

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051922\
 Data File : VU048636.D
 Acq On : 19 May 2022 17:40
 Operator : SY/MD
 Sample : N2883-04ME
 Misc : 5.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4K6ME

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\SFAMULM051622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048636.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	72	80	103	rBV	73589	128820	10.20%	1.231%
2	2.228	273	276	278	rBV2	317	199	0.02%	0.002%
3	2.401	327	330	332	rBV2	312	146	0.01%	0.001%
4	2.539	360	373	384	rBV	236545	387599	30.69%	3.703%
5	2.703	422	424	429	rBV2	242	143	0.01%	0.001%
6	2.851	466	470	472	rBB	180	140	0.01%	0.001%
7	2.893	480	483	486	rBB	202	161	0.01%	0.002%
8	2.935	492	496	498	rBV2	847	621	0.05%	0.006%
9	3.038	515	528	539	rBV5	4029	8602	0.68%	0.082%
10	3.179	557	572	586	rBV2	9981	24975	1.98%	0.239%
11	3.414	643	645	648	rVB	406	201	0.02%	0.002%
12	3.510	672	675	678	rBB	210	150	0.01%	0.001%
13	3.549	685	687	690	rBB	301	162	0.01%	0.002%
14	3.864	782	785	788	rBB	163	136	0.01%	0.001%
15	3.896	791	795	796	rBV	224	150	0.01%	0.001%
16	4.179	880	883	886	rBB	152	126	0.01%	0.001%
17	4.202	886	890	892	rBB	168	137	0.01%	0.001%
18	4.375	940	944	946	rBB	161	130	0.01%	0.001%
19	4.533	989	993	996	rBB2	318	225	0.02%	0.002%
20	4.584	1006	1009	1010	rBV	341	180	0.01%	0.002%
21	4.629	1010	1023	1046	rBV	104346	311191	24.64%	2.973%
22	4.867	1094	1097	1101	rVV2	340	199	0.02%	0.002%
23	4.887	1101	1103	1108	rVB3	350	279	0.02%	0.003%
24	4.909	1108	1110	1113	rBB	271	125	0.01%	0.001%
25	4.967	1126	1128	1131	rBV2	384	209	0.02%	0.002%
26	5.060	1141	1157	1184	rBV	234431	540919	42.83%	5.168%
27	5.295	1223	1230	1232	rBV3	317	376	0.03%	0.004%
28	5.346	1232	1246	1256	rBV4	1917	5274	0.42%	0.050%
29	5.629	1332	1334	1336	rBV	194	120	0.01%	0.001%
30	5.719	1341	1362	1394	rBV2	480903	1262966	100.00%	12.067%
31	5.880	1410	1412	1415	rBV	224	187	0.01%	0.002%
32	5.973	1430	1441	1457	rBV5	6667	15277	1.21%	0.146%
33	6.031	1458	1459	1463	rVB2	381	206	0.02%	0.002%
34	6.108	1480	1483	1488	rVB2	419	298	0.02%	0.003%
35	6.137	1489	1492	1493	rBV	365	187	0.01%	0.002%
36	6.247	1512	1526	1548	rBV	368398	716465	56.73%	6.845%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051922\
 Data File : VU048636.D
 Acq On : 19 May 2022 17:40
 Operator : SY/MD
 Sample : N2883-04ME
 Misc : 5.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4K6ME

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\SFAMULM051622WMA.M
 Title : VOC Analysis

