

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
 Data File : VX039397.D
 Acq On : 20 Dec 2023 13:34
 Operator : JC/MD
 Sample : 05835-16 5X
 Misc : 4.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AR3

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: VX039397.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.368	43	46	58	rBV	51799	59036	9.40%	1.128%
2	1.648	89	92	103	rVB	41828	63401	10.10%	1.212%
3	2.300	194	199	209	rBV	95056	150101	23.90%	2.869%
4	2.502	230	232	233	rBV2	351	235	0.04%	0.004%
5	2.630	251	253	256	rBV2	267	253	0.04%	0.005%
6	2.709	260	266	270	rBV2	1384	2458	0.39%	0.047%
7	2.794	274	280	284	rBV3	2127	4266	0.68%	0.082%
8	2.941	297	304	313	rBV	9391	22781	3.63%	0.435%
9	3.221	348	350	352	rBV	228	227	0.04%	0.004%
10	3.434	383	385	388	rVV	271	260	0.04%	0.005%
11	4.453	541	552	568	rBV	66036	193159	30.76%	3.692%
12	5.056	639	651	670	rBV	79156	252516	40.21%	4.827%
13	5.337	694	697	699	rBV2	198	217	0.03%	0.004%
14	5.379	703	704	707	rBV2	222	230	0.04%	0.004%
15	5.538	728	730	731	rBV2	217	208	0.03%	0.004%
16	5.867	781	784	786	rVB2	198	238	0.04%	0.005%
17	5.964	788	800	817	rBV2	205587	628041	100.00%	12.005%
18	6.245	845	846	848	rBV	301	200	0.03%	0.004%
19	6.269	848	850	852	rBV	246	240	0.04%	0.005%
20	6.611	902	906	907	rBV2	183	252	0.04%	0.005%
21	6.629	907	909	914	rVB2	238	270	0.04%	0.005%
22	6.757	920	930	944	rBV	176993	426718	67.94%	8.157%
23	7.111	983	988	997	rVV5	1221	2639	0.42%	0.050%
24	7.196	1000	1002	1007	rVB2	196	253	0.04%	0.005%
25	7.306	1012	1020	1035	rBV	130184	300722	47.88%	5.748%
26	7.714	1084	1087	1088	rBV	336	280	0.04%	0.005%
27	7.824	1104	1105	1108	rVB	308	212	0.03%	0.004%
28	8.196	1164	1166	1169	rBV	294	219	0.03%	0.004%
29	8.324	1181	1187	1195	rBV	84109	138226	22.01%	2.642%
30	8.562	1223	1226	1227	rBV	301	226	0.04%	0.004%
31	8.586	1227	1230	1234	rVB2	276	300	0.05%	0.006%
32	8.647	1234	1240	1260	rBV	264510	425626	67.77%	8.136%
33	8.854	1272	1274	1276	rVB2	277	213	0.03%	0.004%
34	8.952	1284	1290	1308	rBV	60959	95423	15.19%	1.824%
35	9.074	1308	1310	1313	rVB3	241	282	0.04%	0.005%
36	9.275	1339	1343	1349	rVB3	600	1006	0.16%	0.019%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
 Data File : VX039397.D
 Acq On : 20 Dec 2023 13:34
 Operator : JC/MD
 Sample : 05835-16 5X
 Misc : 4.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AR3

