

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046150.D
 Acq On : 07 Dec 2021 19:34
 Operator : SY/MD
 Sample : M4887-04ME
 Misc : 5.31g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

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: VU046150.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.600	73	81	106	rVB	188520	254188	14.64%	2.039%
2	1.861	157	162	169	rBV3	1991	2396	0.14%	0.019%
3	1.919	169	180	198	rBV	101953	185012	10.65%	1.484%
4	2.546	364	375	389	rBV	258564	430116	24.77%	3.451%
5	3.179	554	572	596	rBV2	12261	33357	1.92%	0.268%
6	3.337	616	621	622	rVB	337	226	0.01%	0.002%
7	3.382	634	635	645	rVB2	239	159	0.01%	0.001%
8	3.928	801	805	807	rBV	164	173	0.01%	0.001%
9	4.012	827	831	836	rBV	167	239	0.01%	0.002%
10	4.057	842	845	848	rVB	170	145	0.01%	0.001%
11	4.092	853	856	859	rBV	160	167	0.01%	0.001%
12	4.237	897	901	905	rBB	152	181	0.01%	0.001%
13	4.269	906	911	912	rBV	160	159	0.01%	0.001%
14	4.436	960	963	966	rBV	145	152	0.01%	0.001%
15	4.475	971	975	978	rBV	179	197	0.01%	0.002%
16	4.523	987	990	993	rBV	150	141	0.01%	0.001%
17	4.658	1014	1032	1100	rBV	84886	423997	24.41%	3.402%
18	5.067	1142	1159	1187	rVB	270180	664951	38.29%	5.335%
19	5.198	1195	1200	1202	rBV2	273	191	0.01%	0.002%
20	5.240	1209	1213	1215	rBV	171	161	0.01%	0.001%
21	5.340	1241	1244	1246	rBV	174	143	0.01%	0.001%
22	5.478	1284	1287	1290	rBV	165	163	0.01%	0.001%
23	5.722	1341	1363	1388	rBV2	684137	1736654	100.00%	13.934%
24	5.848	1400	1402	1407	rBV2	296	227	0.01%	0.002%
25	5.906	1417	1420	1425	rBV2	259	263	0.02%	0.002%
26	5.928	1425	1427	1429	rVV	259	146	0.01%	0.001%
27	5.986	1432	1445	1468	rBV6	5402	17309	1.00%	0.139%
28	6.079	1470	1474	1477	rVV2	349	314	0.02%	0.003%
29	6.112	1481	1484	1492	rVB2	322	484	0.03%	0.004%
30	6.250	1512	1527	1557	rBV	323264	674692	38.85%	5.413%
31	6.539	1605	1617	1628	rBV6	12539	27020	1.56%	0.217%
32	6.581	1628	1630	1631	rBV	400	174	0.01%	0.001%
33	6.690	1650	1664	1693	rVB	365970	764357	44.01%	6.133%
34	6.812	1693	1702	1705	rBV4	849	1314	0.08%	0.011%
35	7.054	1773	1777	1783	rVB	335	386	0.02%	0.003%
36	7.173	1809	1814	1815	rBV	386	295	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046150.D
 Acq On : 07 Dec 2021 19:34
 Operator : SY/MD
 Sample : M4887-04ME
 Misc : 5.31g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

