

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120923\
 Data File : VX039121.D
 Acq On : 08 Dec 2023 21:30
 Operator : JC/MD
 Sample : 05646-17 40X
 Misc : 2.35g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AS4

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

Signal : TIC: VX039121.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	21	26	28	rBV4	3484	5833	0.06%	0.019%
2	1.368	42	46	57	rVB	139079	145415	1.56%	0.477%
3	1.490	65	66	74	rVB	5056	8893	0.10%	0.029%
4	1.569	74	79	80	rBV	2945	3791	0.04%	0.012%
5	1.587	80	82	83	rVV	3394	3147	0.03%	0.010%
6	1.666	87	95	107	rVV	94047	146506	1.57%	0.480%
7	1.746	107	108	111	rVV	1633	2043	0.02%	0.007%
8	2.239	184	189	191	rBV2	4037	6630	0.07%	0.022%
9	2.306	194	200	209	rVB	233188	365118	3.92%	1.197%
10	2.538	234	238	241	rBV	1957	2962	0.03%	0.010%
11	2.623	250	252	254	rBV	2461	2113	0.02%	0.007%
12	2.782	275	278	281	rBV3	2137	3313	0.04%	0.011%
13	2.843	286	288	290	rBV	2003	1420	0.02%	0.005%
14	2.940	299	304	312	rVB	9216	20510	0.22%	0.067%
15	3.001	312	314	316	rBV	1917	1719	0.02%	0.006%
16	3.044	319	321	325	rBV	1203	1947	0.02%	0.006%
17	3.635	416	418	422	rBV	1678	1721	0.02%	0.006%
18	3.904	460	462	463	rBV	1423	1423	0.02%	0.005%
19	4.324	529	531	533	rVB	2474	1712	0.02%	0.006%
20	4.349	533	535	537	rBV	2250	1870	0.02%	0.006%
21	4.452	544	552	566	rBV	100039	284690	3.05%	0.933%
22	4.550	566	568	575	rVB3	3745	7986	0.09%	0.026%
23	4.800	605	609	611	rBV	1385	2037	0.02%	0.007%
24	4.818	611	612	615	rBV	1671	1352	0.01%	0.004%
25	4.922	627	629	630	rBV	1650	1334	0.01%	0.004%
26	5.062	640	652	668	rBV2	135964	429416	4.61%	1.408%
27	5.227	678	679	685	rBV	1586	2083	0.02%	0.007%
28	5.275	685	687	689	rVB	1855	1583	0.02%	0.005%
29	5.336	694	697	699	rBV	1532	1625	0.02%	0.005%
30	5.391	703	706	707	rBV	1708	1311	0.01%	0.004%
31	5.781	768	770	772	rBV	1310	1327	0.01%	0.004%
32	5.970	789	801	819	rBV2	364802	1127958	12.10%	3.698%
33	6.141	827	829	831	rBV	1528	1331	0.01%	0.004%
34	6.367	864	866	868	rVV	1760	1588	0.02%	0.005%
35	6.415	872	874	876	rVB2	1701	1332	0.01%	0.004%
36	6.659	913	914	916	rBV	1681	1414	0.02%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120923\
 Data File : VX039121.D
 Acq On : 08 Dec 2023 21:30
 Operator : JC/MD
 Sample : 05646-17 40X
 Misc : 2.35g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AS4

