

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072524\
 Data File : VX042529.D
 Acq On : 24 Jul 2024 20:05
 Operator : JC/MD
 Sample : VX0725MBL02
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK695

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: VX042529.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	22	26	27	rBV	3672	3617	0.62%	0.081%
2	1.368	43	46	58	rVB	48062	59523	10.24%	1.330%
3	1.502	67	68	69	rBV	292	155	0.03%	0.003%
4	1.544	69	75	76	rVV	1144	1784	0.31%	0.040%
5	1.605	76	85	86	rVV3	3780	9235	1.59%	0.206%
6	1.648	88	92	101	rVV	38842	54812	9.43%	1.225%
7	1.715	101	103	112	rVB2	1863	3114	0.54%	0.070%
8	1.825	119	121	126	rVB3	251	337	0.06%	0.008%
9	1.868	126	128	130	rVB	377	284	0.05%	0.006%
10	1.898	130	133	135	rBV2	237	289	0.05%	0.006%
11	2.020	151	153	156	rVB	179	162	0.03%	0.004%
12	2.124	168	170	174	rVB	262	230	0.04%	0.005%
13	2.160	174	176	180	rVB2	212	262	0.05%	0.006%
14	2.203	180	183	185	rBV2	175	226	0.04%	0.005%
15	2.300	192	199	210	rBV	114604	179024	30.81%	4.001%
16	2.788	275	279	284	rBV2	906	1628	0.28%	0.036%
17	2.947	297	305	313	rVB	2670	5900	1.02%	0.132%
18	3.014	313	316	318	rVB2	136	159	0.03%	0.004%
19	3.483	390	393	398	rBV	170	241	0.04%	0.005%
20	3.520	398	399	402	rVB2	208	210	0.04%	0.005%
21	3.556	402	405	407	rBV2	186	271	0.05%	0.006%
22	3.648	419	420	423	rVB	225	216	0.04%	0.005%
23	3.684	423	426	428	rBV	184	232	0.04%	0.005%
24	3.946	463	469	470	rBV2	91	157	0.03%	0.004%
25	4.020	478	481	483	rBV2	121	155	0.03%	0.003%
26	4.276	522	523	526	rBV2	166	149	0.03%	0.003%
27	4.471	546	555	573	rBV	43066	128921	22.19%	2.882%
28	4.739	597	599	602	rBV3	223	330	0.06%	0.007%
29	4.812	609	611	615	rVB	128	169	0.03%	0.004%
30	4.855	615	618	620	rVB2	165	196	0.03%	0.004%
31	4.891	622	624	627	rVB	129	154	0.03%	0.003%
32	5.056	639	651	668	rBV	77089	231385	39.82%	5.172%
33	5.190	671	673	677	rVV3	161	176	0.03%	0.004%
34	5.263	683	685	687	rVB	185	165	0.03%	0.004%
35	5.336	693	697	700	rBV2	95	149	0.03%	0.003%
36	5.550	729	732	733	rBV	150	154	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072524\
 Data File : VX042529.D
 Acq On : 24 Jul 2024 20:05
 Operator : JC/MD
 Sample : VX0725MBL02
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK695