37	6.382	1565	1568	1571	rBV2	363	303	0.02%	0.003%
38	6.523	1601	1612	1624	rVB5	7134	13773	1.09%	0.132%
39	6.594	1625	1634	1650	rBV5	2946	7079	0.56%	0.068%
40	6.690	1650	1664	1686	rVV	271917	558151	44.19%	5.333%
41	6.803	1695	1699	1700	rBV2	347	267	0.02%	0.003%
42	6.890	1721	1726	1728	rBB	217	190	0.02%	0.002%
43	6.932	1735	1739	1740	rBV	367	246	0.02%	0.002%
44	6.957	1745	1747	1750	rVB	340	179	0.01%	0.002%
45	6.980	1750	1754	1755	rBV	272	182	0.01%	0.002%
46	6.989	1755	1757	1759	rVB	425	225	0.02%	0.002%
47	7.005	1760	1762	1765	rBB	262	135	0.01%	0.001%
48	7.031	1768	1770	1773	rBB	223	139	0.01%	0.001%
49	7.050	1773	1776	1779	rBV	504	433	0.03%	0.004%
50	7.192	1808	1820	1826	rBV5	5837	11116	0.88%	0.106%
51	7.301	1852	1854	1855	rBV	272	149	0.01%	0.001%
52	7.340	1863	1866	1868	rBV	338	220	0.02%	0.002%
53	7.446	1895	1899	1902	rBB	250	172	0.01%	0.002%
54	7.497	1912	1915	1917	rBV	267	133	0.01%	0.001%
55	7.565	1924	1936	1955	rBV	160264	309086	24.47%	2.953%
56	7.684	1968	1973	1974	rBV3	1213	1038	0.08%	0.010%
57	7.790	1994	2006	2015	rBV2	6380	12270	0.97%	0.117%
58	7.896	2026	2039	2056	rBV	577036	1028825	81.46%	9.830%
59	8.070	2086	2093	2099	rVB5	603	827	0.07%	0.008%
60	8.108	2101	2105	2107	rBV	179	136	0.01%	0.001%
61	8.182	2116	2128	2150	rVV	109719	223860	17.72%	2.139%
62	8.327	2170	2173	2176	rVB3	333	199	0.02%	0.002%
63	8.346	2176	2179	2180	rBV	503	304	0.02%	0.003%
64	8.385	2190	2191	2193	rBV	363	134	0.01%	0.001%
65	8.423	2201	2203	2207	rVB	304	180	0.01%	0.002%
66	8.472	2213	2218	2220	rBV	561	472	0.04%	0.005%
67	8.552	2241	2243	2245	rVB	300	138	0.01%	0.001%
68	8.652	2257	2274	2302	rBV	352734	780803	61.82%	7.460%
69	8.861	2337	2339	2340	rBV	495	196	0.02%	0.002%
70	8.928	2351	2360	2366	rBV5	1988	3416	0.27%	0.033%
71	9.044	2393	2396	2399	rVB	239	157	0.01%	0.002%
72	9.163	2430	2433	2434	rBV	508	322	0.03%	0.003%
73	9.211	2440	2448	2455	rBV4	1140	1268	0.10%	0.012%
74	9.269	2462	2466	2470	rVB2	308	255	0.02%	0.002%
75	9.304	2473	2477	2478	rBV	174	150	0.01%	0.001%
76	9.327	2481	2484	2486	rBV	703	496	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051922\
 Data File : VU048636.D
 Acq On : 19 May 2022 17:40
 Operator : SY/MD
 Sample : N2883-04ME
 Misc : 5.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 EW4K6ME

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\SFAMULM051622WMA.M
 Title : VOC Analysis

77	9.420	2498	2513	2530	rBV	484173	912909	72.28%	8.722%
78	9.571	2554	2560	2568	rBV3	892	1356	0.11%	0.013%
79	9.648	2578	2584	2587	rBV	396	308	0.02%	0.003%
80	9.697	2591	2599	2601	rBV3	2641	2995	0.24%	0.029%
81	9.854	2644	2648	2650	rBV	204	199	0.02%	0.002%
82	10.025	2694	2701	2706	rBV5	1271	1716	0.14%	0.016%
83	10.070	2714	2715	2720	rVB2	215	126	0.01%	0.001%
84	10.108	2722	2727	2731	rVV4	1279	1316	0.10%	0.013%
85	10.144	2735	2738	2739	rBV	302	198	0.02%	0.002%
86	10.173	2745	2747	2749	rBV2	301	189	0.01%	0.002%
87	10.256	2761	2773	2781	rBV9	3820	8012	0.63%	0.077%
88	10.308	2785	2789	2790	rBV	327	185	0.01%	0.002%
89	10.359	2797	2805	2807	rBV6	2448	3145	0.25%	0.030%
90	10.465	2832	2838	2842	rBV5	1246	1760	0.14%	0.017%
91	10.542	2855	2862	2864	rBV5	1681	1821	0.14%	0.017%
92	10.719	2914	2917	2918	rBV2	473	269	0.02%	0.003%
93	10.764	2918	2931	2953	rVV	479238	794190	62.88%	7.588%
94	10.954	2981	2990	2995	rBV7	1502	2513	0.20%	0.024%
95	11.002	3000	3005	3006	rBV3	1553	1206	0.10%	0.012%
96	11.115	3032	3040	3055	rVB4	21101	35502	2.81%	0.339%
97	11.417	3128	3134	3142	rVB5	11481	14981	1.19%	0.143%
98	11.578	3173	3184	3188	rBV4	3242	5489	0.43%	0.052%
99	11.816	3246	3258	3272	rBV	705347	1109360	87.84%	10.599%
100	12.195	3364	3376	3392	rBV	736420	1201890	95.16%	11.483%

