

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121123\
 Data File : VX039147.D
 Acq On : 11 Dec 2023 16:31
 Operator : JC/MD
 Sample : 05752-01 100X
 Misc : 4.22g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AS9

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\SFAMXML120523WMA.M
 Title : VOC Analysis

Signal : TIC: VX039147.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.246	23	26	28	rBV	2809	3757	0.34%	0.043%
2	1.368	42	46	55	rBV	130169	133302	12.21%	1.530%
3	1.666	91	95	109	rVB	84418	119779	10.97%	1.374%
4	2.306	194	200	213	rVB	228325	354476	32.46%	4.068%
5	2.788	273	279	285	rVB3	1156	2192	0.20%	0.025%
6	2.947	300	305	310	rBV2	951	1788	0.16%	0.021%
7	3.117	331	333	334	rBV	345	222	0.02%	0.003%
8	3.136	334	336	338	rVB2	256	189	0.02%	0.002%
9	3.251	352	355	356	rBV	339	290	0.03%	0.003%
10	3.611	411	414	416	rBV2	251	316	0.03%	0.004%
11	3.690	425	427	428	rVB2	222	140	0.01%	0.002%
12	3.703	428	429	431	rBV	254	201	0.02%	0.002%
13	3.721	431	432	434	rBV	259	142	0.01%	0.002%
14	3.837	449	451	452	rVV	252	141	0.01%	0.002%
15	3.904	460	462	465	rBV2	380	394	0.04%	0.005%
16	4.074	487	490	492	rVB2	357	362	0.03%	0.004%
17	4.117	494	497	499	rVV2	193	201	0.02%	0.002%
18	4.269	520	522	523	rBV	203	185	0.02%	0.002%
19	4.324	529	531	532	rVB	242	146	0.01%	0.002%
20	4.337	532	533	536	rBV	343	289	0.03%	0.003%
21	4.446	542	551	569	rBV	99290	284946	26.10%	3.270%
22	4.830	612	614	617	rVB3	325	214	0.02%	0.002%
23	5.056	638	651	671	rBV	132286	422362	38.68%	4.846%
24	5.373	702	703	704	rBV	456	187	0.02%	0.002%
25	5.531	728	729	730	rBV	290	167	0.02%	0.002%
26	5.818	774	776	777	rBV	212	156	0.01%	0.002%
27	5.964	788	800	810	rBV2	350332	1091888	100.00%	12.529%
28	6.306	854	856	858	rBV2	263	174	0.02%	0.002%
29	6.324	858	859	863	rVB2	230	199	0.02%	0.002%
30	6.452	877	880	881	rBV2	304	309	0.03%	0.004%
31	6.501	886	888	889	rVB	228	142	0.01%	0.002%
32	6.562	896	898	899	rBV	356	245	0.02%	0.003%
33	6.659	913	914	918	rBV	227	225	0.02%	0.003%
34	6.757	921	930	944	rBV	266504	656097	60.09%	7.529%
35	7.117	983	989	995	rVB3	1837	3425	0.31%	0.039%
36	7.214	1003	1005	1009	rBV2	241	267	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121123\
 Data File : VX039147.D
 Acq On : 11 Dec 2023 16:31
 Operator : JC/MD
 Sample : 05752-01 100X
 Misc : 4.22g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AS9

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\SFAMXML120523WMA.M
 Title : VOC Analysis

