

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111324\
 Data File : VX043829.D
 Acq On : 13 Nov 2024 11:58
 Operator : JC/MD
 Sample : VX1113MBL01
 Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK725

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: VX043829.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.240	22	25	27	rBV	5270	6156	0.88%	0.106%
2	1.368	43	46	58	rBV	62976	80999	11.64%	1.391%
3	1.642	88	91	108	rVB	58845	113043	16.25%	1.941%
4	2.294	192	198	206	rBV	138036	210954	30.32%	3.623%
5	2.380	210	212	214	rVB3	713	530	0.08%	0.009%
6	2.495	229	231	237	rVB	1534	2161	0.31%	0.037%
7	2.782	272	278	285	rVB7	1438	3416	0.49%	0.059%
8	2.831	285	286	289	rBV3	289	335	0.05%	0.006%
9	2.940	296	304	310	rBV3	3530	8780	1.26%	0.151%
10	3.087	324	328	335	rVV5	1424	2996	0.43%	0.051%
11	3.136	335	336	340	rVB4	617	550	0.08%	0.009%
12	3.270	357	358	363	rBV2	209	361	0.05%	0.006%
13	3.428	378	384	394	rVV5	2873	7119	1.02%	0.122%
14	3.666	421	423	426	rBV2	224	318	0.05%	0.005%
15	3.751	434	437	440	rVB2	299	321	0.05%	0.006%
16	3.794	442	444	447	rBV	288	311	0.04%	0.005%
17	4.020	479	481	484	rVB2	331	298	0.04%	0.005%
18	4.166	502	505	507	rVB2	688	546	0.08%	0.009%
19	4.294	524	526	530	rBV	257	433	0.06%	0.007%
20	4.452	544	552	568	rBV	44177	139132	20.00%	2.389%
21	4.843	614	616	619	rBV	337	380	0.05%	0.007%
22	5.050	637	650	670	rBV	94641	295101	42.41%	5.068%
23	5.233	677	680	683	rVB2	324	315	0.05%	0.005%
24	5.318	692	694	696	rBV3	328	314	0.05%	0.005%
25	5.379	700	704	705	rBV2	497	628	0.09%	0.011%
26	5.397	705	707	711	rVB3	643	650	0.09%	0.011%
27	5.544	727	731	732	rVV3	475	544	0.08%	0.009%
28	5.660	746	750	755	rBV4	360	754	0.11%	0.013%
29	5.775	766	769	771	rBV2	321	377	0.05%	0.006%
30	5.830	776	778	782	rBV3	244	298	0.04%	0.005%
31	5.958	788	799	824	rVV2	229061	695769	100.00%	11.949%
32	6.336	859	861	863	rVB2	355	321	0.05%	0.006%
33	6.373	865	867	870	rVV2	378	317	0.05%	0.005%
34	6.403	870	872	875	rVV3	333	306	0.04%	0.005%
35	6.446	877	879	882	rVV	306	354	0.05%	0.006%
36	6.647	909	912	915	rVB3	266	389	0.06%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111324\
 Data File : VX043829.D
 Acq On : 13 Nov 2024 11:58
 Operator : JC/MD
 Sample : VX1113MBL01
 Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK725