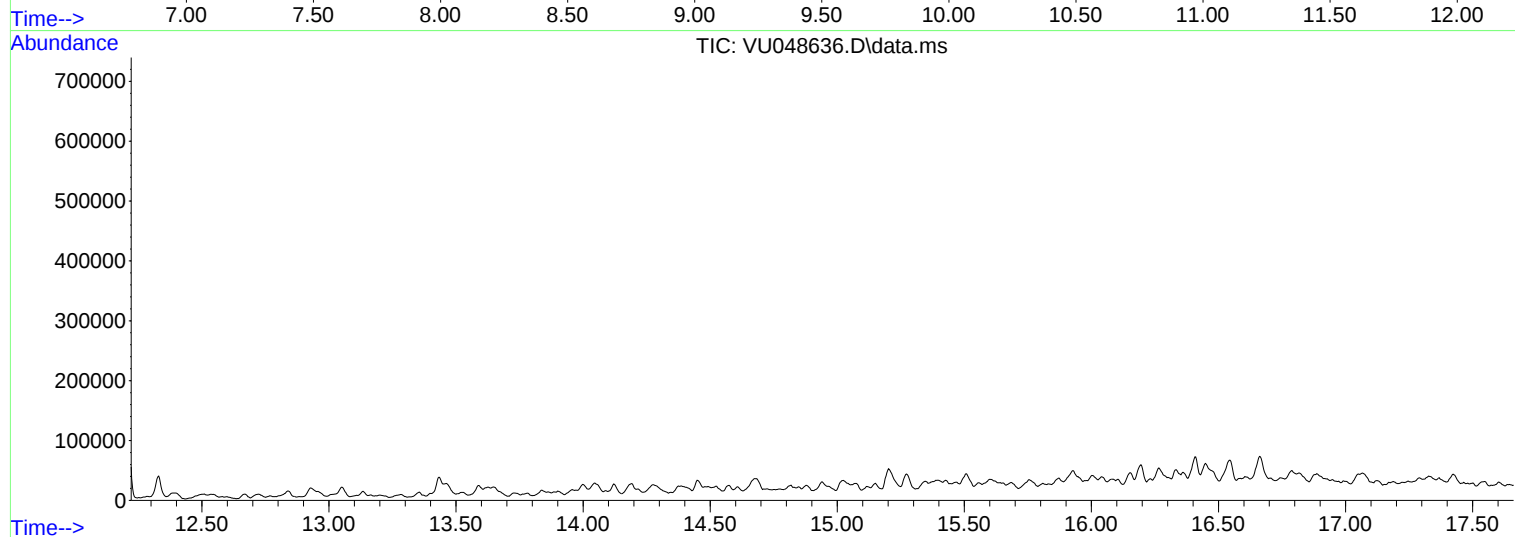
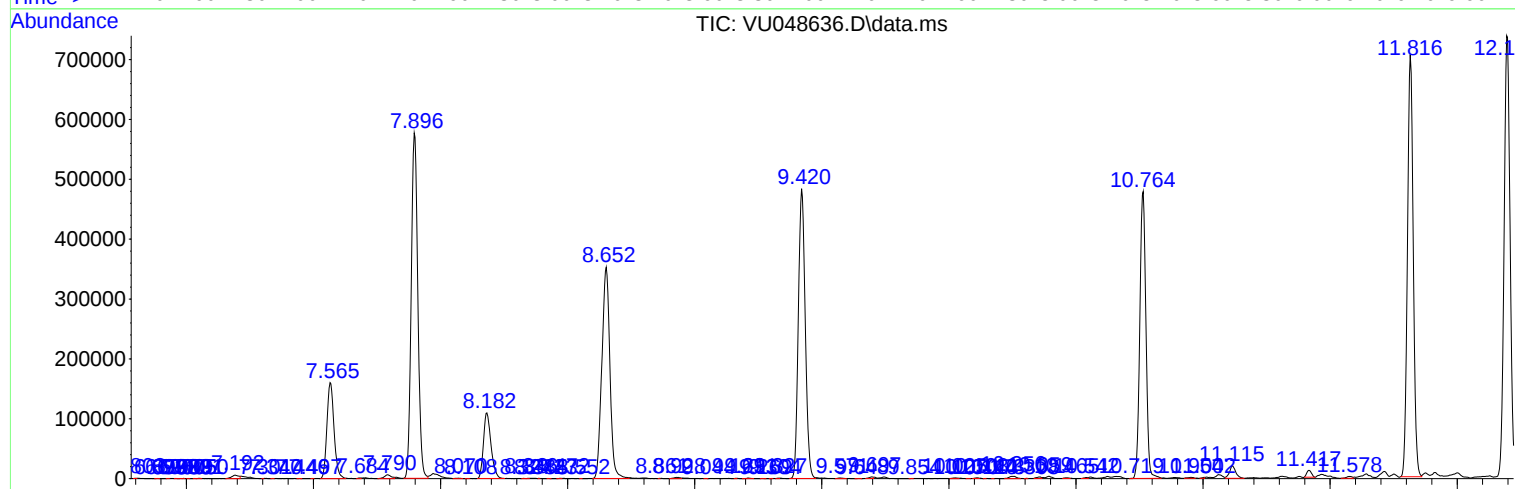
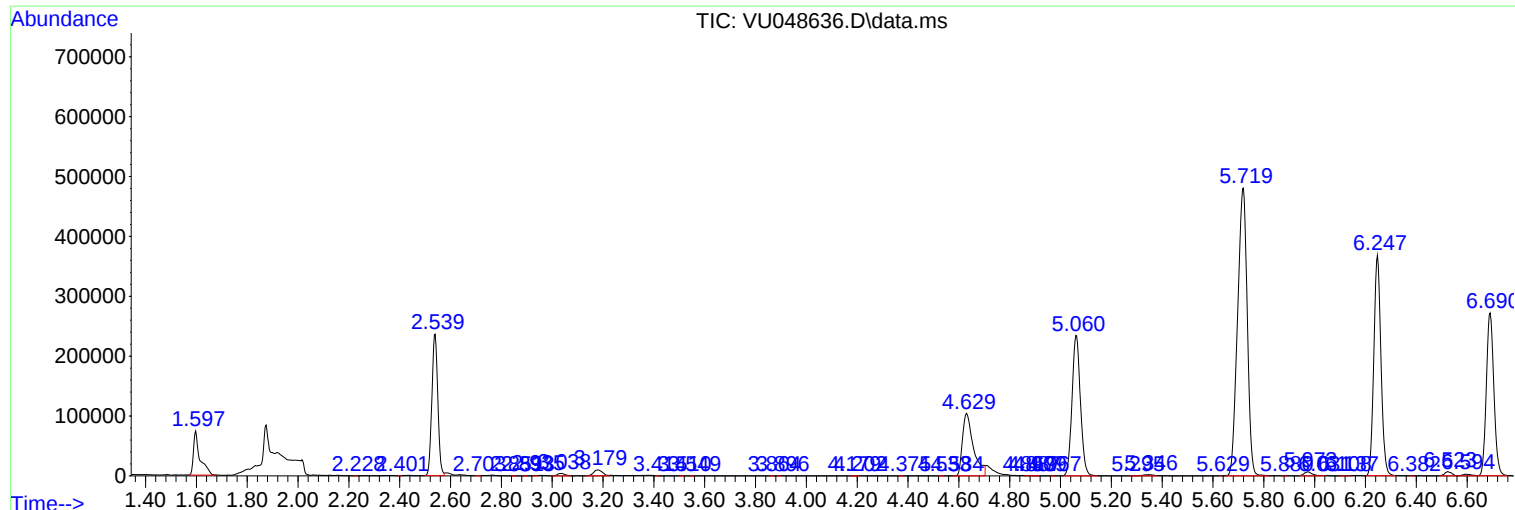
Sum of corrected areas: 10466540

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051922\
Data File : VU048636.D
Acq On : 19 May 2022 17:40
Operator : SY/MD
Sample : N2883-04ME
Misc : 5.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4K6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU051922\
Data File : VU048636.D
Acq On : 19 May 2022 17:40
Operator : SY/MD
Sample : N2883-04ME
Misc : 5.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4K6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.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\VU051922\
Data File : VU048636.D
Acq On : 19 May 2022 17:40
Operator : SY/MD
Sample : N2883-04ME
Misc : 5.73g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 16 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
EW4K6ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM051622WMA.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