

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121721\
 Data File : VU046479.D
 Acq On : 17 Dec 2021 17:56
 Operator : SY/MD
 Sample : M5102-02ME
 Misc : 6.20g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL45ME

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\SFAMULM112921WMA.M
 Title : VOC Analysis

Signal : TIC: VU046479.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.601	73	81	111	rVB	38050	79096	13.36%	1.689%
2	1.880	165	168	170	rBV	301	183	0.03%	0.004%
3	1.916	170	179	190	rBV	22496	44215	7.47%	0.944%
4	2.546	364	375	392	rBV	95039	173153	29.25%	3.697%
5	2.764	440	443	448	rVV4	433	360	0.06%	0.008%
6	2.790	448	451	454	rVB3	302	180	0.03%	0.004%
7	2.883	479	480	483	rVB	382	165	0.03%	0.004%
8	2.906	483	487	493	rVB2	212	243	0.04%	0.005%
9	3.035	520	527	528	rBV3	743	661	0.11%	0.014%
10	3.182	564	573	588	rVB4	2499	5168	0.87%	0.110%
11	3.282	598	604	606	rBV	144	197	0.03%	0.004%
12	3.363	625	629	632	rBB2	283	208	0.04%	0.004%
13	3.446	652	655	658	rBB	143	119	0.02%	0.003%
14	3.684	727	729	732	rBV	140	120	0.02%	0.003%
15	3.755	748	751	754	rBB	148	123	0.02%	0.003%
16	3.864	782	785	787	rBB	255	158	0.03%	0.003%
17	3.945	806	810	813	rBB	144	125	0.02%	0.003%
18	4.330	927	930	935	rBB	125	159	0.03%	0.003%
19	4.366	938	941	946	rBB	148	174	0.03%	0.004%
20	4.655	1016	1031	1088	rBV2	29903	141499	23.90%	3.021%
21	4.944	1119	1121	1124	rBV2	217	120	0.02%	0.003%
22	5.063	1141	1158	1181	rBV	101644	235969	39.86%	5.038%
23	5.308	1226	1234	1246	rBB6	2204	4704	0.79%	0.100%
24	5.395	1258	1261	1263	rBV	142	124	0.02%	0.003%
25	5.597	1322	1324	1328	rBB	139	120	0.02%	0.003%
26	5.719	1343	1362	1386	rBV2	232792	591934	100.00%	12.638%
27	5.980	1434	1443	1462	rBV6	3305	8032	1.36%	0.171%
28	6.250	1512	1527	1558	rBV	171837	342882	57.93%	7.321%
29	6.539	1607	1617	1628	rBV5	7504	13748	2.32%	0.294%
30	6.604	1628	1637	1648	rVV5	1264	2399	0.41%	0.051%
31	6.694	1651	1665	1686	rVB	127665	263371	44.49%	5.623%
32	6.806	1697	1700	1703	rBV2	323	264	0.04%	0.006%
33	7.054	1774	1777	1781	rBB	146	122	0.02%	0.003%
34	7.186	1815	1818	1820	rBV	232	181	0.03%	0.004%
35	7.234	1829	1833	1837	rBV2	271	293	0.05%	0.006%
36	7.488	1909	1912	1914	rBV	147	129	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121721\
 Data File : VU046479.D
 Acq On : 17 Dec 2021 17:56
 Operator : SY/MD
 Sample : M5102-02ME
 Misc : 6.20g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL45ME

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\SFAMULM112921WMA.M
 Title : VOC Analysis