37	7.306	1011	1020	1035	rBV	221385	490810	44.95%	5.632%
38	7.757	1092	1094	1095	rVB2	269	196	0.02%	0.002%
39	7.799	1100	1101	1105	rBV2	247	253	0.02%	0.003%
40	7.946	1123	1125	1126	rBV2	266	168	0.02%	0.002%
41	8.324	1181	1187	1200	rBV	163237	270769	24.80%	3.107%
42	8.647	1233	1240	1256	rBV	531497	848525	77.71%	9.737%
43	8.848	1271	1273	1274	rVB2	447	265	0.02%	0.003%
44	8.952	1282	1290	1301	rBV	117106	181004	16.58%	2.077%
45	9.202	1330	1331	1333	rBV	203	165	0.02%	0.002%
46	9.275	1341	1343	1347	rVB	502	364	0.03%	0.004%
47	9.342	1351	1354	1355	rBV	177	178	0.02%	0.002%
48	9.384	1355	1361	1384	rBV	445825	657690	60.23%	7.547%
49	9.695	1409	1412	1419	rVB3	511	986	0.09%	0.011%
50	9.750	1419	1421	1423	rBV	325	250	0.02%	0.003%
51	9.921	1448	1449	1452	rVB	166	146	0.01%	0.002%
52	9.945	1452	1453	1455	rBV	303	223	0.02%	0.003%
53	10.055	1465	1471	1473	rBV	589265	927843	84.98%	10.647%
54	10.293	1508	1510	1511	rVB2	334	221	0.02%	0.003%
55	10.311	1511	1513	1514	rBV	242	195	0.02%	0.002%
56	10.561	1550	1554	1555	rBV	192	161	0.01%	0.002%
57	10.628	1562	1565	1568	rVB2	213	288	0.03%	0.003%
58	10.707	1577	1578	1581	rVB	295	143	0.01%	0.002%
59	10.799	1590	1593	1595	rBV	345	264	0.02%	0.003%
60	10.957	1617	1619	1622	rBV2	183	194	0.02%	0.002%
61	10.988	1622	1624	1628	rBV2	240	329	0.03%	0.004%
62	11.061	1635	1636	1638	rBV	203	140	0.01%	0.002%
63	11.091	1638	1641	1648	rVB2	592	1034	0.09%	0.012%
64	11.189	1652	1657	1670	rVV	418712	530723	48.61%	6.090%
65	11.299	1673	1675	1677	rBV2	394	229	0.02%	0.003%
66	11.372	1684	1687	1691	rVB2	805	941	0.09%	0.011%
67	11.457	1699	1701	1706	rVV3	370	562	0.05%	0.006%
68	11.524	1709	1712	1713	rBV	361	298	0.03%	0.003%
69	11.683	1736	1738	1739	rBV	189	139	0.01%	0.002%
70	11.762	1749	1751	1754	rVB	251	213	0.02%	0.002%
71	11.969	1782	1785	1788	rBV4	4152	5358	0.49%	0.061%
72	12.018	1788	1793	1806	rVB2	613924	906658	83.04%	10.404%
73	12.280	1834	1836	1837	rBV	294	240	0.02%	0.003%
74	12.317	1837	1842	1853	rVV	586076	753065	68.97%	8.641%
75	12.518	1874	1875	1878	rBV	268	194	0.02%	0.002%
76	12.542	1878	1879	1881	rVV2	195	168	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121123\
 Data File : VX039147.D
 Acq On : 11 Dec 2023 16:31
 Operator : JC/MD
 Sample : 05752-01 100X
 Misc : 4.22g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AS9

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\SFAMXML120523WMA.M
 Title : VOC Analysis

77	12.567	1881	1883	1885	rVB2	272	222	0.02%	0.003%
78	12.628	1890	1893	1894	rVV2	242	200	0.02%	0.002%
79	12.750	1911	1913	1917	rVB3	460	636	0.06%	0.007%
80	12.786	1917	1919	1920	rBV2	330	347	0.03%	0.004%
81	12.908	1938	1939	1941	rBV	327	221	0.02%	0.003%
82	13.073	1959	1966	1970	rBV5	1260	2310	0.21%	0.027%
83	13.432	2023	2025	2026	rBV	235	140	0.01%	0.002%
84	13.487	2032	2034	2036	rVB2	302	181	0.02%	0.002%
85	13.591	2046	2051	2059	rVB	22369	30839	2.82%	0.354%
86	13.652	2059	2061	2063	rBV	312	276	0.03%	0.003%
87	13.780	2077	2082	2085	rBV3	284	516	0.05%	0.006%
88	13.810	2085	2087	2090	rVB2	186	160	0.01%	0.002%
89	13.963	2107	2112	2118	rVV	9748	12362	1.13%	0.142%
90	14.060	2125	2128	2129	rBV2	174	157	0.01%	0.002%
91	14.073	2129	2130	2133	rVB	331	224	0.02%	0.003%
92	14.127	2138	2139	2144	rVB2	378	284	0.03%	0.003%
93	14.487	2196	2198	2203	rBV	226	298	0.03%	0.003%
94	14.780	2244	2246	2248	rVB2	296	158	0.01%	0.002%
95	14.890	2262	2264	2266	rBV2	214	192	0.02%	0.002%
96	15.219	2316	2318	2319	rBV2	258	178	0.02%	0.002%
97	15.249	2319	2323	2328	rVV4	1897	2752	0.25%	0.032%
98	15.310	2331	2333	2335	rBV2	304	281	0.03%	0.003%
99	15.932	2433	2435	2437	rBV2	476	412	0.04%	0.005%
100	16.627	2547	2549	2552	rVB2	360	341	0.03%	0.004%

