

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041822\
 Data File : VU048117.D
 Acq On : 18 Apr 2022 13:44
 Operator : SY/MD
 Sample : N2373-12ME
 Misc : 3.35g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFF3ME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs : 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU048117.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	73	80	102	rVB	61381	108080	9.23%	1.139%
2	2.549	363	376	387	rBV	162844	277473	23.70%	2.925%
3	2.832	461	464	467	rBV	423	320	0.03%	0.003%
4	2.855	467	471	473	rBV	506	390	0.03%	0.004%
5	2.916	488	490	491	rVV	444	224	0.02%	0.002%
6	2.957	492	503	520	rVV	14090	29609	2.53%	0.312%
7	3.038	521	528	544	rVB6	2293	4485	0.38%	0.047%
8	3.183	552	573	590	rBV	13207	34116	2.91%	0.360%
9	3.440	649	653	657	rBV	235	256	0.02%	0.003%
10	3.578	689	696	700	rBV4	772	1001	0.09%	0.011%
11	3.633	710	713	718	rVB2	303	259	0.02%	0.003%
12	3.668	718	724	728	rBV2	323	381	0.03%	0.004%
13	3.787	757	761	763	rVB2	352	303	0.03%	0.003%
14	3.890	791	793	800	rVB3	327	270	0.02%	0.003%
15	4.025	829	835	840	rBV2	277	439	0.04%	0.005%
16	4.218	890	895	897	rBV	275	251	0.02%	0.003%
17	4.385	943	947	952	rVB3	487	485	0.04%	0.005%
18	4.417	952	957	959	rBV2	486	439	0.04%	0.005%
19	4.433	959	962	965	rVV2	391	265	0.02%	0.003%
20	4.453	965	968	972	rVV2	271	215	0.02%	0.002%
21	4.568	1001	1004	1006	rBV2	336	251	0.02%	0.003%
22	4.636	1012	1025	1078	rVV	103021	367046	31.36%	3.869%
23	5.063	1140	1158	1182	rBV	187917	425067	36.31%	4.480%
24	5.170	1188	1191	1194	rVB2	307	217	0.02%	0.002%
25	5.205	1198	1202	1206	rVB2	454	429	0.04%	0.005%
26	5.285	1222	1227	1230	rBV3	484	530	0.05%	0.006%
27	5.359	1241	1250	1251	rBV3	639	782	0.07%	0.008%
28	5.555	1305	1311	1315	rBV2	244	337	0.03%	0.004%
29	5.719	1339	1362	1385	rBV2	388340	1023581	87.45%	10.789%
30	5.970	1429	1440	1456	rBV4	9779	23522	2.01%	0.248%
31	6.121	1485	1487	1491	rVB3	294	219	0.02%	0.002%
32	6.163	1497	1500	1503	rVB3	387	241	0.02%	0.003%
33	6.247	1511	1526	1555	rVV	415314	811212	69.30%	8.550%
34	6.395	1571	1572	1577	rVB2	560	203	0.02%	0.002%
35	6.459	1589	1592	1595	rVB3	324	246	0.02%	0.003%
36	6.526	1603	1613	1625	rVV8	4149	7963	0.68%	0.084%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041822\
 Data File : VU048117.D
 Acq On : 18 Apr 2022 13:44
 Operator : SY/MD
 Sample : N2373-12ME
 Misc : 3.35g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFF3ME