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	5.970	789	801	822	rBV2	194763	581030	100.00%	12.987%
38	6.367	864	866	870	rVB3	145	162	0.03%	0.004%
39	6.470	880	883	886	rBV	133	177	0.03%	0.004%
40	6.763	922	931	952	rBV	166663	402468	69.27%	8.996%
41	7.068	978	981	982	rBV2	164	185	0.03%	0.004%
42	7.129	983	991	1002	rVB6	2727	6990	1.20%	0.156%
43	7.214	1002	1005	1011	rBV3	381	465	0.08%	0.010%
44	7.312	1012	1021	1037	rBV	116639	259884	44.73%	5.809%
45	7.586	1064	1066	1069	rVB2	150	145	0.02%	0.003%
46	7.958	1123	1127	1128	rBV2	357	433	0.07%	0.010%
47	8.330	1181	1188	1203	rVV	65343	114669	19.74%	2.563%
48	8.507	1215	1217	1218	rBV	343	221	0.04%	0.005%
49	8.647	1234	1240	1256	rBV	290621	465676	80.15%	10.408%
50	8.952	1285	1290	1305	rBV	48501	73486	12.65%	1.642%
51	9.281	1340	1344	1350	rVB4	1142	1728	0.30%	0.039%
52	9.324	1350	1351	1355	rBV2	126	172	0.03%	0.004%
53	9.385	1356	1361	1374	rBV	179310	276752	47.63%	6.186%
54	9.561	1388	1390	1392	rVB2	376	207	0.04%	0.005%
55	9.641	1401	1403	1405	rVB2	183	156	0.03%	0.003%
56	9.708	1411	1414	1416	rVB2	462	502	0.09%	0.011%
57	9.732	1416	1418	1421	rBV	205	204	0.04%	0.005%
58	9.927	1449	1450	1453	rBV	193	228	0.04%	0.005%
59	10.055	1465	1471	1486	rVV	343268	464126	79.88%	10.374%
60	10.177	1490	1491	1492	rVV	385	230	0.04%	0.005%
61	10.208	1495	1496	1498	rVV	610	337	0.06%	0.008%
62	10.311	1508	1513	1520	rBV3	561	1092	0.19%	0.024%
63	10.646	1565	1568	1570	rVV2	267	276	0.05%	0.006%
64	10.665	1570	1571	1574	rVB2	282	226	0.04%	0.005%
65	10.970	1618	1621	1623	rVB	202	170	0.03%	0.004%
66	11.092	1637	1641	1643	rBV	144	175	0.03%	0.004%
67	11.189	1652	1657	1668	rVV	224045	303262	52.19%	6.778%
68	11.268	1668	1670	1673	rVB3	321	310	0.05%	0.007%
69	11.299	1673	1675	1676	rBV2	225	175	0.03%	0.004%
70	11.311	1676	1677	1682	rVB	480	387	0.07%	0.009%
71	11.427	1693	1696	1698	rVV2	118	152	0.03%	0.003%
72	11.457	1698	1701	1705	rVV4	287	480	0.08%	0.011%
73	11.494	1705	1707	1711	rVV	192	155	0.03%	0.003%
74	11.555	1714	1717	1719	rBV2	200	237	0.04%	0.005%
75	11.756	1748	1750	1754	rVB2	368	393	0.07%	0.009%
76	11.969	1783	1785	1788	rBV	414	483	0.08%	0.011%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072524\
 Data File : VX042529.D
 Acq On : 24 Jul 2024 20:05
 Operator : JC/MD
 Sample : VX0725MBL02
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK695

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	12.024	1788	1794	1806	rBV	313323	409195	70.43%	9.146%
78	12.317	1837	1842	1852	rBV	321627	413383	71.15%	9.239%
79	12.762	1912	1915	1920	rVV3	667	855	0.15%	0.019%
80	12.847	1928	1929	1931	rBV2	245	183	0.03%	0.004%
81	13.024	1957	1958	1962	rBV	119	146	0.03%	0.003%
82	13.122	1971	1974	1977	rVB3	354	496	0.09%	0.011%
83	13.591	2046	2051	2053	rBV3	351	528	0.09%	0.012%
84	13.786	2079	2083	2086	rBV	418	589	0.10%	0.013%
85	13.957	2110	2111	2119	rVB4	427	693	0.12%	0.015%
86	14.128	2136	2139	2143	rVB2	821	944	0.16%	0.021%
87	14.390	2179	2182	2185	rBV3	214	309	0.05%	0.007%
88	14.438	2187	2190	2191	rVB2	154	158	0.03%	0.004%
89	14.688	2229	2231	2233	rBV2	190	191	0.03%	0.004%
90	14.780	2243	2246	2248	rBV3	183	231	0.04%	0.005%
91	14.841	2253	2256	2258	rBV3	241	304	0.05%	0.007%
92	15.036	2286	2288	2294	rBV4	193	265	0.05%	0.006%
93	15.170	2308	2310	2311	rBV	182	166	0.03%	0.004%
94	15.359	2338	2341	2342	rBV2	311	346	0.06%	0.008%
95	15.383	2342	2345	2350	rVB3	694	1195	0.21%	0.027%
96	16.176	2473	2475	2477	rVB2	380	213	0.04%	0.005%
97	16.225	2482	2483	2486	rBV3	268	249	0.04%	0.006%
98	16.341	2499	2502	2503	rBV2	254	296	0.05%	0.007%
99	16.511	2528	2530	2531	rBV2	264	168	0.03%	0.004%
100	16.548	2535	2536	2538	rBV	299	212	0.04%	0.005%

