

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052424\
 Data File : VU058977.D
 Acq On : 24 May 2024 17:45
 Operator : MD/SY
 Sample : P2568-03ME
 Misc : 6.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH5Q6ME

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_U\Method\SFAMULM052324WMA.M

Title : VOC Analysis

Signal : TIC: VU058977.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.476	54	58	65	rVB2	6190	6470	0.74%	0.098%
2	1.592	86	94	121	rVB	69234	122872	14.14%	1.863%
3	1.843	136	172	174	rBV5	57771	267733	30.81%	4.060%
4	2.531	374	386	406	rBV	167246	274478	31.59%	4.162%
5	3.026	531	540	551	rVB5	4780	8800	1.01%	0.133%
6	3.171	570	585	601	rBV2	10177	26508	3.05%	0.402%
7	3.312	628	629	635	rVV3	447	401	0.05%	0.006%
8	3.338	635	637	639	rVV2	483	242	0.03%	0.004%
9	3.370	643	647	650	rVB2	854	723	0.08%	0.011%
10	3.396	650	655	659	rBV2	316	292	0.03%	0.004%
11	3.669	734	740	745	rVB3	775	899	0.10%	0.014%
12	3.769	768	771	776	rVB2	315	273	0.03%	0.004%
13	3.836	789	792	796	rVB2	274	221	0.03%	0.003%
14	4.020	843	849	855	rBV	305	384	0.04%	0.006%
15	4.177	892	898	901	rBV2	207	255	0.03%	0.004%
16	4.264	921	925	929	rVB2	253	207	0.02%	0.003%
17	4.367	954	957	961	rVB2	302	248	0.03%	0.004%
18	4.412	967	971	975	rVB2	295	208	0.02%	0.003%
19	4.441	975	980	982	rBV	295	219	0.03%	0.003%
20	4.624	1027	1037	1076	rBV	72061	231724	26.67%	3.514%
21	4.891	1117	1120	1125	rVB2	450	369	0.04%	0.006%
22	4.936	1131	1134	1140	rVB3	279	255	0.03%	0.004%
23	5.052	1153	1170	1192	rBV2	146522	337517	38.84%	5.118%
24	5.447	1289	1293	1296	rBV	351	223	0.03%	0.003%
25	5.541	1319	1322	1328	rBV2	199	212	0.02%	0.003%
26	5.608	1340	1343	1346	rVB	319	209	0.02%	0.003%
27	5.631	1346	1350	1356	rBV2	326	295	0.03%	0.004%
28	5.711	1356	1375	1402	rBV2	330774	868987	100.00%	13.177%
29	5.971	1447	1456	1457	rBV3	2146	2504	0.29%	0.038%
30	6.052	1476	1481	1486	rVB2	229	272	0.03%	0.004%
31	6.110	1494	1499	1502	rBV2	322	277	0.03%	0.004%
32	6.238	1526	1539	1561	rBV	239870	472866	54.42%	7.170%
33	6.367	1576	1579	1582	rBV2	423	249	0.03%	0.004%
34	6.460	1605	1608	1613	rVB2	324	245	0.03%	0.004%
35	6.531	1618	1630	1642	rBV8	8786	18061	2.08%	0.274%
36	6.592	1642	1649	1653	rBV5	3271	4605	0.53%	0.070%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052424\
 Data File : VU058977.D
 Acq On : 24 May 2024 17:45
 Operator : MD/SY
 Sample : P2568-03ME
 Misc : 6.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH5Q6ME

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_U\Method\SFAMULM052324WMA.M
 Title : VOC Analysis