37	7.568	1925	1937	1960	rBV	64172	130538	22.05%	2.787%
38	7.787	1999	2005	2006	rBV	1091	833	0.14%	0.018%
39	7.899	2026	2040	2058	rBV	258906	469346	79.29%	10.021%
40	7.973	2058	2063	2073	rVB2	3000	4727	0.80%	0.101%
41	8.038	2081	2083	2091	rVB2	315	299	0.05%	0.006%
42	8.185	2115	2129	2150	rBV	36993	88203	14.90%	1.883%
43	8.359	2180	2183	2186	rBB	162	131	0.02%	0.003%
44	8.391	2189	2193	2196	rBV	172	181	0.03%	0.004%
45	8.478	2211	2220	2221	rBV	462	507	0.09%	0.011%
46	8.552	2231	2243	2259	rVB2	54973	94610	15.98%	2.020%
47	8.681	2262	2283	2306	rBV2	99952	293568	49.59%	6.268%
48	8.806	2320	2322	2329	rVB2	467	466	0.08%	0.010%
49	8.893	2346	2349	2353	rBV	142	137	0.02%	0.003%
50	8.947	2362	2366	2372	rBV2	410	511	0.09%	0.011%
51	8.989	2376	2379	2385	rVB	198	225	0.04%	0.005%
52	9.057	2397	2400	2405	rBV	128	176	0.03%	0.004%
53	9.192	2439	2442	2445	rBB	193	154	0.03%	0.003%
54	9.227	2450	2453	2455	rBV	158	131	0.02%	0.003%
55	9.269	2463	2466	2468	rBV	141	122	0.02%	0.003%
56	9.427	2501	2515	2535	rBV	210735	455387	76.93%	9.723%
57	9.568	2556	2559	2560	rBV	210	133	0.02%	0.003%
58	9.581	2560	2563	2570	rVB2	365	484	0.08%	0.010%
59	9.616	2571	2574	2577	rBV	195	171	0.03%	0.004%
60	9.703	2595	2601	2604	rBV2	397	612	0.10%	0.013%
61	9.742	2609	2613	2615	rBV	160	129	0.02%	0.003%
62	9.874	2651	2654	2656	rBV	153	133	0.02%	0.003%
63	9.973	2682	2685	2689	rBB	147	150	0.03%	0.003%
64	10.044	2703	2707	2710	rBB	127	136	0.02%	0.003%
65	10.108	2723	2727	2731	rBB2	280	273	0.05%	0.006%
66	10.156	2739	2742	2746	rVB	162	166	0.03%	0.004%
67	10.182	2747	2750	2752	rBV	144	124	0.02%	0.003%
68	10.304	2783	2788	2794	rBB	183	238	0.04%	0.005%
69	10.337	2795	2798	2801	rBB	182	145	0.02%	0.003%
70	10.362	2801	2806	2808	rBV	160	187	0.03%	0.004%
71	10.494	2844	2847	2853	rVB2	319	359	0.06%	0.008%
72	10.645	2892	2894	2897	rBV	258	208	0.04%	0.004%
73	10.668	2897	2901	2904	rBV2	991	939	0.16%	0.020%
74	10.774	2919	2934	2948	rVV	190532	319395	53.96%	6.819%
75	10.902	2965	2974	2980	rBV2	469	771	0.13%	0.016%
76	11.021	3007	3011	3013	rBV	149	151	0.03%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121721\
 Data File : VU046479.D
 Acq On : 17 Dec 2021 17:56
 Operator : SY/MD
 Sample : M5102-02ME
 Misc : 6.20g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BGL45ME

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\SFAMULM112921WMA.M
 Title : VOC Analysis

77	11.095	3032	3034	3035	rBV	255	121	0.02%	0.003%
78	11.115	3035	3040	3047	rVV3	723	835	0.14%	0.018%
79	11.195	3061	3065	3068	rBV	165	158	0.03%	0.003%
80	11.298	3095	3097	3101	rBV	148	132	0.02%	0.003%
81	11.410	3125	3132	3135	rBV	217	339	0.06%	0.007%
82	11.459	3141	3147	3148	rBV	593	557	0.09%	0.012%
83	11.607	3190	3193	3199	rVB	204	245	0.04%	0.005%
84	11.636	3199	3202	3205	rBV	167	152	0.03%	0.003%
85	11.722	3225	3229	3231	rBV	140	150	0.03%	0.003%
86	11.751	3236	3238	3243	rVV2	226	194	0.03%	0.004%
87	11.819	3247	3259	3278	rVB	288022	455612	76.97%	9.728%
88	11.976	3304	3308	3313	rVB3	641	787	0.13%	0.017%
89	12.201	3364	3378	3396	rVV	277381	441337	74.56%	9.423%
90	12.774	3549	3556	3563	rBV	797	1176	0.20%	0.025%
91	13.516	3784	3787	3789	rBV	196	159	0.03%	0.003%
92	13.600	3809	3813	3819	rBV	134	129	0.02%	0.003%
93	14.098	3962	3968	3974	rVB2	238	350	0.06%	0.007%
94	14.578	4109	4117	4126	rVB2	1207	1790	0.30%	0.038%
95	15.079	4271	4273	4279	rVB2	200	141	0.02%	0.003%
96	15.211	4312	4314	4316	rBV	250	122	0.02%	0.003%
97	15.606	4434	4437	4440	rBV2	183	163	0.03%	0.003%
98	15.883	4517	4523	4530	rBV2	342	577	0.10%	0.012%
99	16.192	4612	4619	4631	rVB3	1198	2202	0.37%	0.047%
100	17.204	4930	4934	4935	rBV	421	311	0.05%	0.007%