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	1923	1937	1965	rBV	207207	415678	23.94%	3.335%
38	7.790	1997	2006	2019	rBV5	3097	5760	0.33%	0.046%
39	7.899	2024	2040	2057	rBV	771398	1473349	84.84%	11.821%
40	8.182	2115	2128	2160	rVB	120599	281786	16.23%	2.261%
41	8.468	2210	2217	2227	rBV	375	781	0.04%	0.006%
42	8.555	2231	2244	2259	rBV	84341	146060	8.41%	1.172%
43	8.684	2259	2284	2316	rBV2	272252	892266	51.38%	7.159%
44	8.951	2359	2367	2378	rVB3	1205	2264	0.13%	0.018%
45	9.298	2468	2475	2481	rBV	176	360	0.02%	0.003%
46	9.423	2498	2514	2542	rVB	360614	844027	48.60%	6.772%
47	9.581	2553	2563	2570	rBV2	760	1225	0.07%	0.010%
48	9.700	2590	2600	2611	rVV	1958	3393	0.20%	0.027%
49	10.111	2720	2728	2729	rBV	518	565	0.03%	0.005%
50	10.221	2759	2762	2767	rBV2	170	172	0.01%	0.001%
51	10.285	2779	2782	2784	rBV	200	166	0.01%	0.001%
52	10.539	2857	2861	2862	rBV2	325	227	0.01%	0.002%
53	10.671	2892	2902	2912	rBV2	5320	7912	0.46%	0.063%
54	10.774	2919	2934	2949	rBV	519600	882099	50.79%	7.077%
55	10.828	2949	2951	2955	rVB3	456	265	0.02%	0.002%
56	10.870	2959	2964	2966	rBV2	814	797	0.05%	0.006%
57	10.883	2966	2968	2969	rBV2	445	170	0.01%	0.001%
58	11.002	3000	3005	3014	rBV	320	579	0.03%	0.005%
59	11.105	3029	3037	3039	rBV5	944	1092	0.06%	0.009%
60	11.208	3063	3069	3073	rBV3	375	461	0.03%	0.004%
61	11.301	3095	3098	3101	rVV	352	251	0.01%	0.002%
62	11.375	3117	3121	3128	rBV	350	467	0.03%	0.004%
63	11.459	3138	3147	3160	rVB5	4530	8129	0.47%	0.065%
64	11.574	3179	3183	3184	rBV5	681	433	0.02%	0.003%
65	11.697	3213	3221	3229	rBV3	2514	3708	0.21%	0.030%
66	11.819	3245	3259	3279	rBV	557526	883128	50.85%	7.086%
67	11.902	3281	3285	3287	rBV2	277	230	0.01%	0.002%
68	11.947	3287	3299	3302	rVV4	2050	3543	0.20%	0.028%
69	11.973	3302	3307	3316	rVB4	4288	6071	0.35%	0.049%
70	12.008	3316	3318	3322	rBV	291	194	0.01%	0.002%
71	12.086	3337	3342	3345	rVB3	389	341	0.02%	0.003%
72	12.201	3357	3378	3394	rBV	820484	1341632	77.25%	10.764%
73	12.275	3394	3401	3407	rVV4	1072	1386	0.08%	0.011%
74	12.330	3410	3418	3426	rVB3	1812	2653	0.15%	0.021%
75	12.391	3431	3437	3438	rBV	523	518	0.03%	0.004%
76	12.600	3494	3502	3504	rBV2	267	346	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
 Data File : VU046150.D
 Acq On : 07 Dec 2021 19:34
 Operator : SY/MD
 Sample : M4887-04ME
 Misc : 5.31g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

