

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039373.D
 Acq On : 19 Dec 2023 21:38
 Operator : JC/MD
 Sample : 05807-04 5X
 Misc : 2.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AX6

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: VX039373.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.367	43	46	56	rBV	89263	103658	13.00%	1.689%
2	1.648	89	92	102	rVB	60243	88284	11.07%	1.439%
3	2.306	193	200	208	rBV	161160	261447	32.78%	4.261%
4	2.508	228	233	235	rBV3	616	952	0.12%	0.016%
5	2.562	238	242	247	rVB4	457	795	0.10%	0.013%
6	2.703	260	265	272	rBV2	3021	5387	0.68%	0.088%
7	2.788	274	279	285	rBV2	3144	6020	0.75%	0.098%
8	2.946	297	305	315	rVV	4083	10056	1.26%	0.164%
9	3.117	331	333	339	rVB2	291	260	0.03%	0.004%
10	3.166	339	341	343	rBV2	235	188	0.02%	0.003%
11	3.318	364	366	368	rVV2	425	447	0.06%	0.007%
12	3.416	379	382	384	rVB	216	194	0.02%	0.003%
13	3.452	384	388	390	rBV2	231	343	0.04%	0.006%
14	3.727	431	433	436	rBV2	157	204	0.03%	0.003%
15	4.050	483	486	488	rBV2	203	229	0.03%	0.004%
16	4.135	499	500	503	rBV2	158	167	0.02%	0.003%
17	4.452	544	552	568	rBV	69406	201022	25.20%	3.276%
18	4.757	601	602	604	rBV	252	195	0.02%	0.003%
19	4.800	607	609	612	rBV2	245	238	0.03%	0.004%
20	5.056	640	651	668	rBV	97227	308217	38.64%	5.023%
21	5.348	697	699	703	rBV2	185	212	0.03%	0.003%
22	5.403	706	708	712	rVB2	318	268	0.03%	0.004%
23	5.964	789	800	824	rBV2	260850	797624	100.00%	12.998%
24	6.367	864	866	870	rBV	154	251	0.03%	0.004%
25	6.757	920	930	947	rBV	190273	465206	58.32%	7.581%
26	7.116	983	989	990	rBV4	989	1641	0.21%	0.027%
27	7.305	1011	1020	1032	rBV2	160935	355940	44.63%	5.800%
28	7.781	1096	1098	1101	rBV2	200	251	0.03%	0.004%
29	7.872	1110	1113	1116	rVB2	250	273	0.03%	0.004%
30	7.952	1124	1126	1128	rVV2	216	193	0.02%	0.003%
31	8.031	1136	1139	1141	rBV2	149	211	0.03%	0.003%
32	8.080	1144	1147	1150	rVV2	136	176	0.02%	0.003%
33	8.324	1181	1187	1204	rVV	101940	171592	21.51%	2.796%
34	8.647	1234	1240	1261	rBV	384834	600802	75.32%	9.791%
35	8.951	1284	1290	1304	rBV	72272	114679	14.38%	1.869%
36	9.073	1308	1310	1311	rVV	364	181	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039373.D
 Acq On : 19 Dec 2023 21:38
 Operator : JC/MD
 Sample : 05807-04 5X
 Misc : 2.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AX6

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\SFAMXLM120523WMA.M
 Title : VOC Analysis

