

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070824\
 Data File : VX042229.D
 Acq On : 08 Jul 2024 11:27
 Operator : JC/MD
 Sample : P3100-16ME
 Misc : 4.48g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D07ME

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\SFAMXML070324WMA.M
 Title : VOC Analysis

Signal : TIC: VX042229.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.264	23	29	40	rBV2	13851	18611	2.66%	0.295%
2	1.367	42	46	48	rBV	18335	23346	3.34%	0.370%
3	1.575	70	80	81	rBV5	4068	8392	1.20%	0.133%
4	1.599	81	84	85	rBV2	3077	2917	0.42%	0.046%
5	1.648	85	92	94	rBV3	14865	28811	4.12%	0.457%
6	2.276	189	195	211	rBV	106964	193530	27.71%	3.069%
7	2.721	262	268	275	rBV	11532	25362	3.63%	0.402%
8	2.946	299	305	316	rVB	2805	7302	1.05%	0.116%
9	3.075	320	326	332	rVB4	1353	2943	0.42%	0.047%
10	3.416	377	382	391	rBV5	1455	3555	0.51%	0.056%
11	4.282	516	524	533	rVB5	1846	5311	0.76%	0.084%
12	4.489	550	558	577	rBV	41007	144710	20.72%	2.295%
13	5.056	638	651	667	rBV2	83531	260700	37.32%	4.134%
14	5.391	696	706	709	rBV4	1497	4002	0.57%	0.063%
15	5.458	710	717	726	rVB5	4257	13505	1.93%	0.214%
16	5.964	789	800	825	rBV2	241951	698479	100.00%	11.076%
17	6.336	856	861	862	rBV3	1348	1918	0.27%	0.030%
18	6.604	898	905	912	rBV3	1428	3156	0.45%	0.050%
19	6.757	921	930	951	rBV	238975	579047	82.90%	9.182%
20	7.110	983	988	996	rVV4	1318	2852	0.41%	0.045%
21	7.305	1011	1020	1027	rVV	135551	303374	43.43%	4.811%
22	7.373	1027	1031	1042	rVV2	24289	54102	7.75%	0.858%
23	7.769	1090	1096	1101	rVB6	989	2189	0.31%	0.035%
24	7.946	1119	1125	1133	rBV6	1365	2949	0.42%	0.047%
25	8.275	1174	1179	1182	rBV	1338	2140	0.31%	0.034%
26	8.324	1182	1187	1202	rVV	78313	139798	20.01%	2.217%
27	8.433	1202	1205	1215	rVB5	895	2091	0.30%	0.033%
28	8.592	1227	1231	1234	rBV2	4159	6996	1.00%	0.111%
29	8.647	1234	1240	1248	rVV	360092	571279	81.79%	9.059%
30	8.720	1249	1252	1257	rVB	8970	13286	1.90%	0.211%
31	8.909	1278	1283	1286	rBV3	2044	3181	0.46%	0.050%
32	8.951	1286	1290	1305	rVB	60520	97712	13.99%	1.549%
33	9.098	1310	1314	1319	rVB2	1631	2484	0.36%	0.039%
34	9.275	1337	1343	1357	rVB	47668	72686	10.41%	1.153%
35	9.390	1357	1362	1378	rBV	168352	340536	48.75%	5.400%
36	9.561	1386	1390	1394	rVB3	5388	8444	1.21%	0.134%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070824\
 Data File : VX042229.D
 Acq On : 08 Jul 2024 11:27
 Operator : JC/MD
 Sample : P3100-16ME
 Misc : 4.48g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D07ME

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\SFAMXML070324WMA.M
 Title : VOC Analysis

