

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050622\
 Data File : VU048459.D
 Acq On : 06 May 2022 16:55
 Operator : SY/MD
 Sample : VU0506MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK117

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\SFAMULM050622WMA.M
 Title : VOC Analysis

Signal : TIC: VU048459.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	98	rBV	182216	236088	14.78%	1.937%
2	1.900	167	174	190	rVB	123733	177647	11.12%	1.457%
3	2.565	368	381	401	rBV	342493	562290	35.20%	4.612%
4	2.793	442	452	461	rBV	2840	5051	0.32%	0.041%
5	3.018	519	522	524	rBV2	480	325	0.02%	0.003%
6	3.047	524	531	538	rVV4	1303	1830	0.11%	0.015%
7	3.186	563	574	583	rBV5	2952	6792	0.43%	0.056%
8	3.353	620	626	634	rBV5	1013	1485	0.09%	0.012%
9	3.449	653	656	661	rVB2	352	302	0.02%	0.002%
10	3.475	661	664	670	rVB3	420	337	0.02%	0.003%
11	3.549	683	687	688	rBV	263	164	0.01%	0.001%
12	3.642	714	716	719	rVB2	360	172	0.01%	0.001%
13	3.662	719	722	723	rBV	338	188	0.01%	0.002%
14	3.764	750	754	757	rBV	183	150	0.01%	0.001%
15	3.780	757	759	765	rBV2	186	150	0.01%	0.001%
16	3.858	779	783	784	rBV2	298	188	0.01%	0.002%
17	3.912	794	800	804	rBV2	188	217	0.01%	0.002%
18	3.941	807	809	812	rVB2	356	158	0.01%	0.001%
19	3.996	823	826	829	rBV2	233	161	0.01%	0.001%
20	4.079	850	852	855	rBV	197	164	0.01%	0.001%
21	4.215	890	894	898	rBV	190	126	0.01%	0.001%
22	4.240	898	902	904	rBV2	310	215	0.01%	0.002%
23	4.321	925	927	932	rVB	543	345	0.02%	0.003%
24	4.353	932	937	939	rBV	174	163	0.01%	0.001%
25	4.456	964	969	971	rBV2	222	193	0.01%	0.002%
26	4.488	975	979	981	rBV	277	176	0.01%	0.001%
27	4.526	987	991	994	rVB3	286	192	0.01%	0.002%
28	4.623	1007	1021	1050	rBV2	178381	440707	27.59%	3.615%
29	5.063	1137	1158	1182	rBV	280480	612173	38.32%	5.022%
30	5.195	1196	1199	1203	rBV	518	469	0.03%	0.004%
31	5.253	1215	1217	1221	rVB	234	151	0.01%	0.001%
32	5.285	1222	1227	1231	rBV2	794	888	0.06%	0.007%
33	5.385	1254	1258	1259	rBV	371	279	0.02%	0.002%
34	5.436	1272	1274	1279	rVB2	168	132	0.01%	0.001%
35	5.539	1303	1306	1309	rVB2	360	207	0.01%	0.002%
36	5.594	1314	1323	1326	rBV2	311	380	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050622\
 Data File : VU048459.D
 Acq On : 06 May 2022 16:55
 Operator : SY/MD
 Sample : VU0506MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK117

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\SFAMULM050622WMA.M
 Title : VOC Analysis

