

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111224\
 Data File : VX043804.D
 Acq On : 12 Nov 2024 12:42
 Operator : JC/MD
 Sample : VX1112MBL01
 Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK723

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\SFAMXML110424WMA.M
 Title : VOC Analysis

Signal : TIC: VX043804.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.239	22	25	32	rVB2	8396	10363	1.24%	0.162%
2	1.367	42	46	57	rBV	72453	99059	11.81%	1.547%
3	1.642	88	91	104	rVB	53668	105173	12.54%	1.642%
4	2.294	192	198	207	rBV	167014	258940	30.88%	4.044%
5	2.733	267	270	274	rBV2	404	676	0.08%	0.011%
6	2.940	300	304	311	rVB	2350	5175	0.62%	0.081%
7	3.129	333	335	339	rVB2	351	494	0.06%	0.008%
8	3.203	345	347	351	rVB2	298	394	0.05%	0.006%
9	3.434	378	385	394	rVB3	3481	8413	1.00%	0.131%
10	3.507	394	397	398	rVV2	381	335	0.04%	0.005%
11	3.526	398	400	403	rVB	329	304	0.04%	0.005%
12	3.623	411	416	420	rBV3	300	502	0.06%	0.008%
13	3.672	422	424	426	rVB2	358	294	0.04%	0.005%
14	3.739	433	435	440	rVB	440	528	0.06%	0.008%
15	3.776	440	441	444	rBV2	406	374	0.04%	0.006%
16	3.824	447	449	453	rVB2	367	419	0.05%	0.007%
17	3.995	475	477	478	rBV2	417	373	0.04%	0.006%
18	4.093	490	493	496	rBV3	283	487	0.06%	0.008%
19	4.178	503	507	508	rBV2	342	323	0.04%	0.005%
20	4.464	546	554	574	rBV	48733	161861	19.31%	2.528%
21	4.830	612	614	615	rBV	346	290	0.03%	0.005%
22	4.940	629	632	637	rVB2	374	479	0.06%	0.007%
23	5.050	639	650	663	rBV	110176	336866	40.18%	5.261%
24	5.379	700	704	708	rBV3	733	1620	0.19%	0.025%
25	5.544	724	731	733	rBV3	623	1269	0.15%	0.020%
26	5.702	756	757	761	rVB2	359	410	0.05%	0.006%
27	5.848	779	781	783	rBV2	355	344	0.04%	0.005%
28	5.964	788	800	817	rBV3	283136	838427	100.00%	13.093%
29	6.385	868	869	871	rBV	383	308	0.04%	0.005%
30	6.501	886	888	890	rVV	369	329	0.04%	0.005%
31	6.543	893	895	898	rVV2	365	338	0.04%	0.005%
32	6.574	898	900	902	rVB2	285	298	0.04%	0.005%
33	6.757	920	930	949	rBV	229383	563107	67.16%	8.794%
34	7.123	983	990	1004	rBV5	14404	35443	4.23%	0.553%
35	7.305	1011	1020	1036	rBV2	170915	379250	45.23%	5.922%
36	7.440	1041	1042	1044	rVV2	493	424	0.05%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111224\
 Data File : VX043804.D
 Acq On : 12 Nov 2024 12:42
 Operator : JC/MD
 Sample : VX1112MBL01
 Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK723

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\SFAMXLM110424WMA.M
 Title : VOC Analysis

