

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039358.D
 Acq On : 19 Dec 2023 15:56
 Operator : JC/MD
 Sample : 05834-05ME
 Misc : 3.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGQZ8ME

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: VX039358.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.374	43	47	63	rVB	66605	122021	13.75%	1.735%
2	1.569	73	79	81	rBV4	4858	10147	1.14%	0.144%
3	1.648	89	92	98	rBV	22041	37881	4.27%	0.539%
4	2.288	191	197	209	rBV	160206	283351	31.92%	4.029%
5	2.550	239	240	243	rVB2	491	406	0.05%	0.006%
6	2.611	248	250	253	rBV2	401	456	0.05%	0.006%
7	2.788	274	279	285	rVB5	1957	4216	0.47%	0.060%
8	2.934	298	303	311	rBV	4316	10472	1.18%	0.149%
9	3.184	341	344	347	rVB	254	288	0.03%	0.004%
10	3.349	369	371	372	rVV2	308	211	0.02%	0.003%
11	3.434	381	385	391	rVV2	1008	1795	0.20%	0.026%
12	3.483	391	393	396	rVV2	405	314	0.04%	0.004%
13	3.532	399	401	403	rVB2	280	220	0.02%	0.003%
14	3.556	403	405	407	rBV2	230	223	0.03%	0.003%
15	3.757	436	438	441	rBV2	182	226	0.03%	0.003%
16	3.953	465	470	471	rBV	193	208	0.02%	0.003%
17	4.020	477	481	483	rBV2	184	258	0.03%	0.004%
18	4.142	499	501	505	rVB	374	331	0.04%	0.005%
19	4.361	536	537	540	rBV	223	257	0.03%	0.004%
20	4.483	547	557	593	rBV2	38315	204681	23.06%	2.911%
21	4.794	599	608	614	rVB6	1573	4562	0.51%	0.065%
22	4.958	633	635	638	rVB3	269	214	0.02%	0.003%
23	5.062	639	652	671	rVV	98635	330527	37.24%	4.700%
24	5.367	700	702	706	rVB2	276	289	0.03%	0.004%
25	5.446	713	715	717	rBV2	230	225	0.03%	0.003%
26	5.562	732	734	738	rVB2	269	329	0.04%	0.005%
27	5.806	771	774	777	rBV2	229	339	0.04%	0.005%
28	5.964	788	800	823	rBV2	295445	880106	99.15%	12.515%
29	6.220	840	842	848	rVB3	232	336	0.04%	0.005%
30	6.373	860	867	872	rBV7	1006	2943	0.33%	0.042%
31	6.464	880	882	887	rVB3	202	259	0.03%	0.004%
32	6.513	887	890	893	rBV2	188	276	0.03%	0.004%
33	6.574	898	900	903	rVB2	187	209	0.02%	0.003%
34	6.757	921	930	948	rBV	199693	508583	57.29%	7.232%
35	7.117	983	989	998	rBV8	1618	4978	0.56%	0.071%
36	7.306	1012	1020	1036	rVB	166841	385247	43.40%	5.478%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039358.D
 Acq On : 19 Dec 2023 15:56
 Operator : JC/MD
 Sample : 05834-05ME
 Misc : 3.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGQZ8ME