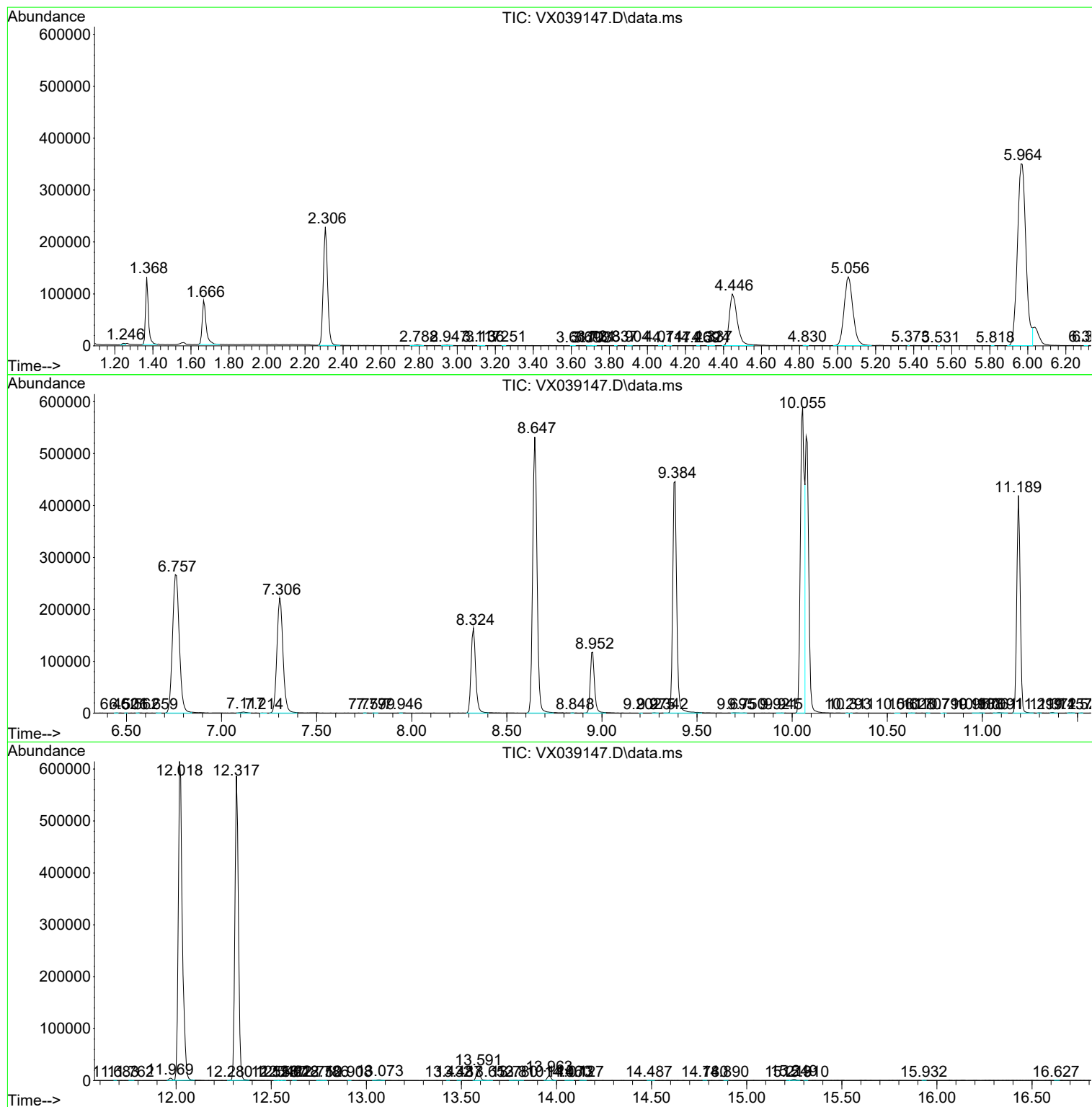
Sum of corrected areas: 8714794

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121123\
Data File : VX039147.D
Acq On : 11 Dec 2023 16:31
Operator : JC/MD
Sample : 05752-01 100X
Misc : 4.22g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AS9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121123\
Data File : VX039147.D
Acq On : 11 Dec 2023 16:31
Operator : JC/MD
Sample : 05752-01 100X
Misc : 4.22g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AS9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.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\VX121123\
Data File : VX039147.D
Acq On : 11 Dec 2023 16:31
Operator : JC/MD
Sample : 05752-01 100X
Misc : 4.22g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AS9

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML120523WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

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