

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081121\
 Data File : VX023653.D
 Acq On : 11 Aug 2021 16:53
 Operator : JC/MD
 Sample : M3364-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DBK82

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\SFAMXML081121WMA.M
 Title : VOC Analysis

Signal : TIC: VX023653.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.367	43	46	55	rVB	120940	127533	11.33%	1.477%
2	1.666	91	95	106	rVB	95508	126916	11.28%	1.470%
3	2.306	194	200	209	rBV	226081	375563	33.37%	4.350%
4	2.501	230	232	233	rBV	325	334	0.03%	0.004%
5	2.782	275	278	279	rBV2	495	497	0.04%	0.006%
6	2.946	300	305	308	rBV2	709	1356	0.12%	0.016%
7	3.050	319	322	324	rBV2	267	336	0.03%	0.004%
8	3.074	324	326	328	rVV2	240	309	0.03%	0.004%
9	3.123	328	334	343	rVV2	2619	6272	0.56%	0.073%
10	3.392	376	378	382	rVB3	253	314	0.03%	0.004%
11	3.434	382	385	388	rBV3	376	570	0.05%	0.007%
12	3.574	406	408	411	rBV2	306	412	0.04%	0.005%
13	3.611	411	414	417	rVV3	499	781	0.07%	0.009%
14	4.026	480	482	484	rVV2	299	286	0.03%	0.003%
15	4.166	500	505	507	rBV2	257	319	0.03%	0.004%
16	4.251	515	519	520	rVB2	251	271	0.02%	0.003%
17	4.355	532	536	538	rBV	303	329	0.03%	0.004%
18	4.464	544	554	569	rBV	93302	264375	23.49%	3.062%
19	4.842	614	616	621	rVV	362	446	0.04%	0.005%
20	5.068	642	653	671	rVV	145937	442011	39.28%	5.120%
21	5.397	704	707	709	rBV3	477	463	0.04%	0.005%
22	5.861	779	783	786	rBV3	368	511	0.05%	0.006%
23	5.976	789	802	818	rBV2	382356	1125313	100.00%	13.035%
24	6.318	856	858	860	rBV	325	267	0.02%	0.003%
25	6.354	860	864	869	rVB3	505	852	0.08%	0.010%
26	6.397	869	871	873	rBV2	301	316	0.03%	0.004%
27	6.769	922	932	945	rBV	319376	750118	66.66%	8.689%
28	6.934	957	959	961	rBV2	330	347	0.03%	0.004%
29	7.116	982	989	998	rVB5	4674	10729	0.95%	0.124%
30	7.318	1012	1022	1033	rBV	235706	513105	45.60%	5.943%
31	7.476	1043	1048	1055	rVB4	1082	2144	0.19%	0.025%
32	7.580	1063	1065	1067	rBV	282	286	0.03%	0.003%
33	7.805	1099	1102	1107	rVV4	575	1068	0.09%	0.012%
34	7.933	1117	1123	1130	rVV3	2386	4647	0.41%	0.054%
35	8.330	1181	1188	1197	rBV	155644	246397	21.90%	2.854%
36	8.470	1208	1211	1217	rVB2	1801	2612	0.23%	0.030%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081121\
 Data File : VX023653.D
 Acq On : 11 Aug 2021 16:53
 Operator : JC/MD
 Sample : M3364-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DBK82

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\SFAMXML081121WMA.M
 Title : VOC Analysis