37	9.616	1394	1399	1402	rBV2	3426	4962	0.71%	0.079%
38	9.817	1428	1432	1438	rBV4	3095	4792	0.69%	0.076%
39	10.055	1465	1471	1481	rBV	486016	674853	96.62%	10.702%
40	10.201	1488	1495	1498	rBV	2967	4417	0.63%	0.070%
41	10.244	1498	1502	1505	rVV2	2300	3374	0.48%	0.054%
42	10.305	1507	1512	1517	rVV	15621	24965	3.57%	0.396%
43	10.360	1517	1521	1527	rVB2	3802	5685	0.81%	0.090%
44	10.585	1551	1558	1564	rBV4	2236	4536	0.65%	0.072%
45	10.646	1564	1568	1577	rVV	10076	15145	2.17%	0.240%
46	10.780	1587	1590	1594	rVB2	4265	5167	0.74%	0.082%
47	10.854	1598	1602	1605	rVV3	3000	4105	0.59%	0.065%
48	10.896	1605	1609	1613	rVB2	3399	5231	0.75%	0.083%
49	10.963	1613	1620	1624	rBV4	2936	4470	0.64%	0.071%
50	11.085	1637	1640	1642	rBV4	1635	2178	0.31%	0.035%
51	11.195	1652	1658	1670	rVB	272323	371003	53.12%	5.883%
52	11.311	1671	1677	1685	rBV2	5023	8848	1.27%	0.140%
53	11.384	1685	1689	1694	rBV2	4013	6153	0.88%	0.098%
54	11.457	1698	1701	1702	rVV	2620	3415	0.49%	0.054%
55	11.475	1702	1704	1709	rVB3	5884	7278	1.04%	0.115%
56	11.616	1723	1727	1733	rVB3	2754	4250	0.61%	0.067%
57	11.731	1733	1746	1748	rBV5	13256	30781	4.41%	0.488%
58	11.847	1760	1765	1767	rBV5	1322	2038	0.29%	0.032%
59	11.890	1769	1772	1777	rVV5	2317	4003	0.57%	0.063%
60	11.945	1777	1781	1783	rVV5	2404	3422	0.49%	0.054%
61	11.975	1783	1786	1788	rVV4	1925	2271	0.33%	0.036%
62	12.024	1788	1794	1801	rVV	528736	672350	96.26%	10.662%
63	12.085	1801	1804	1813	rVB4	4494	9228	1.32%	0.146%
64	12.177	1813	1819	1822	rVB4	1251	2015	0.29%	0.032%
65	12.323	1837	1843	1850	rBV	411362	545637	78.12%	8.652%
66	12.426	1855	1860	1864	rBV	7159	9230	1.32%	0.146%
67	12.469	1864	1867	1873	rVB4	1879	2971	0.43%	0.047%
68	12.536	1874	1878	1879	rBV2	1477	1799	0.26%	0.029%
69	12.683	1899	1902	1905	rBV4	1288	1736	0.25%	0.028%
70	12.719	1905	1908	1912	rVV4	1340	2011	0.29%	0.032%
71	12.762	1912	1915	1920	rVV4	1864	2587	0.37%	0.041%
72	12.884	1933	1935	1946	rVB9	2052	4863	0.70%	0.077%
73	12.969	1946	1949	1955	rVB4	2550	3916	0.56%	0.062%
74	13.042	1955	1961	1964	rVB4	1306	1779	0.25%	0.028%
75	13.268	1992	1998	2001	rBV	7573	10037	1.44%	0.159%
76	13.384	2014	2017	2024	rBV5	5255	10134	1.45%	0.161%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070824\
 Data File : VX042229.D
 Acq On : 08 Jul 2024 11:27
 Operator : JC/MD
 Sample : P3100-16ME
 Misc : 4.48g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 A4D07ME

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\SFAMXML070324WMA.M
 Title : VOC Analysis

77	13.591	2046	2051	2055	rBV5	1151	2530	0.36%	0.040%
78	13.688	2063	2067	2071	rBV7	1349	2491	0.36%	0.040%
79	13.737	2071	2075	2077	rBV3	1832	2581	0.37%	0.041%
80	13.780	2077	2082	2088	rVV	17657	25515	3.65%	0.405%
81	13.841	2088	2092	2097	rVV	7509	9294	1.33%	0.147%
82	14.036	2121	2124	2128	rBV2	6413	7988	1.14%	0.127%
83	14.194	2143	2150	2157	rBV9	1798	4103	0.59%	0.065%
84	14.432	2181	2189	2194	rBV5	1897	3851	0.55%	0.061%
85	14.609	2215	2218	2220	rBV3	2653	3151	0.45%	0.050%
86	14.639	2220	2223	2227	rVB	12143	13524	1.94%	0.214%
87	14.755	2237	2242	2243	rBV	5247	6018	0.86%	0.095%
88	14.780	2243	2246	2250	rVV	16411	22237	3.18%	0.353%
89	14.822	2250	2253	2260	rVB3	9598	12909	1.85%	0.205%
90	14.987	2278	2280	2286	rVB6	1055	1747	0.25%	0.028%
91	15.182	2309	2312	2313	rVV3	1607	1792	0.26%	0.028%
92	15.213	2313	2317	2322	rVV5	4688	6938	0.99%	0.110%
93	15.274	2322	2327	2331	rVB6	1519	2794	0.40%	0.044%
94	15.383	2340	2345	2347	rBV5	1990	3254	0.47%	0.052%
95	15.408	2347	2349	2353	rVV5	2120	2870	0.41%	0.046%
96	15.487	2357	2362	2368	rVB4	4860	8640	1.24%	0.137%
97	15.615	2378	2383	2386	rBV	6175	10270	1.47%	0.163%
98	15.652	2386	2389	2395	rVB2	3584	5438	0.78%	0.086%
99	15.847	2417	2421	2430	rVB8	2110	4191	0.60%	0.066%
100	16.182	2474	2476	2484	rVB7	1805	2664	0.38%	0.042%

