

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102921\
 Data File : VX025020.D
 Acq On : 29 Oct 2021 12:36
 Operator : JC/MD
 Sample : VX1029MBL05
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK626

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\SFAMXML102821WMA.M
 Title : VOC Analysis

Signal : TIC: VX025020.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	55	rVB	66087	71022	10.37%	1.356%
2	1.618	85	87	91	rBV3	1023	1581	0.23%	0.030%
3	1.666	91	95	105	rVB	47969	62914	9.19%	1.201%
4	1.807	116	118	120	rVB	767	462	0.07%	0.009%
5	2.313	194	201	214	rVB	134416	227582	33.23%	4.346%
6	2.441	221	222	228	rVB2	667	778	0.11%	0.015%
7	2.514	228	234	241	rBV2	749	1722	0.25%	0.033%
8	2.672	259	260	264	rVV2	710	659	0.10%	0.013%
9	2.788	275	279	285	rVV5	2048	3562	0.52%	0.068%
10	2.837	285	287	290	rVB	682	680	0.10%	0.013%
11	2.947	300	305	306	rBV4	1025	862	0.13%	0.016%
12	3.014	313	316	318	rBV	882	821	0.12%	0.016%
13	3.087	325	328	329	rVB2	520	520	0.08%	0.010%
14	3.410	379	381	384	rVB	429	500	0.07%	0.010%
15	3.483	391	393	396	rVB	704	563	0.08%	0.011%
16	3.514	396	398	403	rBV2	455	683	0.10%	0.013%
17	3.562	403	406	408	rBV	674	534	0.08%	0.010%
18	3.617	412	415	417	rBV	471	597	0.09%	0.011%
19	3.727	431	433	435	rVB2	530	456	0.07%	0.009%
20	4.020	479	481	483	rBV	485	559	0.08%	0.011%
21	4.123	496	498	500	rVB	611	488	0.07%	0.009%
22	4.166	500	505	506	rBV	573	884	0.13%	0.017%
23	4.306	525	528	530	rVV	393	556	0.08%	0.011%
24	4.465	545	554	571	rVV	57120	168958	24.67%	3.227%
25	4.757	597	602	604	rBV2	743	1170	0.17%	0.022%
26	4.898	622	625	627	rBV2	648	679	0.10%	0.013%
27	5.062	641	652	669	rVB	100293	303089	44.26%	5.788%
28	5.324	691	695	699	rVB2	712	1275	0.19%	0.024%
29	5.544	728	731	732	rBV2	590	534	0.08%	0.010%
30	5.635	744	746	750	rBV	407	641	0.09%	0.012%
31	5.885	783	787	788	rBV	563	681	0.10%	0.013%
32	5.977	790	802	820	rVV4	228671	684780	100.00%	13.077%
33	6.373	864	867	869	rBV	587	767	0.11%	0.015%
34	6.409	871	873	876	rVB	645	559	0.08%	0.011%
35	6.769	921	932	943	rBV2	181051	433787	63.35%	8.284%
36	7.062	978	980	982	rVB	846	605	0.09%	0.012%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102921\
 Data File : VX025020.D
 Acq On : 29 Oct 2021 12:36
 Operator : JC/MD
 Sample : VX1029MBL05
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK626

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\SFAMXLM102821WMA.M
 Title : VOC Analysis