37	8.580	1227	1229	1234	rVB3	733	717	0.06%	0.008%
38	8.653	1234	1241	1248	rBV	600618	917335	81.52%	10.626%
39	8.720	1249	1252	1260	rVV	14404	23193	2.06%	0.269%
40	8.775	1260	1261	1266	rVV3	457	495	0.04%	0.006%
41	8.836	1266	1271	1272	rVB	267	384	0.03%	0.004%
42	8.951	1284	1290	1300	rBV	113231	164680	14.63%	1.907%
43	9.037	1303	1304	1308	rVB3	295	331	0.03%	0.004%
44	9.171	1325	1326	1330	rVB2	498	474	0.04%	0.005%
45	9.287	1340	1345	1349	rVB3	1885	2862	0.25%	0.033%
46	9.390	1356	1362	1380	rVV	418872	596647	53.02%	6.911%
47	9.525	1380	1384	1389	rVB5	1901	3279	0.29%	0.038%
48	9.616	1397	1399	1402	rBV2	321	291	0.03%	0.003%
49	9.677	1405	1409	1412	rBV3	260	448	0.04%	0.005%
50	9.732	1415	1418	1420	rBV3	231	312	0.03%	0.004%
51	10.055	1465	1471	1487	rVB	646288	881231	78.31%	10.207%
52	10.201	1491	1495	1499	rVB4	828	1129	0.10%	0.013%
53	10.305	1508	1512	1516	rBV3	1221	1739	0.15%	0.020%
54	10.640	1564	1567	1568	rBV2	636	700	0.06%	0.008%
55	10.689	1573	1575	1578	rVB	302	269	0.02%	0.003%
56	10.860	1601	1603	1610	rVV2	782	1090	0.10%	0.013%
57	10.963	1618	1620	1622	rVV2	425	318	0.03%	0.004%
58	11.122	1642	1646	1652	rVB	3922	5040	0.45%	0.058%
59	11.195	1652	1658	1669	rBV	409392	515323	45.79%	5.969%
60	11.463	1697	1702	1703	rBV3	1013	1376	0.12%	0.016%
61	11.542	1713	1715	1718	rBV2	508	510	0.05%	0.006%
62	11.616	1724	1727	1728	rBV2	248	260	0.02%	0.003%
63	11.689	1737	1739	1742	rBV3	419	365	0.03%	0.004%
64	11.750	1745	1749	1753	rVB2	4825	5540	0.49%	0.064%
65	11.847	1761	1765	1769	rVB4	706	1248	0.11%	0.014%
66	11.939	1775	1780	1783	rBV2	2546	3254	0.29%	0.038%
67	11.975	1783	1786	1789	rBV2	486	441	0.04%	0.005%
68	12.024	1789	1794	1806	rBV	612460	753085	66.92%	8.723%
69	12.128	1809	1811	1812	rVV2	2075	1636	0.15%	0.019%
70	12.152	1812	1815	1820	rVB3	3636	4531	0.40%	0.052%
71	12.225	1823	1827	1829	rBV3	876	1276	0.11%	0.015%
72	12.323	1835	1843	1850	rBV	565633	718759	63.87%	8.325%
73	12.426	1856	1860	1864	rBV7	1199	1547	0.14%	0.018%
74	12.597	1885	1888	1889	rBV3	332	350	0.03%	0.004%
75	12.664	1897	1899	1902	rVB2	1089	930	0.08%	0.011%
76	12.762	1911	1915	1916	rBV3	397	529	0.05%	0.006%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081121\
 Data File : VX023653.D
 Acq On : 11 Aug 2021 16:53
 Operator : JC/MD
 Sample : M3364-03
 Misc : 5.0mL/MSVOA_X/WATER
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 DBK82

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\SFAMXML081121WMA.M
 Title : VOC Analysis

77	12.859	1930	1931	1934	rVB	732	505	0.04%	0.006%
78	12.975	1946	1950	1954	rBV2	600	912	0.08%	0.011%
79	13.006	1954	1955	1959	rVV	317	331	0.03%	0.004%
80	13.054	1959	1963	1966	rVB3	848	1256	0.11%	0.015%
81	13.115	1971	1973	1975	rVV2	399	381	0.03%	0.004%
82	13.158	1977	1980	1981	rVV2	445	350	0.03%	0.004%
83	13.176	1981	1983	1987	rVB3	307	411	0.04%	0.005%
84	13.493	2032	2035	2036	rBV	232	301	0.03%	0.003%
85	13.676	2061	2065	2066	rVV2	243	272	0.02%	0.003%
86	13.695	2066	2068	2071	rVB2	460	383	0.03%	0.004%
87	13.780	2079	2082	2085	rBV2	727	865	0.08%	0.010%
88	13.969	2109	2113	2117	rVB3	363	582	0.05%	0.007%
89	14.048	2124	2126	2127	rBV	350	274	0.02%	0.003%
90	14.115	2135	2137	2139	rVV3	304	361	0.03%	0.004%
91	14.133	2139	2140	2143	rVB2	501	358	0.03%	0.004%
92	14.201	2149	2151	2153	rVB	501	321	0.03%	0.004%
93	14.243	2154	2158	2160	rVB2	325	318	0.03%	0.004%
94	14.316	2168	2170	2172	rBV	364	314	0.03%	0.004%
95	14.761	2240	2243	2244	rVB2	325	263	0.02%	0.003%
96	14.780	2244	2246	2249	rBV2	335	348	0.03%	0.004%
97	15.530	2366	2369	2373	rVB3	551	724	0.06%	0.008%
98	15.591	2377	2379	2380	rVB2	492	317	0.03%	0.004%
99	16.145	2467	2470	2471	rBV3	504	544	0.05%	0.006%
100	16.401	2511	2512	2514	rBV2	456	279	0.02%	0.003%

