

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072022\
 Data File : VU049810.D
 Acq On : 20 Jul 2022 18:01
 Operator : SY/MD
 Sample : N3743-15ME
 Misc : 6.17g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5D13ME

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\SFAMULM071122WMA.M
 Title : VOC Analysis

Signal : TIC: VU049810.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.514	50	54	58	rBV4	1812	2066	0.33%	0.040%
2	1.594	71	79	85	rBV	35012	46303	7.46%	0.885%
3	2.218	270	273	276	rBV3	769	513	0.08%	0.010%
4	2.350	311	314	317	rVB2	583	331	0.05%	0.006%
5	2.514	354	365	382	rVB	106881	171318	27.60%	3.276%
6	2.584	384	387	394	rVB3	384	307	0.05%	0.006%
7	2.629	398	401	404	rBV2	398	351	0.06%	0.007%
8	2.652	406	408	415	rVB2	707	617	0.10%	0.012%
9	2.739	432	435	438	rBV2	363	244	0.04%	0.005%
10	2.758	439	441	445	rVB2	402	236	0.04%	0.005%
11	2.780	445	448	450	rBV2	245	181	0.03%	0.003%
12	2.928	489	494	497	rBV3	370	365	0.06%	0.007%
13	3.022	512	523	536	rVB4	3961	7558	1.22%	0.145%
14	3.124	550	555	558	rBV2	219	186	0.03%	0.004%
15	3.166	561	568	583	rBV2	1703	3786	0.61%	0.072%
16	3.478	659	665	667	rBV2	189	193	0.03%	0.004%
17	3.665	719	723	725	rVB2	592	439	0.07%	0.008%
18	3.687	725	730	735	rBV2	157	211	0.03%	0.004%
19	3.790	755	762	765	rBV	307	285	0.05%	0.005%
20	4.542	992	996	1001	rVB2	311	353	0.06%	0.007%
21	4.568	1001	1004	1009	rBV2	267	330	0.05%	0.006%
22	4.645	1014	1028	1072	rBV2	65567	209639	33.77%	4.008%
23	5.060	1141	1157	1182	rVV	108095	251761	40.56%	4.814%
24	5.282	1217	1226	1231	rBV3	916	1308	0.21%	0.025%
25	5.372	1247	1254	1260	rVB2	508	774	0.12%	0.015%
26	5.481	1280	1288	1291	rVV2	182	269	0.04%	0.005%
27	5.713	1337	1360	1387	rBV2	244887	620756	100.00%	11.869%
28	5.976	1431	1442	1463	rBV5	8113	20435	3.29%	0.391%
29	6.112	1481	1484	1489	rVB2	256	192	0.03%	0.004%
30	6.144	1489	1494	1497	rBV2	240	221	0.04%	0.004%
31	6.243	1510	1525	1549	rBV	243173	481223	77.52%	9.201%
32	6.533	1604	1615	1627	rVV8	14693	28676	4.62%	0.548%
33	6.607	1627	1638	1649	rVV4	4278	9573	1.54%	0.183%
34	6.687	1649	1663	1685	rVB	144076	292441	47.11%	5.591%
35	6.816	1699	1703	1706	rBV2	309	231	0.04%	0.004%
36	6.874	1718	1721	1725	rBV2	236	207	0.03%	0.004%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072022\
 Data File : VU049810.D
 Acq On : 20 Jul 2022 18:01
 Operator : SY/MD
 Sample : N3743-15ME
 Misc : 6.17g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5D13ME

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\SFAMULM071122WMA.M
 Title : VOC Analysis