37	6.682	1664	1677	1698	rBV	196552	392689	45.19%	5.954%
38	6.807	1709	1716	1720	rVB4	553	605	0.07%	0.009%
39	7.052	1788	1792	1797	rVB2	289	252	0.03%	0.004%
40	7.084	1797	1802	1805	rVB2	270	257	0.03%	0.004%
41	7.116	1805	1812	1816	rBV2	223	279	0.03%	0.004%
42	7.139	1816	1819	1824	rBV2	215	210	0.02%	0.003%
43	7.222	1841	1845	1850	rBV4	658	738	0.08%	0.011%
44	7.270	1855	1860	1865	rBV2	303	302	0.03%	0.005%
45	7.360	1886	1888	1893	rVB2	422	237	0.03%	0.004%
46	7.434	1907	1911	1916	rBV	341	263	0.03%	0.004%
47	7.495	1925	1930	1935	rVB3	629	572	0.07%	0.009%
48	7.560	1935	1950	1973	rBV	94834	179254	20.63%	2.718%
49	7.724	1997	2001	2006	rBV3	391	451	0.05%	0.007%
50	7.782	2014	2019	2024	rVB3	436	446	0.05%	0.007%
51	7.891	2040	2053	2075	rBV	359173	638357	73.46%	9.680%
52	8.174	2130	2141	2167	rVB	64204	120580	13.88%	1.828%
53	8.267	2167	2170	2172	rBV2	388	248	0.03%	0.004%
54	8.338	2187	2192	2194	rBV	411	331	0.04%	0.005%
55	8.351	2194	2196	2199	rVB	479	281	0.03%	0.004%
56	8.457	2221	2229	2235	rBV2	517	871	0.10%	0.013%
57	8.643	2271	2287	2323	rBV	174512	474601	54.62%	7.197%
58	9.007	2398	2400	2406	rVB2	320	249	0.03%	0.004%
59	9.235	2468	2471	2477	rVB	207	235	0.03%	0.004%
60	9.267	2477	2481	2486	rBV2	282	236	0.03%	0.004%
61	9.415	2514	2527	2548	rBV	328325	598962	68.93%	9.082%
62	9.540	2562	2566	2570	rVB4	339	275	0.03%	0.004%
63	9.569	2570	2575	2580	rBV4	628	668	0.08%	0.010%
64	9.656	2599	2602	2605	rVV2	391	258	0.03%	0.004%
65	9.698	2607	2615	2630	rVB3	2050	3621	0.42%	0.055%
66	9.833	2654	2657	2662	rVV2	247	256	0.03%	0.004%
67	9.978	2699	2702	2707	rVB2	310	256	0.03%	0.004%
68	10.007	2707	2711	2716	rVB2	351	398	0.05%	0.006%
69	10.058	2722	2727	2731	rVB2	284	285	0.03%	0.004%
70	10.100	2735	2740	2750	rBV3	537	874	0.10%	0.013%
71	10.142	2750	2753	2755	rVV	371	224	0.03%	0.003%
72	10.319	2805	2808	2810	rBV	312	221	0.03%	0.003%
73	10.502	2861	2865	2871	rBV2	245	317	0.04%	0.005%
74	10.756	2924	2944	2960	rBV	277338	475759	54.75%	7.214%
75	10.884	2980	2984	2987	rBV3	531	445	0.05%	0.007%
76	11.109	3050	3054	3059	rVB3	374	334	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052424\
 Data File : VU058977.D
 Acq On : 24 May 2024 17:45
 Operator : MD/SY
 Sample : P2568-03ME
 Misc : 6.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BH5Q6ME

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_U\Method\SFAMULM052324WMA.M
 Title : VOC Analysis

77	11.267	3098	3103	3106	rBV2	261	264	0.03%	0.004%
78	11.380	3135	3138	3144	rVB2	251	218	0.03%	0.003%
79	11.810	3260	3272	3300	rBV	317214	517848	59.59%	7.852%
80	12.190	3378	3390	3417	rBV	309798	521715	60.04%	7.911%
81	12.380	3447	3449	3453	rBV2	434	294	0.03%	0.004%
82	12.502	3482	3487	3490	rBV2	434	371	0.04%	0.006%
83	12.617	3520	3523	3528	rBV	380	293	0.03%	0.004%
84	12.701	3546	3549	3556	rVB2	390	394	0.05%	0.006%
85	12.753	3562	3565	3567	rBV	579	402	0.05%	0.006%
86	12.823	3581	3587	3590	rBV2	273	340	0.04%	0.005%
87	13.138	3682	3685	3688	rBV	317	217	0.02%	0.003%
88	13.315	3737	3740	3743	rBV2	263	207	0.02%	0.003%
89	13.714	3861	3864	3866	rBV	415	283	0.03%	0.004%
90	13.855	3904	3908	3915	rBV2	595	660	0.08%	0.010%
91	14.122	3986	3991	3992	rBV2	559	472	0.05%	0.007%
92	14.396	4070	4076	4079	rBV2	443	529	0.06%	0.008%
93	14.469	4095	4099	4102	rBV2	521	372	0.04%	0.006%
94	14.743	4181	4184	4186	rBV2	403	254	0.03%	0.004%
95	15.418	4392	4394	4398	rBV2	600	363	0.04%	0.006%
96	15.859	4528	4531	4532	rBV2	566	330	0.04%	0.005%
97	15.910	4543	4547	4555	rBV3	1069	1437	0.17%	0.022%
98	16.164	4623	4626	4629	rVB2	862	500	0.06%	0.008%
99	16.183	4629	4632	4634	rBV2	782	567	0.07%	0.009%
100	16.318	4671	4674	4679	rBV2	582	507	0.06%	0.008%

