

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121123\
 Data File : VX039143.D
 Acq On : 11 Dec 2023 14:59
 Operator : JC/MD
 Sample : 05646-16DL 400X
 Misc : 2.63g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AS3DL

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: VX039143.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	42	46	57	rVB	139303	144160	7.40%	1.226%
2	1.666	91	95	108	rVB	90362	130600	6.71%	1.111%
3	2.306	194	200	216	rVB	242234	381244	19.57%	3.242%
4	2.788	277	279	283	rVB	1125	1068	0.05%	0.009%
5	3.148	337	338	340	rVB	403	240	0.01%	0.002%
6	3.885	458	459	462	rVB2	195	157	0.01%	0.001%
7	4.081	489	491	494	rVB2	217	212	0.01%	0.002%
8	4.306	526	528	531	rVB2	286	322	0.02%	0.003%
9	4.446	543	551	568	rBV	104573	298752	15.34%	2.540%
10	4.965	634	636	639	rVB	382	195	0.01%	0.002%
11	5.056	639	651	668	rBV	144350	453762	23.30%	3.858%
12	5.397	705	707	710	rVB2	606	645	0.03%	0.005%
13	5.623	740	744	745	rBV2	199	234	0.01%	0.002%
14	5.641	745	747	750	rVB2	241	279	0.01%	0.002%
15	5.684	750	754	756	rBV2	260	274	0.01%	0.002%
16	5.727	759	761	763	rVB	225	147	0.01%	0.001%
17	5.818	775	776	780	rBV2	172	210	0.01%	0.002%
18	5.970	789	801	817	rBV2	376186	1148102	58.95%	9.763%
19	6.361	861	865	866	rBV2	247	344	0.02%	0.003%
20	6.409	872	873	877	rBV	261	286	0.01%	0.002%
21	6.452	877	880	883	rVV2	256	351	0.02%	0.003%
22	6.550	891	896	899	rVB2	228	405	0.02%	0.003%
23	6.586	901	902	904	rBV2	200	148	0.01%	0.001%
24	6.641	909	911	913	rVB	339	187	0.01%	0.002%
25	6.757	921	930	947	rBV	287335	698704	35.87%	5.941%
26	7.110	984	988	995	rVB4	1675	3413	0.18%	0.029%
27	7.306	1011	1020	1034	rBV	233444	523085	26.86%	4.448%
28	7.458	1044	1045	1046	rBV	352	200	0.01%	0.002%
29	7.708	1084	1086	1087	rBV	266	150	0.01%	0.001%
30	7.775	1095	1097	1099	rBV2	252	297	0.02%	0.003%
31	7.860	1110	1111	1112	rBV	331	147	0.01%	0.001%
32	8.037	1138	1140	1143	rBV	129	183	0.01%	0.002%
33	8.062	1143	1144	1146	rVB	289	155	0.01%	0.001%
34	8.153	1157	1159	1161	rBV	189	145	0.01%	0.001%
35	8.196	1163	1166	1167	rBV2	141	144	0.01%	0.001%
36	8.251	1173	1175	1177	rVB2	261	203	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121123\
 Data File : VX039143.D
 Acq On : 11 Dec 2023 14:59
 Operator : JC/MD
 Sample : 05646-16DL 400X
 Misc : 2.63g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AS3DL

