

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046178.D
 Acq On : 08 Dec 2021 16:11
 Operator : SY/MD
 Sample : M4887-11ME
 Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8A6ME

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: VU046178.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	94	rBV	72988	93877	12.94%	1.521%
2	1.861	158	162	164	rBV2	900	818	0.11%	0.013%
3	1.916	171	179	197	rVB	43462	74421	10.26%	1.206%
4	2.160	251	255	259	rVB6	509	502	0.07%	0.008%
5	2.192	259	265	268	rBV4	1044	1203	0.17%	0.019%
6	2.244	277	281	287	rBV5	421	440	0.06%	0.007%
7	2.446	340	344	348	rBV7	467	457	0.06%	0.007%
8	2.549	362	376	392	rBV	131368	220115	30.34%	3.566%
9	2.774	443	446	448	rBV3	650	496	0.07%	0.008%
10	2.826	460	462	466	rVB	788	473	0.07%	0.008%
11	2.890	479	482	486	rVB2	818	520	0.07%	0.008%
12	3.060	533	535	539	rVB2	1453	845	0.12%	0.014%
13	3.183	560	573	584	rBV2	6673	15423	2.13%	0.250%
14	3.440	649	653	661	rBV	829	1242	0.17%	0.020%
15	3.729	741	743	749	rVB	651	567	0.08%	0.009%
16	4.038	835	839	844	rVB	654	690	0.10%	0.011%
17	4.289	915	917	921	rVB2	675	463	0.06%	0.008%
18	4.655	1017	1031	1068	rBV	36405	160501	22.12%	2.600%
19	5.067	1143	1159	1180	rBV2	109005	272132	37.51%	4.409%
20	5.195	1196	1199	1206	rVB	590	555	0.08%	0.009%
21	5.481	1284	1288	1294	rVB	658	612	0.08%	0.010%
22	5.723	1340	1363	1385	rBV2	273766	703783	97.01%	11.402%
23	5.899	1415	1418	1423	rBV	576	511	0.07%	0.008%
24	5.980	1433	1443	1459	rBV5	4638	12199	1.68%	0.198%
25	6.250	1513	1527	1556	rVB	268714	550176	75.84%	8.913%
26	6.539	1607	1617	1629	rBV5	12934	26189	3.61%	0.424%
27	6.690	1651	1664	1685	rVV	152485	310102	42.74%	5.024%
28	6.829	1703	1707	1710	rBV	599	529	0.07%	0.009%
29	6.867	1715	1719	1723	rBV2	415	461	0.06%	0.007%
30	6.903	1727	1730	1735	rBV	682	587	0.08%	0.010%
31	6.983	1751	1755	1758	rBV2	508	508	0.07%	0.008%
32	7.292	1845	1851	1855	rBV2	686	960	0.13%	0.016%
33	7.404	1879	1886	1887	rBV	570	591	0.08%	0.010%
34	7.568	1925	1937	1958	rBV	83078	161373	22.24%	2.614%
35	7.793	1998	2007	2023	rVB3	3055	5796	0.80%	0.094%
36	7.899	2026	2040	2058	rBV	310584	586764	80.88%	9.506%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046178.D
 Acq On : 08 Dec 2021 16:11
 Operator : SY/MD
 Sample : M4887-11ME
 Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8A6ME