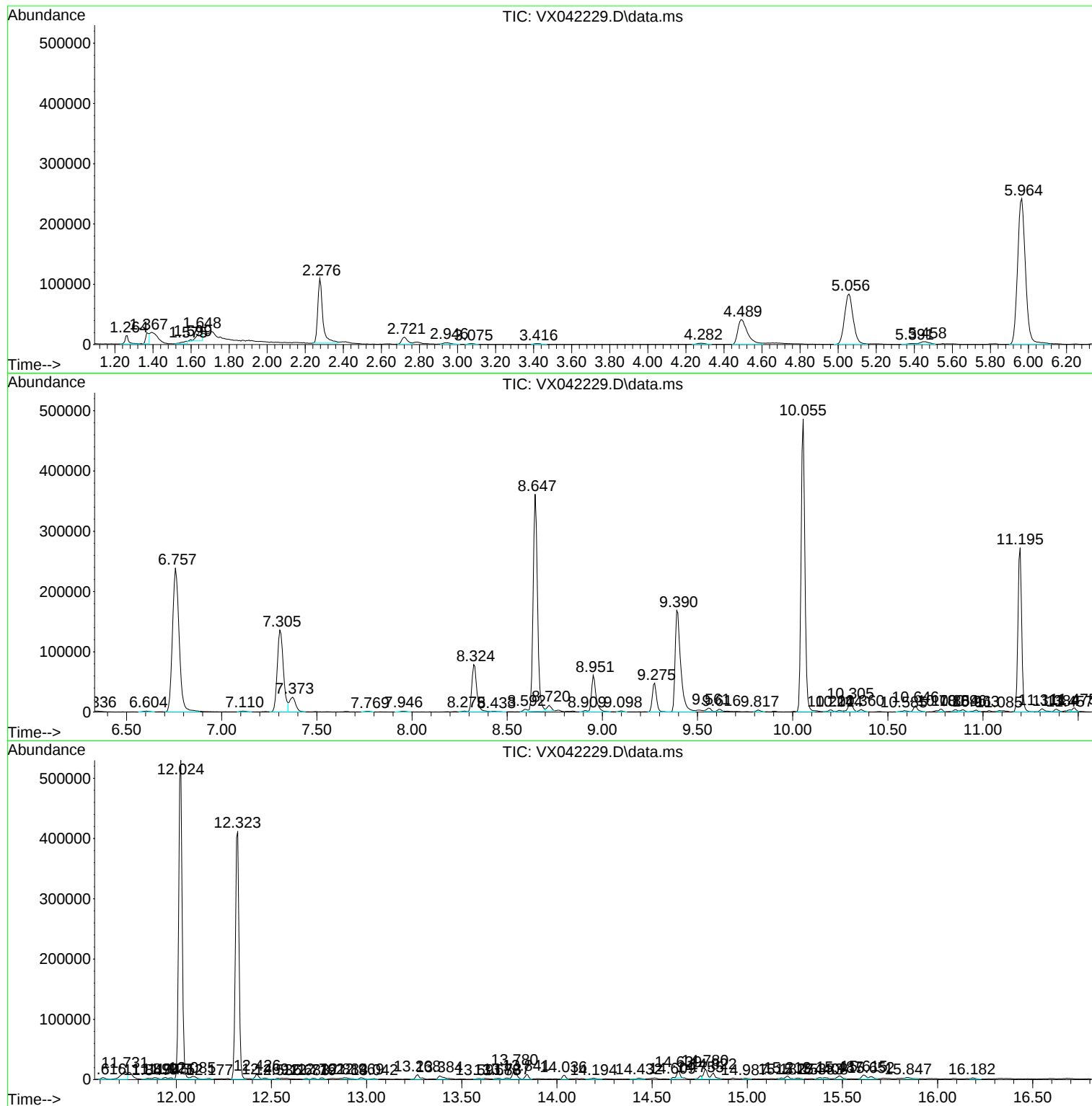
Sum of corrected areas: 6306121

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070824\
Data File : VX042229.D
Acq On : 08 Jul 2024 11:27
Operator : JC/MD
Sample : P3100-16ME
Misc : 4.48g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D07ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX070824\
Data File : VX042229.D
Acq On : 08 Jul 2024 11:27
Operator : JC/MD
Sample : P3100-16ME
Misc : 4.48g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D07ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.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\VX070824\
Data File : VX042229.D
Acq On : 08 Jul 2024 11:27
Operator : JC/MD
Sample : P3100-16ME
Misc : 4.48g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
A4D07ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML070324WMA.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