0.05%	0.006%
11	3.434	378	385	394	rVB6	2793	7729	0.77%	0.105%
12	3.581	407	409	412	rVB3	634	520	0.05%	0.007%
13	3.678	423	425	427	rVV2	547	568	0.06%	0.008%
14	3.715	430	431	434	rVB2	683	543	0.05%	0.007%
15	3.751	434	437	442	rBV2	935	1415	0.14%	0.019%
16	3.794	442	444	447	rBV4	498	535	0.05%	0.007%
17	3.971	469	473	475	rBV3	578	656	0.06%	0.009%
18	4.148	499	502	504	rBV3	673	641	0.06%	0.009%
19	4.294	523	526	527	rBV3	430	477	0.05%	0.006%
20	4.324	529	531	534	rVB3	719	815	0.08%	0.011%
21	4.361	534	537	538	rBV3	549	631	0.06%	0.009%
22	4.465	544	554	571	rBV	63155	202700	20.07%	2.755%
23	4.958	633	635	639	rBV3	587	714	0.07%	0.010%
24	5.056	639	651	671	rVV	131332	421936	41.77%	5.735%
25	5.471	715	719	722	rBV3	702	1136	0.11%	0.015%
26	5.501	722	724	727	rBV4	647	662	0.07%	0.009%
27	5.538	727	730	731	rBV3	747	788	0.08%	0.011%
28	5.788	769	771	774	rVB2	809	650	0.06%	0.009%
29	5.964	789	800	822	rBV2	348888	1010160	100.00%	13.731%
30	6.281	847	852	853	rBV4	470	679	0.07%	0.009%
31	6.312	855	857	861	rVB4	750	1013	0.10%	0.014%
32	6.373	865	867	873	rVB4	810	1444	0.14%	0.020%
33	6.428	873	876	877	rBV2	766	854	0.08%	0.012%
34	6.525	890	892	897	rVB4	737	512	0.05%	0.007%
35	6.757	921	930	949	rVV	245266	587400	58.15%	7.985%
36	7.056	977	979	981	rBV2	507	601	0.06%	0.008%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120524\
 Data File : VX044148.D
 Acq On : 05 Dec 2024 15:30
 Operator : JC/MD
 Sample : P5066-03 100X
 Misc : 6.19g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28M2

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	7.117	984	989	995	rBV7	2544	5128	0.51%	0.070%
38	7.184	998	1000	1002	rBV2	599	497	0.05%	0.007%
39	7.306	1011	1020	1035	rBV	211886	460389	45.58%	6.258%
40	7.708	1084	1086	1089	rBV2	463	540	0.05%	0.007%
41	8.037	1137	1140	1142	rBV2	685	893	0.09%	0.012%
42	8.324	1181	1187	1202	rBV	129025	220106	21.79%	2.992%
43	8.476	1210	1212	1214	rBV2	752	668	0.07%	0.009%
44	8.647	1233	1240	1255	rBV	467516	757862	75.02%	10.302%
45	8.860	1273	1275	1278	rVB3	574	643	0.06%	0.009%
46	8.952	1285	1290	1305	rVB	91379	139729	13.83%	1.899%
47	9.275	1338	1343	1352	rVB6	5832	10558	1.05%	0.144%
48	9.336	1352	1353	1355	rBV2	767	506	0.05%	0.007%
49	9.384	1356	1361	1375	rBV	278735	435530	43.11%	5.920%
50	9.836	1433	1435	1436	rBV2	710	557	0.06%	0.008%
51	9.890	1443	1444	1448	rBV2	686	774	0.08%	0.011%
52	9.933	1448	1451	1454	rBV3	569	853	0.08%	0.012%
53	9.988	1457	1460	1463	rBV3	605	734	0.07%	0.010%
54	10.055	1465	1471	1482	rBV	468523	681077	67.42%	9.258%
55	10.262	1503	1505	1506	rBV2	781	585	0.06%	0.008%
56	10.354	1518	1520	1525	rVB5	1848	2136	0.21%	0.029%
57	10.476	1538	1540	1541	rBV	621	563	0.06%	0.008%
58	10.585	1550	1558	1561	rBV6	1755	3461	0.34%	0.047%
59	10.750	1583	1585	1587	rBV3	898	819	0.08%	0.011%
60	10.781	1587	1590	1594	rVB4	2468	3190	0.32%	0.043%
61	10.829	1594	1598	1599	rBV3	666	739	0.07%	0.010%
62	10.860	1599	1603	1605	rBV4	2055	3291	0.33%	0.045%
63	10.927	1612	1614	1615	rVB2	784	474	0.05%	0.006%
64	10.945	1615	1617	1618	rBV	1081	838	0.08%	0.011%
65	11.189	1652	1657	1669	rVV	357225	467268	46.26%	6.352%
66	11.335	1680	1681	1686	rVB4	923	1170	0.12%	0.016%
67	11.433	1693	1697	1698	rBV3	1281	1527	0.15%	0.021%
68	11.476	1701	1704	1709	rVV3	6573	8781	0.87%	0.119%
69	11.591	1721	1723	1724	rBV2	809	481	0.05%	0.007%
70	11.719	1739	1744	1747	rBV5	2315	3422	0.34%	0.047%
71	11.756	1747	1750	1755	rVV5	1801	2998	0.30%	0.041%
72	11.975	1784	1786	1788	rBV3	790	744	0.07%	0.010%
73	12.018	1788	1793	1805	rBV	442312	579053	57.32%	7.871%
74	12.238	1827	1829	1834	rBV4	556	678	0.07%	0.009%
75	12.317	1837	1842	1856	rVV	478229	617617	61.14%	8.395%
76	12.427	1856	1860	1863	rVB3	5406	6842	0.68%	0.093%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120524\
 Data File : VX044148.D
 Acq On : 05 Dec 2024 15:30
 Operator : JC/MD
 Sample : P5066-03 100X
 Misc : 6.19g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 14 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 E28M2