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	8.324	1180	1187	1198	rBV	179329	289737	14.88%	2.464%
38	8.647	1234	1240	1257	rVV	582545	900907	46.25%	7.661%
39	8.860	1273	1275	1278	rBV2	267	287	0.01%	0.002%
40	8.952	1284	1290	1305	rVV	125243	194555	9.99%	1.654%
41	9.104	1313	1315	1320	rVB3	458	705	0.04%	0.006%
42	9.256	1337	1340	1344	rBV2	316	395	0.02%	0.003%
43	9.384	1355	1361	1376	rBV	463717	687510	35.30%	5.846%
44	9.592	1393	1395	1398	rBV2	334	279	0.01%	0.002%
45	9.695	1409	1412	1420	rVB3	1512	2677	0.14%	0.023%
46	9.769	1420	1424	1427	rBV3	343	623	0.03%	0.005%
47	9.848	1434	1437	1439	rBV2	383	407	0.02%	0.003%
48	9.878	1439	1442	1443	rBV3	206	286	0.01%	0.002%
49	10.006	1459	1463	1465	rBV2	310	384	0.02%	0.003%
50	10.055	1465	1471	1490	rBV	597092	888989	45.64%	7.559%
51	10.268	1504	1506	1508	rBV2	302	189	0.01%	0.002%
52	10.360	1519	1521	1525	rBV	240	305	0.02%	0.003%
53	10.543	1549	1551	1556	rVB2	363	378	0.02%	0.003%
54	10.695	1573	1576	1580	rVB2	276	342	0.02%	0.003%
55	10.774	1586	1589	1592	rVB2	181	246	0.01%	0.002%
56	10.817	1595	1596	1599	rVB2	299	224	0.01%	0.002%
57	10.957	1616	1619	1621	rBV2	205	237	0.01%	0.002%
58	11.091	1635	1641	1646	rVB4	921	1527	0.08%	0.013%
59	11.189	1652	1657	1667	rBV	440214	560432	28.77%	4.766%
60	11.317	1677	1678	1681	rBV2	241	256	0.01%	0.002%
61	11.348	1681	1683	1684	rVV	293	146	0.01%	0.001%
62	11.415	1691	1694	1697	rBV	187	315	0.02%	0.003%
63	11.604	1723	1725	1727	rVB	249	150	0.01%	0.001%
64	11.817	1759	1760	1762	rBV2	278	169	0.01%	0.001%
65	11.969	1780	1785	1789	rBV	25876	33959	1.74%	0.289%
66	12.036	1789	1796	1810	rVB2	965278	1947735	100.00%	16.562%
67	12.317	1837	1842	1854	rBV3	653604	1003305	51.51%	8.531%
68	12.579	1883	1885	1886	rBV	339	268	0.01%	0.002%
69	12.762	1913	1915	1917	rBV2	246	208	0.01%	0.002%
70	12.951	1945	1946	1949	rBV	275	299	0.02%	0.003%
71	13.061	1959	1964	1971	rVV3	5992	10798	0.55%	0.092%
72	13.109	1971	1972	1978	rVB	1057	950	0.05%	0.008%
73	13.164	1978	1981	1982	rBV	272	237	0.01%	0.002%
74	13.335	2007	2009	2012	rVB2	186	169	0.01%	0.001%
75	13.384	2016	2017	2020	rVB	711	583	0.03%	0.005%
76	13.463	2029	2030	2033	rBV	244	150	0.01%	0.001%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121123\
 Data File : VX039143.D
 Acq On : 11 Dec 2023 14:59
 Operator : JC/MD
 Sample : 05646-16DL 400X
 Misc : 2.63g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AS3DL

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	13.487	2033	2034	2036	rVB	304	169	0.01%	0.001%
78	13.518	2036	2039	2040	rBV	200	174	0.01%	0.001%
79	13.585	2045	2050	2063	rVV	905211	1113123	57.15%	9.465%
80	13.707	2068	2070	2072	rBV2	317	257	0.01%	0.002%
81	13.774	2080	2081	2083	rBV2	211	149	0.01%	0.001%
82	13.865	2094	2096	2100	rVB2	181	190	0.01%	0.002%
83	13.957	2106	2111	2124	rVV	208666	270912	13.91%	2.304%
84	14.073	2128	2130	2132	rVB2	220	150	0.01%	0.001%
85	14.103	2132	2135	2137	rBV2	220	294	0.02%	0.002%
86	14.128	2137	2139	2144	rVB3	291	435	0.02%	0.004%
87	14.225	2153	2155	2156	rBV	345	250	0.01%	0.002%
88	14.341	2173	2174	2178	rBV2	193	213	0.01%	0.002%
89	14.481	2194	2197	2201	rBV2	221	363	0.02%	0.003%
90	14.524	2201	2204	2205	rBV2	195	197	0.01%	0.002%
91	14.627	2220	2221	2223	rVB2	278	159	0.01%	0.001%
92	14.780	2240	2246	2251	rBV2	6965	11047	0.57%	0.094%
93	14.865	2258	2260	2262	rBV3	324	368	0.02%	0.003%
94	15.012	2283	2284	2289	rBV2	408	433	0.02%	0.004%
95	15.249	2318	2323	2329	rVB	28766	39755	2.04%	0.338%
96	15.828	2416	2418	2419	rBV	379	174	0.01%	0.001%
97	16.121	2464	2466	2467	rBV	282	224	0.01%	0.002%
98	16.316	2496	2498	2500	rVB2	361	230	0.01%	0.002%
99	16.487	2524	2526	2527	rBV2	336	183	0.01%	0.002%
100	16.773	2571	2573	2574	rVB	298	148	0.01%	0.001%