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	7.720	1084	1088	1092	rVB2	250	459	0.05%	0.007%
38	7.964	1125	1128	1129	rBV2	386	462	0.05%	0.007%
39	8.080	1145	1147	1150	rVB2	302	291	0.03%	0.004%
40	8.208	1165	1168	1172	rVB2	140	214	0.02%	0.003%
41	8.324	1181	1187	1204	rBV	100514	187275	21.10%	2.663%
42	8.598	1228	1232	1233	rBV2	331	330	0.04%	0.005%
43	8.647	1233	1240	1256	rBV	417107	672561	75.77%	9.564%
44	8.952	1285	1290	1307	rBV	72799	123822	13.95%	1.761%
45	9.275	1337	1343	1349	rBV4	4929	8054	0.91%	0.115%
46	9.397	1357	1363	1379	rBV	237419	465899	52.49%	6.625%
47	9.647	1402	1404	1407	rBV4	448	373	0.04%	0.005%
48	9.714	1412	1415	1420	rBV2	1179	1377	0.16%	0.020%
49	9.909	1444	1447	1451	rBV2	274	385	0.04%	0.005%
50	10.055	1465	1471	1486	rBV2	420985	820962	92.49%	11.674%
51	10.293	1508	1510	1511	rBV	507	352	0.04%	0.005%
52	10.421	1529	1531	1533	rBV	221	211	0.02%	0.003%
53	10.451	1534	1536	1539	rVV2	241	253	0.03%	0.004%
54	10.518	1545	1547	1548	rVB	389	231	0.03%	0.003%
55	10.610	1557	1562	1565	rBV2	183	294	0.03%	0.004%
56	10.653	1565	1569	1571	rBV2	575	683	0.08%	0.010%
57	10.744	1581	1584	1587	rVB	223	248	0.03%	0.004%
58	10.963	1615	1620	1621	rBV2	363	450	0.05%	0.006%
59	11.098	1639	1642	1646	rBV3	512	555	0.06%	0.008%
60	11.195	1652	1658	1671	rBV	287789	382708	43.11%	5.442%
61	11.335	1680	1681	1684	rVB2	310	239	0.03%	0.003%
62	11.372	1684	1687	1689	rBV	278	319	0.04%	0.005%
63	11.451	1696	1700	1702	rBV3	504	540	0.06%	0.008%
64	11.683	1736	1738	1741	rBV3	285	275	0.03%	0.004%
65	11.811	1756	1759	1762	rBV2	234	282	0.03%	0.004%
66	11.969	1780	1785	1789	rBV	11963	16576	1.87%	0.236%
67	12.024	1789	1794	1806	rVB2	505339	887661	100.00%	12.622%
68	12.225	1825	1827	1829	rBV	328	221	0.02%	0.003%
69	12.323	1837	1843	1853	rBV	430749	586377	66.06%	8.338%
70	12.512	1871	1874	1875	rBV2	261	267	0.03%	0.004%
71	12.634	1892	1894	1898	rVB2	359	361	0.04%	0.005%
72	12.707	1905	1906	1911	rVV2	296	340	0.04%	0.005%
73	12.762	1911	1915	1919	rVV	1776	2275	0.26%	0.032%
74	12.823	1922	1925	1927	rVV2	226	288	0.03%	0.004%
75	12.847	1927	1929	1932	rVV2	209	216	0.02%	0.003%
76	12.951	1944	1946	1947	rVB	355	218	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
 Data File : VX039358.D
 Acq On : 19 Dec 2023 15:56
 Operator : JC/MD
 Sample : 05834-05ME
 Misc : 3.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 BGQZ8ME

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	12.969	1947	1949	1952	rBV2	171	240	0.03%	0.003%
78	13.061	1960	1964	1970	rVV4	3047	5200	0.59%	0.074%
79	13.109	1970	1972	1977	rVV3	604	912	0.10%	0.013%
80	13.591	2046	2051	2059	rVB2	16198	22390	2.52%	0.318%
81	13.707	2066	2070	2071	rBV2	272	217	0.02%	0.003%
82	13.780	2080	2082	2087	rBV2	424	603	0.07%	0.009%
83	13.847	2090	2093	2094	rBV2	358	308	0.03%	0.004%
84	13.963	2108	2112	2117	rBV	11268	14661	1.65%	0.208%
85	14.042	2123	2125	2127	rBV2	266	251	0.03%	0.004%
86	14.079	2127	2131	2135	rVV2	274	462	0.05%	0.007%
87	14.128	2135	2139	2143	rVV	2788	3631	0.41%	0.052%
88	14.262	2159	2161	2164	rBV2	164	215	0.02%	0.003%
89	14.481	2191	2197	2200	rBV3	294	546	0.06%	0.008%
90	14.603	2215	2217	2218	rBV	273	214	0.02%	0.003%
91	14.627	2219	2221	2224	rVV2	702	678	0.08%	0.010%
92	14.768	2240	2244	2251	rBV5	1408	2411	0.27%	0.034%
93	15.249	2319	2323	2328	rBV2	7291	9470	1.07%	0.135%
94	15.444	2354	2355	2357	rBV2	363	224	0.03%	0.003%
95	15.804	2411	2414	2415	rBV2	285	278	0.03%	0.004%
96	15.969	2439	2441	2442	rBV2	279	224	0.03%	0.003%
97	16.334	2500	2501	2504	rVB	326	225	0.03%	0.003%
98	16.359	2504	2505	2507	rBV2	382	249	0.03%	0.004%
99	16.505	2525	2529	2536	rVB6	4255	6234	0.70%	0.089%
100	16.743	2565	2568	2570	rBV2	280	324	0.04%	0.005%

