

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
 Data File : VU050539.D
 Acq On : 31 Aug 2022 00:50
 Operator : SY/MD
 Sample : N4345-19ME 50X
 Misc : 5.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVT7ME

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\SFAMULM083022WMA.M

Title : VOC Analysis

Signal : TIC: VU050539.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.482	39	44	50	rBV2	4418	5441	0.41%	0.058%
2	1.517	52	55	59	rVV2	2594	2305	0.17%	0.025%
3	1.597	72	80	101	rBV	131043	170360	12.90%	1.817%
4	1.900	166	174	195	rVB	125794	169756	12.85%	1.810%
5	2.562	367	380	395	rBV	226402	364350	27.59%	3.886%
6	2.781	445	448	449	rBV	617	295	0.02%	0.003%
7	2.890	478	482	484	rBV3	522	374	0.03%	0.004%
8	2.974	506	508	514	rVB2	315	180	0.01%	0.002%
9	3.041	518	529	543	rVB	7845	13311	1.01%	0.142%
10	3.186	559	574	589	rBV	18739	42430	3.21%	0.452%
11	3.282	600	604	607	rBV3	308	214	0.02%	0.002%
12	3.314	610	614	622	rVB2	254	289	0.02%	0.003%
13	3.369	628	631	634	rVB2	276	204	0.02%	0.002%
14	3.414	640	645	647	rBV2	156	165	0.01%	0.002%
15	3.501	669	672	676	rVV2	259	221	0.02%	0.002%
16	3.523	676	679	683	rVB	374	275	0.02%	0.003%
17	3.797	759	764	767	rVB2	305	211	0.02%	0.002%
18	3.932	803	806	809	rVB	311	167	0.01%	0.002%
19	3.961	813	815	824	rVB2	283	337	0.03%	0.004%
20	4.118	858	864	870	rBV2	380	359	0.03%	0.004%
21	4.221	894	896	899	rBV	293	226	0.02%	0.002%
22	4.244	900	903	904	rVV	299	194	0.01%	0.002%
23	4.276	908	913	917	rVB2	245	254	0.02%	0.003%
24	4.327	923	929	932	rBV	227	226	0.02%	0.002%
25	4.401	948	952	955	rBV2	311	289	0.02%	0.003%
26	4.459	965	970	972	rBV2	248	249	0.02%	0.003%
27	4.523	986	990	994	rVB2	190	168	0.01%	0.002%
28	4.546	994	997	1004	rVB2	229	234	0.02%	0.002%
29	4.581	1004	1008	1010	rBV2	340	248	0.02%	0.003%
30	4.629	1010	1023	1067	rBV	144080	390479	29.57%	4.164%
31	4.948	1119	1122	1126	rBV2	343	247	0.02%	0.003%
32	5.064	1141	1158	1183	rBV	228622	506917	38.38%	5.406%
33	5.231	1206	1210	1218	rVB4	648	895	0.07%	0.010%
34	5.292	1218	1229	1237	rVV4	1081	2141	0.16%	0.023%
35	5.330	1238	1241	1244	rVB2	266	155	0.01%	0.002%
36	5.369	1250	1253	1258	rBV	579	463	0.04%	0.005%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
 Data File : VU050539.D
 Acq On : 31 Aug 2022 00:50
 Operator : SY/MD
 Sample : N4345-19ME 50X
 Misc : 5.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVT7ME

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\SFAMULM083022WMA.M
 Title : VOC Analysis