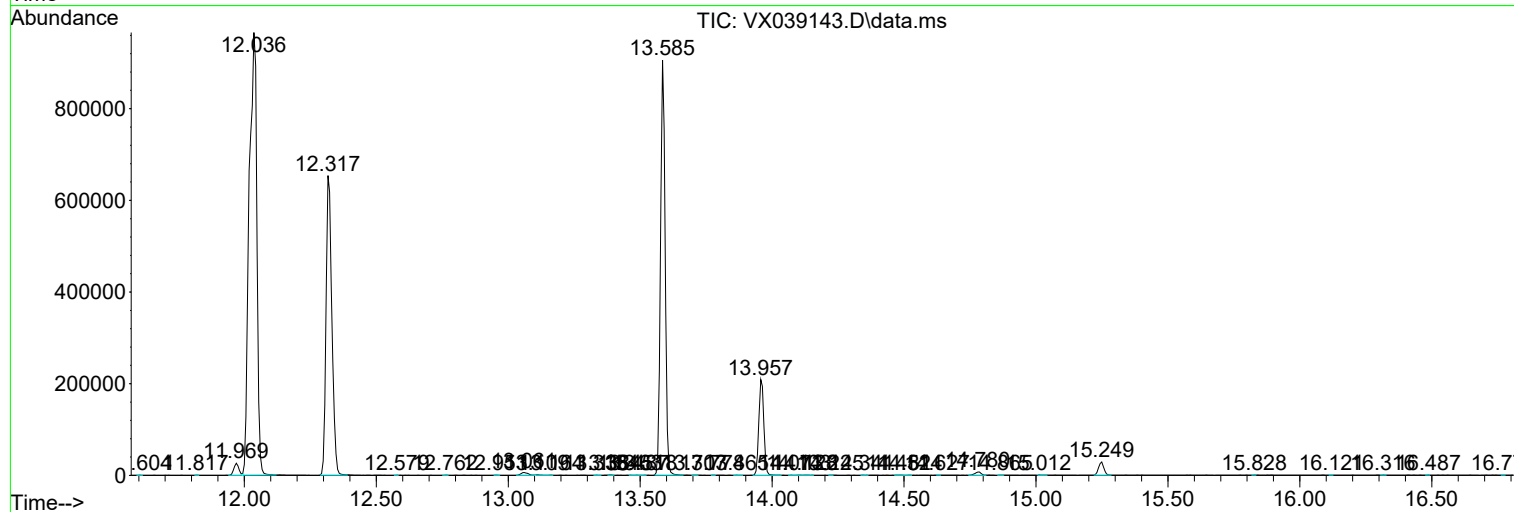
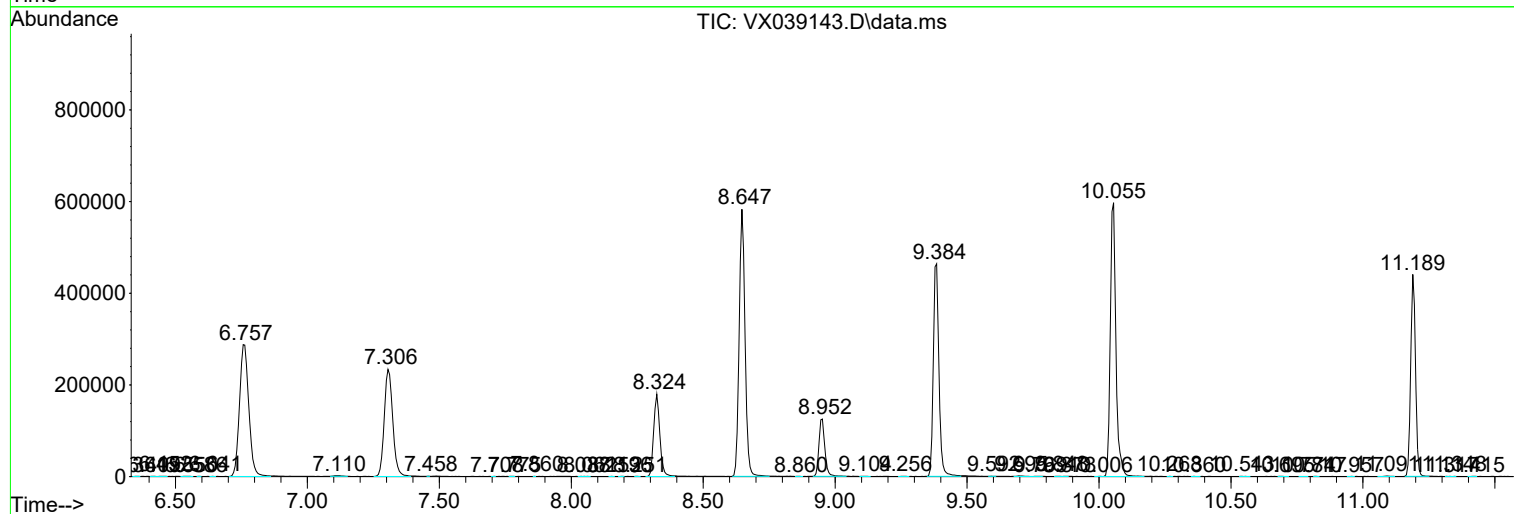
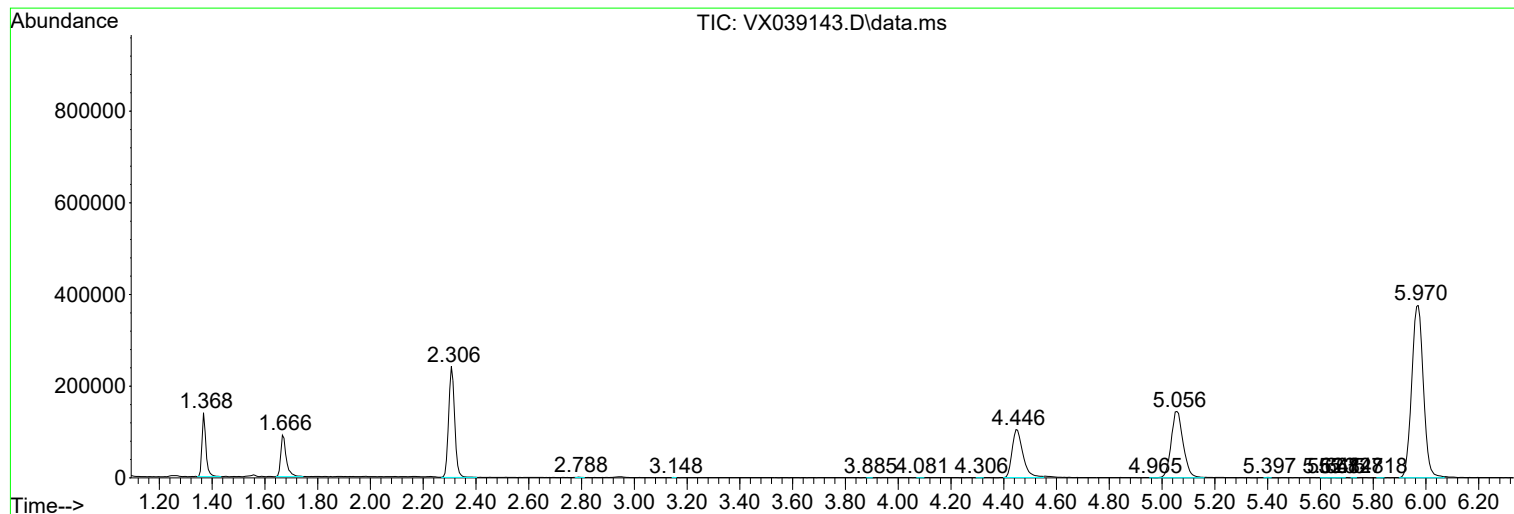
Sum of corrected areas: 11760065

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX121123\
Data File : VX039143.D
Acq On : 11 Dec 2023 14:59
Operator : JC/MD
Sample : 05646-16DL 400X
Misc : 2.63g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AS3DL

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\VX121123\
Data File : VX039143.D
Acq On : 11 Dec 2023 14:59
Operator : JC/MD
Sample : 05646-16DL 400X
Misc : 2.63g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AS3DL

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 : VX039143.D
Acq On : 11 Dec 2023 14:59
Operator : JC/MD
Sample : 05646-16DL 400X
Misc : 2.63g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AS3DL

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	--Internal Standard--			
					#	RT	Resp	Conc