

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
 Data File : VU050534.D
 Acq On : 30 Aug 2022 22:51
 Operator : SY/MD
 Sample : N4363-06ME
 Misc : 5.81g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVW1ME

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: VU050534.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.478	37	43	49	rBV3	5429	7152	0.31%	0.063%
2	1.514	50	54	69	rVB4	3550	6026	0.26%	0.053%
3	1.591	71	78	87	rBV	65144	87696	3.85%	0.777%
4	2.520	356	367	388	rVB	206351	337591	14.82%	2.993%
5	2.854	468	471	478	rVV3	626	632	0.03%	0.006%
6	2.922	488	492	496	rBV5	714	826	0.04%	0.007%
7	3.025	514	524	539	rVB2	11928	23480	1.03%	0.208%
8	3.182	558	573	588	rBV2	23219	63008	2.77%	0.559%
9	3.452	655	657	661	rVV	320	193	0.01%	0.002%
10	3.552	684	688	690	rBV2	232	182	0.01%	0.002%
11	3.665	713	723	730	rVV6	1423	2366	0.10%	0.021%
12	3.935	800	807	810	rBV	359	422	0.02%	0.004%
13	3.957	810	814	821	rVV2	706	862	0.04%	0.008%
14	4.317	921	926	930	rVB2	267	263	0.01%	0.002%
15	4.391	946	949	953	rBV	212	210	0.01%	0.002%
16	4.417	953	957	960	rVV	346	271	0.01%	0.002%
17	4.478	971	976	979	rBV2	170	194	0.01%	0.002%
18	4.513	984	987	992	rBV2	248	245	0.01%	0.002%
19	4.649	1016	1029	1076	rBV	74677	277331	12.17%	2.459%
20	4.970	1127	1129	1134	rBV	250	197	0.01%	0.002%
21	5.060	1140	1157	1182	rBV	168483	397295	17.44%	3.522%
22	5.192	1194	1198	1202	rBV4	687	560	0.02%	0.005%
23	5.250	1214	1216	1219	rBV	288	201	0.01%	0.002%
24	5.292	1219	1229	1239	rVB3	1167	2260	0.10%	0.020%
25	5.353	1244	1248	1249	rBV	300	195	0.01%	0.002%
26	5.366	1249	1252	1254	rBV	442	367	0.02%	0.003%
27	5.716	1342	1361	1385	rBV2	423343	1053656	46.25%	9.341%
28	5.938	1425	1430	1432	rBV	317	252	0.01%	0.002%
29	5.980	1432	1443	1463	rBV3	13403	34792	1.53%	0.308%
30	6.092	1473	1478	1479	rBV	312	201	0.01%	0.002%
31	6.182	1500	1506	1509	rBV2	285	268	0.01%	0.002%
32	6.247	1511	1526	1551	rBV	526046	1049952	46.09%	9.308%
33	6.394	1568	1572	1574	rBV3	345	276	0.01%	0.002%
34	6.468	1591	1595	1596	rBV	298	204	0.01%	0.002%
35	6.526	1604	1613	1625	rBV8	5280	11013	0.48%	0.098%
36	6.607	1628	1638	1649	rVV4	6539	14504	0.64%	0.129%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
 Data File : VU050534.D
 Acq On : 30 Aug 2022 22:51
 Operator : SY/MD
 Sample : N4363-06ME
 Misc : 5.81g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVW1ME