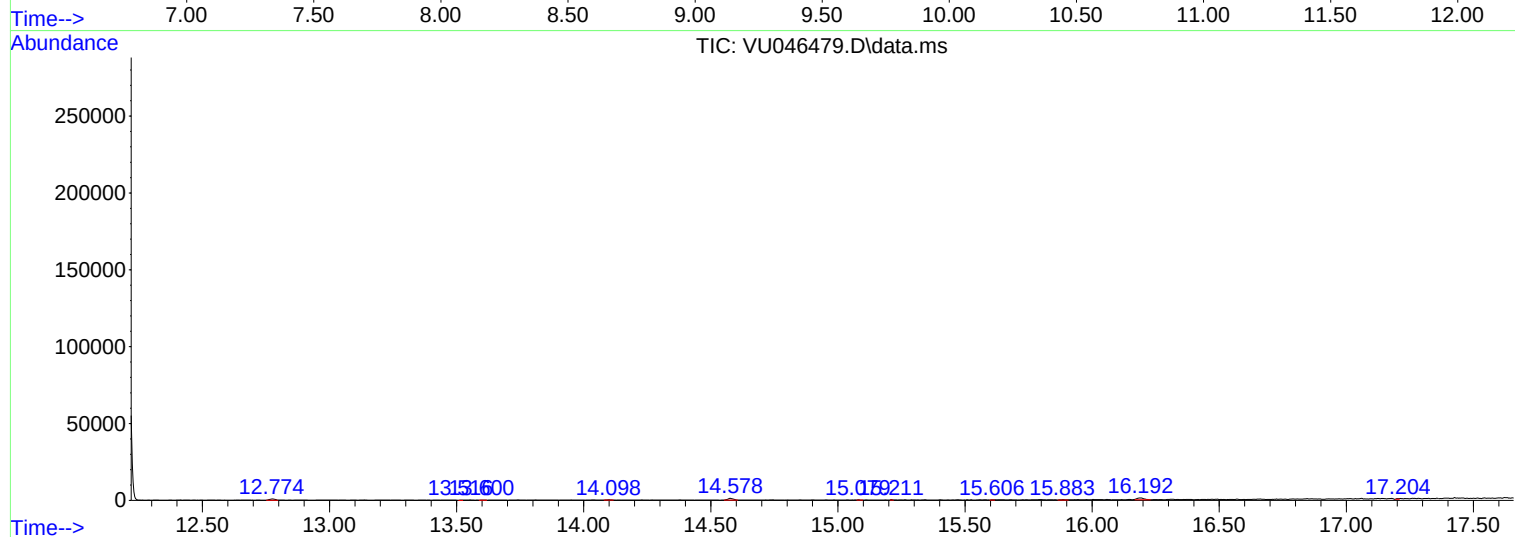
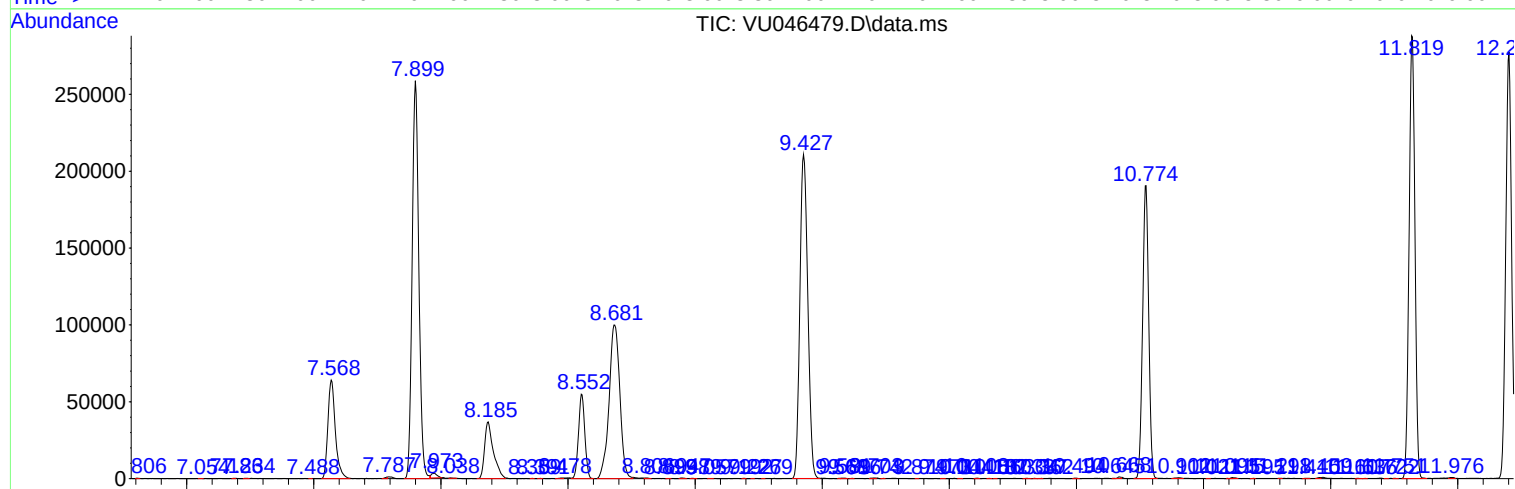
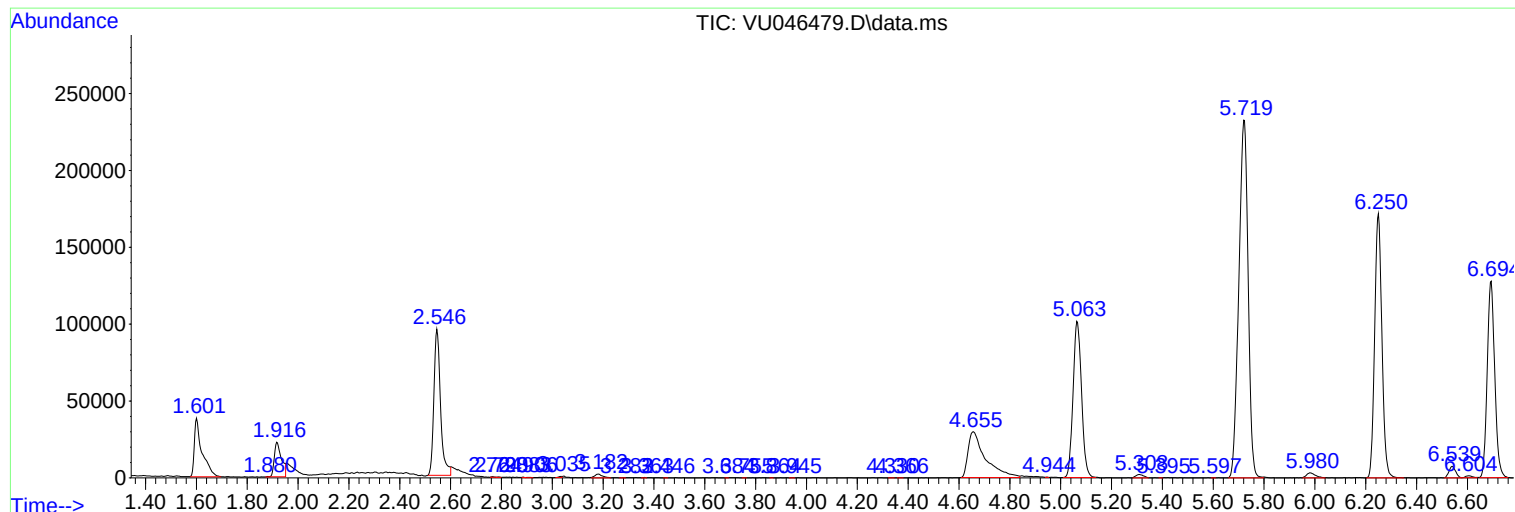
Sum of corrected areas: 4683593

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121721\
Data File : VU046479.D
Acq On : 17 Dec 2021 17:56
Operator : SY/MD
Sample : M5102-02ME
Misc : 6.20g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL45ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU121721\
Data File : VU046479.D
Acq On : 17 Dec 2021 17:56
Operator : SY/MD
Sample : M5102-02ME
Misc : 6.20g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL45ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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\VU121721\
Data File : VU046479.D
Acq On : 17 Dec 2021 17:56
Operator : SY/MD
Sample : M5102-02ME
Misc : 6.20g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 19 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BGL45ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM112921WMA.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
------------------	----	---------	-------	----------	---	----	------	------