

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052524\
 Data File : VU058990.D
 Acq On : 25 May 2024 11:40
 Operator : MD/SY
 Sample : VU0525MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK053

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: VU058990.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.477	54	58	64	rVB3	3474	3694	0.52%	0.071%
2	1.592	87	94	112	rVB	78303	100086	14.01%	1.931%
3	1.856	133	176	179	rBV5	70838	331113	46.34%	6.388%
4	2.454	359	362	365	rBV	277	161	0.02%	0.003%
5	2.550	380	392	408	rBV	134680	218735	30.61%	4.220%
6	2.775	458	462	471	rVB2	984	1421	0.20%	0.027%
7	2.936	508	512	515	rBV2	181	176	0.02%	0.003%
8	2.956	515	518	525	rVB3	352	383	0.05%	0.007%
9	3.029	532	541	552	rBV5	3325	6326	0.89%	0.122%
10	3.174	574	586	598	rBV	3019	5958	0.83%	0.115%
11	3.573	707	710	712	rBV2	280	191	0.03%	0.004%
12	3.634	725	729	731	rBV	236	171	0.02%	0.003%
13	3.705	746	751	755	rVB2	144	148	0.02%	0.003%
14	3.750	760	765	769	rBV2	269	308	0.04%	0.006%
15	4.113	871	878	883	rBV2	269	363	0.05%	0.007%
16	4.367	954	957	961	rBV2	175	140	0.02%	0.003%
17	4.528	1001	1007	1010	rBV2	142	166	0.02%	0.003%
18	4.611	1023	1033	1066	rBV	65980	170206	23.82%	3.284%
19	4.936	1130	1134	1137	rVB	383	300	0.04%	0.006%
20	4.959	1137	1141	1142	rBV2	268	169	0.02%	0.003%
21	5.052	1153	1170	1198	rVB	125168	280353	39.24%	5.409%
22	5.152	1198	1201	1203	rBV2	306	225	0.03%	0.004%
23	5.164	1203	1205	1207	rVV	322	184	0.03%	0.004%
24	5.219	1219	1222	1227	rBV2	431	385	0.05%	0.007%
25	5.277	1234	1240	1241	rBV	820	620	0.09%	0.012%
26	5.409	1276	1281	1284	rBV	286	229	0.03%	0.004%
27	5.602	1336	1341	1344	rBV	237	239	0.03%	0.005%
28	5.714	1355	1376	1404	rBV2	261240	714521	100.00%	13.786%
29	5.856	1418	1420	1423	rVB2	381	225	0.03%	0.004%
30	5.875	1423	1426	1429	rBV2	338	205	0.03%	0.004%
31	5.894	1429	1432	1436	rVB2	317	228	0.03%	0.004%
32	5.917	1436	1439	1442	rBV	329	230	0.03%	0.004%
33	5.968	1452	1455	1458	rVV2	619	423	0.06%	0.008%
34	6.062	1480	1484	1485	rBV	247	152	0.02%	0.003%
35	6.103	1494	1497	1505	rVB	234	223	0.03%	0.004%
36	6.238	1521	1539	1565	rBV	168308	325166	45.51%	6.274%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052524\
 Data File : VU058990.D
 Acq On : 25 May 2024 11:40
 Operator : MD/SY
 Sample : VU0525MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK053