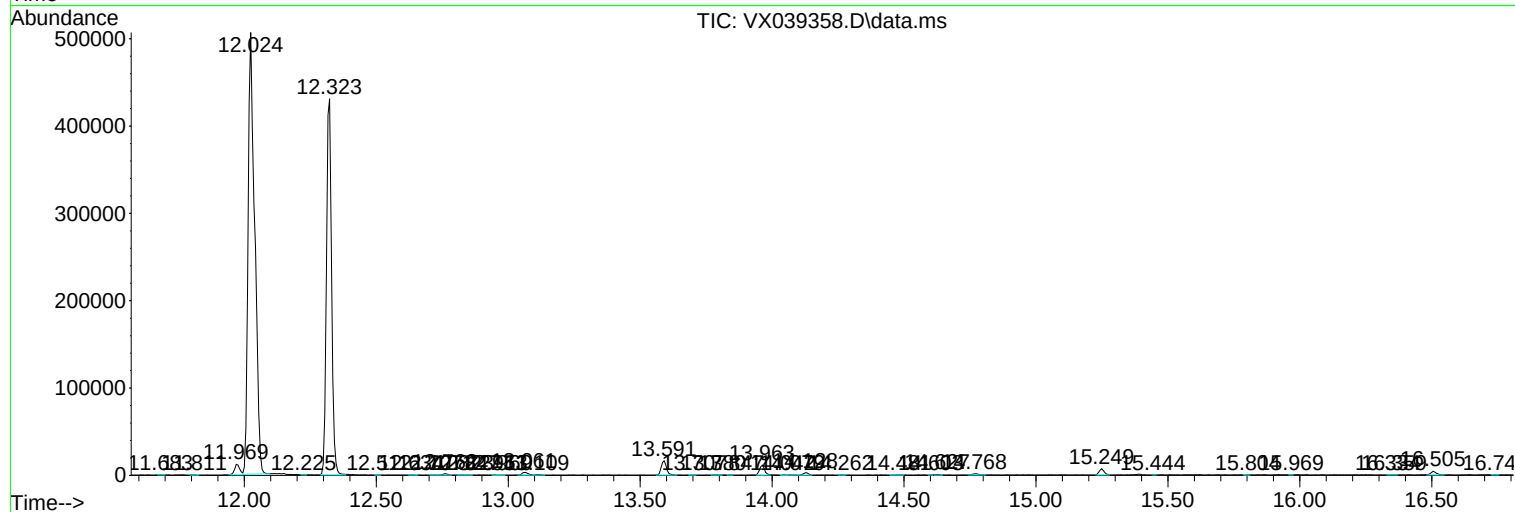
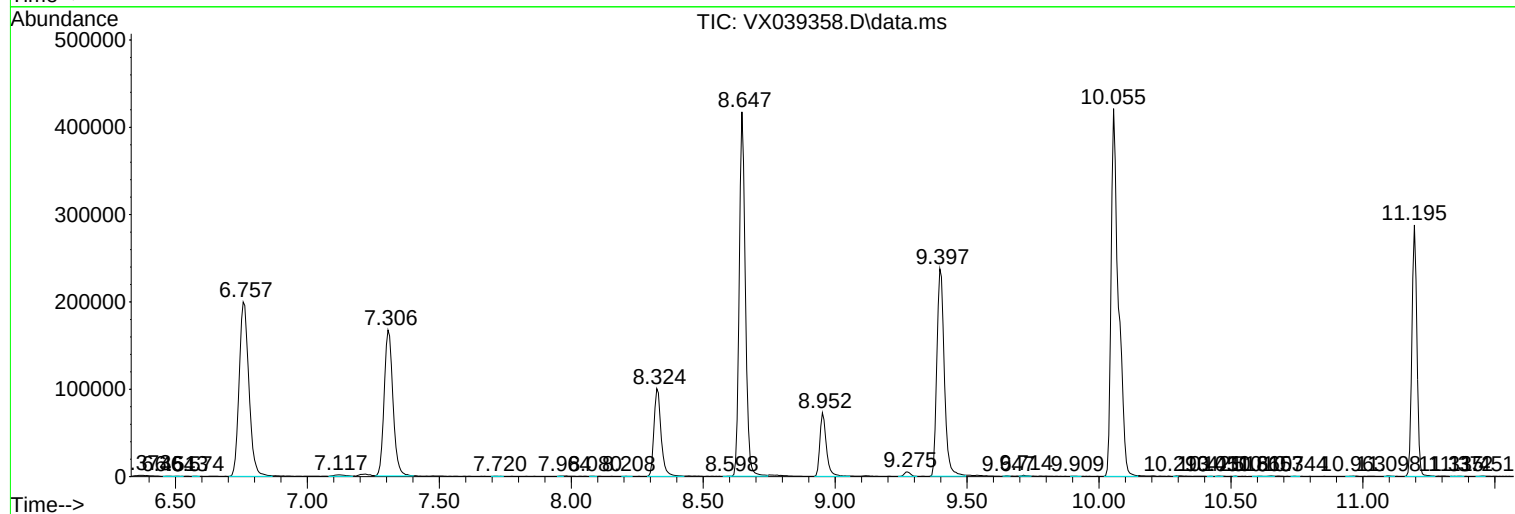
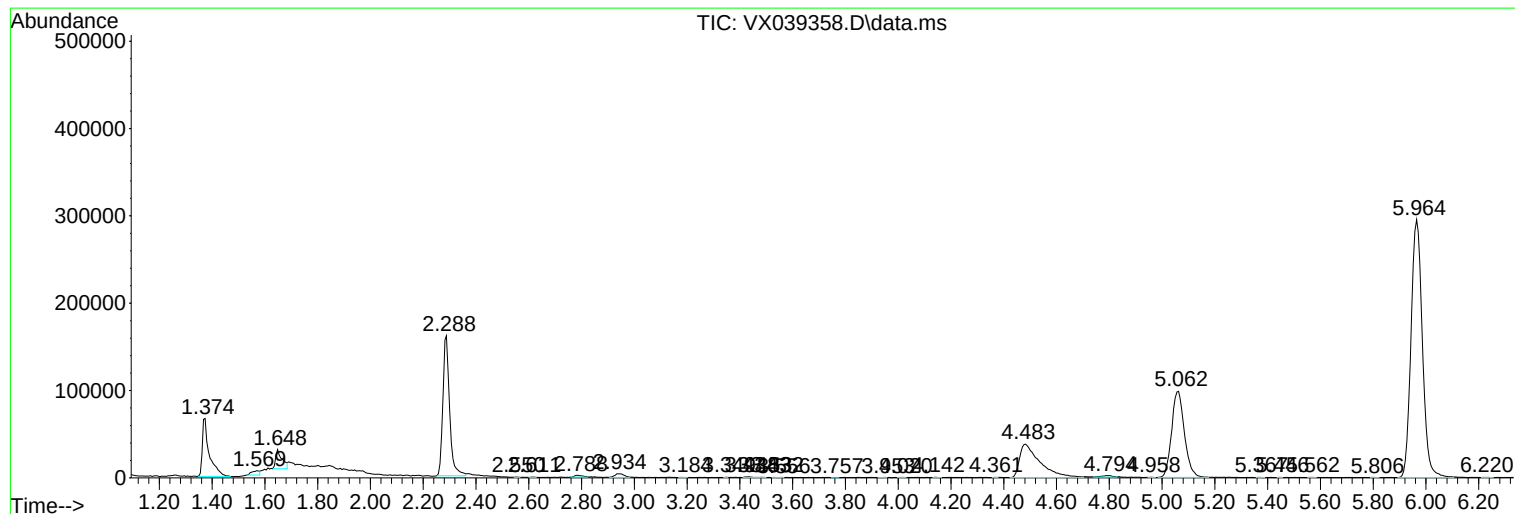
Sum of corrected areas: 7032455

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121923\
Data File : VX039358.D
Acq On : 19 Dec 2023 15:56
Operator : JC/MD
Sample : 05834-05ME
Misc : 3.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGQZ8ME

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\VX121923\
Data File : VX039358.D
Acq On : 19 Dec 2023 15:56
Operator : JC/MD
Sample : 05834-05ME
Misc : 3.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGQZ8ME

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 : VX039358.D
Acq On : 19 Dec 2023 15:56
Operator : JC/MD
Sample : 05834-05ME
Misc : 3.13g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 18 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
BGQZ8ME

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