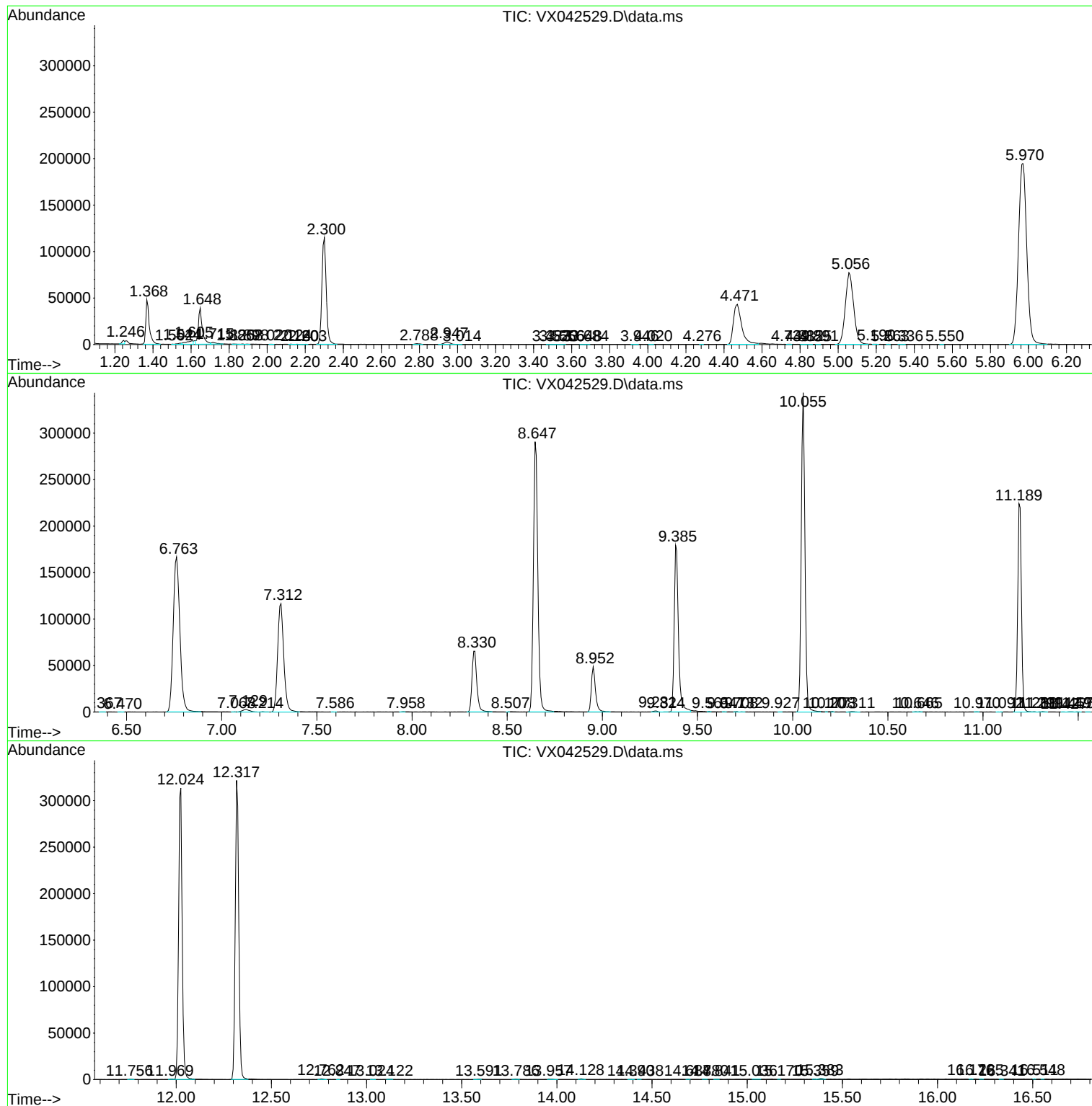
Sum of corrected areas: 4474092

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX072524\
Data File : VX042529.D
Acq On : 24 Jul 2024 20:05
Operator : JC/MD
Sample : VX0725MBL02
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK695

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\VX072524\
Data File : VX042529.D
Acq On : 24 Jul 2024 20:05
Operator : JC/MD
Sample : VX0725MBL02
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK695

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\VX072524\
Data File : VX042529.D
Acq On : 24 Jul 2024 20:05
Operator : JC/MD
Sample : VX0725MBL02
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK695

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