37	7.476	1047	1048	1051	rVV2	771	692	0.08%	0.011%
38	7.525	1054	1056	1060	rBV2	525	836	0.10%	0.013%
39	7.714	1081	1087	1090	rBV2	312	729	0.09%	0.011%
40	7.878	1111	1114	1118	rBV2	514	676	0.08%	0.011%
41	7.952	1125	1126	1128	rBV	382	363	0.04%	0.006%
42	8.189	1163	1165	1167	rVB	369	351	0.04%	0.005%
43	8.214	1167	1169	1172	rBV	360	538	0.06%	0.008%
44	8.324	1181	1187	1203	rBV	106737	182385	21.75%	2.848%
45	8.598	1229	1232	1233	rBV	716	398	0.05%	0.006%
46	8.647	1233	1240	1256	rBV	414949	673382	80.31%	10.516%
47	8.951	1284	1290	1303	rBV	70891	115339	13.76%	1.801%
48	9.043	1303	1305	1307	rVV2	506	518	0.06%	0.008%
49	9.092	1311	1313	1316	rVB2	376	338	0.04%	0.005%
50	9.275	1340	1343	1345	rBV2	377	430	0.05%	0.007%
51	9.384	1356	1361	1384	rBV	221715	371707	44.33%	5.805%
52	9.646	1402	1404	1406	rVB2	543	466	0.06%	0.007%
53	9.701	1409	1413	1417	rVV5	743	1430	0.17%	0.022%
54	9.872	1438	1441	1442	rVV	432	383	0.05%	0.006%
55	10.012	1462	1464	1465	rBV2	458	335	0.04%	0.005%
56	10.055	1465	1471	1483	rBV	434656	637367	76.02%	9.953%
57	10.244	1498	1502	1507	rBV2	420	716	0.09%	0.011%
58	10.287	1507	1509	1511	rBV2	378	294	0.04%	0.005%
59	10.384	1522	1525	1526	rVB2	431	381	0.05%	0.006%
60	10.476	1539	1540	1543	rVV2	331	305	0.04%	0.005%
61	10.543	1546	1551	1552	rVB2	259	341	0.04%	0.005%
62	10.640	1563	1567	1568	rBV	323	354	0.04%	0.006%
63	10.744	1581	1584	1586	rBV2	321	383	0.05%	0.006%
64	10.890	1606	1608	1613	rVB2	418	660	0.08%	0.010%
65	10.927	1613	1614	1617	rVB	414	285	0.03%	0.004%
66	11.061	1635	1636	1640	rVV2	356	384	0.05%	0.006%
67	11.189	1652	1657	1667	rBV	332367	430134	51.30%	6.717%
68	11.317	1676	1678	1682	rVB3	495	492	0.06%	0.008%
69	11.360	1682	1685	1686	rBV2	253	281	0.03%	0.004%
70	11.378	1686	1688	1689	rBV2	348	347	0.04%	0.005%
71	11.506	1707	1709	1712	rVB2	360	319	0.04%	0.005%
72	11.707	1740	1742	1746	rBV	388	370	0.04%	0.006%
73	11.744	1746	1748	1751	rVB2	583	596	0.07%	0.009%
74	11.829	1761	1762	1763	rBV	557	320	0.04%	0.005%
75	12.018	1788	1793	1803	rBV	428255	560622	66.87%	8.755%
76	12.317	1837	1842	1855	rBV	463438	589830	70.35%	9.211%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111224\
 Data File : VX043804.D
 Acq On : 12 Nov 2024 12:42
 Operator : JC/MD
 Sample : VX1112MBL01
 Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK723

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\SFAMXML110424WMA.M
 Title : VOC Analysis

77	12.646	1895	1896	1900	rVB2	479	405	0.05%	0.006%
78	12.689	1900	1903	1904	rBV	446	506	0.06%	0.008%
79	12.762	1910	1915	1918	rBV2	759	1314	0.16%	0.021%
80	13.134	1973	1976	1977	rBV2	405	373	0.04%	0.006%
81	13.426	2022	2024	2026	rVB2	421	301	0.04%	0.005%
82	13.469	2029	2031	2033	rVV	340	292	0.03%	0.005%
83	13.566	2043	2047	2049	rBV2	287	485	0.06%	0.008%
84	13.792	2082	2084	2086	rVV2	444	311	0.04%	0.005%
85	13.944	2106	2109	2112	rVB2	738	695	0.08%	0.011%
86	13.981	2112	2115	2118	rBV3	413	611	0.07%	0.010%
87	14.024	2120	2122	2125	rVV2	459	348	0.04%	0.005%
88	14.060	2125	2128	2132	rVV2	347	416	0.05%	0.006%
89	14.127	2136	2139	2145	rVB	1516	1988	0.24%	0.031%
90	14.170	2145	2146	2148	rVB2	512	347	0.04%	0.005%
91	14.201	2148	2151	2153	rBV3	288	446	0.05%	0.007%
92	14.316	2168	2170	2174	rVB2	668	890	0.11%	0.014%
93	14.682	2229	2230	2232	rVB2	489	344	0.04%	0.005%
94	14.737	2236	2239	2240	rBV2	402	352	0.04%	0.005%
95	14.786	2245	2247	2248	rBV	465	318	0.04%	0.005%
96	15.011	2280	2284	2286	rBV2	460	710	0.08%	0.011%
97	15.371	2342	2343	2346	rBV3	829	852	0.10%	0.013%
98	15.749	2402	2405	2407	rBV2	480	470	0.06%	0.007%
99	16.517	2528	2531	2532	rVV2	646	499	0.06%	0.008%
100	16.584	2541	2542	2544	rBV2	721	611	0.07%	0.010%