37	6.970	1747	1751	1753	rBV3	209	183	0.03%	0.003%
38	7.044	1763	1774	1776	rBV2	341	324	0.05%	0.006%
39	7.195	1812	1821	1822	rBV4	2123	2155	0.35%	0.041%
40	7.314	1852	1858	1861	rVB4	692	655	0.11%	0.013%
41	7.417	1884	1890	1894	rBV2	266	296	0.05%	0.006%
42	7.494	1911	1914	1918	rVB2	453	369	0.06%	0.007%
43	7.565	1918	1936	1953	rBV	70210	130867	21.08%	2.502%
44	7.700	1972	1978	1987	rVV3	743	975	0.16%	0.019%
45	7.896	2026	2039	2059	rBV	245123	433214	69.79%	8.283%
46	7.992	2059	2069	2084	rVB4	5075	11354	1.83%	0.217%
47	8.066	2087	2092	2095	rBV2	388	369	0.06%	0.007%
48	8.182	2117	2128	2145	rVB2	46359	88119	14.20%	1.685%
49	8.353	2174	2181	2191	rBV5	761	1035	0.17%	0.020%
50	8.552	2232	2243	2254	rVB2	44862	76035	12.25%	1.454%
51	8.652	2258	2274	2302	rBV2	175686	423043	68.15%	8.088%
52	8.800	2313	2320	2329	rVB5	2645	4746	0.76%	0.091%
53	9.099	2409	2413	2417	rBV2	253	189	0.03%	0.004%
54	9.163	2430	2433	2436	rBV	290	211	0.03%	0.004%
55	9.234	2451	2455	2459	rVB	320	241	0.04%	0.005%
56	9.420	2497	2513	2536	rVV	334364	593863	95.67%	11.354%
57	9.568	2555	2559	2560	rBV	385	240	0.04%	0.005%
58	9.697	2594	2599	2605	rBV2	420	420	0.07%	0.008%
59	9.825	2635	2639	2645	rBV2	289	412	0.07%	0.008%
60	10.044	2702	2707	2709	rBV	259	236	0.04%	0.005%
61	10.217	2756	2761	2766	rVB2	207	220	0.04%	0.004%
62	10.243	2766	2769	2773	rBV2	319	277	0.04%	0.005%
63	10.430	2822	2827	2831	rBV2	227	256	0.04%	0.005%
64	10.484	2839	2844	2847	rBV	331	286	0.05%	0.005%
65	10.626	2885	2888	2891	rBV2	419	372	0.06%	0.007%
66	10.655	2895	2897	2905	rVB3	422	363	0.06%	0.007%
67	10.700	2905	2911	2915	rBV2	208	260	0.04%	0.005%
68	10.764	2916	2931	2954	rVV	216607	366534	59.05%	7.008%
69	10.851	2954	2958	2962	rVV3	319	289	0.05%	0.006%
70	10.989	2997	3001	3006	rVB2	272	273	0.04%	0.005%
71	11.050	3017	3020	3029	rVB2	354	431	0.07%	0.008%
72	11.118	3035	3041	3050	rVB3	1072	1489	0.24%	0.028%
73	11.314	3099	3102	3104	rBV2	321	186	0.03%	0.004%
74	11.578	3181	3184	3188	rVB	418	285	0.05%	0.005%
75	11.770	3238	3244	3246	rBV2	414	423	0.07%	0.008%
76	11.815	3246	3258	3274	rVV	339278	534099	86.04%	10.212%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072022\
 Data File : VU049810.D
 Acq On : 20 Jul 2022 18:01
 Operator : SY/MD
 Sample : N3743-15ME
 Misc : 6.17g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5D13ME

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\SFAMULM071122WMA.M
 Title : VOC Analysis

77	11.960	3299	3303	3304	rBV	250	194	0.03%	0.004%
78	11.989	3310	3312	3316	rVB2	336	199	0.03%	0.004%
79	12.198	3364	3377	3398	rBV	240714	394408	63.54%	7.541%
80	12.327	3415	3417	3421	rVB2	331	235	0.04%	0.004%
81	12.516	3470	3476	3478	rBV2	265	292	0.05%	0.006%
82	12.693	3529	3531	3536	rVB2	410	217	0.03%	0.004%
83	12.770	3553	3555	3560	rVB2	398	329	0.05%	0.006%
84	12.922	3599	3602	3606	rBV	261	212	0.03%	0.004%
85	13.024	3631	3634	3637	rVB	349	200	0.03%	0.004%
86	13.195	3683	3687	3691	rVB2	369	311	0.05%	0.006%
87	13.359	3736	3738	3741	rVB2	333	192	0.03%	0.004%
88	13.381	3741	3745	3748	rBV2	302	314	0.05%	0.006%
89	13.542	3792	3795	3799	rBV2	287	231	0.04%	0.004%
90	13.651	3827	3829	3836	rVB3	323	313	0.05%	0.006%
91	13.758	3859	3862	3865	rBV	312	260	0.04%	0.005%
92	13.870	3895	3897	3904	rBV2	299	325	0.05%	0.006%
93	14.053	3951	3954	3957	rVB3	375	253	0.04%	0.005%
94	14.372	4048	4053	4058	rBV3	281	344	0.06%	0.007%
95	14.503	4089	4094	4099	rBV3	361	489	0.08%	0.009%
96	14.700	4152	4155	4157	rBV3	389	266	0.04%	0.005%
97	15.060	4265	4267	4271	rVB	466	306	0.05%	0.006%
98	15.082	4271	4274	4277	rBV3	474	293	0.05%	0.006%
99	15.819	4501	4503	4506	rBV2	463	278	0.04%	0.005%
100	16.384	4677	4679	4682	rBV4	583	270	0.04%	0.005%