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

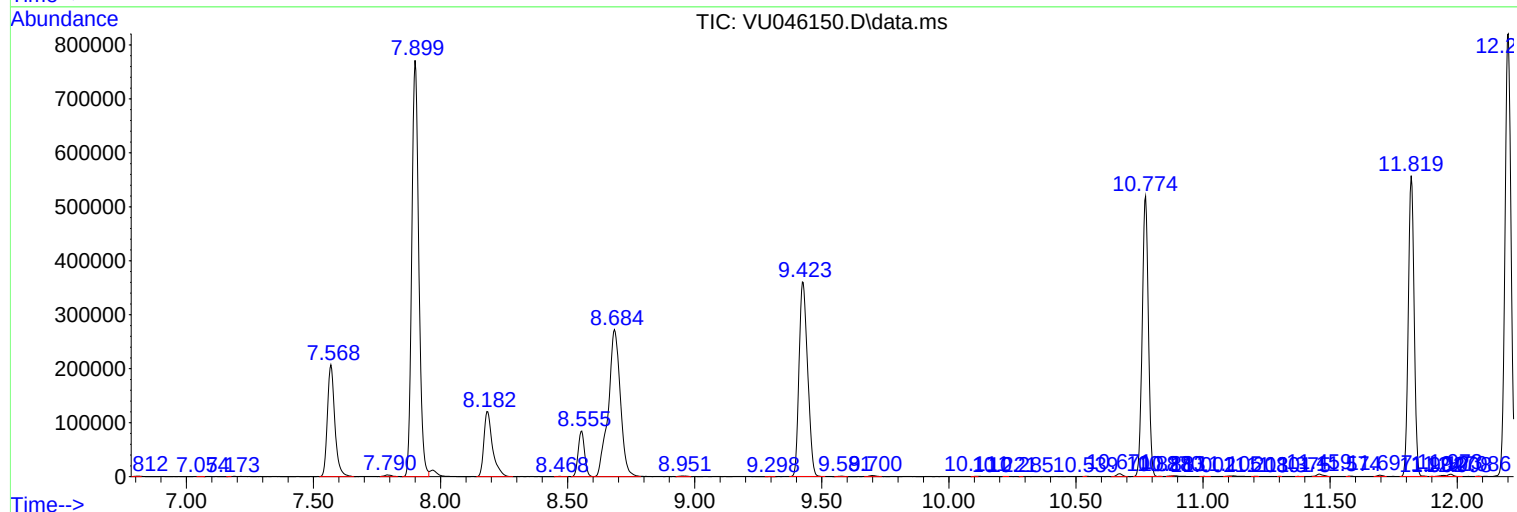
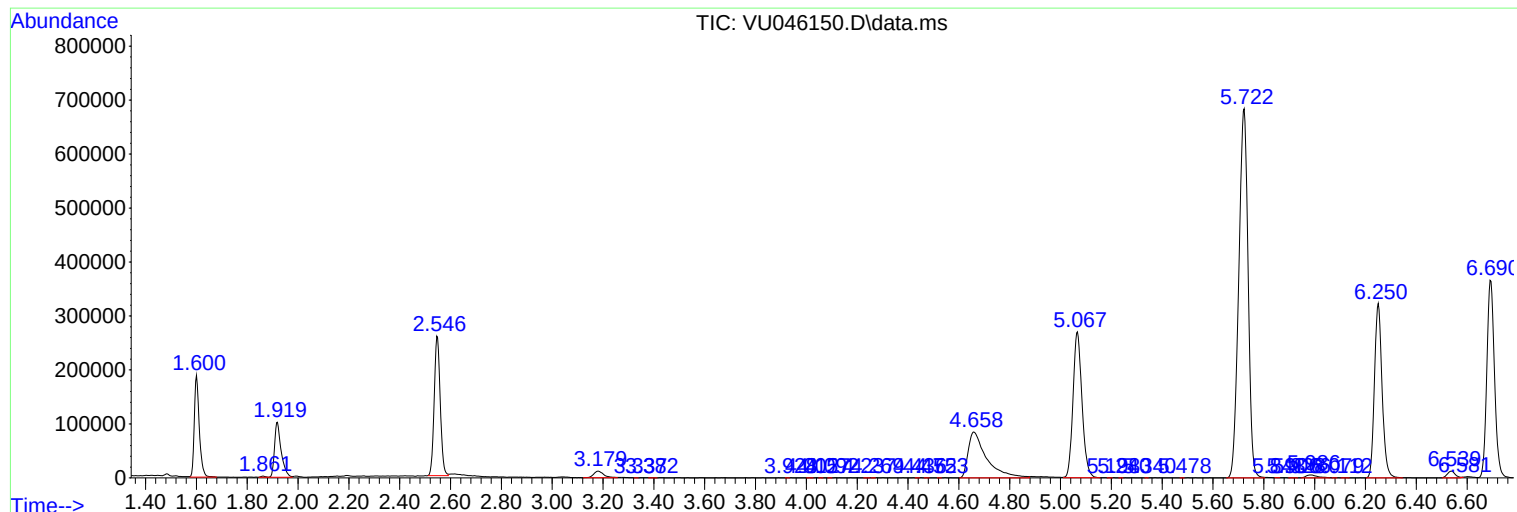
77	12.889	3588	3592	3597	rBV2	220	239	0.01%	0.002%
78	13.057	3640	3644	3648	rVB3	304	210	0.01%	0.002%
79	13.082	3648	3652	3657	rBV2	212	250	0.01%	0.002%
80	13.140	3663	3670	3671	rBV2	539	455	0.03%	0.004%
81	13.227	3693	3697	3701	rVB	446	403	0.02%	0.003%
82	13.275	3708	3712	3716	rVV3	348	348	0.02%	0.003%
83	13.426	3753	3759	3762	rBV3	539	610	0.04%	0.005%
84	13.581	3804	3807	3808	rBV3	254	145	0.01%	0.001%
85	13.751	3857	3860	3868	rVB	246	278	0.02%	0.002%
86	13.841	3884	3888	3894	rBV2	513	619	0.04%	0.005%
87	14.092	3956	3966	3976	rBV	4580	6179	0.36%	0.050%
88	14.182	3991	3994	3995	rBV	601	294	0.02%	0.002%
89	14.330	4037	4040	4046	rVV3	497	576	0.03%	0.005%
90	14.449	4071	4077	4085	rVV3	1896	2581	0.15%	0.021%
91	14.581	4108	4118	4126	rVB3	1755	3230	0.19%	0.026%
92	14.635	4132	4135	4141	rVV4	465	492	0.03%	0.004%
93	14.716	4157	4160	4163	rBV	235	175	0.01%	0.001%
94	15.217	4309	4316	4325	rVB4	1087	1973	0.11%	0.016%
95	15.378	4359	4366	4367	rBV6	1521	1389	0.08%	0.011%
96	15.497	4402	4403	4406	rVB2	423	161	0.01%	0.001%
97	15.976	4545	4552	4560	rBV6	1547	1817	0.10%	0.015%
98	16.188	4610	4618	4625	rBV6	2106	3355	0.19%	0.027%
99	16.288	4646	4649	4657	rVB4	2058	2274	0.13%	0.018%
100	16.401	4681	4684	4690	rBV4	845	820	0.05%	0.007%

Sum of corrected areas: 12463606

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU120721\
Data File : VU046150.D
Acq On : 07 Dec 2021 19:34
Operator : SY/MD
Sample : M4887-04ME
Misc : 5.31g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

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\VU120721\
Data File : VU046150.D
Acq On : 07 Dec 2021 19:34
Operator : SY/MD
Sample : M4887-04ME
Misc : 5.31g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

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\VU120721\
Data File : VU046150.D
Acq On : 07 Dec 2021 19:34
Operator : SY/MD
Sample : M4887-04ME
Misc : 5.31g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

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
