

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042522\
 Data File : VU048266.D
 Acq On : 25 Apr 2022 14:04
 Operator : SY/MD
 Sample : VU0425MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK110

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\SFAMULM042522WMA.M

Title : VOC Analysis

Signal : TIC: VU048266.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.485	41	45	51	rBV4	3109	2908	0.16%	0.021%
2	1.601	73	81	100	rBV	213733	274718	15.27%	2.013%
3	1.890	163	171	189	rVB	143677	216758	12.05%	1.588%
4	2.562	367	380	397	rBV	373642	617541	34.32%	4.525%
5	2.794	442	452	460	rBV2	1458	2690	0.15%	0.020%
6	2.877	475	478	482	rBV2	225	221	0.01%	0.002%
7	2.900	482	485	488	rBV3	251	216	0.01%	0.002%
8	2.958	499	503	511	rVV4	759	1024	0.06%	0.008%
9	3.044	516	530	538	rBV5	2563	4610	0.26%	0.034%
10	3.105	544	549	551	rBV2	235	226	0.01%	0.002%
11	3.183	561	573	591	rBV2	2951	7742	0.43%	0.057%
12	3.311	611	613	620	rVB2	326	389	0.02%	0.003%
13	3.343	620	623	625	rBV2	664	418	0.02%	0.003%
14	3.440	649	653	657	rVB	234	209	0.01%	0.002%
15	3.469	657	662	666	rVB3	318	351	0.02%	0.003%
16	3.498	666	671	673	rBV3	384	321	0.02%	0.002%
17	3.951	807	812	813	rBV	320	272	0.02%	0.002%
18	4.179	879	883	885	rBV3	257	219	0.01%	0.002%
19	4.414	948	956	964	rVB2	275	462	0.03%	0.003%
20	4.504	974	984	990	rBV2	215	369	0.02%	0.003%
21	4.620	1006	1020	1065	rBV	208887	516980	28.73%	3.788%
22	5.064	1141	1158	1183	rBV	317007	695642	38.67%	5.097%
23	5.247	1213	1215	1219	rVB	315	179	0.01%	0.001%
24	5.289	1223	1228	1230	rBV3	361	359	0.02%	0.003%
25	5.594	1319	1323	1330	rBV	251	312	0.02%	0.002%
26	5.723	1342	1363	1396	rBV2	668993	1799150	100.00%	13.182%
27	5.970	1436	1440	1444	rBV3	697	620	0.03%	0.005%
28	6.041	1456	1462	1463	rVV2	274	290	0.02%	0.002%
29	6.096	1476	1479	1482	rVV2	251	181	0.01%	0.001%
30	6.125	1482	1488	1492	rVB3	648	729	0.04%	0.005%
31	6.173	1498	1503	1507	rVB3	321	404	0.02%	0.003%
32	6.250	1511	1527	1550	rBV	427523	812137	45.14%	5.950%
33	6.523	1605	1612	1613	rBV3	1822	1498	0.08%	0.011%
34	6.588	1629	1632	1634	rBV3	629	525	0.03%	0.004%
35	6.620	1640	1642	1647	rVB2	345	215	0.01%	0.002%
36	6.690	1649	1664	1695	rVV	419303	810962	45.07%	5.942%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042522\
 Data File : VU048266.D
 Acq On : 25 Apr 2022 14:04
 Operator : SY/MD
 Sample : VU0425MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK110

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\SFAMULM042522WMA.M
 Title : VOC Analysis