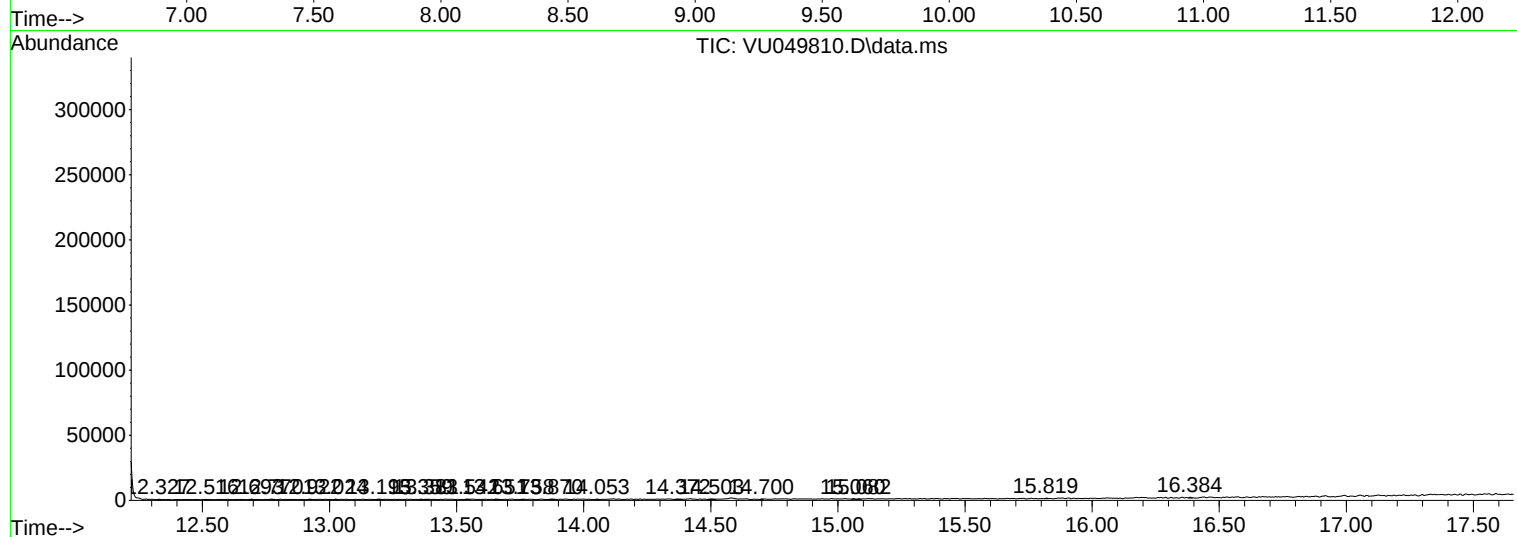
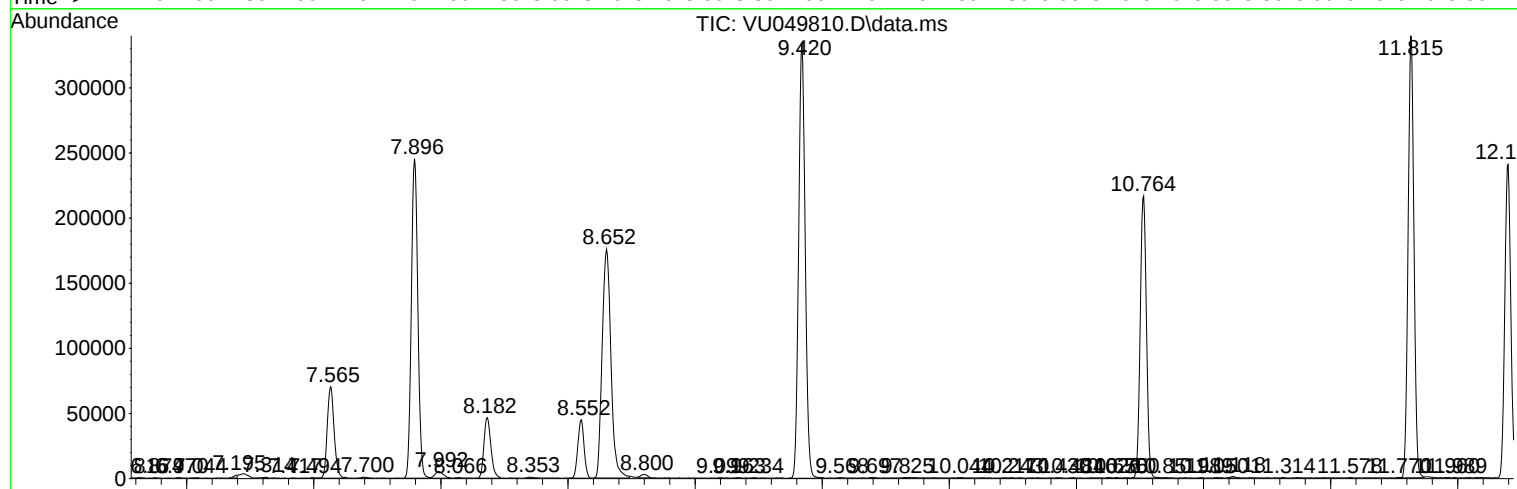
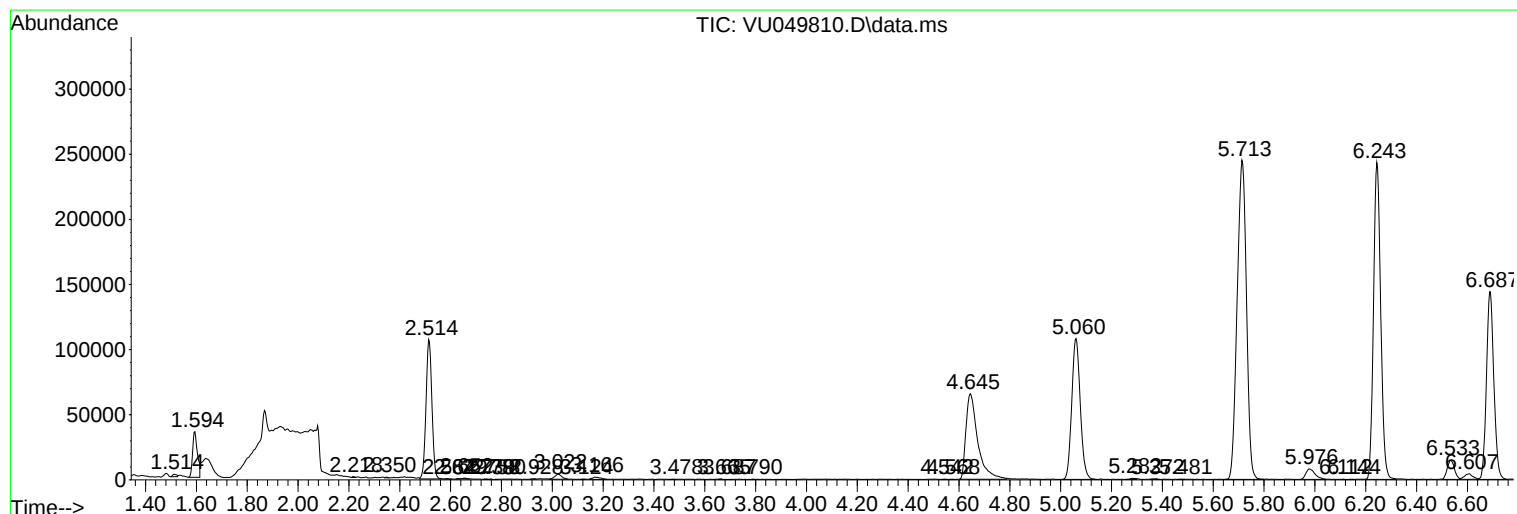
Sum of corrected areas: 5230204

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072022\
Data File : VU049810.D
Acq On : 20 Jul 2022 18:01
Operator : SY/MD
Sample : N3743-15ME
Misc : 6.17g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5D13ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU072022\
Data File : VU049810.D
Acq On : 20 Jul 2022 18:01
Operator : SY/MD
Sample : N3743-15ME
Misc : 6.17g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5D13ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.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\VU072022\
Data File : VU049810.D
Acq On : 20 Jul 2022 18:01
Operator : SY/MD
Sample : N3743-15ME
Misc : 6.17g/5.0mL/100ul/5.0mL/MSVOA_U/MEOH
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5D13ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.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