37	9.189	1327	1329	1331	rVB	416	209	0.03%	0.003%
38	9.275	1340	1343	1348	rVB2	609	613	0.08%	0.010%
39	9.384	1356	1361	1376	rBV	335216	484892	60.79%	7.902%
40	9.701	1411	1413	1416	rVB2	289	319	0.04%	0.005%
41	9.738	1416	1419	1421	rBV2	206	188	0.02%	0.003%
42	9.848	1435	1437	1438	rVV2	320	176	0.02%	0.003%
43	9.945	1449	1453	1455	rVB3	238	293	0.04%	0.005%
44	10.055	1465	1471	1472	rBV	428745	544116	68.22%	8.867%
45	10.311	1507	1513	1516	rBV4	772	1248	0.16%	0.020%
46	10.445	1533	1535	1538	rBV2	197	262	0.03%	0.004%
47	10.506	1542	1545	1547	rBV2	189	191	0.02%	0.003%
48	10.665	1565	1571	1574	rBV3	231	478	0.06%	0.008%
49	10.957	1617	1619	1620	rBV2	271	268	0.03%	0.004%
50	11.006	1626	1627	1630	rVB	207	177	0.02%	0.003%
51	11.189	1652	1657	1671	rBV	300254	390364	48.94%	6.361%
52	11.311	1674	1677	1683	rVB3	604	844	0.11%	0.014%
53	11.390	1689	1690	1694	rVB2	208	185	0.02%	0.003%
54	11.451	1697	1700	1704	rBV4	368	540	0.07%	0.009%
55	11.756	1748	1750	1753	rBV2	603	511	0.06%	0.008%
56	11.969	1781	1785	1789	rBV2	4883	6752	0.85%	0.110%
57	12.024	1789	1794	1805	rVB	447454	644945	80.86%	10.510%
58	12.317	1837	1842	1853	rBV	409819	541685	67.91%	8.827%
59	12.585	1883	1886	1889	rBV	133	192	0.02%	0.003%
60	12.731	1908	1910	1911	rBV	237	184	0.02%	0.003%
61	12.762	1911	1915	1925	rVB2	1632	2509	0.31%	0.041%
62	12.932	1940	1943	1948	rBV2	238	353	0.04%	0.006%
63	12.993	1951	1953	1955	rBV2	229	180	0.02%	0.003%
64	13.121	1970	1974	1978	rBV2	458	611	0.08%	0.010%
65	13.335	2003	2009	2010	rBV2	268	385	0.05%	0.006%
66	13.390	2014	2018	2019	rBV2	173	165	0.02%	0.003%
67	13.451	2025	2028	2031	rBV	227	268	0.03%	0.004%
68	13.506	2034	2037	2039	rBV2	195	193	0.02%	0.003%
69	13.536	2039	2042	2045	rBV	306	346	0.04%	0.006%
70	13.597	2047	2052	2054	rBV2	1126	1350	0.17%	0.022%
71	13.749	2074	2077	2079	rBV2	217	309	0.04%	0.005%
72	13.780	2079	2082	2085	rBV2	523	658	0.08%	0.011%
73	13.890	2095	2100	2102	rBV2	241	384	0.05%	0.006%
74	13.908	2102	2103	2106	rVV2	345	275	0.03%	0.004%
75	13.944	2106	2109	2110	rVV2	212	189	0.02%	0.003%
76	13.963	2110	2112	2117	rVV2	478	726	0.09%	0.012%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039373.D
 Acq On : 19 Dec 2023 21:38
 Operator : JC/MD
 Sample : 05807-04 5X
 Misc : 2.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 33 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AX6

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\SFAMXLM120523WMA.M
 Title : VOC Analysis

77	14.048	2123	2126	2128	rBV	212	208	0.03%	0.003%
78	14.133	2135	2140	2144	rVB	2198	3284	0.41%	0.054%
79	14.207	2149	2152	2153	rBV2	212	221	0.03%	0.004%
80	14.255	2157	2160	2165	rBV2	189	309	0.04%	0.005%
81	14.341	2172	2174	2179	rBV	235	383	0.05%	0.006%
82	14.390	2179	2182	2184	rVV	254	241	0.03%	0.004%
83	14.499	2198	2200	2201	rBV2	201	185	0.02%	0.003%
84	14.542	2205	2207	2208	rVV2	384	223	0.03%	0.004%
85	14.597	2212	2216	2217	rBV3	227	234	0.03%	0.004%
86	14.646	2221	2224	2226	rBV2	198	203	0.03%	0.003%
87	14.749	2239	2241	2244	rBV2	297	337	0.04%	0.005%
88	14.822	2251	2253	2254	rBV	325	185	0.02%	0.003%
89	14.841	2254	2256	2259	rBV3	240	288	0.04%	0.005%
90	14.914	2267	2268	2271	rVB2	353	235	0.03%	0.004%
91	14.950	2272	2274	2277	rBV3	297	335	0.04%	0.005%
92	15.011	2283	2284	2287	rBV	278	225	0.03%	0.004%
93	15.395	2341	2347	2348	rBV3	602	970	0.12%	0.016%
94	15.530	2367	2369	2372	rVB2	344	256	0.03%	0.004%
95	15.859	2421	2423	2426	rVB3	396	405	0.05%	0.007%
96	15.883	2426	2427	2430	rBV	491	343	0.04%	0.006%
97	15.920	2430	2433	2434	rVB2	316	281	0.04%	0.005%
98	15.950	2436	2438	2439	rBV	309	203	0.03%	0.003%
99	16.078	2457	2459	2462	rVB	315	286	0.04%	0.005%
100	16.139	2467	2469	2472	rBV2	248	286	0.04%	0.005%