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	8.182	2115	2128	2156	rVB	48846	110508	15.23%	1.790%
38	8.555	2233	2244	2260	rVB2	59208	104105	14.35%	1.687%
39	8.681	2260	2283	2319	rBV2	110436	366938	50.58%	5.945%
40	9.427	2500	2515	2538	rVB	309561	694744	95.76%	11.255%
41	9.684	2590	2595	2596	rBV2	948	696	0.10%	0.011%
42	9.954	2675	2679	2686	rVB	690	756	0.10%	0.012%
43	10.060	2710	2712	2717	rBV	489	473	0.07%	0.008%
44	10.134	2727	2735	2740	rBV	840	1291	0.18%	0.021%
45	10.189	2747	2752	2755	rBV	550	569	0.08%	0.009%
46	10.211	2755	2759	2766	rVB	682	952	0.13%	0.015%
47	10.430	2823	2827	2829	rBV	577	478	0.07%	0.008%
48	10.668	2896	2901	2902	rBV	801	669	0.09%	0.011%
49	10.771	2921	2933	2949	rVB	219271	366240	50.48%	5.933%
50	10.886	2965	2969	2973	rBV2	743	655	0.09%	0.011%
51	10.925	2978	2981	2985	rBV2	724	583	0.08%	0.009%
52	10.986	2996	3000	3003	rBV	806	694	0.10%	0.011%
53	11.031	3003	3014	3016	rBV2	720	1113	0.15%	0.018%
54	11.359	3112	3116	3120	rBV	457	445	0.06%	0.007%
55	11.459	3141	3147	3150	rBV3	1069	1326	0.18%	0.021%
56	11.819	3246	3259	3272	rBV	457939	725471	100.00%	11.753%
57	11.973	3303	3307	3310	rBV2	972	823	0.11%	0.013%
58	12.066	3330	3336	3338	rBV3	1031	1008	0.14%	0.016%
59	12.198	3363	3377	3393	rVV	335678	551269	75.99%	8.931%
60	12.333	3413	3419	3425	rVB3	1226	1701	0.23%	0.028%
61	12.562	3487	3490	3495	rVB	516	490	0.07%	0.008%
62	12.590	3495	3499	3503	rBV2	608	587	0.08%	0.010%
63	12.726	3537	3541	3550	rBV	681	812	0.11%	0.013%
64	12.764	3550	3553	3555	rBV2	705	520	0.07%	0.008%
65	12.880	3584	3589	3592	rBV2	655	663	0.09%	0.011%
66	13.192	3683	3686	3689	rBV	642	556	0.08%	0.009%
67	13.295	3712	3718	3723	rVB2	684	945	0.13%	0.015%
68	13.430	3756	3760	3767	rBV5	842	768	0.11%	0.012%
69	13.494	3775	3780	3785	rBV2	513	713	0.10%	0.012%
70	13.767	3861	3865	3871	rVB	616	617	0.09%	0.010%
71	13.934	3913	3917	3920	rBV	624	565	0.08%	0.009%
72	14.092	3959	3966	3967	rBV2	787	765	0.11%	0.012%
73	14.369	4050	4052	4056	rVB	785	438	0.06%	0.007%
74	14.452	4070	4078	4082	rVB4	1448	1706	0.24%	0.028%
75	14.510	4093	4096	4099	rVB	732	458	0.06%	0.007%
76	14.578	4110	4117	4125	rVB2	2129	3021	0.42%	0.049%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
 Data File : VU046178.D
 Acq On : 08 Dec 2021 16:11
 Operator : SY/MD
 Sample : M4887-11ME
 Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EX8A6ME

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	14.639	4132	4136	4140	rBV5	715	731	0.10%	0.012%
78	14.764	4171	4175	4179	rBV	540	561	0.08%	0.009%
79	14.928	4219	4226	4227	rBV2	582	590	0.08%	0.010%
80	15.024	4253	4256	4260	rVB2	622	539	0.07%	0.009%
81	15.053	4260	4265	4267	rBV2	821	810	0.11%	0.013%
82	15.111	4280	4283	4289	rVV	522	567	0.08%	0.009%
83	15.137	4289	4291	4296	rVB	636	457	0.06%	0.007%
84	15.179	4296	4304	4306	rBV2	919	1003	0.14%	0.016%
85	15.198	4306	4310	4313	rVV2	420	485	0.07%	0.008%
86	15.224	4316	4318	4324	rVB4	828	753	0.10%	0.012%
87	15.397	4368	4372	4374	rBV2	1278	1159	0.16%	0.019%
88	15.619	4438	4441	4443	rBV	624	440	0.06%	0.007%
89	15.642	4443	4448	4450	rVV2	410	438	0.06%	0.007%
90	15.761	4480	4485	4486	rBV2	651	609	0.08%	0.010%
91	15.787	4489	4493	4499	rVB	608	727	0.10%	0.012%
92	15.860	4512	4516	4518	rBV	561	470	0.06%	0.008%
93	16.188	4613	4618	4624	rVB3	2356	2368	0.33%	0.038%
94	16.291	4646	4650	4658	rVB5	978	1137	0.16%	0.018%
95	16.343	4662	4666	4669	rVB3	542	432	0.06%	0.007%
96	16.381	4671	4678	4685	rBV3	707	1357	0.19%	0.022%
97	16.516	4717	4720	4723	rBV	828	633	0.09%	0.010%
98	16.812	4808	4812	4815	rBV2	678	669	0.09%	0.011%
99	16.864	4825	4828	4833	rBV5	712	685	0.09%	0.011%
100	17.227	4938	4941	4946	rBV4	856	883	0.12%	0.014%