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	9.385	1356	1361	1375	rBV	320721	460123	73.26%	8.795%
38	9.628	1399	1401	1407	rVB3	284	510	0.08%	0.010%
39	9.702	1409	1413	1418	rBV5	850	1616	0.26%	0.031%
40	9.799	1427	1429	1433	rBV2	224	331	0.05%	0.006%
41	9.945	1452	1453	1456	rVB2	316	241	0.04%	0.005%
42	10.055	1465	1471	1473	rBV	397422	609702	97.08%	11.654%
43	10.195	1492	1494	1499	rVB2	849	976	0.16%	0.019%
44	10.311	1509	1513	1516	rVV4	372	617	0.10%	0.012%
45	10.781	1588	1590	1595	rVB	209	253	0.04%	0.005%
46	10.836	1597	1599	1603	rVB2	241	266	0.04%	0.005%
47	10.964	1618	1620	1622	rVV2	318	270	0.04%	0.005%
48	11.104	1641	1643	1646	rVB2	286	287	0.05%	0.005%
49	11.189	1652	1657	1666	rBV	274270	355206	56.56%	6.790%
50	11.305	1674	1676	1681	rBV4	338	582	0.09%	0.011%
51	11.366	1681	1686	1691	rVV2	12820	16979	2.70%	0.325%
52	11.457	1698	1701	1708	rVB4	3659	4516	0.72%	0.086%
53	11.665	1733	1735	1740	rBV2	160	198	0.03%	0.004%
54	11.750	1746	1749	1750	rBV	168	194	0.03%	0.004%
55	11.927	1777	1778	1781	rVB	304	193	0.03%	0.004%
56	11.969	1781	1785	1788	rBV2	1139	1374	0.22%	0.026%
57	12.018	1788	1793	1806	rBV	408451	552544	87.98%	10.562%
58	12.171	1817	1818	1821	rVB3	286	262	0.04%	0.005%
59	12.317	1837	1842	1854	rBV	320174	415820	66.21%	7.948%
60	12.475	1866	1868	1869	rBV	222	222	0.04%	0.004%
61	12.512	1872	1874	1876	rVB2	268	218	0.03%	0.004%
62	12.640	1892	1895	1898	rBV2	231	332	0.05%	0.006%
63	12.762	1910	1915	1919	rBV	2364	3276	0.52%	0.063%
64	12.890	1932	1936	1937	rBV2	339	295	0.05%	0.006%
65	12.908	1937	1939	1942	rBV	212	230	0.04%	0.004%
66	13.067	1961	1965	1970	rVV	6324	9290	1.48%	0.178%
67	13.110	1970	1972	1973	rVV	284	200	0.03%	0.004%
68	13.286	2000	2001	2005	rVB3	383	383	0.06%	0.007%
69	13.390	2015	2018	2019	rBV3	449	540	0.09%	0.010%
70	13.512	2037	2038	2041	rVB2	431	265	0.04%	0.005%
71	13.585	2048	2050	2056	rVB4	525	852	0.14%	0.016%
72	13.701	2067	2069	2072	rVB3	565	430	0.07%	0.008%
73	13.731	2072	2074	2078	rVB3	443	457	0.07%	0.009%
74	13.792	2080	2084	2088	rVB3	875	1469	0.23%	0.028%
75	13.841	2088	2092	2097	rVB6	924	1426	0.23%	0.027%
76	13.945	2107	2109	2110	rBV2	214	202	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
 Data File : VX039397.D
 Acq On : 20 Dec 2023 13:34
 Operator : JC/MD
 Sample : 05835-16 5X
 Misc : 4.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AR3

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	14.128	2135	2139	2144	rVB	4644	5973	0.95%	0.114%
78	14.164	2144	2145	2146	rBV	451	249	0.04%	0.005%
79	14.219	2151	2154	2157	rVB2	474	497	0.08%	0.010%
80	14.250	2157	2159	2160	rBV	350	253	0.04%	0.005%
81	14.329	2171	2172	2173	rBV	339	231	0.04%	0.004%
82	14.420	2182	2187	2190	rBV6	469	897	0.14%	0.017%
83	14.609	2216	2218	2222	rVB2	878	822	0.13%	0.016%
84	14.676	2227	2229	2230	rBV2	402	206	0.03%	0.004%
85	14.749	2240	2241	2244	rBV2	631	376	0.06%	0.007%
86	14.890	2262	2264	2265	rVB2	367	212	0.03%	0.004%
87	14.920	2265	2269	2270	rVB3	517	507	0.08%	0.010%
88	14.951	2270	2274	2275	rBV3	522	694	0.11%	0.013%
89	15.237	2319	2321	2324	rBV	356	300	0.05%	0.006%
90	15.603	2379	2381	2382	rBV2	343	327	0.05%	0.006%
91	15.701	2395	2397	2398	rBV	359	239	0.04%	0.005%
92	15.847	2419	2421	2422	rBV2	557	343	0.05%	0.007%
93	15.883	2426	2427	2429	rVB	504	250	0.04%	0.005%
94	16.005	2442	2447	2452	rBV6	1021	2070	0.33%	0.040%
95	16.213	2479	2481	2483	rBV	429	359	0.06%	0.007%
96	16.255	2486	2488	2490	rBV	499	395	0.06%	0.008%
97	16.475	2523	2524	2528	rBV3	483	530	0.08%	0.010%
98	16.554	2534	2537	2538	rBV	634	604	0.10%	0.012%
99	16.572	2538	2540	2542	rBV3	584	647	0.10%	0.012%
100	16.767	2570	2572	2574	rBV3	586	451	0.07%	0.009%