37	5.616	1326	1330	1332	rBV	232	194	0.01%	0.002%
38	5.726	1341	1364	1388	rBV2	600024	1597511	100.00%	13.104%
39	5.919	1422	1424	1428	rBV2	270	268	0.02%	0.002%
40	6.022	1452	1456	1458	rBV2	436	263	0.02%	0.002%
41	6.102	1479	1481	1482	rBV	295	156	0.01%	0.001%
42	6.198	1507	1511	1512	rBV2	341	218	0.01%	0.002%
43	6.250	1512	1527	1548	rVV	489937	931595	58.32%	7.642%
44	6.423	1578	1581	1588	rVB4	375	325	0.02%	0.003%
45	6.491	1599	1602	1605	rBV2	464	287	0.02%	0.002%
46	6.533	1605	1615	1621	rBV8	2659	4067	0.25%	0.033%
47	6.604	1634	1637	1639	rBV	355	233	0.01%	0.002%
48	6.690	1648	1664	1687	rBV	369935	723503	45.29%	5.935%
49	6.941	1739	1742	1746	rVB2	313	185	0.01%	0.002%
50	7.018	1763	1766	1768	rBV	204	165	0.01%	0.001%
51	7.140	1801	1804	1806	rBV2	211	127	0.01%	0.001%
52	7.185	1806	1818	1830	rVB4	3660	7506	0.47%	0.062%
53	7.337	1861	1865	1866	rBV2	251	175	0.01%	0.001%
54	7.430	1891	1894	1895	rBV	254	120	0.01%	0.001%
55	7.565	1922	1936	1957	rBV	198046	348234	21.80%	2.857%
56	7.729	1984	1987	1990	rBV2	319	208	0.01%	0.002%
57	7.758	1993	1996	2000	rBV	492	403	0.03%	0.003%
58	7.803	2002	2010	2013	rBV4	1100	1678	0.11%	0.014%
59	7.899	2026	2040	2056	rBV	689485	1205985	75.49%	9.893%
60	8.140	2106	2115	2116	rBV3	507	560	0.04%	0.005%
61	8.179	2116	2127	2145	rVV2	135033	227690	14.25%	1.868%
62	8.475	2216	2219	2221	rBV	303	164	0.01%	0.001%
63	8.488	2221	2223	2225	rBV2	232	129	0.01%	0.001%
64	8.552	2239	2243	2244	rBV3	934	728	0.05%	0.006%
65	8.636	2256	2269	2302	rBV2	533161	994692	62.27%	8.159%
66	8.861	2337	2339	2342	rBV	408	210	0.01%	0.002%
67	8.880	2342	2345	2346	rBV3	345	200	0.01%	0.002%
68	8.954	2365	2368	2374	rBV3	435	443	0.03%	0.004%
69	9.044	2392	2396	2400	rVB3	394	316	0.02%	0.003%
70	9.066	2400	2403	2406	rBV3	333	220	0.01%	0.002%
71	9.147	2425	2428	2429	rBV	278	151	0.01%	0.001%
72	9.163	2429	2433	2435	rVV2	604	424	0.03%	0.003%
73	9.282	2468	2470	2475	rBV2	372	295	0.02%	0.002%
74	9.417	2499	2512	2550	rBV	679744	1125096	70.43%	9.229%
75	9.571	2555	2560	2562	rBV3	1249	1113	0.07%	0.009%
76	9.616	2571	2574	2576	rBV2	361	260	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050622\
 Data File : VU048459.D
 Acq On : 06 May 2022 16:55
 Operator : SY/MD
 Sample : VU0506MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 12 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK117

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\SFAMULM050622WMA.M
 Title : VOC Analysis

77	9.697	2592	2599	2606	rVB4	2160	2620	0.16%	0.021%
78	9.838	2638	2643	2646	rBV	384	306	0.02%	0.003%
79	9.967	2680	2683	2688	rVB2	452	410	0.03%	0.003%
80	10.095	2719	2723	2724	rVV3	916	719	0.05%	0.006%
81	10.111	2724	2728	2740	rVB5	2768	3836	0.24%	0.031%
82	10.330	2793	2796	2798	rBV2	202	152	0.01%	0.001%
83	10.558	2865	2867	2870	rBV2	266	200	0.01%	0.002%
84	10.610	2875	2883	2885	rBV2	349	492	0.03%	0.004%
85	10.671	2895	2902	2911	rVB4	2364	2964	0.19%	0.024%
86	10.758	2915	2929	2946	rBV	517626	848848	53.14%	6.963%
87	10.967	2990	2994	2995	rBV2	313	191	0.01%	0.002%
88	11.163	3053	3055	3058	rBV2	443	301	0.02%	0.002%
89	11.272	3086	3089	3091	rBV2	284	179	0.01%	0.001%
90	11.369	3116	3119	3124	rVB3	603	513	0.03%	0.004%
91	11.398	3124	3128	3133	rBV2	463	456	0.03%	0.004%
92	11.745	3229	3236	3245	rBV6	3267	4908	0.31%	0.040%
93	11.812	3245	3257	3277	rBV	634899	1004419	62.87%	8.239%
94	12.008	3316	3318	3321	rBV2	490	334	0.02%	0.003%
95	12.073	3336	3338	3342	rBV2	522	309	0.02%	0.003%
96	12.192	3363	3375	3394	rBV	617464	996631	62.39%	8.175%
97	13.224	3690	3696	3708	rVB7	4660	7273	0.46%	0.060%
98	13.841	3880	3888	3902	rVB2	12044	17936	1.12%	0.147%
99	14.089	3956	3965	3980	rBV	28671	47637	2.98%	0.391%
100	14.333	4032	4041	4051	rVB4	14515	22386	1.40%	0.184%