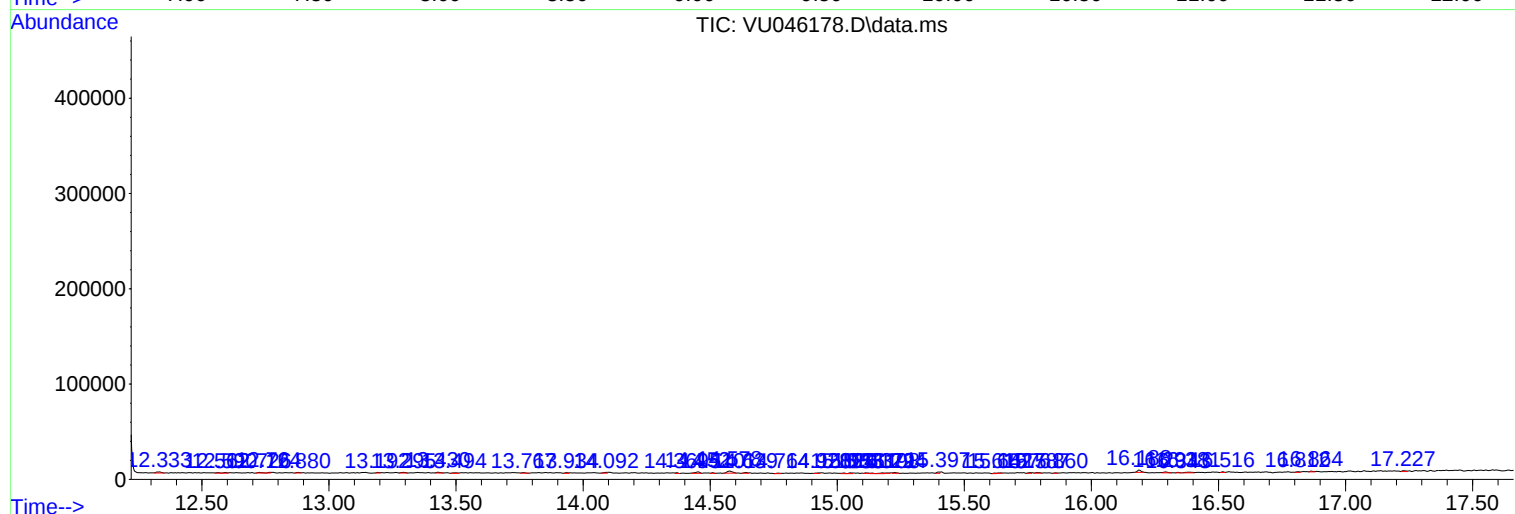
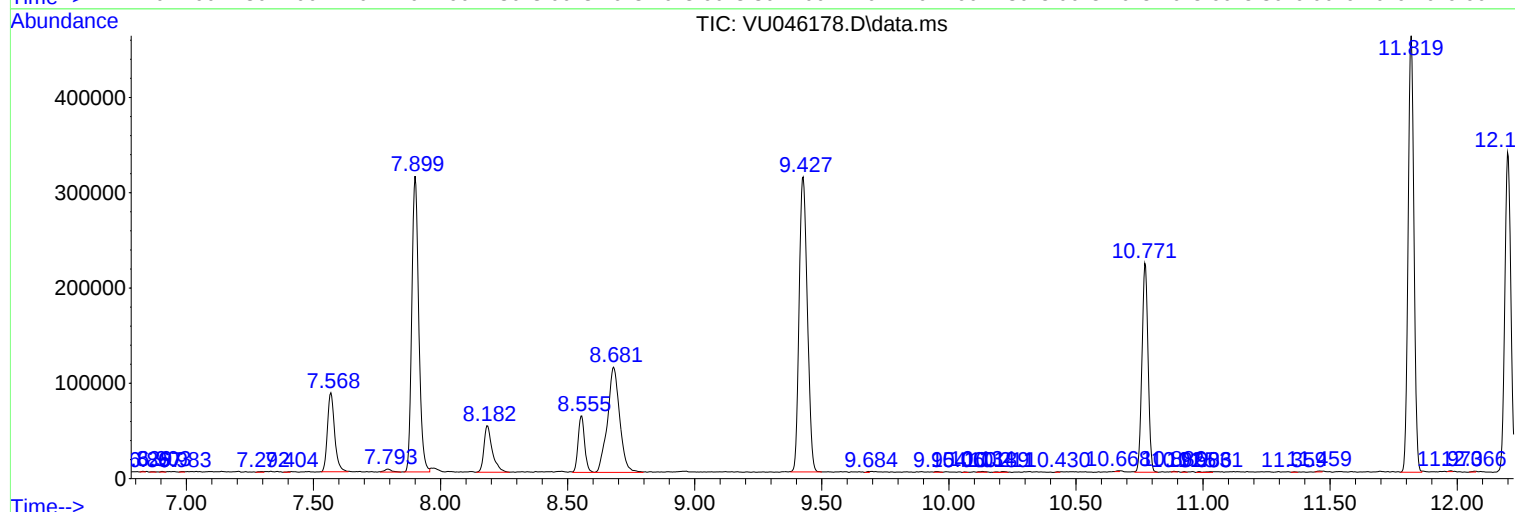
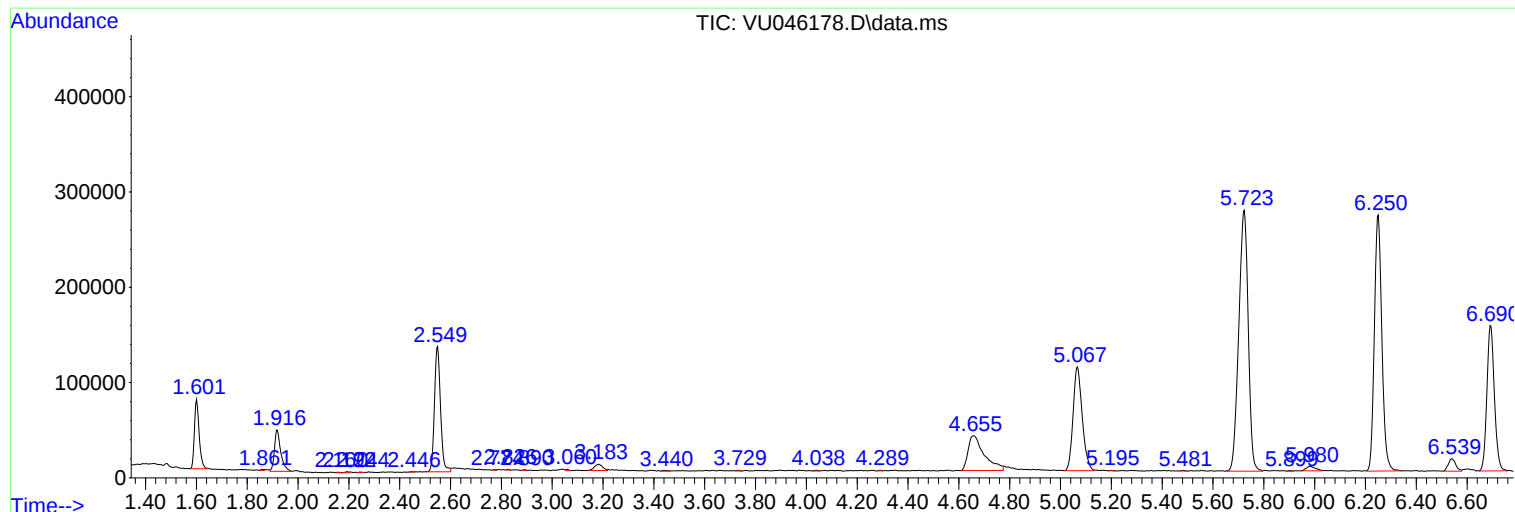
Sum of corrected areas: 6172515

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120821\
Data File : VU046178.D
Acq On : 08 Dec 2021 16:11
Operator : SY/MD
Sample : M4887-11ME
Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8A6ME

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\VU120821\
Data File : VU046178.D
Acq On : 08 Dec 2021 16:11
Operator : SY/MD
Sample : M4887-11ME
Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8A6ME

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\VU120821\
Data File : VU046178.D
Acq On : 08 Dec 2021 16:11
Operator : SY/MD
Sample : M4887-11ME
Misc : 5.74g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EX8A6ME

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	--Internal Standard--
				#	RT Resp Conc