

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059308.D
 Acq On : 18 Jun 2024 13:40
 Operator : MD/SY
 Sample : P2775-09ME
 Misc : 3.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4C87ME

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\SFAMULM052924WMA.M
 Title : VOC Analysis

Signal : TIC: VU059308.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	87	95	111	rVB	59659	70037	12.73%	1.599%
2	1.679	119	121	124	rBV2	813	458	0.08%	0.010%
3	1.759	140	146	156	rBV2	3928	5356	0.97%	0.122%
4	1.907	184	192	208	rBV	54310	74937	13.62%	1.711%
5	2.560	383	395	410	rBV	97504	159986	29.09%	3.653%
6	2.727	439	447	448	rBV	300	333	0.06%	0.008%
7	3.039	533	544	556	rVB3	6568	12791	2.33%	0.292%
8	3.091	556	560	563	rVB2	279	204	0.04%	0.005%
9	3.139	571	575	577	rBV	295	204	0.04%	0.005%
10	3.174	582	586	588	rBV2	380	337	0.06%	0.008%
11	3.345	635	639	644	rBV2	338	384	0.07%	0.009%
12	3.573	705	710	714	rBV2	220	294	0.05%	0.007%
13	3.717	752	755	758	rBV	207	197	0.04%	0.004%
14	3.859	796	799	805	rVB2	199	199	0.04%	0.005%
15	3.926	812	820	822	rBV2	302	447	0.08%	0.010%
16	4.026	848	851	853	rBV	251	206	0.04%	0.005%
17	4.219	905	911	915	rVB2	359	443	0.08%	0.010%
18	4.242	915	918	920	rBV2	269	223	0.04%	0.005%
19	4.441	976	980	984	rBV2	333	329	0.06%	0.008%
20	4.486	989	994	996	rBV2	317	309	0.06%	0.007%
21	4.615	1024	1034	1069	rBV	56396	144402	26.25%	3.297%
22	5.000	1151	1154	1156	rBV	431	337	0.06%	0.008%
23	5.055	1156	1171	1200	rVB	100682	225105	40.92%	5.140%
24	5.467	1296	1299	1304	rBV2	236	292	0.05%	0.007%
25	5.576	1329	1333	1338	rBV2	320	389	0.07%	0.009%
26	5.624	1342	1348	1351	rBV	296	327	0.06%	0.007%
27	5.717	1357	1377	1402	rBV2	198226	550048	100.00%	12.560%
28	5.872	1422	1425	1429	rVB2	435	334	0.06%	0.008%
29	5.930	1439	1443	1447	rVB2	322	341	0.06%	0.008%
30	5.962	1451	1453	1455	rBV	290	194	0.04%	0.004%
31	6.007	1460	1467	1471	rBV	179	256	0.05%	0.006%
32	6.245	1528	1541	1565	rBV	194674	379689	69.03%	8.670%
33	6.377	1575	1582	1586	rVV2	323	441	0.08%	0.010%
34	6.399	1586	1589	1592	rVB2	287	227	0.04%	0.005%
35	6.531	1620	1630	1641	rBV6	4107	8175	1.49%	0.187%
36	6.685	1665	1678	1709	rBV	127670	253292	46.05%	5.784%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059308.D
 Acq On : 18 Jun 2024 13:40
 Operator : MD/SY
 Sample : P2775-09ME
 Misc : 3.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4C87ME

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\SFAMULM052924WMA.M
 Title : VOC Analysis