37	5.581	1315	1319	1323	rBV2	261	273	0.02%	0.003%
38	5.649	1333	1340	1342	rBV	228	257	0.02%	0.003%
39	5.723	1342	1363	1386	rBV2	489740	1320633	100.00%	14.084%
40	5.973	1437	1441	1449	rBV4	730	1075	0.08%	0.011%
41	6.118	1482	1486	1490	rVV3	289	299	0.02%	0.003%
42	6.163	1496	1500	1503	rBV	230	157	0.01%	0.002%
43	6.250	1512	1527	1551	rBV	414991	792786	60.03%	8.455%
44	6.488	1598	1601	1604	rBV2	281	222	0.02%	0.002%
45	6.530	1607	1614	1615	rBV3	1263	1165	0.09%	0.012%
46	6.578	1625	1629	1631	rBV3	307	216	0.02%	0.002%
47	6.594	1631	1634	1639	rVB3	341	351	0.03%	0.004%
48	6.690	1650	1664	1689	rBV	312813	612155	46.35%	6.528%
49	6.874	1716	1721	1722	rBV	313	258	0.02%	0.003%
50	6.999	1755	1760	1763	rBV2	311	219	0.02%	0.002%
51	7.198	1820	1822	1827	rVB4	297	228	0.02%	0.002%
52	7.462	1901	1904	1907	rBV	209	159	0.01%	0.002%
53	7.507	1915	1918	1924	rBV2	204	180	0.01%	0.002%
54	7.565	1924	1936	1953	rBV	121952	216638	16.40%	2.310%
55	7.649	1959	1962	1964	rVB2	409	265	0.02%	0.003%
56	7.899	2026	2040	2060	rBV	525586	909694	68.88%	9.701%
57	8.179	2116	2127	2150	rVV	81078	140672	10.65%	1.500%
58	8.260	2150	2152	2155	rVV2	645	464	0.04%	0.005%
59	8.276	2155	2157	2163	rVV2	705	570	0.04%	0.006%
60	8.305	2164	2166	2169	rVB	429	252	0.02%	0.003%
61	8.472	2214	2218	2224	rBV2	372	398	0.03%	0.004%
62	8.555	2234	2244	2255	rVB2	17117	27749	2.10%	0.296%
63	8.636	2257	2269	2311	rBV3	326124	742043	56.19%	7.914%
64	8.851	2333	2336	2340	rVB2	593	479	0.04%	0.005%
65	8.883	2343	2346	2347	rBV2	314	197	0.01%	0.002%
66	9.092	2407	2411	2413	rBV	356	279	0.02%	0.003%
67	9.124	2419	2421	2429	rVB2	317	252	0.02%	0.003%
68	9.195	2440	2443	2446	rBV2	257	201	0.02%	0.002%
69	9.237	2455	2456	2463	rVB	246	174	0.01%	0.002%
70	9.279	2466	2469	2471	rBV2	252	162	0.01%	0.002%
71	9.417	2499	2512	2538	rBV	563700	949258	71.88%	10.123%
72	9.694	2595	2598	2600	rBV	332	220	0.02%	0.002%
73	9.745	2612	2614	2617	rBV	245	183	0.01%	0.002%
74	9.893	2658	2660	2667	rVB2	308	226	0.02%	0.002%
75	10.118	2727	2730	2732	rBV3	347	201	0.02%	0.002%
76	10.211	2755	2759	2762	rBV	309	221	0.02%	0.002%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
 Data File : VU050539.D
 Acq On : 31 Aug 2022 00:50
 Operator : SY/MD
 Sample : N4345-19ME 50X
 Misc : 5.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 29 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVT7ME

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\SFAMULM083022WMA.M
 Title : VOC Analysis

77	10.231	2762	2765	2770	rBV2	165	161	0.01%	0.002%
78	10.423	2821	2825	2830	rBV	229	251	0.02%	0.003%
79	10.758	2916	2929	2950	rBV	423664	692789	52.46%	7.388%
80	10.893	2968	2971	2973	rBV	254	160	0.01%	0.002%
81	11.198	3063	3066	3069	rBV	283	202	0.02%	0.002%
82	11.330	3104	3107	3110	rVB2	239	175	0.01%	0.002%
83	11.349	3110	3113	3116	rBV2	388	299	0.02%	0.003%
84	11.700	3219	3222	3225	rVB	267	171	0.01%	0.002%
85	11.719	3225	3228	3231	rVB	336	202	0.02%	0.002%
86	11.812	3245	3257	3285	rBV	395285	636147	48.17%	6.784%
87	11.989	3310	3312	3317	rVB2	468	303	0.02%	0.003%
88	12.195	3363	3376	3401	rBV	384815	645800	48.90%	6.887%
89	12.571	3490	3493	3497	rBV3	289	263	0.02%	0.003%
90	12.636	3510	3513	3515	rBV3	291	166	0.01%	0.002%
91	12.722	3538	3540	3546	rVB2	395	269	0.02%	0.003%
92	12.854	3578	3581	3587	rBV2	289	268	0.02%	0.003%
93	12.922	3598	3602	3610	rVB3	636	777	0.06%	0.008%
94	12.986	3618	3622	3624	rBV2	285	258	0.02%	0.003%
95	13.073	3646	3649	3651	rBV	396	250	0.02%	0.003%
96	13.105	3657	3659	3663	rBB2	280	163	0.01%	0.002%
97	13.369	3734	3741	3743	rBV4	642	692	0.05%	0.007%
98	13.896	3902	3905	3907	rBV3	351	259	0.02%	0.003%
99	14.099	3965	3968	3970	rBV2	405	293	0.02%	0.003%
100	14.491	4086	4090	4094	rBV2	418	473	0.04%	0.005%