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	12.542	1878	1879	1882	rBV3	854	737	0.07%	0.010%
78	12.878	1932	1934	1935	rBV	855	765	0.08%	0.010%
79	12.969	1947	1949	1956	rVB5	1471	1909	0.19%	0.026%
80	13.122	1972	1974	1979	rBV6	807	712	0.07%	0.010%
81	13.207	1985	1988	1994	rVB6	909	1645	0.16%	0.022%
82	13.268	1994	1998	2006	rBV7	7473	13254	1.31%	0.180%
83	13.384	2014	2017	2020	rVB3	2411	2858	0.28%	0.039%
84	13.701	2065	2069	2071	rBV4	908	1457	0.14%	0.020%
85	13.786	2079	2083	2087	rVB4	3251	5554	0.55%	0.075%
86	13.969	2110	2113	2116	rBV3	1081	1163	0.12%	0.016%
87	14.036	2121	2124	2131	rBV3	5601	7796	0.77%	0.106%
88	14.609	2216	2218	2222	rBV4	1359	2228	0.22%	0.030%
89	14.755	2239	2242	2247	rBV5	3582	4838	0.48%	0.066%
90	14.890	2262	2264	2267	rBV3	740	558	0.06%	0.008%
91	14.914	2267	2268	2270	rBV2	618	482	0.05%	0.007%
92	15.249	2321	2323	2325	rBV3	829	676	0.07%	0.009%
93	15.335	2336	2337	2339	rBV2	661	553	0.05%	0.008%
94	15.493	2360	2363	2365	rVB4	1681	1815	0.18%	0.025%
95	15.578	2375	2377	2379	rBV2	721	608	0.06%	0.008%
96	15.615	2381	2383	2387	rVB4	1714	1595	0.16%	0.022%
97	16.078	2457	2459	2460	rBV3	841	628	0.06%	0.009%
98	16.286	2491	2493	2495	rBV3	839	760	0.08%	0.010%
99	16.353	2502	2504	2506	rBV	827	482	0.05%	0.007%
100	16.651	2551	2553	2556	rBV2	900	1099	0.11%	0.015%