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	6.757	920	930	942	rBV	266905	658687	7.07%	2.160%
38	7.074	980	982	984	rBV	1713	1456	0.02%	0.005%
39	7.092	984	985	987	rBV	1972	1373	0.01%	0.005%
40	7.202	1000	1003	1004	rBV	1922	1639	0.02%	0.005%
41	7.306	1012	1020	1032	rBV	224512	497277	5.34%	1.630%
42	7.574	1062	1064	1065	rBV	2128	1405	0.02%	0.005%
43	7.860	1107	1111	1113	rVB	1232	1778	0.02%	0.006%
44	8.275	1177	1179	1182	rVV	1513	1836	0.02%	0.006%
45	8.324	1182	1187	1196	rVV	163921	267747	2.87%	0.878%
46	8.647	1234	1240	1254	rVV	551740	863531	9.26%	2.831%
47	8.952	1284	1290	1302	rBV	122043	183251	1.97%	0.601%
48	9.037	1302	1304	1308	rVB2	1193	1444	0.02%	0.005%
49	9.299	1345	1347	1349	rBV	1524	1698	0.02%	0.006%
50	9.384	1356	1361	1369	rBV	459637	659508	7.08%	2.162%
51	9.701	1409	1413	1416	rVV2	2351	3497	0.04%	0.011%
52	9.756	1418	1422	1427	rBV	2743	4722	0.05%	0.015%
53	10.055	1465	1471	1473	rBV	573620	836963	8.98%	2.744%
54	10.305	1509	1512	1513	rBV	1269	1339	0.01%	0.004%
55	10.354	1518	1520	1523	rVB	2116	1826	0.02%	0.006%
56	10.378	1523	1524	1528	rBV	1588	1869	0.02%	0.006%
57	10.628	1561	1565	1566	rBV	1671	2210	0.02%	0.007%
58	10.646	1566	1568	1570	rVB	1712	1609	0.02%	0.005%
59	10.823	1594	1597	1598	rBV	1883	1677	0.02%	0.005%
60	10.970	1620	1621	1625	rBV	1621	1292	0.01%	0.004%
61	11.189	1652	1657	1666	rVV	420326	534190	5.73%	1.751%
62	11.347	1681	1683	1687	rBV2	1284	1653	0.02%	0.005%
63	11.494	1705	1707	1709	rVB	1540	1483	0.02%	0.005%
64	11.969	1779	1785	1789	rBV	241866	311163	3.34%	1.020%
65	12.042	1789	1797	1808	rVB	6936387	9320779	100.00%	30.559%
66	12.329	1837	1844	1858	rVB2	1484197	2501198	26.83%	8.200%
67	12.524	1872	1876	1878	rBV	1353	2247	0.02%	0.007%
68	12.664	1898	1899	1901	rBV	2012	1368	0.01%	0.004%
69	12.707	1903	1906	1909	rVB3	2737	4212	0.05%	0.014%
70	12.744	1909	1912	1914	rBV	2269	3185	0.03%	0.010%
71	12.792	1917	1920	1924	rBV	1532	2650	0.03%	0.009%
72	12.914	1938	1940	1942	rBV	2306	1458	0.02%	0.005%
73	13.012	1954	1956	1958	rVV	1584	1781	0.02%	0.006%
74	13.055	1958	1963	1969	rVV2	54812	104540	1.12%	0.343%
75	13.115	1969	1973	1977	rVB2	10376	14923	0.16%	0.049%
76	13.152	1977	1979	1980	rBV	1268	1357	0.01%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120923\
 Data File : VX039121.D
 Acq On : 08 Dec 2023 21:30
 Operator : JC/MD
 Sample : 05646-17 40X
 Misc : 2.35g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0AS4

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	13.329	2006	2008	2010	rBV	1192	1407	0.02%	0.005%
78	13.384	2012	2017	2021	rVV	12289	15710	0.17%	0.052%
79	13.439	2024	2026	2028	rVB	2036	1329	0.01%	0.004%
80	13.469	2028	2031	2036	rBV	2953	3889	0.04%	0.013%
81	13.506	2036	2037	2039	rBV	2119	1346	0.01%	0.004%
82	13.591	2045	2051	2067	rVB	6330352	8459140	90.76%	27.734%
83	13.780	2078	2082	2083	rBV	1527	1514	0.02%	0.005%
84	13.957	2106	2111	2121	rBV	1688613	2155495	23.13%	7.067%
85	14.054	2123	2127	2128	rBV	1327	1564	0.02%	0.005%
86	14.176	2146	2147	2150	rVB	2873	2193	0.02%	0.007%
87	14.201	2150	2151	2154	rBV	2147	2124	0.02%	0.007%
88	14.536	2204	2206	2213	rVB3	4362	5634	0.06%	0.018%
89	14.627	2217	2221	2225	rVB3	5644	7739	0.08%	0.025%
90	14.780	2240	2246	2250	rBV2	67004	104126	1.12%	0.341%
91	15.115	2299	2301	2303	rVB	2239	1413	0.02%	0.005%
92	15.249	2317	2323	2330	rVV	213307	316490	3.40%	1.038%
93	15.609	2378	2382	2384	rBV	1382	1831	0.02%	0.006%
94	15.719	2397	2400	2402	rBV	2038	2051	0.02%	0.007%
95	15.767	2404	2408	2409	rBV	1995	2370	0.03%	0.008%
96	15.834	2417	2419	2421	rVB	2215	1694	0.02%	0.006%
97	16.243	2483	2486	2488	rBV2	1364	1737	0.02%	0.006%
98	16.322	2497	2499	2502	rVB	2736	2694	0.03%	0.009%
99	16.359	2502	2505	2506	rBV2	1643	1908	0.02%	0.006%
100	16.420	2513	2515	2517	rVB	1901	1349	0.01%	0.004%