37	7.111	982	988	994	rBV4	3165	6746	0.99%	0.129%
38	7.318	1011	1022	1033	rVV	140770	309108	45.14%	5.903%
39	7.940	1121	1124	1128	rVB3	511	734	0.11%	0.014%
40	8.056	1140	1143	1145	rBV	468	481	0.07%	0.009%
41	8.135	1152	1156	1158	rVB2	428	576	0.08%	0.011%
42	8.330	1182	1188	1197	rBV	99133	161518	23.59%	3.085%
43	8.470	1208	1211	1212	rBV2	580	605	0.09%	0.012%
44	8.653	1234	1241	1249	rVV	337440	522889	76.36%	9.986%
45	8.726	1249	1253	1260	rVB2	5025	8323	1.22%	0.159%
46	8.830	1267	1270	1272	rBV2	602	649	0.09%	0.012%
47	8.952	1284	1290	1303	rBV	79805	115741	16.90%	2.210%
48	9.269	1340	1342	1347	rVB2	767	1120	0.16%	0.021%
49	9.391	1353	1362	1376	rBV	247776	371976	54.32%	7.104%
50	9.750	1418	1421	1422	rBV2	602	487	0.07%	0.009%
51	10.055	1466	1471	1480	rBV	354007	492616	71.94%	9.408%
52	10.299	1508	1511	1516	rBV2	1072	1527	0.22%	0.029%
53	10.543	1549	1551	1553	rVB	523	477	0.07%	0.009%
54	10.653	1566	1569	1571	rVV	688	637	0.09%	0.012%
55	10.683	1571	1574	1576	rVV2	593	505	0.07%	0.010%
56	10.957	1616	1619	1620	rBV	504	473	0.07%	0.009%
57	11.122	1643	1646	1650	rVB3	2190	2766	0.40%	0.053%
58	11.195	1650	1658	1666	rBV	269379	331958	48.48%	6.339%
59	11.378	1684	1688	1690	rBV3	635	966	0.14%	0.018%
60	11.463	1699	1702	1703	rVB2	639	603	0.09%	0.012%
61	11.610	1721	1726	1727	rVB	667	755	0.11%	0.014%
62	11.634	1727	1730	1733	rBV2	667	758	0.11%	0.014%
63	11.933	1775	1779	1782	rBV2	1249	1600	0.23%	0.031%
64	11.976	1784	1786	1788	rVV2	819	658	0.10%	0.013%
65	12.024	1789	1794	1802	rVB	357668	448909	65.56%	8.573%
66	12.128	1808	1811	1812	rBV2	860	757	0.11%	0.014%
67	12.201	1820	1823	1826	rBV	542	652	0.10%	0.012%
68	12.323	1837	1843	1849	rBV	359472	449932	65.70%	8.592%
69	12.421	1856	1859	1860	rBV2	1017	930	0.14%	0.018%
70	12.463	1863	1866	1867	rVV	714	688	0.10%	0.013%
71	12.494	1869	1871	1873	rVV	907	788	0.12%	0.015%
72	12.738	1907	1911	1912	rBV	476	532	0.08%	0.010%
73	12.762	1912	1915	1916	rVV	464	475	0.07%	0.009%
74	12.799	1919	1921	1924	rVB	661	527	0.08%	0.010%
75	12.920	1937	1941	1942	rBV	696	765	0.11%	0.015%
76	13.122	1971	1974	1975	rBV2	574	473	0.07%	0.009%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102921\
 Data File : VX025020.D
 Acq On : 29 Oct 2021 12:36
 Operator : JC/MD
 Sample : VX1029MBL05
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
 ALS Vial : 1 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK626

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\SFAMXML102821WMA.M
 Title : VOC Analysis

77	13.146	1975	1978	1980	rVV2	508	598	0.09%	0.011%
78	13.238	1991	1993	1996	rVB	770	879	0.13%	0.017%
79	13.286	1996	2001	2003	rBV	916	1310	0.19%	0.025%
80	13.414	2020	2022	2024	rBV	453	474	0.07%	0.009%
81	13.701	2066	2069	2071	rBV	513	646	0.09%	0.012%
82	13.865	2092	2096	2098	rBV	459	747	0.11%	0.014%
83	14.085	2129	2132	2134	rVB2	419	481	0.07%	0.009%
84	14.115	2134	2137	2139	rBV	484	460	0.07%	0.009%
85	14.146	2139	2142	2144	rBV	565	759	0.11%	0.014%
86	14.225	2152	2155	2158	rBV	464	813	0.12%	0.016%
87	14.310	2167	2169	2175	rBV	503	842	0.12%	0.016%
88	14.457	2188	2193	2196	rBV	581	1084	0.16%	0.021%
89	14.658	2222	2226	2228	rBV2	776	920	0.13%	0.018%
90	14.695	2230	2232	2237	rVV2	641	877	0.13%	0.017%
91	14.841	2254	2256	2258	rBV2	568	478	0.07%	0.009%
92	14.865	2258	2260	2264	rVB3	641	534	0.08%	0.010%
93	14.957	2274	2275	2280	rVB2	626	483	0.07%	0.009%
94	15.268	2324	2326	2330	rBV2	791	895	0.13%	0.017%
95	15.316	2332	2334	2337	rBV2	587	530	0.08%	0.010%
96	16.011	2446	2448	2451	rBV2	619	744	0.11%	0.014%
97	16.213	2477	2481	2483	rBV2	586	754	0.11%	0.014%
98	16.389	2506	2510	2513	rBV3	526	777	0.11%	0.015%
99	16.463	2521	2522	2524	rBV	573	525	0.08%	0.010%
100	16.682	2557	2558	2561	rVB2	881	580	0.08%	0.011%