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	6.690	1650	1664	1689	rVB	233060	478185	20.99%	4.239%
38	6.864	1713	1718	1721	rBV2	209	191	0.01%	0.002%
39	6.980	1746	1754	1757	rBV3	409	559	0.02%	0.005%
40	7.227	1816	1831	1845	rBV9	5381	14535	0.64%	0.129%
41	7.298	1851	1853	1855	rBV	571	251	0.01%	0.002%
42	7.343	1865	1867	1874	rVB4	229	220	0.01%	0.002%
43	7.459	1899	1903	1908	rVB3	400	375	0.02%	0.003%
44	7.500	1914	1916	1919	rBV	399	188	0.01%	0.002%
45	7.520	1919	1922	1924	rVB	301	197	0.01%	0.002%
46	7.568	1924	1937	1958	rBV	91385	175903	7.72%	1.559%
47	7.719	1981	1984	1988	rVB	384	253	0.01%	0.002%
48	7.800	2003	2009	2014	rBV3	591	593	0.03%	0.005%
49	7.835	2015	2020	2023	rBV	446	464	0.02%	0.004%
50	7.899	2023	2040	2060	rBV	436871	798782	35.06%	7.081%
51	7.992	2061	2069	2085	rVB3	7770	16957	0.74%	0.150%
52	8.127	2109	2111	2115	rVB2	451	250	0.01%	0.002%
53	8.182	2115	2128	2153	rBV	57808	114523	5.03%	1.015%
54	8.353	2172	2181	2191	rVV7	1676	2644	0.12%	0.023%
55	8.552	2229	2243	2261	rVV	1336115	2278217	100.00%	20.196%
56	8.661	2261	2277	2311	rVB2	213513	560759	24.61%	4.971%
57	8.934	2360	2362	2364	rBV	504	312	0.01%	0.003%
58	8.983	2374	2377	2379	rBV2	377	276	0.01%	0.002%
59	9.131	2419	2423	2426	rBV3	306	251	0.01%	0.002%
60	9.275	2464	2468	2471	rBV2	231	206	0.01%	0.002%
61	9.317	2477	2481	2485	rBV2	205	232	0.01%	0.002%
62	9.420	2499	2513	2532	rBV	689599	1261287	55.36%	11.181%
63	9.578	2557	2562	2564	rBV3	1032	944	0.04%	0.008%
64	9.783	2623	2626	2629	rBV3	298	224	0.01%	0.002%
65	9.844	2641	2645	2648	rVB	309	215	0.01%	0.002%
66	9.912	2660	2666	2670	rVB2	166	213	0.01%	0.002%
67	10.156	2737	2742	2744	rBV2	241	224	0.01%	0.002%
68	10.336	2792	2798	2802	rBV2	520	672	0.03%	0.006%
69	10.468	2834	2839	2841	rBV2	373	316	0.01%	0.003%
70	10.645	2891	2894	2897	rBV3	502	347	0.02%	0.003%
71	10.764	2917	2931	2949	rBV	332018	556365	24.42%	4.932%
72	11.118	3031	3041	3053	rVB7	1928	3331	0.15%	0.030%
73	11.182	3058	3061	3064	rBV	278	183	0.01%	0.002%
74	11.314	3098	3102	3104	rBV	348	265	0.01%	0.002%
75	11.349	3109	3113	3116	rVB2	318	236	0.01%	0.002%
76	11.378	3119	3122	3126	rBV2	382	312	0.01%	0.003%

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
 Data File : VU050534.D
 Acq On : 30 Aug 2022 22:51
 Operator : SY/MD
 Sample : N4363-06ME
 Misc : 5.81g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 24 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVW1ME

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	11.497	3156	3159	3162	rVB2	315	192	0.01%	0.002%
78	11.529	3162	3169	3172	rBV2	343	365	0.02%	0.003%
79	11.696	3218	3221	3224	rBV3	272	186	0.01%	0.002%
80	11.748	3234	3237	3242	rBV3	517	462	0.02%	0.004%
81	11.815	3245	3258	3280	rBV	620178	981360	43.08%	8.700%
82	12.137	3355	3358	3360	rBV2	304	229	0.01%	0.002%
83	12.198	3364	3377	3402	rBV	395517	645899	28.35%	5.726%
84	12.497	3467	3470	3476	rBV4	438	390	0.02%	0.003%
85	12.542	3480	3484	3486	rBV2	430	309	0.01%	0.003%
86	12.729	3538	3542	3546	rBV3	414	388	0.02%	0.003%
87	13.012	3626	3630	3633	rBV3	327	269	0.01%	0.002%
88	13.031	3633	3636	3638	rBV2	387	221	0.01%	0.002%
89	13.102	3655	3658	3667	rVB4	380	515	0.02%	0.005%
90	13.150	3671	3673	3679	rVB	339	309	0.01%	0.003%
91	13.182	3681	3683	3689	rBV3	268	274	0.01%	0.002%
92	13.230	3695	3698	3704	rVB4	709	619	0.03%	0.005%
93	13.259	3704	3707	3712	rBV3	423	285	0.01%	0.003%
94	13.285	3712	3715	3720	rVB2	494	398	0.02%	0.004%
95	13.311	3720	3723	3725	rBV	377	280	0.01%	0.002%
96	13.343	3730	3733	3736	rBV3	613	460	0.02%	0.004%
97	13.388	3744	3747	3750	rVB2	481	294	0.01%	0.003%
98	15.265	4328	4331	4336	rVB4	693	577	0.03%	0.005%
99	15.429	4380	4382	4384	rBV	413	247	0.01%	0.002%
100	15.600	4433	4435	4437	rBV3	447	252	0.01%	0.002%