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	6.672	915	916	919	rVB2	366	358	0.05%	0.006%
38	6.751	920	929	955	rBV	228943	559489	80.41%	9.608%
39	7.123	979	990	1004	rBV7	5051	14458	2.08%	0.248%
40	7.299	1009	1019	1036	rBV	144100	322018	46.28%	5.530%
41	7.568	1061	1063	1066	rBV3	406	578	0.08%	0.010%
42	7.726	1087	1089	1096	rVB	281	364	0.05%	0.006%
43	8.031	1135	1139	1142	rVB2	242	339	0.05%	0.006%
44	8.318	1181	1186	1202	rBV	91957	161934	23.27%	2.781%
45	8.580	1226	1229	1233	rBV2	719	1363	0.20%	0.023%
46	8.641	1233	1239	1250	rBV	341683	559428	80.40%	9.607%
47	8.945	1284	1289	1301	rBV	65057	103696	14.90%	1.781%
48	9.067	1307	1309	1311	rBV	334	343	0.05%	0.006%
49	9.275	1339	1343	1347	rVB3	2041	2685	0.39%	0.046%
50	9.384	1356	1361	1379	rBV	208985	319439	45.91%	5.486%
51	9.616	1395	1399	1403	rBV5	683	1267	0.18%	0.022%
52	9.738	1417	1419	1422	rVB2	350	356	0.05%	0.006%
53	9.769	1422	1424	1427	rBV	583	512	0.07%	0.009%
54	10.049	1465	1470	1481	rBV	461620	644438	92.62%	11.067%
55	10.195	1490	1494	1502	rVB3	2071	3802	0.55%	0.065%
56	10.311	1508	1513	1519	rVB2	1949	2925	0.42%	0.050%
57	10.646	1564	1568	1569	rBV4	1882	2448	0.35%	0.042%
58	10.701	1575	1577	1580	rVB2	407	320	0.05%	0.005%
59	10.732	1580	1582	1584	rVB2	463	401	0.06%	0.007%
60	10.902	1607	1610	1613	rBV2	304	417	0.06%	0.007%
61	10.970	1616	1621	1624	rBV2	2095	2660	0.38%	0.046%
62	11.189	1652	1657	1664	rBV	302225	382268	54.94%	6.565%
63	11.317	1676	1678	1679	rBV2	510	414	0.06%	0.007%
64	11.457	1694	1701	1705	rBV4	2061	3242	0.47%	0.056%
65	11.524	1709	1712	1714	rVB2	260	304	0.04%	0.005%
66	11.750	1746	1749	1756	rVB3	1979	2978	0.43%	0.051%
67	11.866	1766	1768	1771	rBV2	347	445	0.06%	0.008%
68	11.975	1781	1786	1788	rBV2	2950	3535	0.51%	0.061%
69	12.018	1788	1793	1805	rVB	464897	591012	84.94%	10.150%
70	12.225	1826	1827	1830	rBV2	426	469	0.07%	0.008%
71	12.317	1837	1842	1852	rBV	406605	523960	75.31%	8.998%
72	12.530	1875	1877	1881	rVB	505	535	0.08%	0.009%
73	12.579	1883	1885	1888	rVV3	438	341	0.05%	0.006%
74	12.609	1888	1890	1894	rVB2	428	409	0.06%	0.007%
75	12.640	1894	1895	1897	rBV	371	331	0.05%	0.006%
76	12.744	1907	1912	1914	rBV4	347	710	0.10%	0.012%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111324\
 Data File : VX043829.D
 Acq On : 13 Nov 2024 11:58
 Operator : JC/MD
 Sample : VX1113MBL01
 Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 3 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 VBLK725

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	12.762	1914	1915	1919	rVV2	583	549	0.08%	0.009%
78	12.896	1934	1937	1939	rBV2	333	360	0.05%	0.006%
79	13.115	1970	1973	1978	rVB3	2344	3120	0.45%	0.054%
80	13.207	1985	1988	1990	rVB	447	352	0.05%	0.006%
81	13.237	1990	1993	1994	rBV	276	302	0.04%	0.005%
82	13.390	2016	2018	2020	rBV	364	330	0.05%	0.006%
83	13.500	2034	2036	2040	rBV3	321	428	0.06%	0.007%
84	13.591	2046	2051	2057	rVB4	2209	4104	0.59%	0.070%
85	13.780	2074	2082	2087	rBV	4378	7644	1.10%	0.131%
86	13.963	2107	2112	2117	rBV3	2883	4180	0.60%	0.072%
87	14.067	2126	2129	2132	rBV2	430	581	0.08%	0.010%
88	14.127	2137	2139	2143	rVV3	1209	1387	0.20%	0.024%
89	14.176	2145	2147	2150	rVV2	412	487	0.07%	0.008%
90	14.256	2156	2160	2162	rBV4	396	438	0.06%	0.008%
91	14.377	2178	2180	2182	rBV3	337	356	0.05%	0.006%
92	14.493	2197	2199	2201	rBV2	353	396	0.06%	0.007%
93	14.640	2221	2223	2224	rBV	388	330	0.05%	0.006%
94	14.896	2262	2265	2266	rBV2	422	528	0.08%	0.009%
95	15.103	2297	2299	2300	rBV	664	471	0.07%	0.008%
96	15.255	2322	2324	2330	rBV4	416	767	0.11%	0.013%
97	15.377	2342	2344	2345	rBV	547	422	0.06%	0.007%
98	15.731	2399	2402	2407	rVB2	718	1053	0.15%	0.018%
99	16.597	2541	2544	2547	rBV3	667	948	0.14%	0.016%
100	16.749	2567	2569	2573	rVB5	887	889	0.13%	0.015%