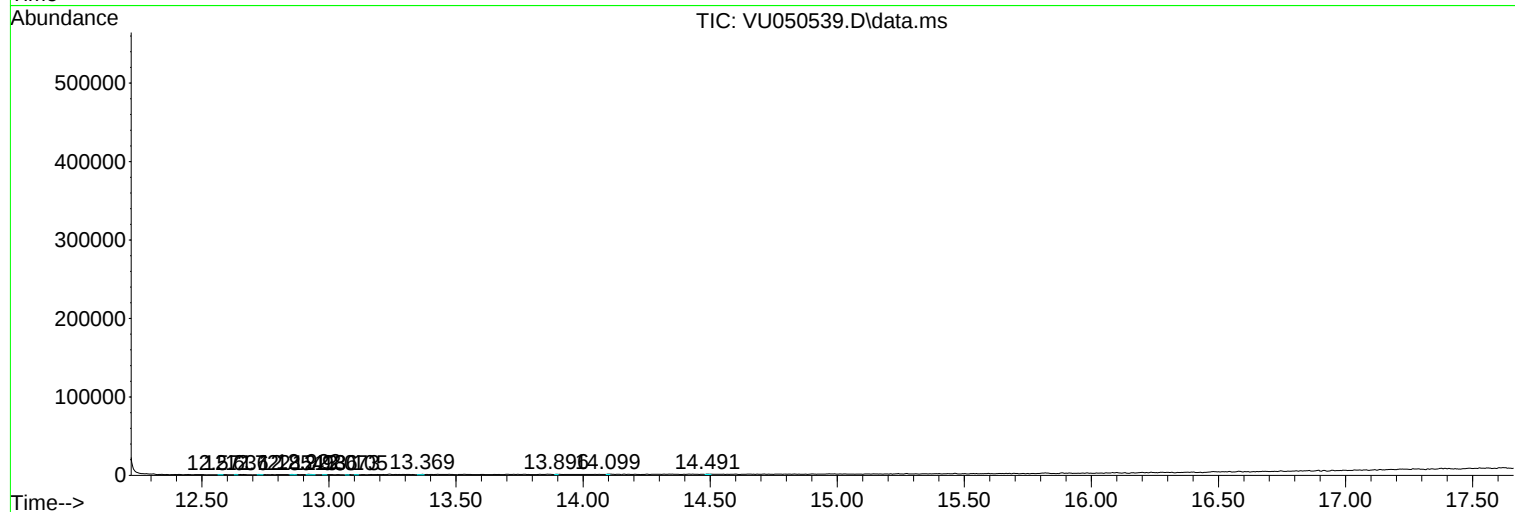
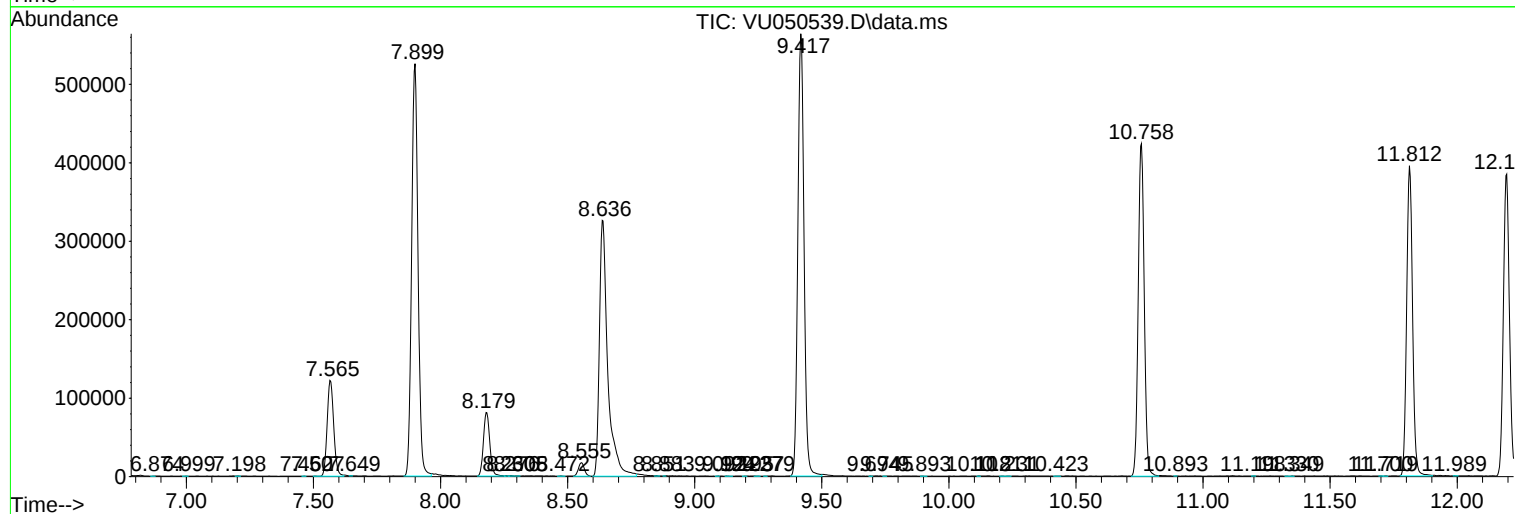
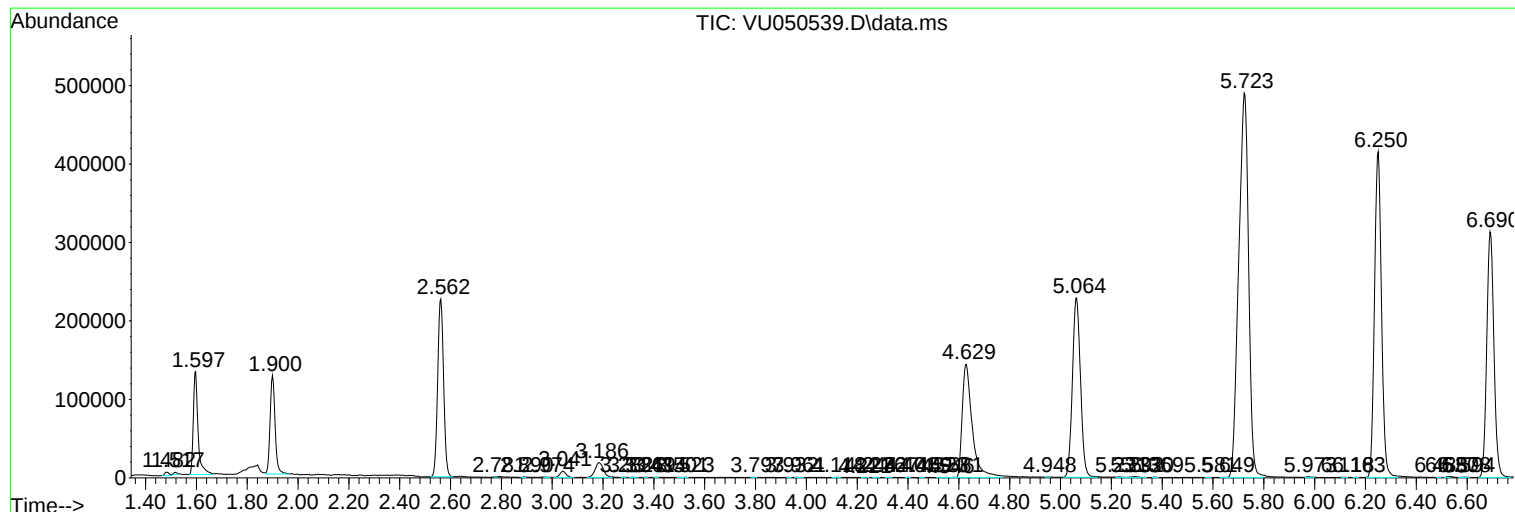
Sum of corrected areas: 9376851

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
Data File : VU050539.D
Acq On : 31 Aug 2022 00:50
Operator : SY/MD
Sample : N4345-19ME 50X
Misc : 5.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVT7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.M
Quant Title : VOC Analysis

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



Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
Data File : VU050539.D
Acq On : 31 Aug 2022 00:50
Operator : SY/MD
Sample : N4345-19ME 50X
Misc : 5.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVT7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.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\VU083022\
Data File : VU050539.D
Acq On : 31 Aug 2022 00:50
Operator : SY/MD
Sample : N4345-19ME 50X
Misc : 5.97g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 29 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVT7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM083022WMA.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