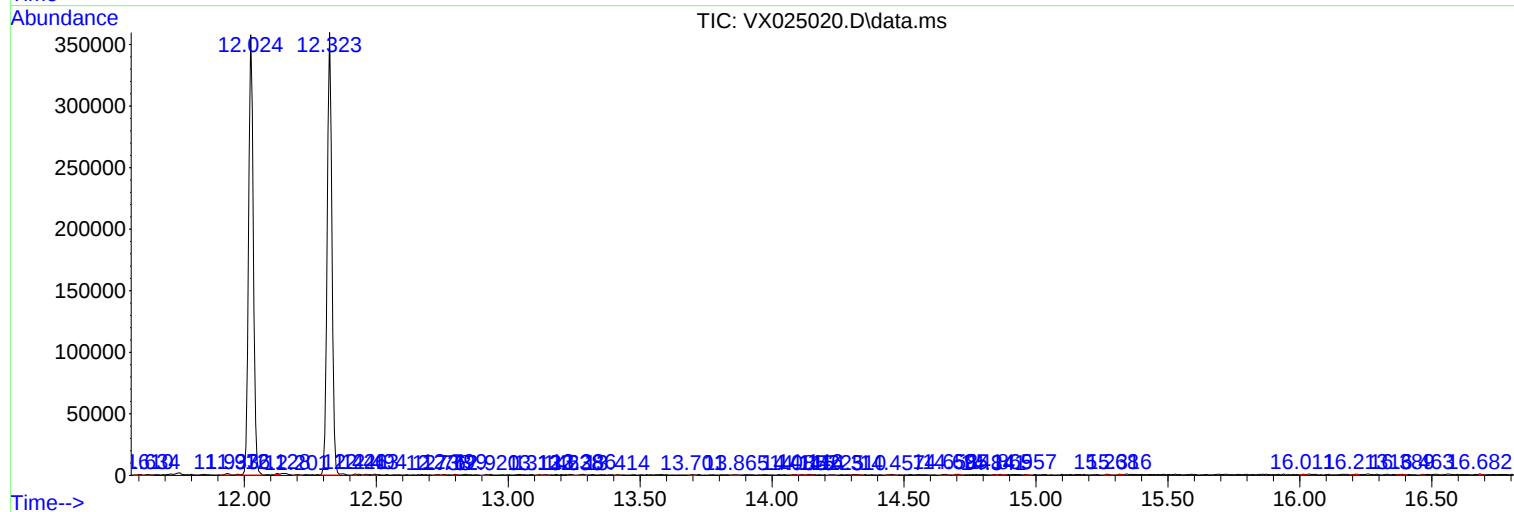
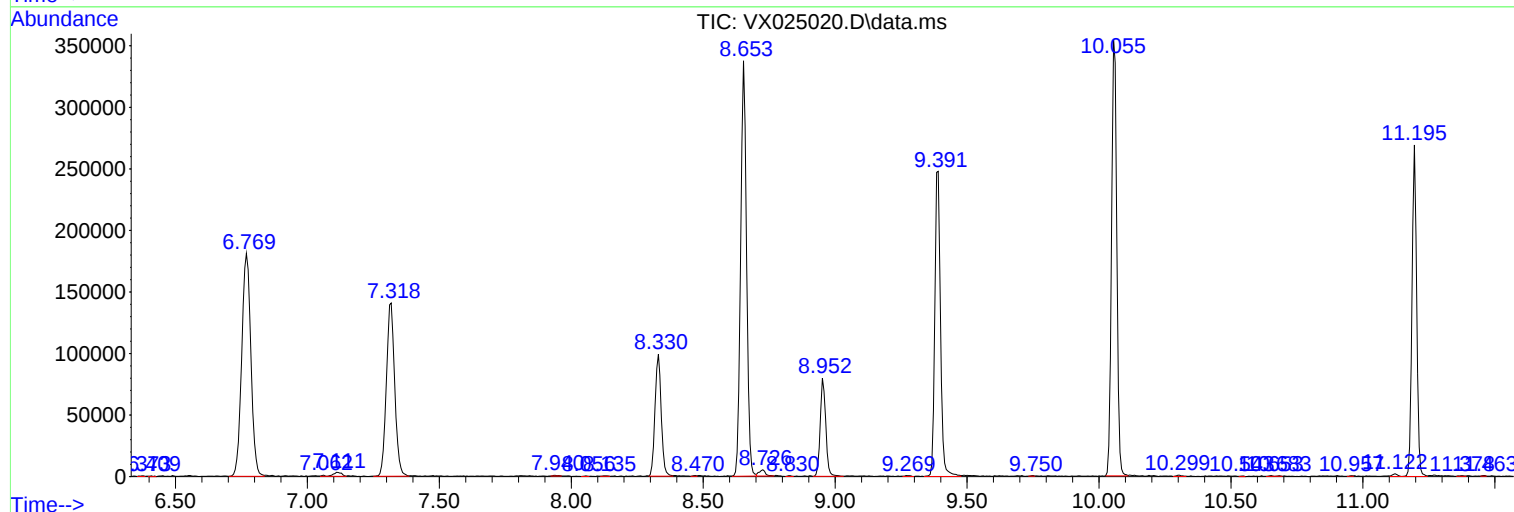
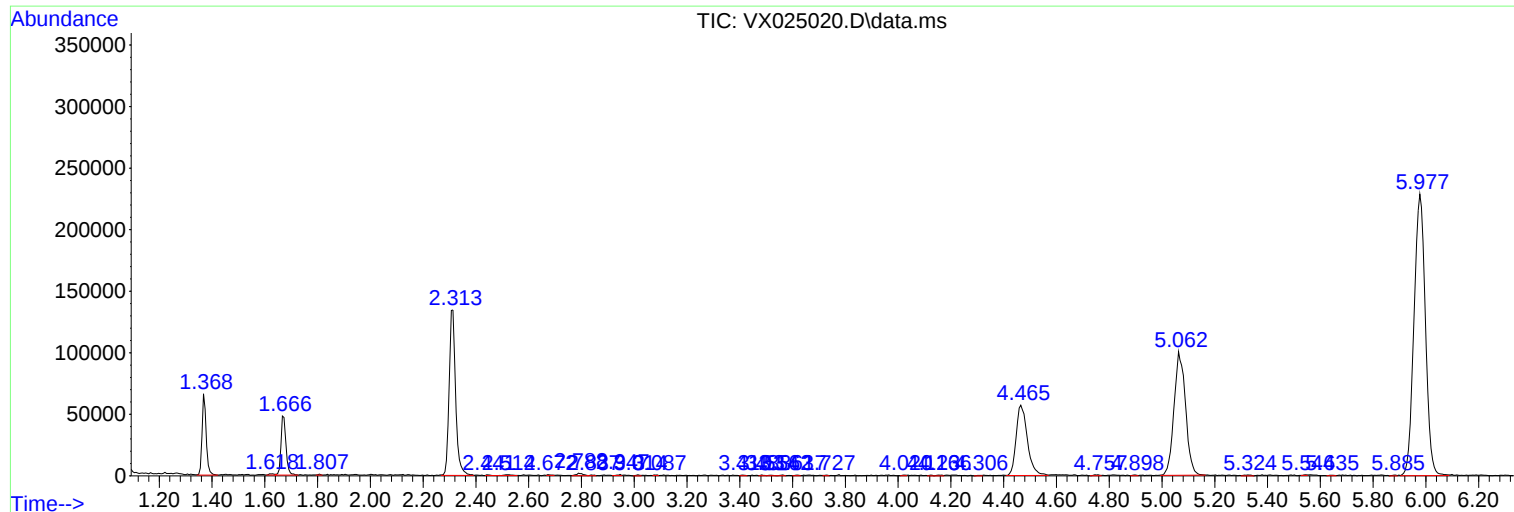
Sum of corrected areas: 5236380

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102921\
Data File : VX025020.D
Acq On : 29 Oct 2021 12:36
Operator : JC/MD
Sample : VX1029MBL05
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK626

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM102821WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX102921\
Data File : VX025020.D
Acq On : 29 Oct 2021 12:36
Operator : JC/MD
Sample : VX1029MBL05
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK626

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML102821WMA.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\VX102921\
Data File : VX025020.D
Acq On : 29 Oct 2021 12:36
Operator : JC/MD
Sample : VX1029MBL05
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_X/MEOH
ALS Vial : 1 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK626

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML102821WMA.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