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	6.418	1590	1595	1601	rVB2	356	450	0.06%	0.009%
38	6.451	1601	1605	1609	rBV2	235	229	0.03%	0.004%
39	6.528	1620	1629	1642	rVB8	3920	7852	1.10%	0.151%
40	6.586	1642	1647	1648	rBV2	564	389	0.05%	0.008%
41	6.679	1662	1676	1702	rBV	165563	329467	46.11%	6.357%
42	6.772	1702	1705	1706	rBV	255	139	0.02%	0.003%
43	6.901	1741	1745	1749	rVV2	175	167	0.02%	0.003%
44	6.920	1749	1751	1758	rVB2	199	168	0.02%	0.003%
45	7.081	1795	1801	1806	rBV2	218	334	0.05%	0.006%
46	7.103	1806	1808	1812	rVV2	246	137	0.02%	0.003%
47	7.132	1813	1817	1820	rVB2	172	170	0.02%	0.003%
48	7.193	1833	1836	1840	rBV3	439	351	0.05%	0.007%
49	7.338	1877	1881	1883	rBV	232	179	0.03%	0.003%
50	7.557	1938	1949	1966	rBV	84527	149500	20.92%	2.884%
51	7.727	1999	2002	2005	rBV	206	139	0.02%	0.003%
52	7.891	2040	2053	2074	rBV	291845	508749	71.20%	9.816%
53	8.081	2110	2112	2114	rBV	334	185	0.03%	0.004%
54	8.174	2130	2141	2158	rBV	56318	98108	13.73%	1.893%
55	8.274	2169	2172	2176	rVV3	300	264	0.04%	0.005%
56	8.315	2182	2185	2190	rVB2	304	191	0.03%	0.004%
57	8.467	2228	2232	2238	rVB2	414	527	0.07%	0.010%
58	8.499	2238	2242	2244	rBV2	180	141	0.02%	0.003%
59	8.627	2272	2282	2309	rBV	183037	358429	50.16%	6.915%
60	8.891	2361	2364	2367	rBV	210	174	0.02%	0.003%
61	9.248	2470	2475	2480	rBV2	282	292	0.04%	0.006%
62	9.319	2494	2497	2500	rVB2	235	146	0.02%	0.003%
63	9.412	2513	2526	2549	rBV	241429	399631	55.93%	7.710%
64	9.534	2561	2564	2569	rVB3	470	485	0.07%	0.009%
65	9.566	2569	2574	2575	rBV2	437	349	0.05%	0.007%
66	9.647	2595	2599	2603	rBV2	234	223	0.03%	0.004%
67	9.698	2608	2615	2621	rBV3	901	1208	0.17%	0.023%
68	9.785	2639	2642	2646	rBV2	170	150	0.02%	0.003%
69	9.930	2684	2687	2690	rBV	210	151	0.02%	0.003%
70	9.984	2702	2704	2712	rVB2	272	285	0.04%	0.005%
71	10.020	2712	2715	2718	rVB2	251	158	0.02%	0.003%
72	10.045	2718	2723	2726	rBV	270	261	0.04%	0.005%
73	10.171	2759	2762	2765	rBV3	249	163	0.02%	0.003%
74	10.351	2815	2818	2823	rVB2	234	189	0.03%	0.004%
75	10.380	2823	2827	2836	rBV	312	425	0.06%	0.008%
76	10.483	2857	2859	2866	rVB3	318	269	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052524\
 Data File : VU058990.D
 Acq On : 25 May 2024 11:40
 Operator : MD/SY
 Sample : VU0525MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK053

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	10.640	2906	2908	2916	rVB3	797	976	0.14%	0.019%
78	10.749	2930	2942	2966	rBV	237312	385834	54.00%	7.444%
79	10.994	3015	3018	3028	rVB2	309	356	0.05%	0.007%
80	11.093	3046	3049	3053	rVB2	338	222	0.03%	0.004%
81	11.216	3084	3087	3090	rBV2	266	203	0.03%	0.004%
82	11.460	3160	3163	3165	rBV2	239	155	0.02%	0.003%
83	11.733	3245	3248	3253	rBV	285	286	0.04%	0.006%
84	11.807	3259	3271	3290	rBV	211249	346526	48.50%	6.686%
85	12.187	3377	3389	3410	rBV	248208	419159	58.66%	8.087%
86	12.470	3474	3477	3479	rBV2	242	161	0.02%	0.003%
87	12.563	3502	3506	3509	rBV2	258	236	0.03%	0.005%
88	12.765	3563	3569	3572	rBV3	649	781	0.11%	0.015%
89	12.878	3602	3604	3607	rVB	341	191	0.03%	0.004%
90	13.196	3700	3703	3707	rVB2	362	266	0.04%	0.005%
91	13.283	3726	3730	3734	rVB2	287	272	0.04%	0.005%
92	13.309	3735	3738	3740	rBV2	208	159	0.02%	0.003%
93	13.849	3903	3906	3908	rBV2	343	222	0.03%	0.004%
94	14.354	4060	4063	4065	rBV	391	243	0.03%	0.005%
95	14.566	4126	4129	4130	rBV	352	236	0.03%	0.005%
96	14.817	4205	4207	4213	rBV3	306	341	0.05%	0.007%
97	14.900	4227	4233	4237	rBV2	483	656	0.09%	0.013%
98	14.994	4259	4262	4263	rBV2	275	145	0.02%	0.003%
99	16.254	4652	4654	4658	rVB2	508	304	0.04%	0.006%
100	16.447	4709	4714	4715	rBV3	448	424	0.06%	0.008%