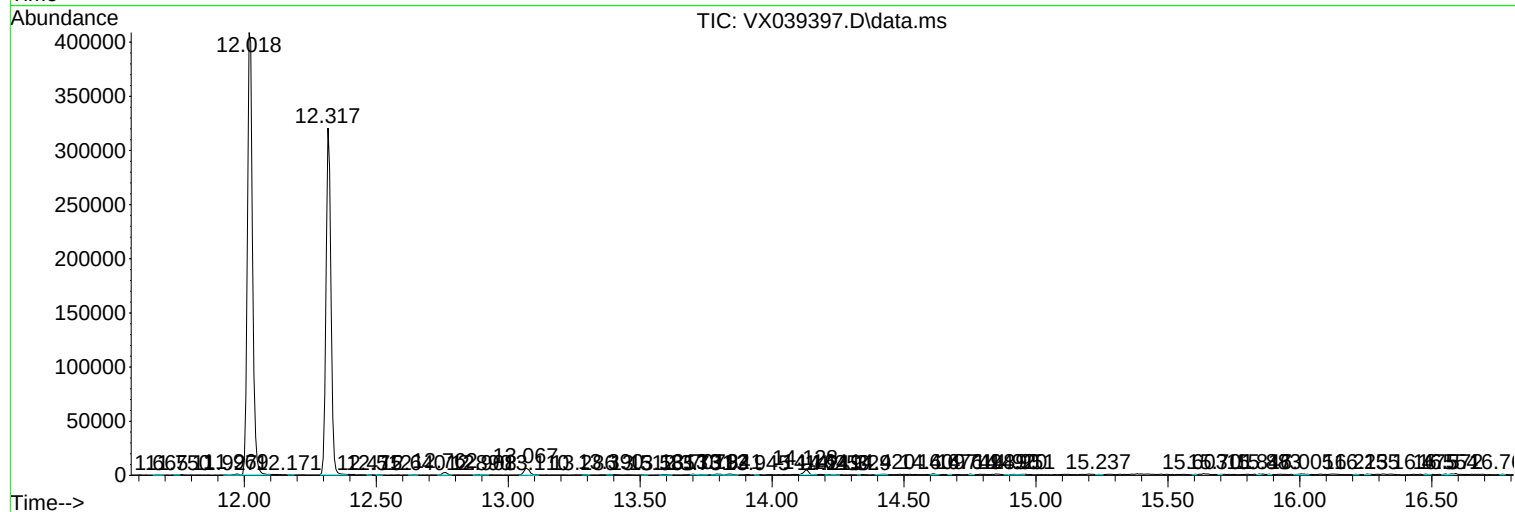
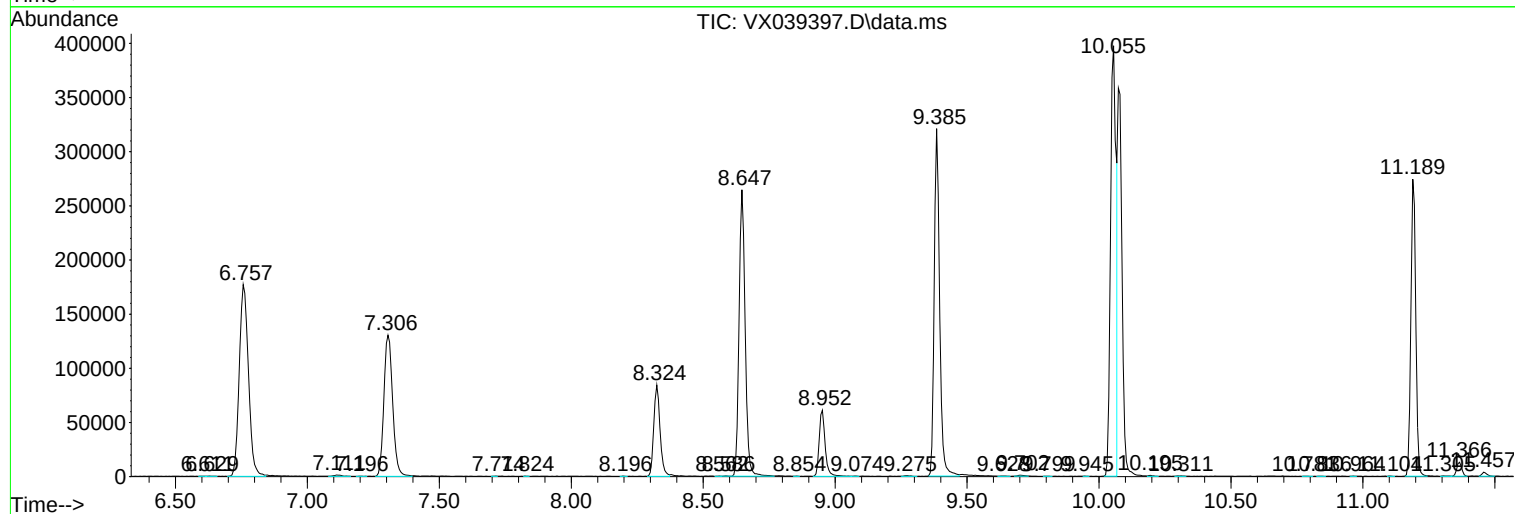
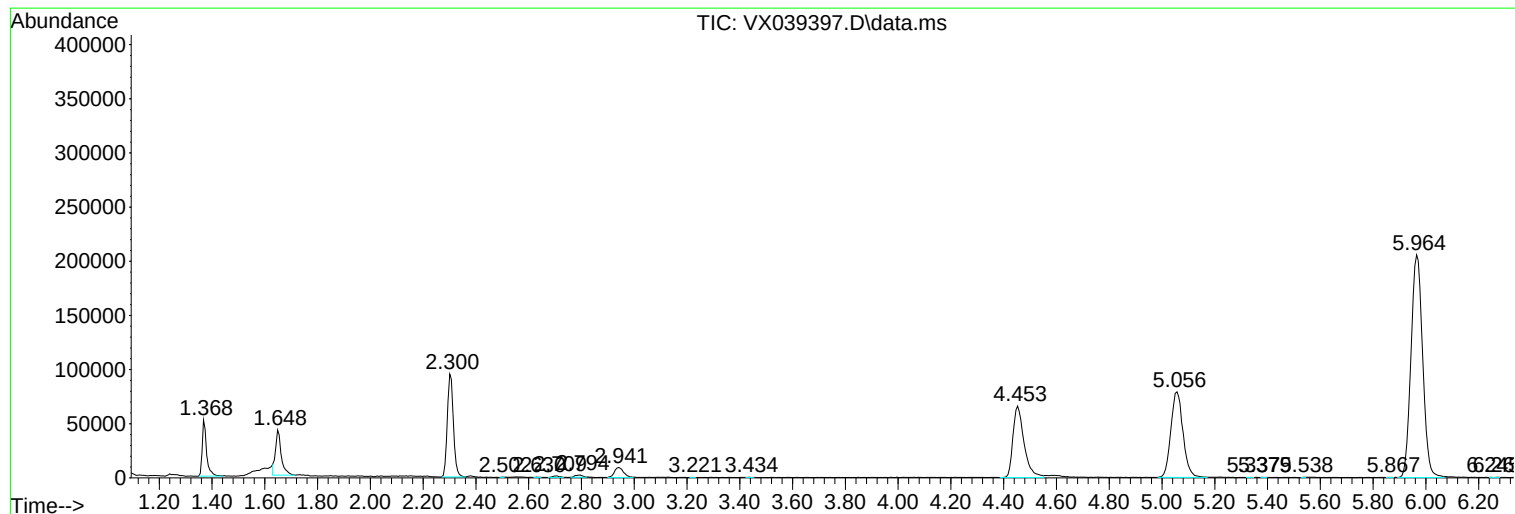
Sum of corrected areas: 5231513

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
Data File : VX039397.D
Acq On : 20 Dec 2023 13:34
Operator : JC/MD
Sample : 05835-16 5X
Misc : 4.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AR3

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM120523WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX122023\
Data File : VX039397.D
Acq On : 20 Dec 2023 13:34
Operator : JC/MD
Sample : 05835-16 5X
Misc : 4.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AR3

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\VX122023\
Data File : VX039397.D
Acq On : 20 Dec 2023 13:34
Operator : JC/MD
Sample : 05835-16 5X
Misc : 4.62g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 13 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AR3

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
------------------	----	---------	-------	----------	---	----	------	------