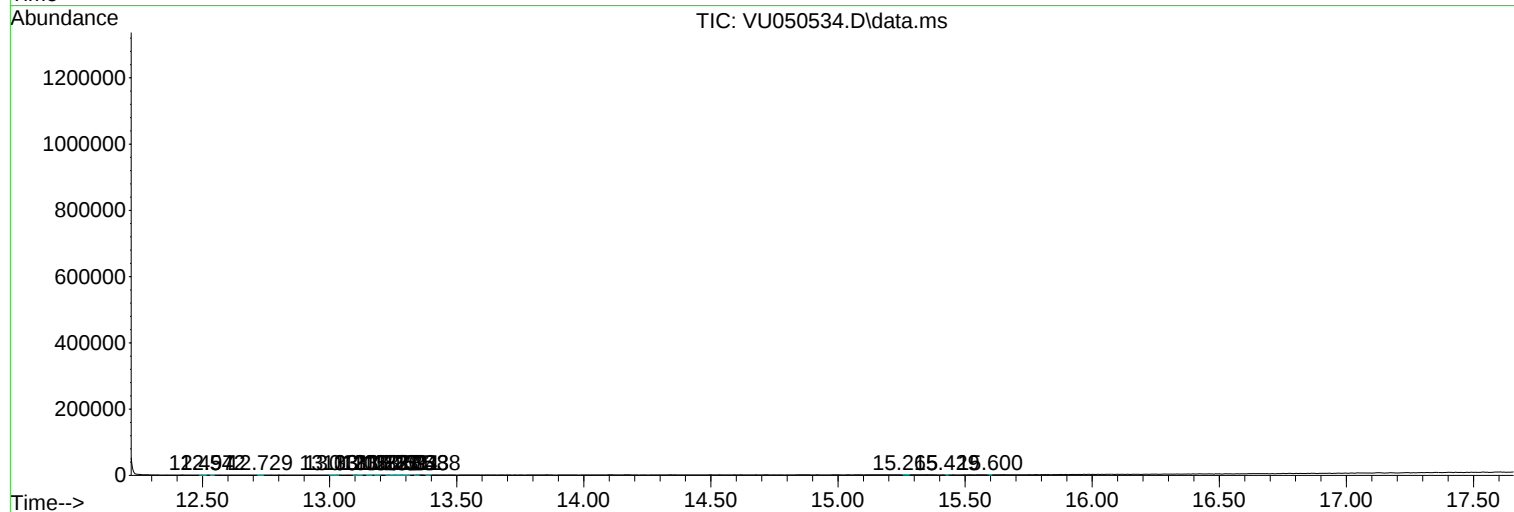
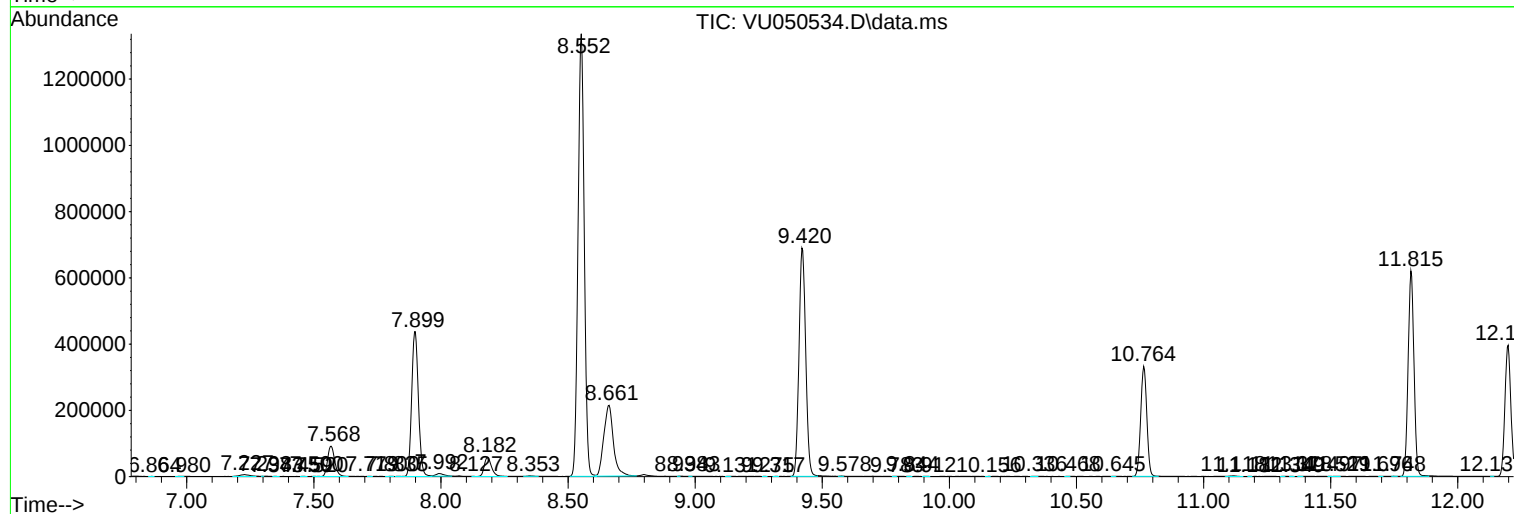
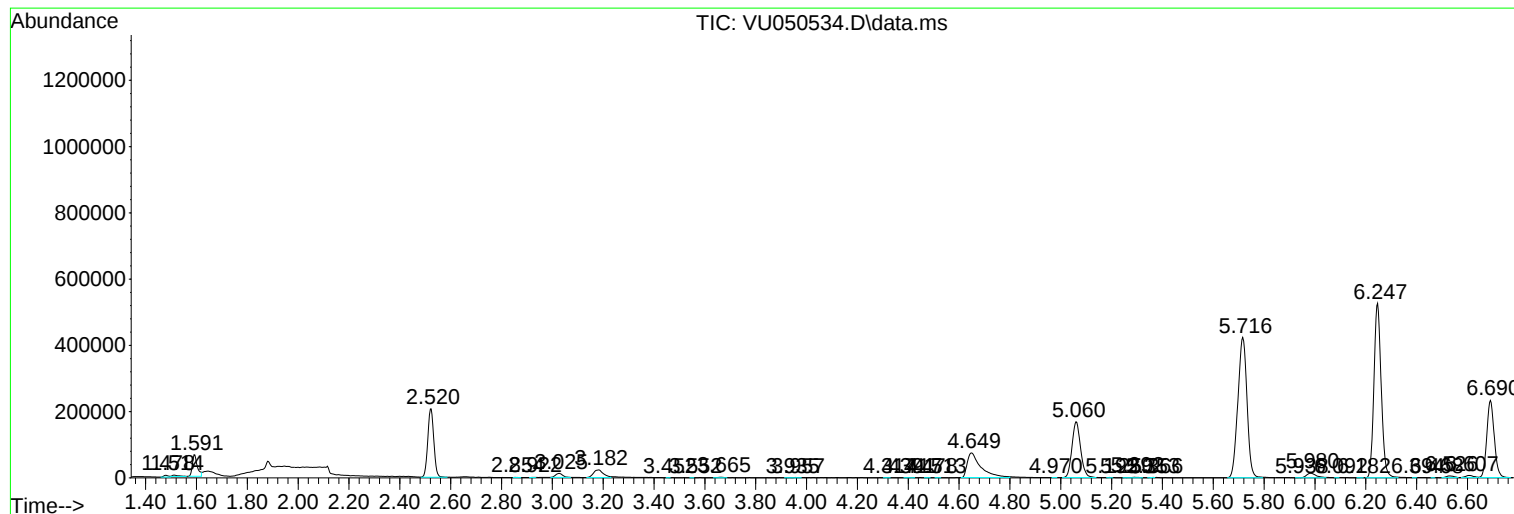
Sum of corrected areas: 11280380

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
Data File : VU050534.D
Acq On : 30 Aug 2022 22:51
Operator : SY/MD
Sample : N4363-06ME
Misc : 5.81g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVW1ME

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 : VU050534.D
Acq On : 30 Aug 2022 22:51
Operator : SY/MD
Sample : N4363-06ME
Misc : 5.81g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVW1ME

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 : VU050534.D
Acq On : 30 Aug 2022 22:51
Operator : SY/MD
Sample : N4363-06ME
Misc : 5.81g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
ALS Vial : 24 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
DBVW1ME

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