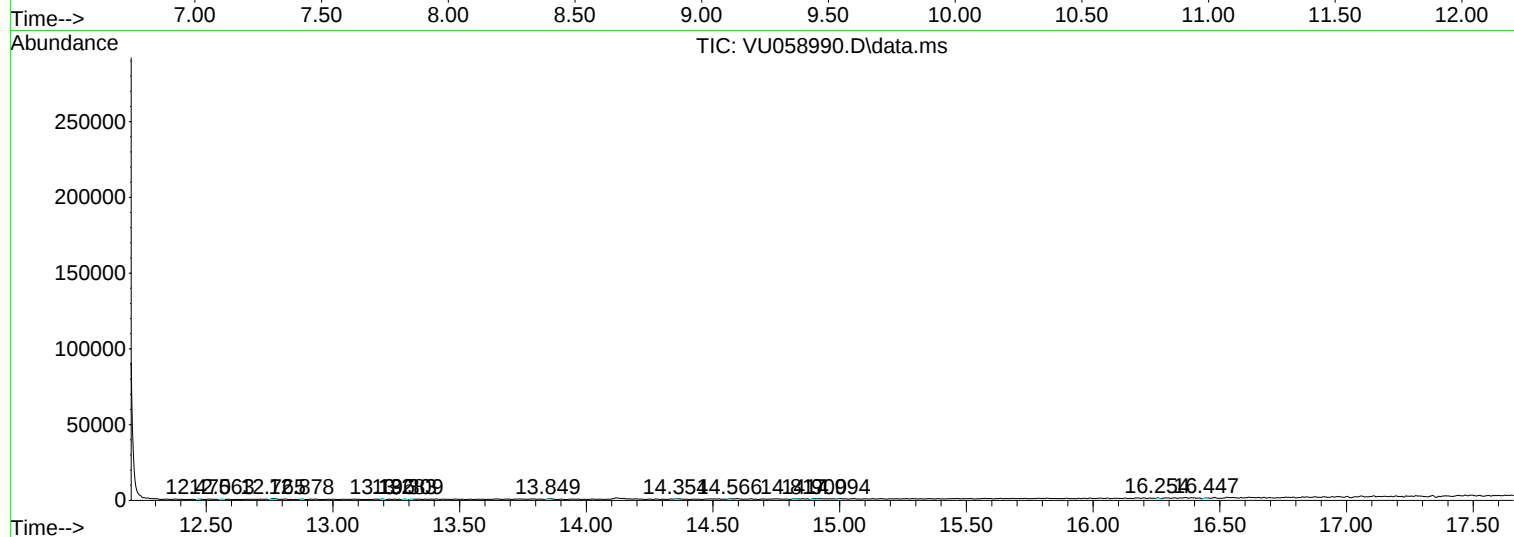
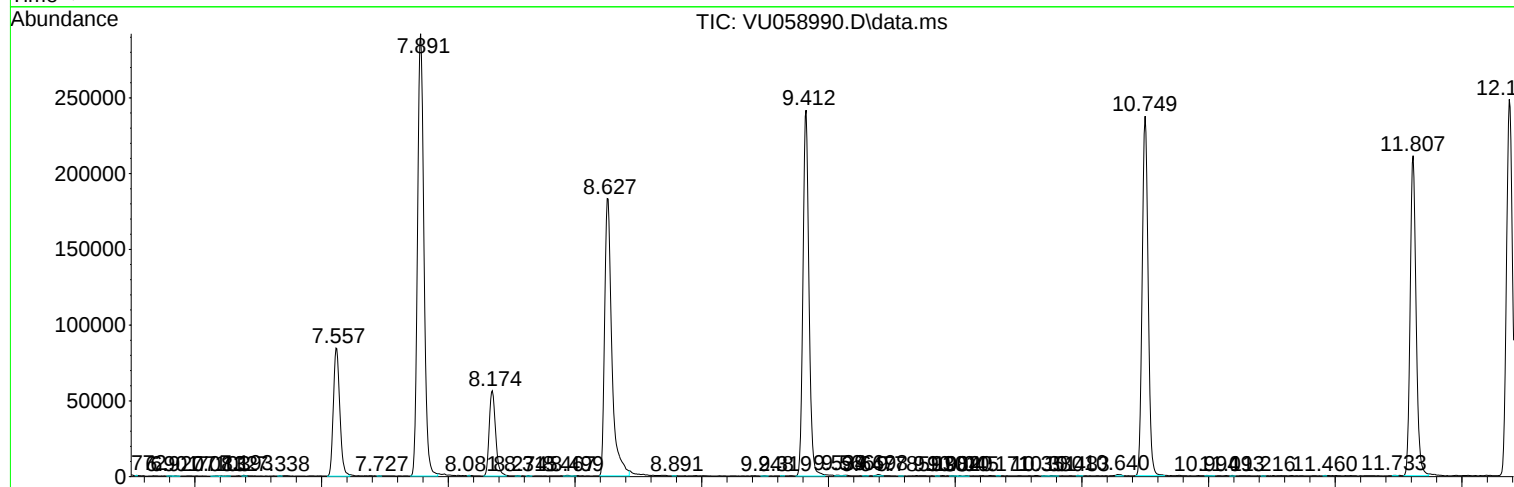
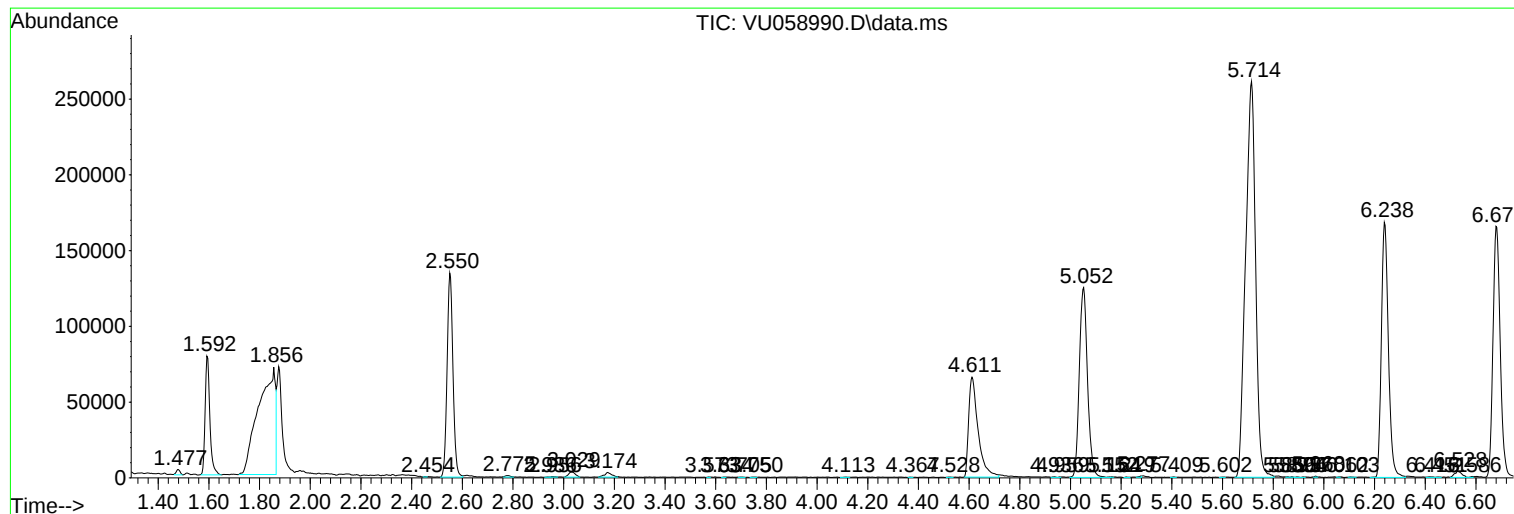
Sum of corrected areas: 5183001

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU052524\
Data File : VU058990.D
Acq On : 25 May 2024 11:40
Operator : MD/SY
Sample : VU0525MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK053

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\VU052524\
Data File : VU058990.D
Acq On : 25 May 2024 11:40
Operator : MD/SY
Sample : VU0525MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK053

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\VU052524\
Data File : VU058990.D
Acq On : 25 May 2024 11:40
Operator : MD/SY
Sample : VU0525MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK053

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	--Internal Standard--			
					#	RT	Resp	Conc