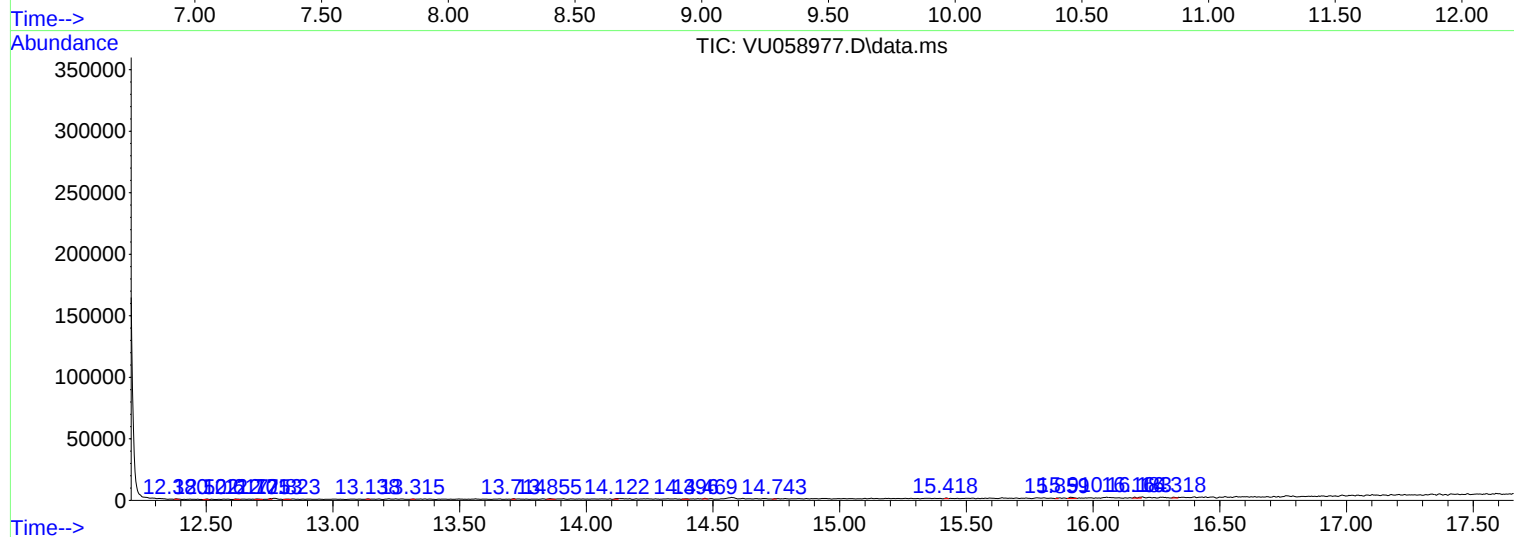
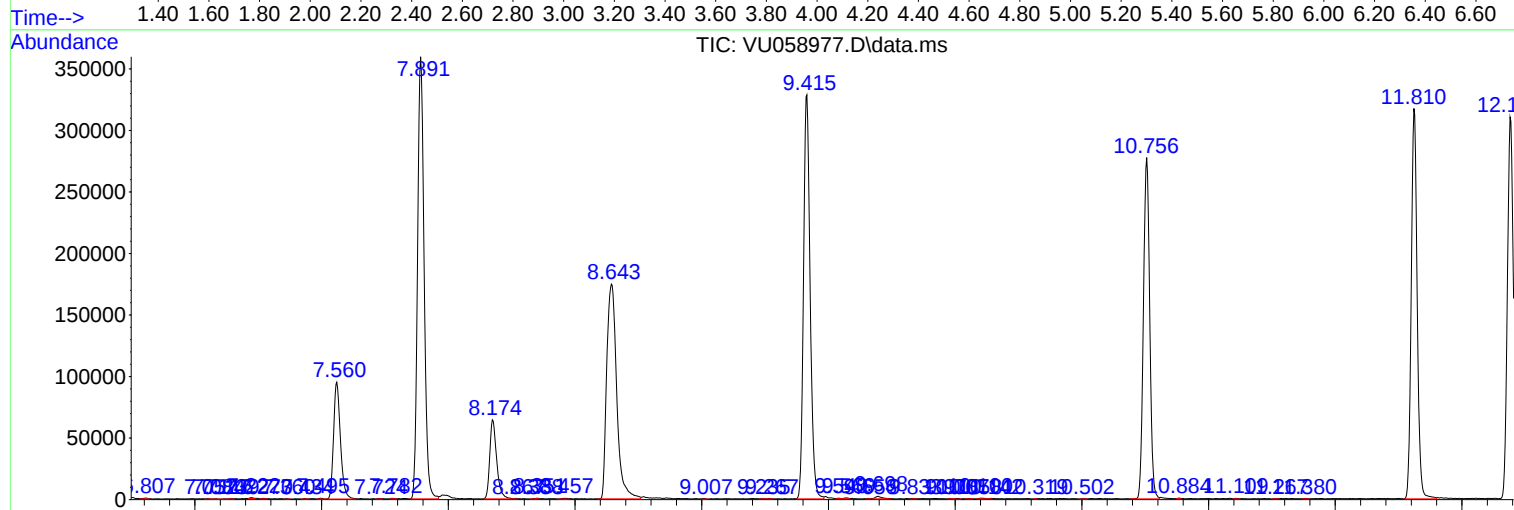
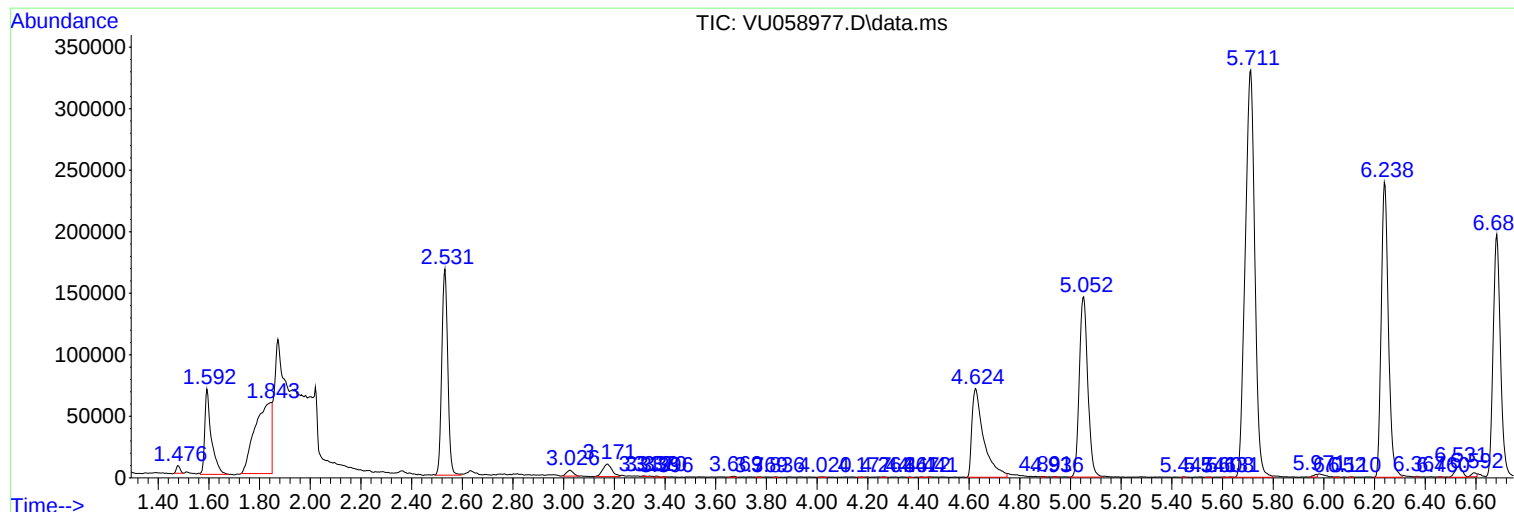
Sum of corrected areas: 6594837

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052424\
Data File : VU058977.D
Acq On : 24 May 2024 17:45
Operator : MD/SY
Sample : P2568-03ME
Misc : 6.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH5Q6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052424\
Data File : VU058977.D
Acq On : 24 May 2024 17:45
Operator : MD/SY
Sample : P2568-03ME
Misc : 6.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH5Q6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.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_U\Data\VU052424\
Data File : VU058977.D
Acq On : 24 May 2024 17:45
Operator : MD/SY
Sample : P2568-03ME
Misc : 6.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BH5Q6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052324WMA.M
Quant Title : VOC Analysis

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

TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
------------------	----	---------	-------	----------	---	----	------	------