Sum of corrected areas: 8633299

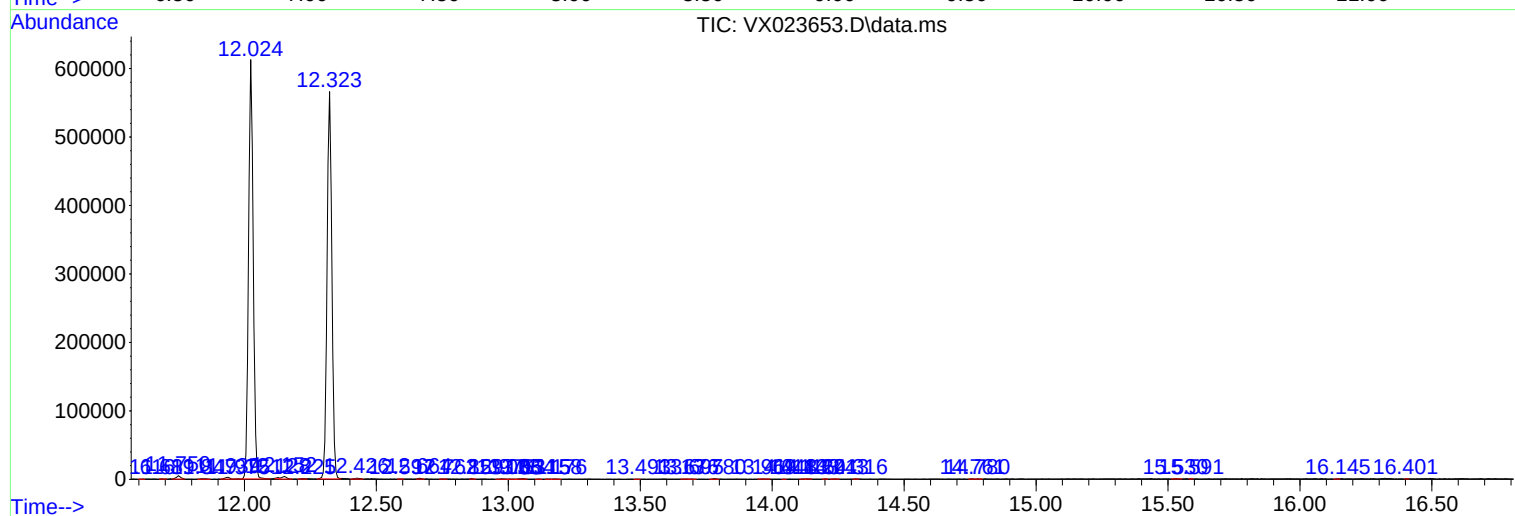
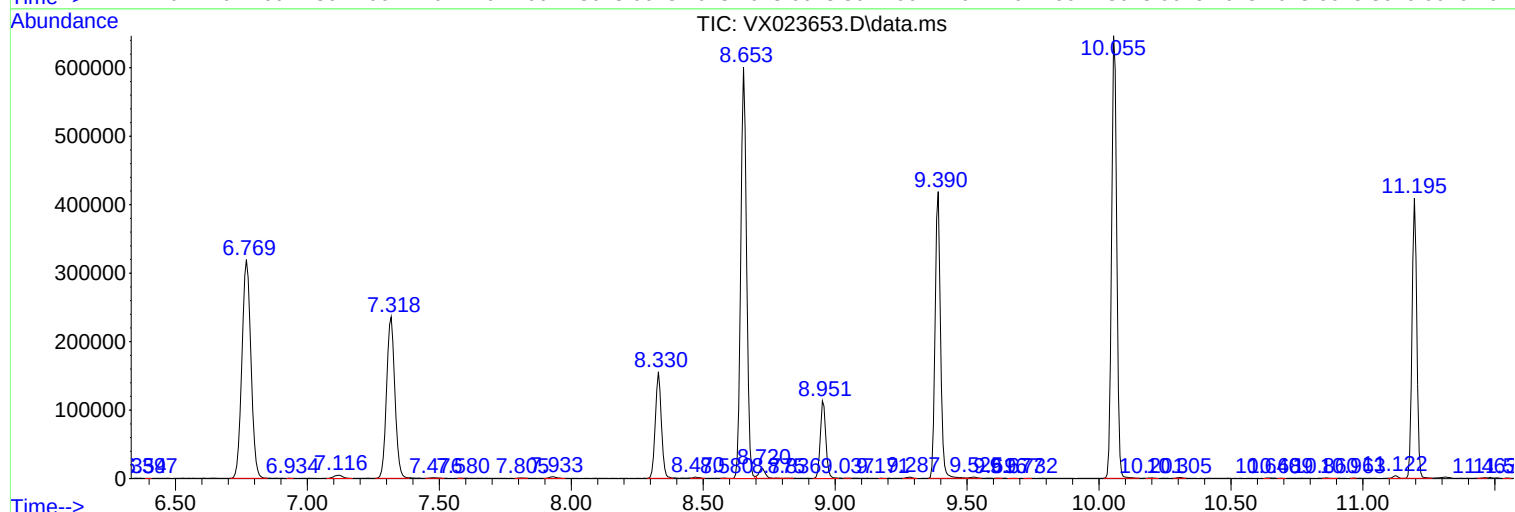
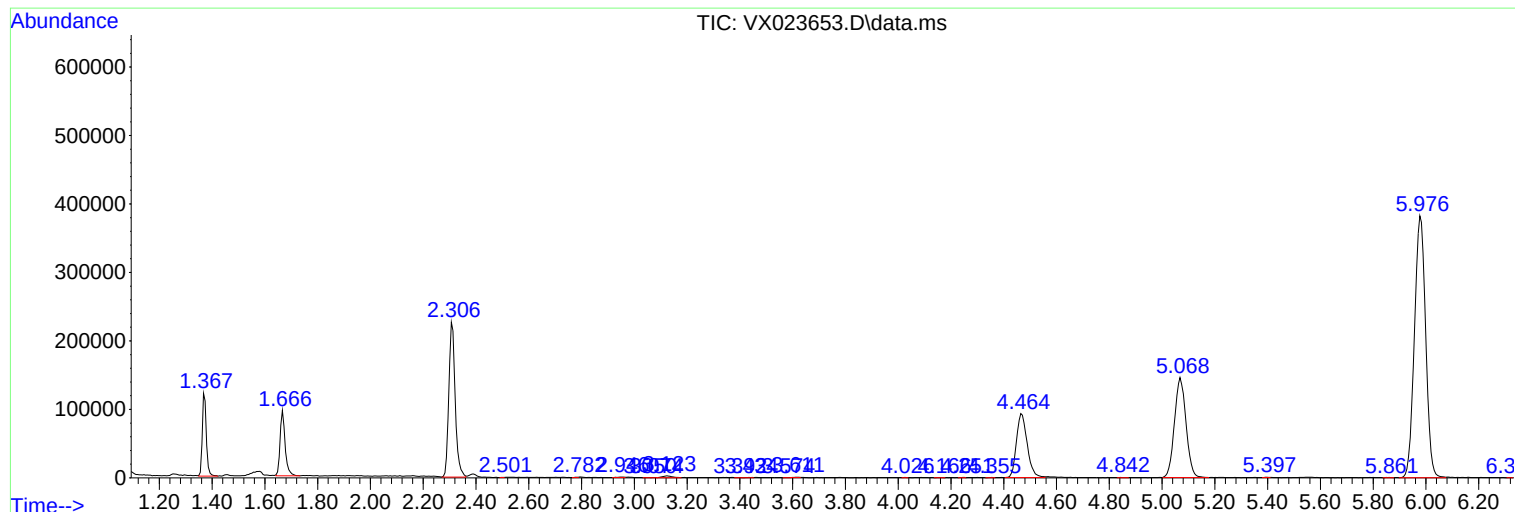
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081121\
Data File : VX023653.D
Acq On : 11 Aug 2021 16:53
Operator : JC/MD
Sample : M3364-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampled :
DBK82

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML081121WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081121\
Data File : VX023653.D
Acq On : 11 Aug 2021 16:53
Operator : JC/MD
Sample : M3364-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DBK82

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML081121WMA.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\VX081121\
Data File : VX023653.D
Acq On : 11 Aug 2021 16:53
Operator : JC/MD
Sample : M3364-03
Misc : 5.0mL/MSVOA_X/WATER
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
DBK82

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML081121WMA.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