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

37	6.600	1625	1636	1650	rBV4	4374	10368	0.89%	0.109%
38	6.690	1650	1664	1688	rVB	240174	483624	41.32%	5.097%
39	6.819	1703	1704	1707	rVB	626	304	0.03%	0.003%
40	7.057	1774	1778	1779	rBV	353	222	0.02%	0.002%
41	7.070	1779	1782	1789	rVB3	514	647	0.06%	0.007%
42	7.189	1808	1819	1847	rBV4	10220	31955	2.73%	0.337%
43	7.305	1851	1855	1856	rVV2	792	554	0.05%	0.006%
44	7.324	1859	1861	1863	rVV	416	205	0.02%	0.002%
45	7.337	1863	1865	1868	rVB	614	263	0.02%	0.003%
46	7.565	1922	1936	1963	rBV	115456	221231	18.90%	2.332%
47	7.690	1966	1975	1976	rBV3	2011	2051	0.18%	0.022%
48	7.784	1996	2004	2006	rBV3	1499	1618	0.14%	0.017%
49	7.899	2026	2040	2056	rBV	425265	758004	64.76%	7.989%
50	8.070	2091	2093	2097	rVB3	727	399	0.03%	0.004%
51	8.182	2115	2128	2146	rBV2	74580	156143	13.34%	1.646%
52	8.346	2177	2179	2184	rVB3	819	567	0.05%	0.006%
53	8.581	2249	2252	2255	rBV	280	228	0.02%	0.002%
54	8.655	2260	2275	2304	rBV	405307	775906	66.29%	8.178%
55	8.906	2351	2353	2356	rVB2	455	289	0.02%	0.003%
56	8.922	2356	2358	2361	rBV2	459	257	0.02%	0.003%
57	8.941	2361	2364	2369	rVB3	650	440	0.04%	0.005%
58	9.005	2380	2384	2385	rBV	440	274	0.02%	0.003%
59	9.144	2424	2427	2430	rBV2	329	225	0.02%	0.002%
60	9.420	2500	2513	2547	rBV	592241	1102665	94.20%	11.622%
61	9.578	2560	2562	2567	rVB2	522	390	0.03%	0.004%
62	9.603	2567	2570	2577	rBV2	432	391	0.03%	0.004%
63	9.690	2594	2597	2601	rBV2	651	571	0.05%	0.006%
64	9.800	2627	2631	2636	rVB3	216	224	0.02%	0.002%
65	9.845	2641	2645	2648	rBV2	228	195	0.02%	0.002%
66	10.430	2822	2827	2830	rBV2	201	230	0.02%	0.002%
67	10.465	2834	2838	2840	rBV3	380	298	0.03%	0.003%
68	10.555	2863	2866	2873	rBV2	236	226	0.02%	0.002%
69	10.645	2890	2894	2896	rVB2	343	234	0.02%	0.002%
70	10.674	2896	2903	2911	rVB6	948	1356	0.12%	0.014%
71	10.764	2917	2931	2950	rVB	448902	723914	61.84%	7.630%
72	10.838	2950	2954	2957	rVB2	342	208	0.02%	0.002%
73	10.896	2964	2972	2976	rBV3	1047	1377	0.12%	0.015%
74	11.092	3031	3033	3036	rVV3	450	295	0.03%	0.003%
75	11.121	3037	3042	3052	rVB4	1149	1677	0.14%	0.018%
76	11.192	3061	3064	3067	rBV	364	248	0.02%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041822\
 Data File : VU048117.D
 Acq On : 18 Apr 2022 13:44
 Operator : SY/MD
 Sample : N2373-12ME
 Misc : 3.35g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFF3ME

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\SFAMULM032422WMA.M
 Title : VOC Analysis

77	11.211	3067	3070	3076	rVV2	387	348	0.03%	0.004%
78	11.420	3130	3135	3138	rBV2	474	451	0.04%	0.005%
79	11.475	3143	3152	3153	rBV4	697	832	0.07%	0.009%
80	11.584	3182	3186	3188	rBV2	310	242	0.02%	0.003%
81	11.700	3216	3222	3229	rVB5	478	652	0.06%	0.007%
82	11.751	3235	3238	3245	rBV2	830	1124	0.10%	0.012%
83	11.816	3245	3258	3278	rVV	750981	1170537	100.00%	12.338%
84	11.919	3282	3290	3301	rVB6	11988	18315	1.56%	0.193%
85	11.967	3302	3305	3307	rBV2	918	496	0.04%	0.005%
86	12.018	3319	3321	3324	rBV	414	289	0.02%	0.003%
87	12.066	3330	3336	3337	rBV	310	304	0.03%	0.003%
88	12.195	3363	3376	3395	rBV	532775	872729	74.56%	9.199%
89	12.353	3421	3425	3427	rBV3	440	304	0.03%	0.003%
90	12.398	3436	3439	3444	rBV2	462	452	0.04%	0.005%
91	12.623	3507	3509	3516	rBV	268	314	0.03%	0.003%
92	12.697	3528	3532	3535	rBV2	468	385	0.03%	0.004%
93	12.915	3591	3600	3610	rBV5	3856	5799	0.50%	0.061%
94	13.153	3670	3674	3676	rBV2	410	329	0.03%	0.003%
95	13.230	3693	3698	3701	rBV2	603	586	0.05%	0.006%
96	13.848	3881	3890	3899	rVB4	3817	5492	0.47%	0.058%
97	14.336	4039	4042	4048	rVB4	1832	1500	0.13%	0.016%
98	14.658	4139	4142	4145	rBV2	445	392	0.03%	0.004%
99	14.963	4232	4237	4245	rBV5	3233	4013	0.34%	0.042%
100	15.024	4254	4256	4260	rBV4	497	300	0.03%	0.003%