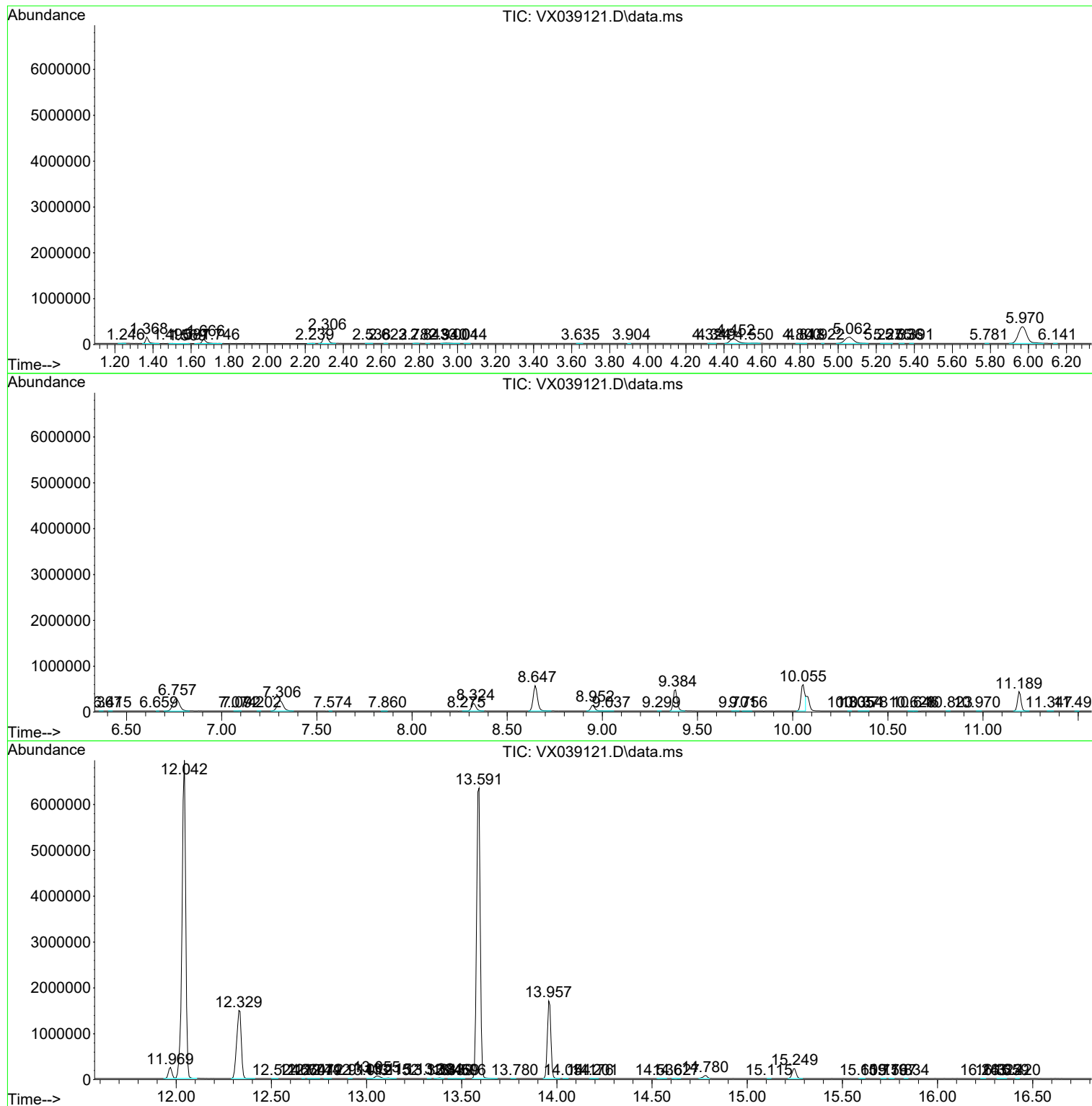
Sum of corrected areas: 30501021

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX120923\
Data File : VX039121.D
Acq On : 08 Dec 2023 21:30
Operator : JC/MD
Sample : 05646-17 40X
Misc : 2.35g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AS4

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\VX120923\
Data File : VX039121.D
Acq On : 08 Dec 2023 21:30
Operator : JC/MD
Sample : 05646-17 40X
Misc : 2.35g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AS4

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\VX120923\
Data File : VX039121.D
Acq On : 08 Dec 2023 21:30
Operator : JC/MD
Sample : 05646-17 40X
Misc : 2.35g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
C0AS4

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

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