Sum of corrected areas: 6403650

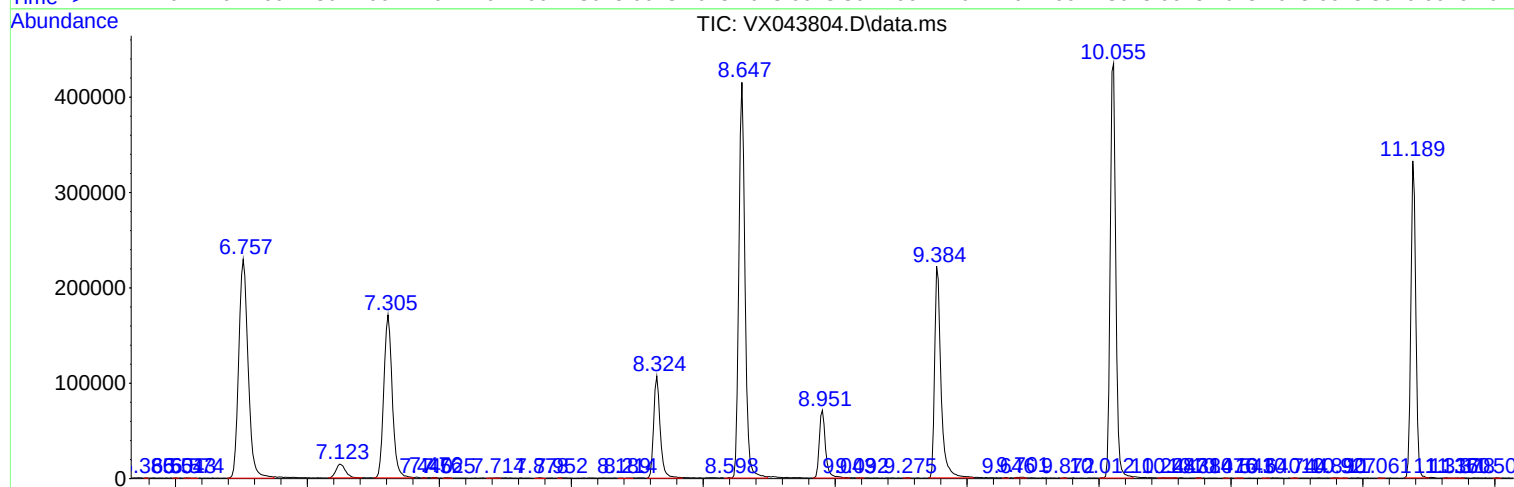
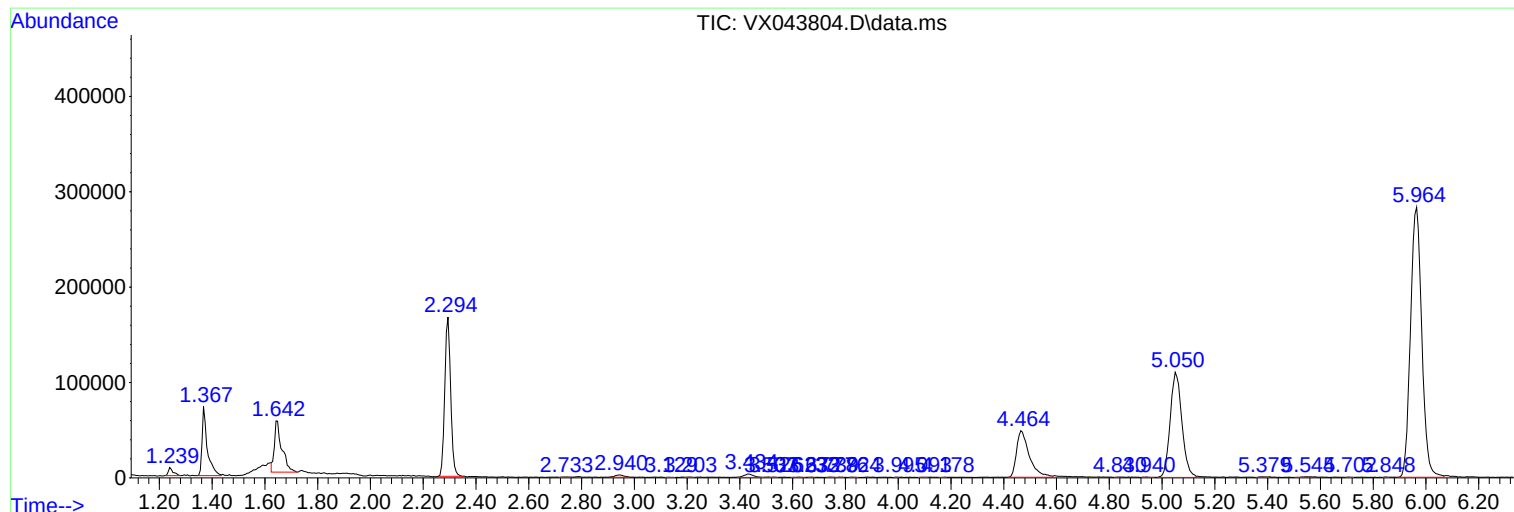
Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111224\
Data File : VX043804.D
Acq On : 12 Nov 2024 12:42
Operator : JC/MD
Sample : VX1112MBL01
Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK723

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXLM110424WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111224\
Data File : VX043804.D
Acq On : 12 Nov 2024 12:42
Operator : JC/MD
Sample : VX1112MBL01
Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK723

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML110424WMA.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\VX111224\
Data File : VX043804.D
Acq On : 12 Nov 2024 12:42
Operator : JC/MD
Sample : VX1112MBL01
Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK723

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML110424WMA.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