37	6.795	1709	1712	1716	rVV2	298	242	0.04%	0.006%
38	6.817	1716	1719	1724	rVV2	506	360	0.07%	0.008%
39	6.910	1744	1748	1752	rBV2	259	353	0.06%	0.008%
40	6.959	1756	1763	1768	rBV2	304	454	0.08%	0.010%
41	7.007	1774	1778	1783	rVB	287	241	0.04%	0.006%
42	7.049	1788	1791	1798	rVB	321	354	0.06%	0.008%
43	7.200	1829	1838	1848	rBV4	1205	2091	0.38%	0.048%
44	7.286	1861	1865	1867	rBV2	251	231	0.04%	0.005%
45	7.338	1877	1881	1885	rBV	344	346	0.06%	0.008%
46	7.518	1933	1937	1940	rBV	321	315	0.06%	0.007%
47	7.563	1940	1951	1971	rVV2	60389	108701	19.76%	2.482%
48	7.679	1985	1987	1990	rBV2	360	249	0.05%	0.006%
49	7.711	1990	1997	2001	rBV4	679	971	0.18%	0.022%
50	7.785	2017	2020	2022	rBV	287	200	0.04%	0.005%
51	7.894	2041	2054	2078	rBV	219957	393312	71.51%	8.981%
52	8.010	2087	2090	2093	rBV3	333	275	0.05%	0.006%
53	8.177	2132	2142	2163	rBV	40832	70702	12.85%	1.614%
54	8.306	2179	2182	2186	rVV	354	251	0.05%	0.006%
55	8.389	2203	2208	2210	rBV2	338	322	0.06%	0.007%
56	8.457	2225	2229	2230	rBV	418	321	0.06%	0.007%
57	8.534	2249	2253	2258	rBV2	250	288	0.05%	0.007%
58	8.630	2270	2283	2310	rBV2	136475	281289	51.14%	6.423%
59	8.823	2341	2343	2349	rVB2	288	276	0.05%	0.006%
60	8.926	2368	2375	2378	rBV	367	466	0.08%	0.011%
61	9.261	2475	2479	2487	rBV2	286	449	0.08%	0.010%
62	9.370	2508	2513	2515	rBV	235	234	0.04%	0.005%
63	9.412	2515	2526	2546	rBV	293629	499912	90.89%	11.415%
64	9.688	2608	2612	2616	rBV	359	309	0.06%	0.007%
65	10.119	2744	2746	2749	rVV	293	209	0.04%	0.005%
66	10.142	2750	2753	2756	rVV	291	244	0.04%	0.006%
67	10.367	2819	2823	2826	rBV2	283	303	0.06%	0.007%
68	10.479	2854	2858	2862	rBV2	293	255	0.05%	0.006%
69	10.605	2890	2897	2900	rBV2	302	410	0.07%	0.009%
70	10.682	2918	2921	2924	rBV	243	241	0.04%	0.006%
71	10.753	2930	2943	2961	rBV	193609	314756	57.22%	7.187%
72	10.888	2974	2985	2992	rBV5	1210	2284	0.42%	0.052%
73	10.939	2996	3001	3004	rBV2	259	290	0.05%	0.007%
74	11.093	3045	3049	3051	rBV2	245	214	0.04%	0.005%
75	11.167	3067	3072	3074	rBV2	224	197	0.04%	0.004%
76	11.245	3093	3096	3101	rVB2	346	324	0.06%	0.007%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
 Data File : VU059308.D
 Acq On : 18 Jun 2024 13:40
 Operator : MD/SY
 Sample : P2775-09ME
 Misc : 3.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 15 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 A4C87ME

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\SFAMULM052924WMA.M
 Title : VOC Analysis

77	11.277	3101	3106	3111	rBV2	325	410	0.07%	0.009%
78	11.740	3246	3250	3253	rBV2	290	271	0.05%	0.006%
79	11.810	3260	3272	3295	rBV	259298	435834	79.24%	9.952%
80	11.971	3319	3322	3328	rVB3	468	514	0.09%	0.012%
81	12.003	3329	3332	3337	rBV3	331	282	0.05%	0.006%
82	12.058	3347	3349	3353	rBV	284	216	0.04%	0.005%
83	12.190	3375	3390	3416	rBV	212573	360841	65.60%	8.239%
84	12.328	3430	3433	3441	rVB2	551	579	0.11%	0.013%
85	12.399	3449	3455	3458	rBV3	396	471	0.09%	0.011%
86	12.624	3522	3525	3527	rBV2	301	203	0.04%	0.005%
87	12.662	3533	3537	3539	rBV2	268	229	0.04%	0.005%
88	12.698	3545	3548	3553	rBV2	355	418	0.08%	0.010%
89	12.759	3564	3567	3569	rBV3	502	362	0.07%	0.008%
90	12.843	3589	3593	3598	rBV2	336	386	0.07%	0.009%
91	13.396	3759	3765	3766	rBV	248	249	0.05%	0.006%
92	13.852	3904	3907	3911	rBV3	327	256	0.05%	0.006%
93	14.257	4030	4033	4036	rBV	393	311	0.06%	0.007%
94	14.560	4123	4127	4128	rBV	431	318	0.06%	0.007%
95	14.685	4163	4166	4170	rBV3	284	196	0.04%	0.004%
96	14.730	4177	4180	4182	rBV2	288	204	0.04%	0.005%
97	15.405	4387	4390	4392	rBV	487	368	0.07%	0.008%
98	15.614	4452	4455	4458	rBV	380	295	0.05%	0.007%
99	15.698	4477	4481	4488	rBV4	643	836	0.15%	0.019%
100	16.891	4849	4852	4854	rBV4	881	626	0.11%	0.014%