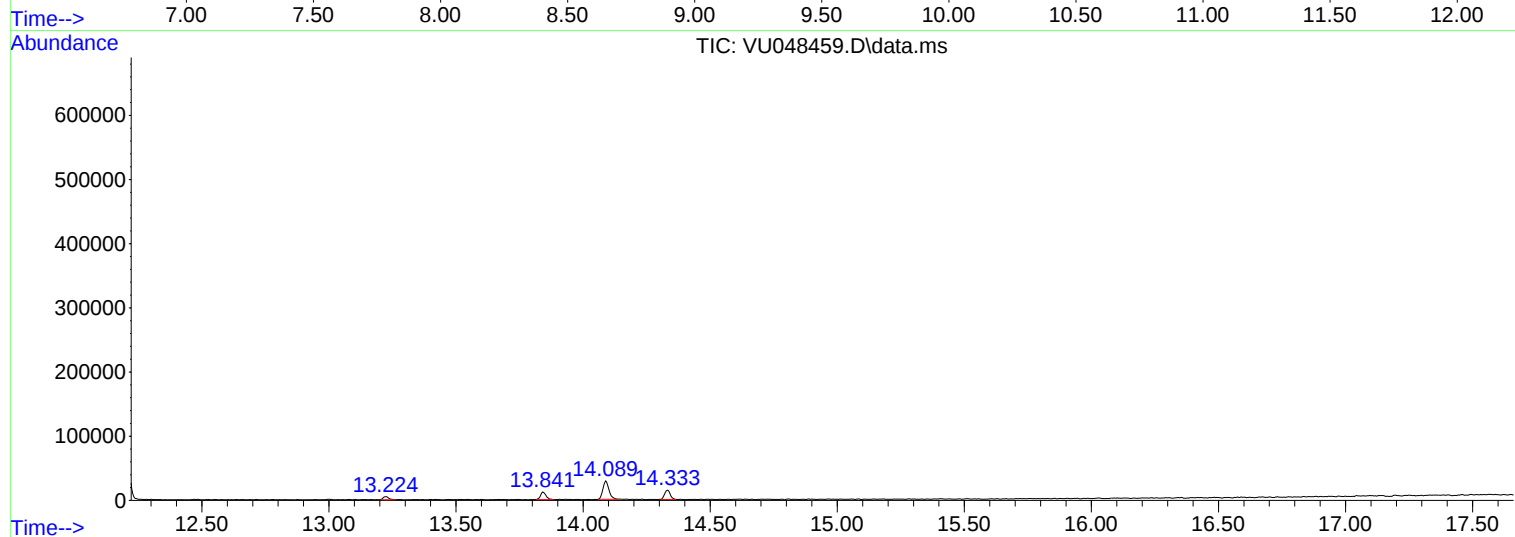
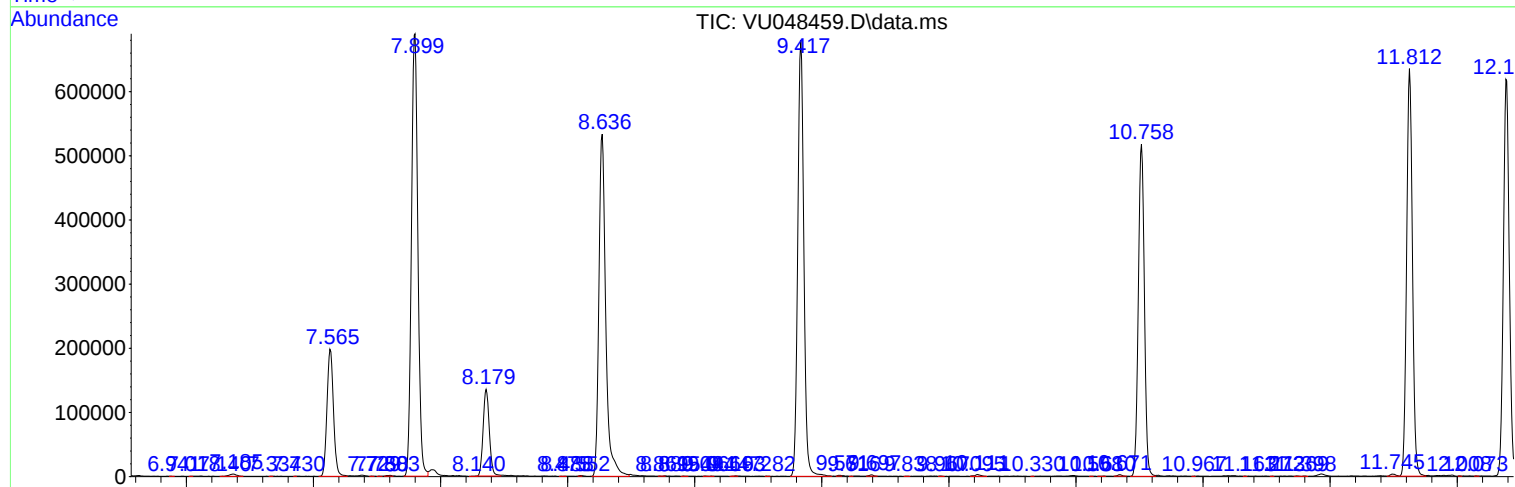
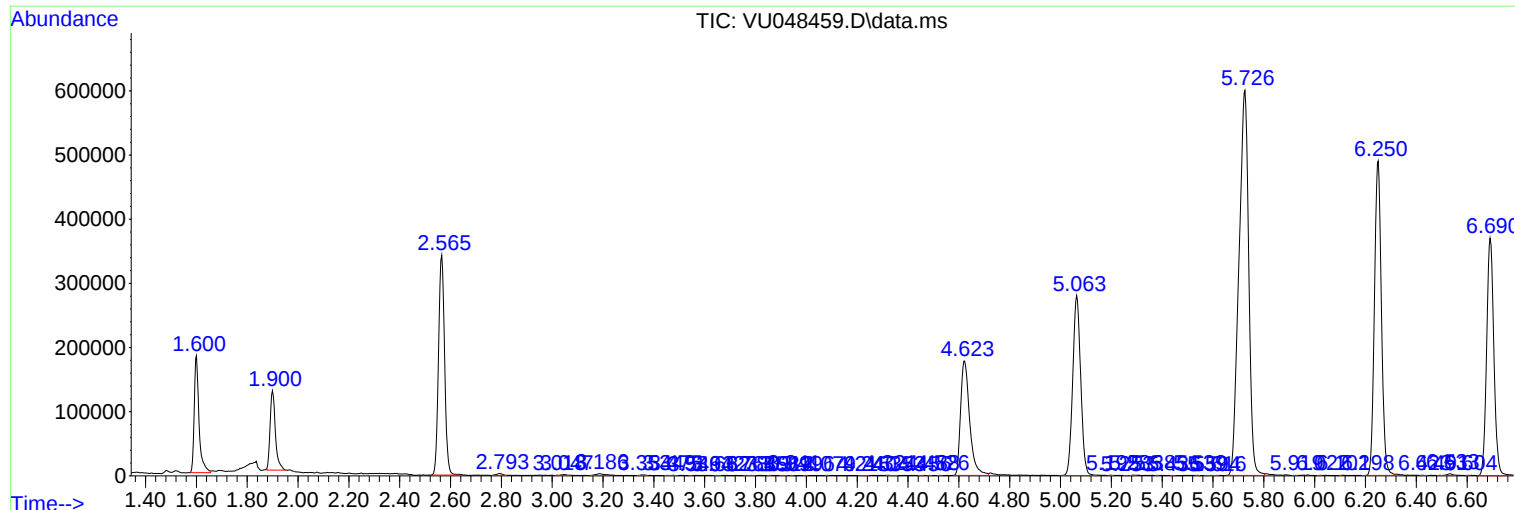
Sum of corrected areas: 12190772

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050622\
Data File : VU048459.D
Acq On : 06 May 2022 16:55
Operator : SY/MD
Sample : VU0506MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK117

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU050622\
Data File : VU048459.D
Acq On : 06 May 2022 16:55
Operator : SY/MD
Sample : VU0506MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK117

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.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\VU050622\
Data File : VU048459.D
Acq On : 06 May 2022 16:55
Operator : SY/MD
Sample : VU0506MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 12 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK117

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM050622WMA.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
------------------	----	---------	-------	----------	---	----	------	------