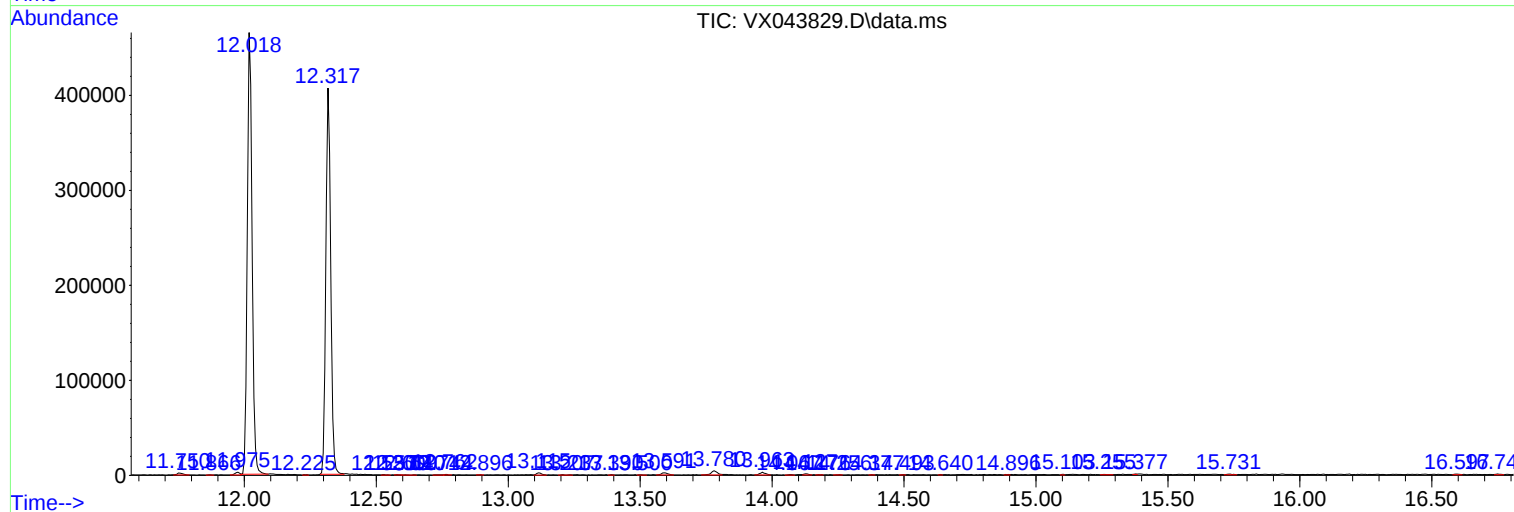
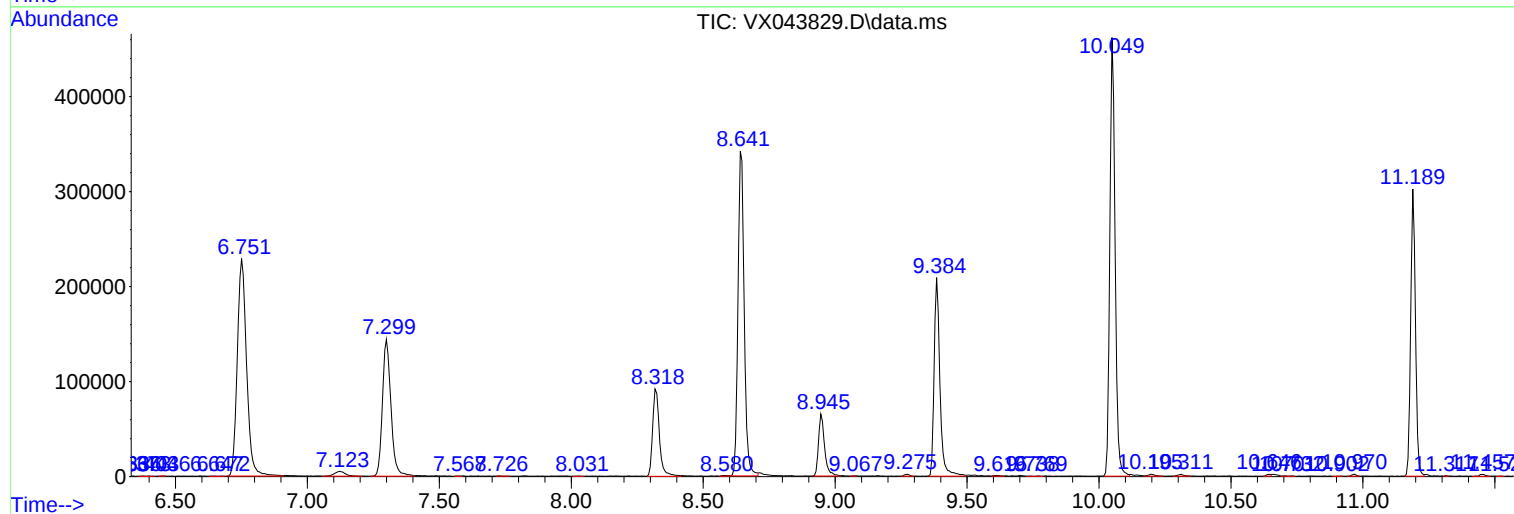
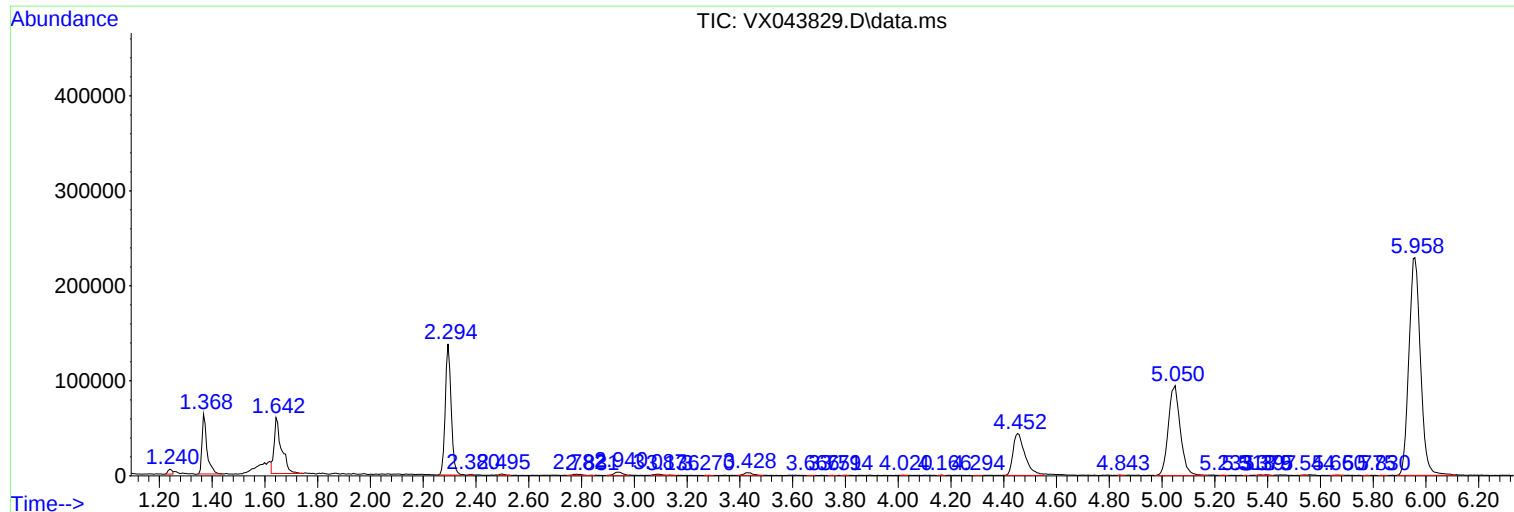
Sum of corrected areas: 5822989

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111324\
Data File : VX043829.D
Acq On : 13 Nov 2024 11:58
Operator : JC/MD
Sample : VX1113MBL01
Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK725

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX111324\
Data File : VX043829.D
Acq On : 13 Nov 2024 11:58
Operator : JC/MD
Sample : VX1113MBL01
Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK725

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\VX111324\
Data File : VX043829.D
Acq On : 13 Nov 2024 11:58
Operator : JC/MD
Sample : VX1113MBL01
Misc : 5.00g/5mL/100uL/5.00mL/MSVOA_X/MEOH
ALS Vial : 3 Sample Multiplier: 1

Instrument :
MSVOA_X
ClientSampleId :
VBLK725

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