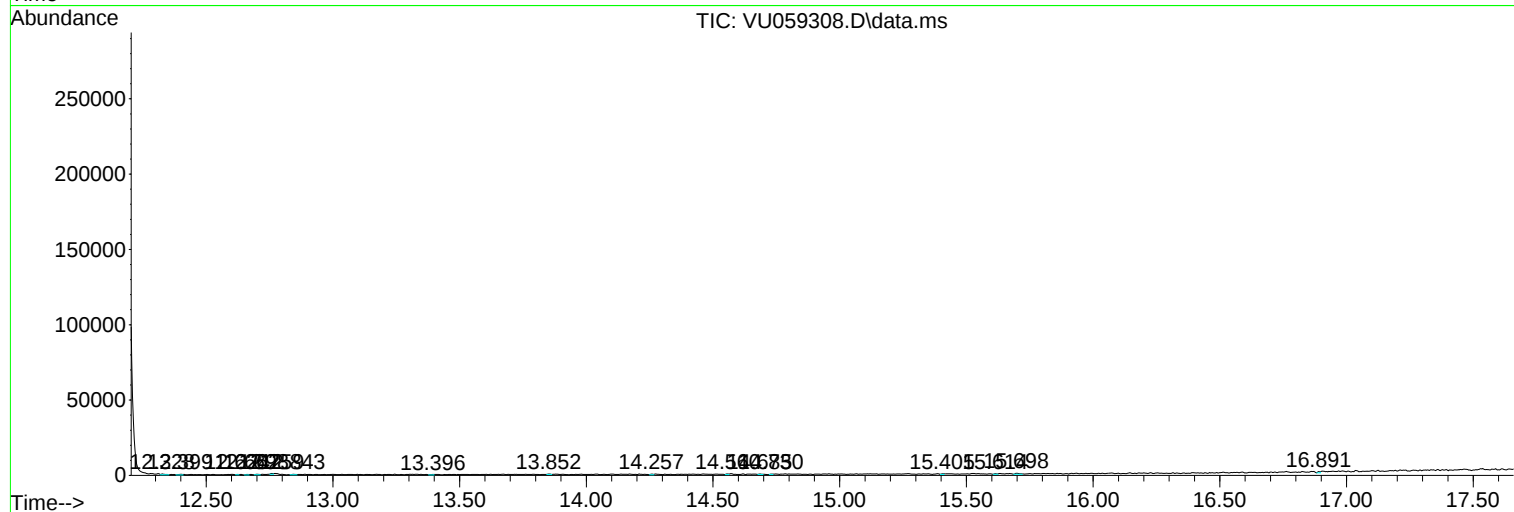
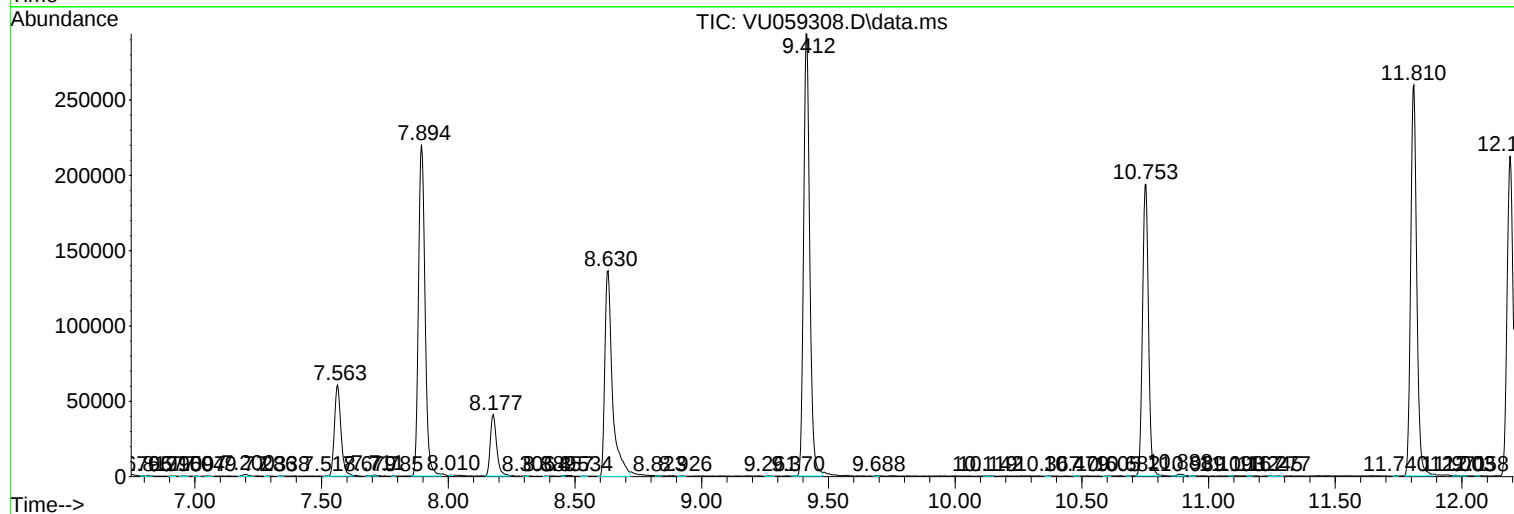
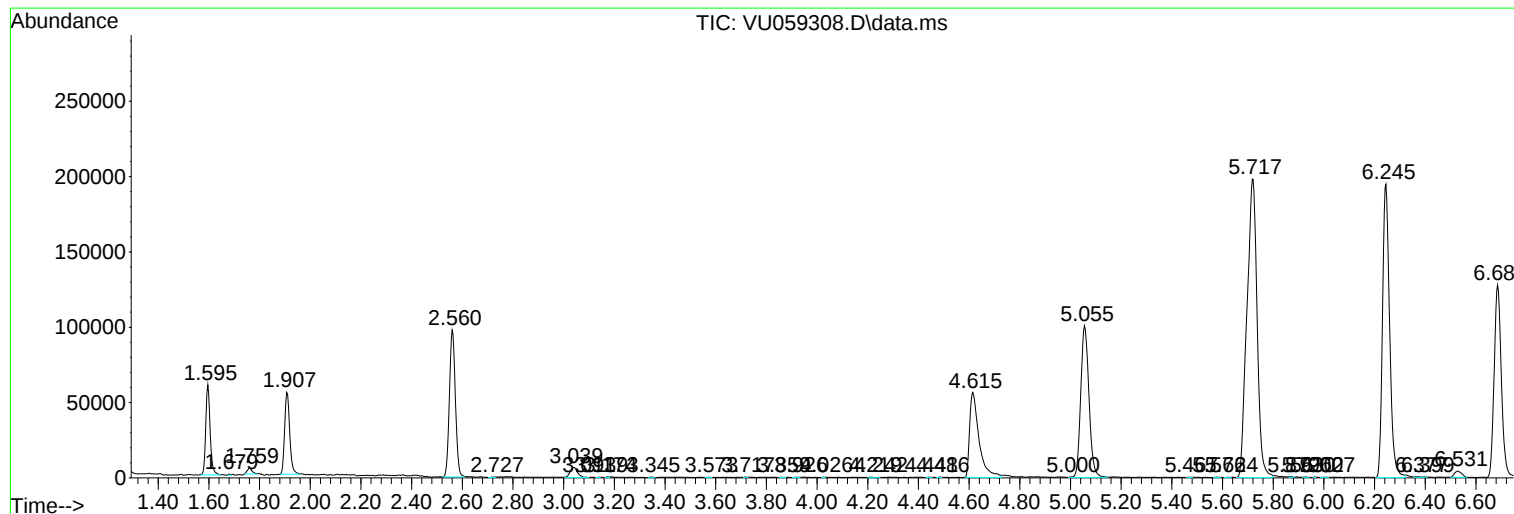
Sum of corrected areas: 4379439

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059308.D
Acq On : 18 Jun 2024 13:40
Operator : MD/SY
Sample : P2775-09ME
Misc : 3.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4C87ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU061824\
Data File : VU059308.D
Acq On : 18 Jun 2024 13:40
Operator : MD/SY
Sample : P2775-09ME
Misc : 3.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4C87ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.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\VU061824\
Data File : VU059308.D
Acq On : 18 Jun 2024 13:40
Operator : MD/SY
Sample : P2775-09ME
Misc : 3.51g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 15 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
A4C87ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM052924WMA.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
------------------	----	---------	-------	----------	---	----	------	------