37	6.803	1695	1699	1712	rVB5	1357	2222	0.12%	0.016%
38	6.912	1727	1733	1739	rVB	278	266	0.01%	0.002%
39	7.047	1763	1775	1779	rBV3	747	1113	0.06%	0.008%
40	7.179	1805	1816	1834	rVB5	5355	11003	0.61%	0.081%
41	7.430	1887	1894	1898	rBV3	298	280	0.02%	0.002%
42	7.565	1922	1936	1962	rBV	220991	385145	21.41%	2.822%
43	7.687	1965	1974	1991	rVB8	2106	4850	0.27%	0.036%
44	7.797	1998	2008	2024	rBV4	3841	7063	0.39%	0.052%
45	7.899	2024	2040	2055	rBV	807477	1402150	77.93%	10.273%
46	8.179	2113	2127	2142	rBV	154926	259293	14.41%	1.900%
47	8.343	2175	2178	2181	rVB2	688	400	0.02%	0.003%
48	8.356	2181	2182	2188	rVB2	500	321	0.02%	0.002%
49	8.388	2188	2192	2194	rBV2	340	237	0.01%	0.002%
50	8.549	2239	2242	2249	rVB4	601	688	0.04%	0.005%
51	8.636	2256	2269	2315	rBV	655906	1220758	67.85%	8.944%
52	8.928	2356	2360	2363	rVB3	459	423	0.02%	0.003%
53	8.999	2379	2382	2387	rVB3	341	303	0.02%	0.002%
54	9.067	2400	2403	2405	rBV2	391	245	0.01%	0.002%
55	9.308	2474	2478	2483	rBV2	325	320	0.02%	0.002%
56	9.340	2483	2488	2491	rVV2	209	223	0.01%	0.002%
57	9.417	2498	2512	2547	rVV	625393	1052158	58.48%	7.709%
58	9.546	2550	2552	2554	rVV	349	222	0.01%	0.002%
59	9.578	2554	2562	2568	rVB3	1368	2017	0.11%	0.015%
60	9.642	2578	2582	2587	rVB4	426	473	0.03%	0.003%
61	9.697	2590	2599	2606	rVV2	2568	3419	0.19%	0.025%
62	9.928	2668	2671	2675	rBV2	323	244	0.01%	0.002%
63	9.986	2684	2689	2692	rVB2	250	235	0.01%	0.002%
64	10.108	2719	2727	2740	rVB4	2088	4461	0.25%	0.033%
65	10.163	2740	2744	2746	rBV2	267	255	0.01%	0.002%
66	10.288	2780	2783	2786	rBV3	367	263	0.01%	0.002%
67	10.485	2836	2844	2851	rBV2	1508	1939	0.11%	0.014%
68	10.636	2885	2891	2897	rBV4	1632	2575	0.14%	0.019%
69	10.671	2897	2902	2911	rVB3	3366	4540	0.25%	0.033%
70	10.758	2915	2929	2946	rBV	688172	1125302	62.55%	8.245%
71	10.864	2958	2962	2964	rBV	421	392	0.02%	0.003%
72	10.893	2969	2971	2977	rVB2	616	482	0.03%	0.004%
73	11.095	3024	3034	3039	rBV4	957	1849	0.10%	0.014%
74	11.153	3048	3052	3056	rBV	446	478	0.03%	0.004%
75	11.202	3065	3067	3070	rVB3	357	187	0.01%	0.001%
76	11.247	3078	3081	3084	rVV	391	221	0.01%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042522\
 Data File : VU048266.D
 Acq On : 25 Apr 2022 14:04
 Operator : SY/MD
 Sample : VU0425MBL01
 Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 VBLK110

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\SFAMULM042522WMA.M
 Title : VOC Analysis

77	11.407	3128	3131	3132	rBV	327	189	0.01%	0.001%
78	11.468	3138	3150	3159	rVB5	4775	8912	0.50%	0.065%
79	11.507	3159	3162	3165	rBV	233	200	0.01%	0.001%
80	11.542	3168	3173	3178	rBV3	330	334	0.02%	0.002%
81	11.581	3178	3185	3189	rBV2	738	782	0.04%	0.006%
82	11.645	3201	3205	3210	rBV3	294	254	0.01%	0.002%
83	11.700	3210	3222	3227	rBV6	1229	1792	0.10%	0.013%
84	11.748	3230	3237	3245	rBV3	3666	4949	0.28%	0.036%
85	11.812	3245	3257	3280	rBV	630047	986060	54.81%	7.225%
86	11.941	3292	3297	3301	rBV4	837	810	0.05%	0.006%
87	12.012	3316	3319	3322	rVB2	458	298	0.02%	0.002%
88	12.050	3329	3331	3336	rVB3	451	394	0.02%	0.003%
89	12.076	3336	3339	3341	rBV	310	201	0.01%	0.001%
90	12.195	3361	3376	3393	rBV	778750	1277433	71.00%	9.359%
91	12.311	3410	3412	3415	rBV4	341	185	0.01%	0.001%
92	12.520	3475	3477	3482	rBV3	291	240	0.01%	0.002%
93	12.700	3530	3533	3536	rBV2	611	479	0.03%	0.004%
94	13.005	3622	3628	3634	rBV5	1173	1629	0.09%	0.012%
95	13.192	3684	3686	3688	rBV3	361	233	0.01%	0.002%
96	13.224	3689	3696	3705	rVB3	5059	7790	0.43%	0.057%
97	13.845	3880	3889	3901	rBV2	11800	17672	0.98%	0.129%
98	14.092	3954	3966	3979	rBV	27254	45600	2.53%	0.334%
99	14.333	4031	4041	4053	rBV2	12946	21186	1.18%	0.155%
100	14.504	4092	4094	4096	rBV	361	206	0.01%	0.002%