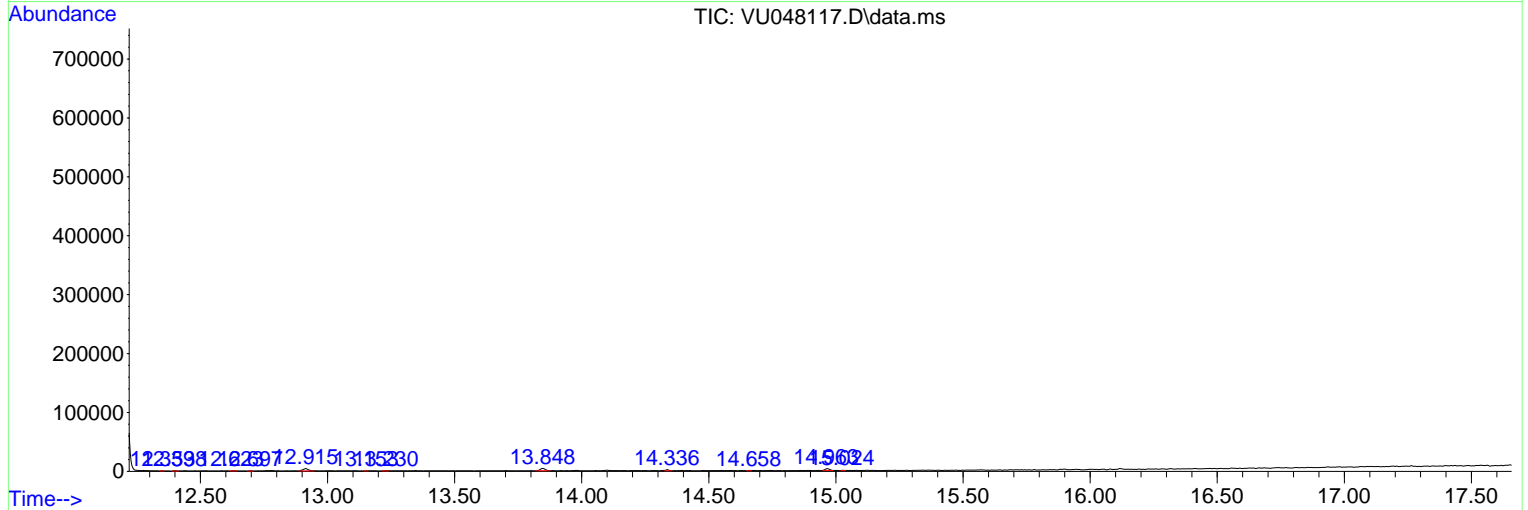
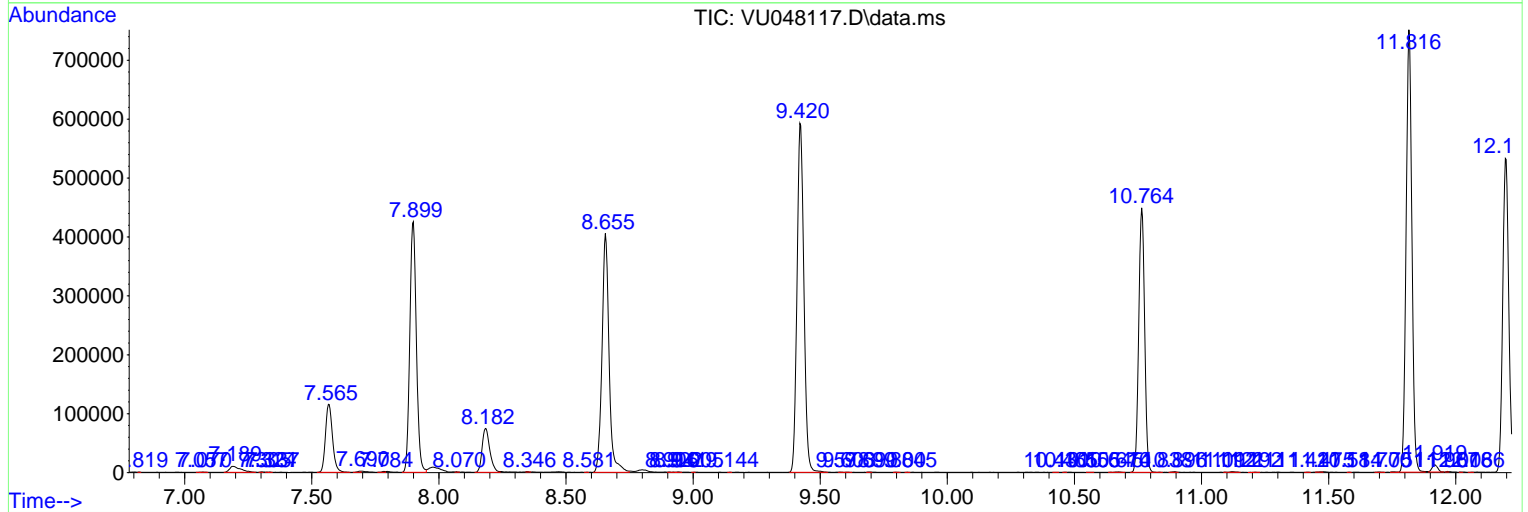
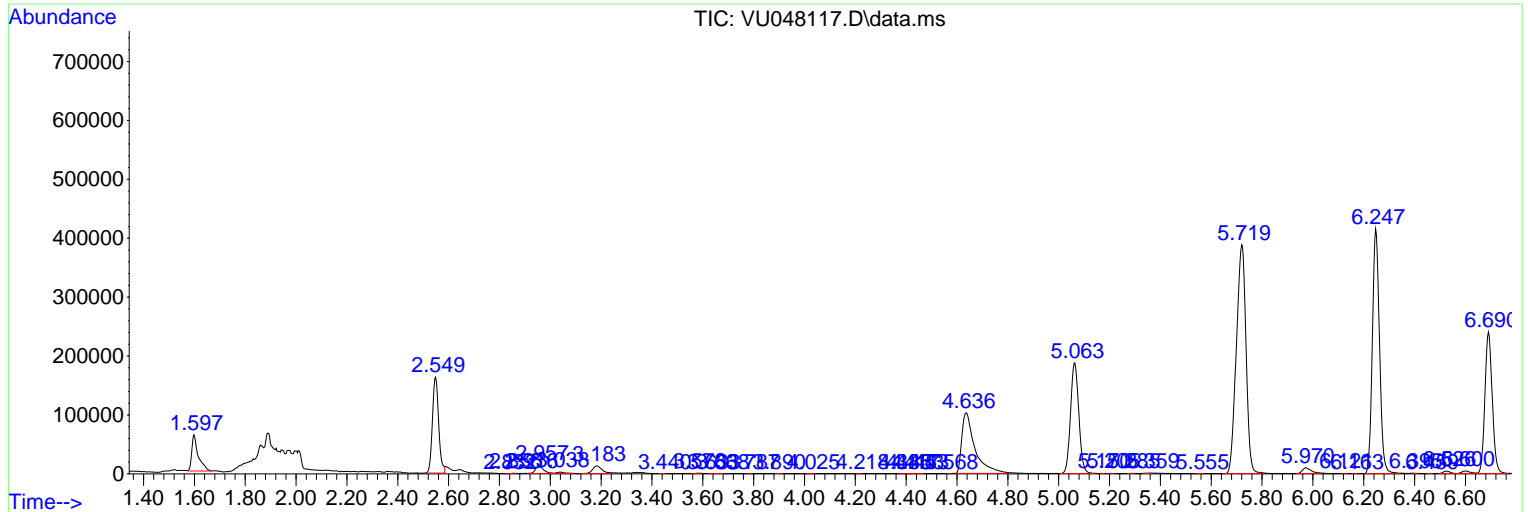
Sum of corrected areas: 9487565

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041822\
 Data File : VU048117.D
 Acq On : 18 Apr 2022 13:44
 Operator : SY/MD
 Sample : N2373-12ME
 Misc : 3.35g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 10 Sample Multiplier: 1

Instrument :
 MSVOA_U
ClientSampleId :
 BFFF3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Quant Title : VOC Analysis

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



Library Search Compound Report

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041822\
Data File : VU048117.D
Acq On : 18 Apr 2022 13:44
Operator : SY/MD
Sample : N2373-12ME
Misc : 3.35g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFF3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.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\VU041822\
Data File : VU048117.D
Acq On : 18 Apr 2022 13:44
Operator : SY/MD
Sample : N2373-12ME
Misc : 3.35g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 10 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFF3ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST0.L
TIC Integration Parameters: LSCINT.P

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--		
					#	RT	Resp Conc