Sum of corrected areas: 7356735

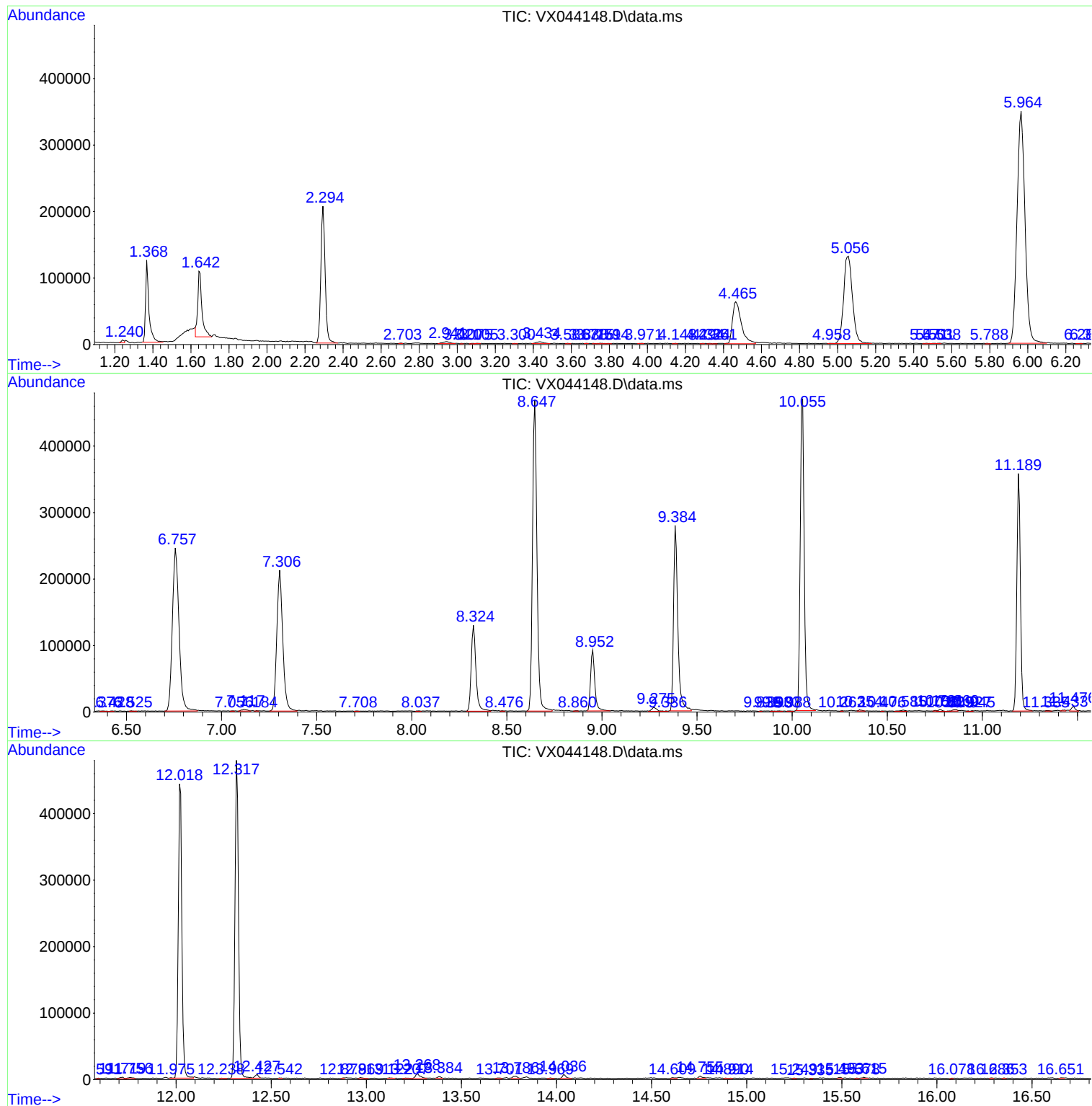
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120524\
Data File : VX044148.D
Acq On : 05 Dec 2024 15:30
Operator : JC/MD
Sample : P5066-03 100X
Misc : 6.19g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28M2

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 : VX044148.D
Acq On : 05 Dec 2024 15:30
Operator : JC/MD
Sample : P5066-03 100X
Misc : 6.19g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28M2

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 : VX044148.D
Acq On : 05 Dec 2024 15:30
Operator : JC/MD
Sample : P5066-03 100X
Misc : 6.19g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 14 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
E28M2

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