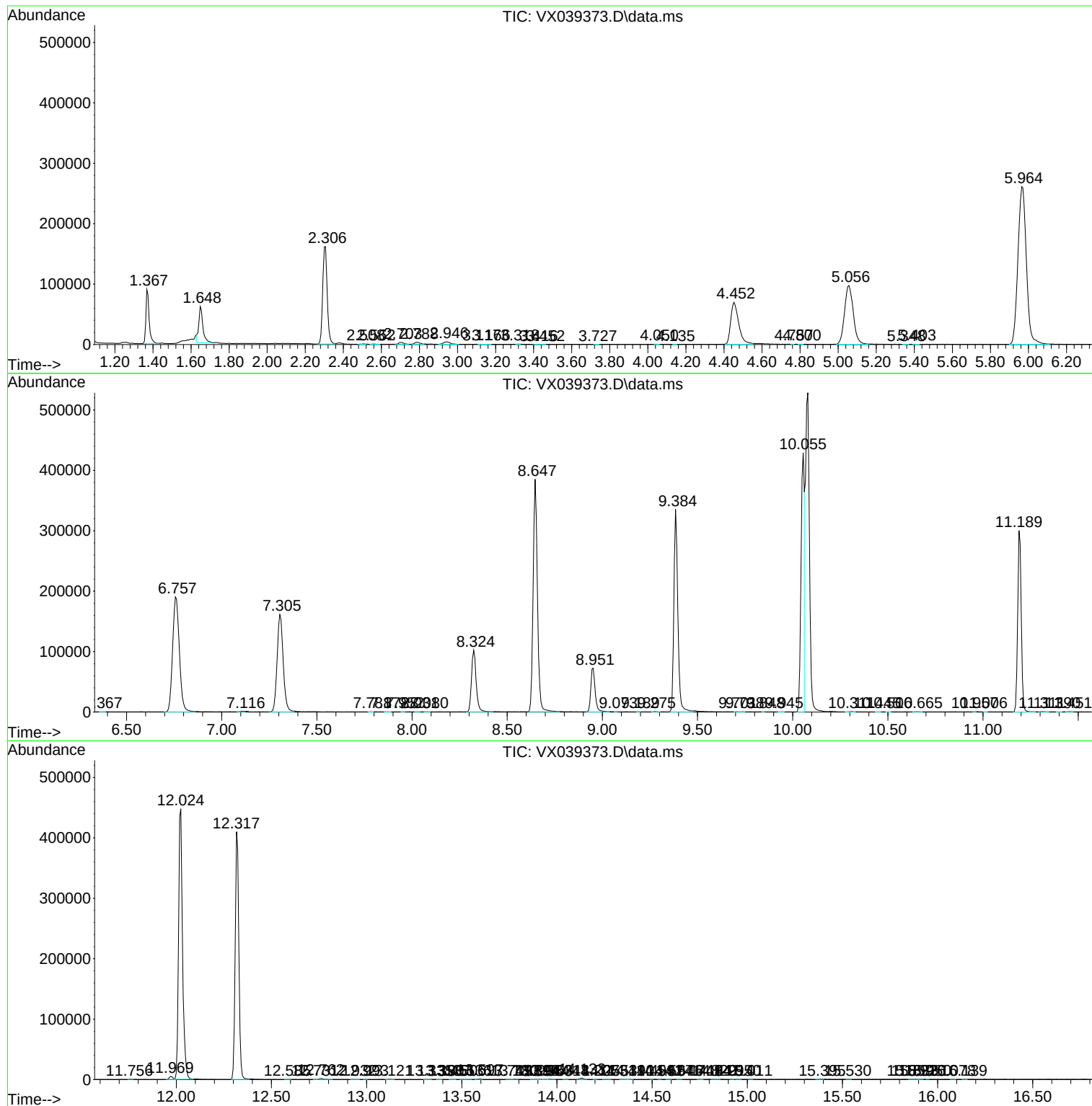
Sum of corrected areas: 6136462

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
Data File : VX039373.D
Acq On : 19 Dec 2023 21:38
Operator : JC/MD
Sample : 05807-04 5X
Misc : 2.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AX6

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\VX121923\
Data File : VX039373.D
Acq On : 19 Dec 2023 21:38
Operator : JC/MD
Sample : 05807-04 5X
Misc : 2.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AX6

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\VX121923\
Data File : VX039373.D
Acq On : 19 Dec 2023 21:38
Operator : JC/MD
Sample : 05807-04 5X
Misc : 2.46g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 33 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AX6

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

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