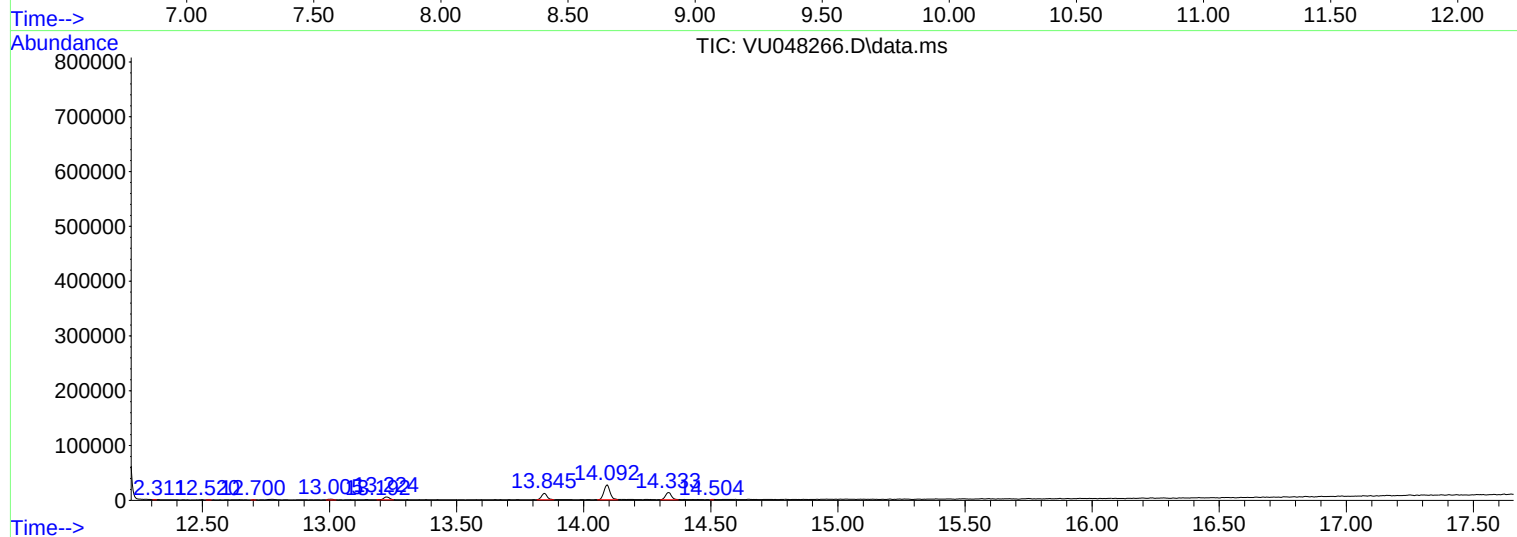
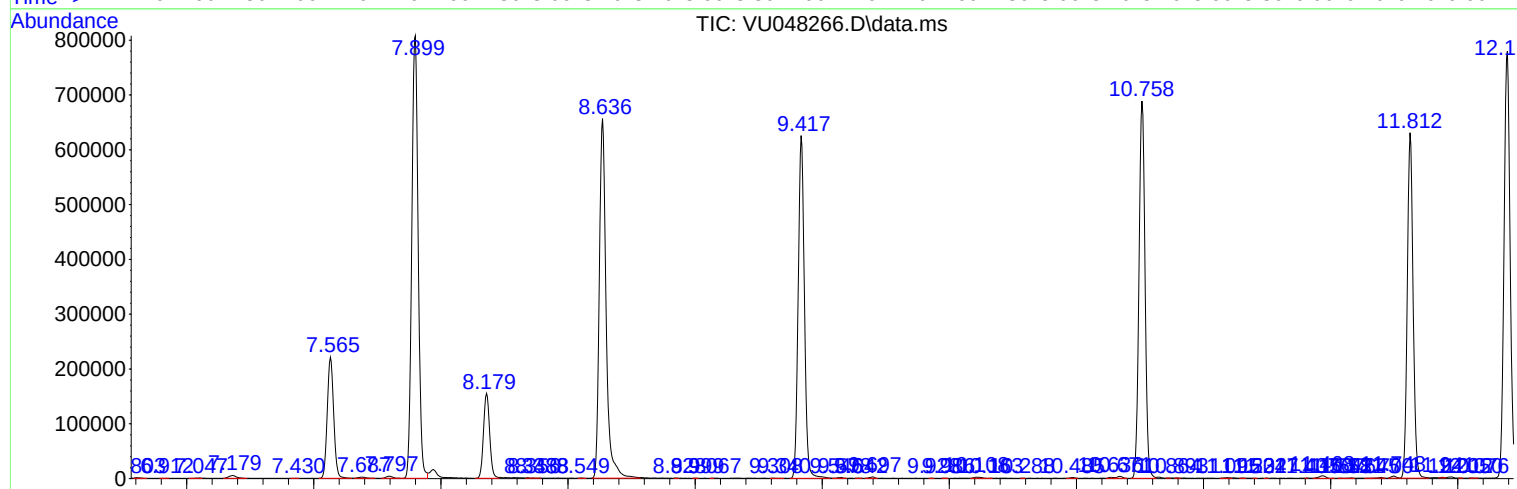
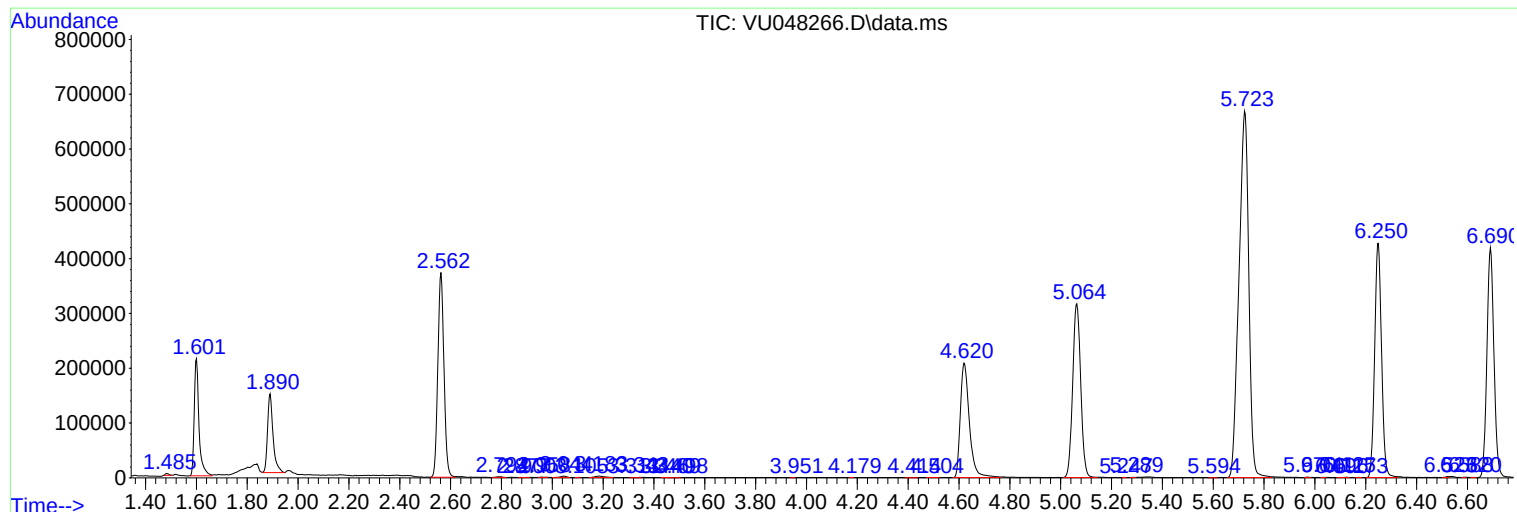
Sum of corrected areas: 13648690

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042522\
Data File : VU048266.D
Acq On : 25 Apr 2022 14:04
Operator : SY/MD
Sample : VU0425MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK110

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU042522\
Data File : VU048266.D
Acq On : 25 Apr 2022 14:04
Operator : SY/MD
Sample : VU0425MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK110

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.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\VU042522\
Data File : VU048266.D
Acq On : 25 Apr 2022 14:04
Operator : SY/MD
Sample : VU0425MBL01
Misc : 5.00g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
VBLK110

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM042522WMA.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