

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU090122\
 Data File : VU050585.D
 Acq On : 01 Sep 2022 16:57
 Operator : SY/MD
 Sample : N4363-04ME
 Misc : 5.78g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 13 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVV9ME

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: VU050585.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	40	44	49	rVB3	4185	3829	0.27%	0.038%
2	1.594	71	79	87	rBV	63916	87110	6.24%	0.872%
3	1.893	167	172	181	rBV2	34367	46285	3.32%	0.463%
4	2.359	314	317	322	rBV3	709	565	0.04%	0.006%
5	2.411	329	333	338	rVB4	907	797	0.06%	0.008%
6	2.456	344	347	350	rVB4	792	532	0.04%	0.005%
7	2.478	350	354	357	rBV2	469	362	0.03%	0.004%
8	2.530	357	370	388	rBV	242657	394571	28.26%	3.951%
9	2.742	433	436	437	rBV2	347	230	0.02%	0.002%
10	2.851	467	470	472	rBV	362	221	0.02%	0.002%
11	2.961	499	504	507	rBV2	273	280	0.02%	0.003%
12	2.977	507	509	514	rVV3	431	403	0.03%	0.004%
13	3.035	514	527	535	rVB4	1637	3622	0.26%	0.036%
14	3.179	559	572	589	rBV3	5655	15699	1.12%	0.157%
15	3.626	706	711	714	rBV	505	481	0.03%	0.005%
16	3.645	714	717	720	rVV2	276	239	0.02%	0.002%
17	3.809	760	768	770	rBV	250	291	0.02%	0.003%
18	3.874	785	788	792	rBV2	301	252	0.02%	0.003%
19	4.108	855	861	866	rBV	381	397	0.03%	0.004%
20	4.305	918	922	925	rBV2	273	245	0.02%	0.002%
21	4.337	928	932	935	rBV	319	307	0.02%	0.003%
22	4.478	970	976	978	rBV	229	210	0.02%	0.002%
23	4.549	994	998	1001	rBV2	233	237	0.02%	0.002%
24	4.649	1015	1029	1050	rBV	89791	312829	22.41%	3.133%
25	4.964	1124	1127	1129	rBV2	286	207	0.01%	0.002%
26	4.999	1135	1138	1140	rBV3	389	278	0.02%	0.003%
27	5.060	1140	1157	1184	rVV2	233151	550232	39.41%	5.510%
28	5.279	1221	1225	1227	rBV	659	633	0.05%	0.006%
29	5.292	1227	1229	1239	rVB3	1198	1503	0.11%	0.015%
30	5.468	1281	1284	1287	rBV	309	269	0.02%	0.003%
31	5.488	1287	1290	1295	rVB2	292	345	0.02%	0.003%
32	5.620	1329	1331	1336	rVB2	284	233	0.02%	0.002%
33	5.716	1341	1361	1385	rBV2	546120	1396041	100.00%	13.980%
34	5.980	1433	1443	1456	rBV3	10294	24932	1.79%	0.250%
35	6.179	1493	1505	1509	rBV3	781	1358	0.10%	0.014%
36	6.247	1511	1526	1559	rVV	419793	854525	61.21%	8.557%

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

37	6.440	1582	1586	1589	rBV4	279	214	0.02%	0.002%
38	6.491	1599	1602	1604	rBV2	397	249	0.02%	0.002%
39	6.533	1604	1615	1623	rBV7	3957	7784	0.56%	0.078%
40	6.607	1628	1638	1649	rBV5	4216	9559	0.68%	0.096%
41	6.690	1650	1664	1686	rVV	305061	631237	45.22%	6.321%
42	6.796	1695	1697	1700	rBV	589	382	0.03%	0.004%
43	6.848	1711	1713	1718	rBV2	286	234	0.02%	0.002%
44	6.948	1738	1744	1747	rVV	310	348	0.02%	0.003%
45	6.980	1751	1754	1757	rVV	482	294	0.02%	0.003%
46	7.031	1767	1770	1774	rBV2	278	207	0.01%	0.002%
47	7.227	1816	1831	1851	rBV8	4713	12260	0.88%	0.123%
48	7.317	1854	1859	1863	rVV4	814	812	0.06%	0.008%
49	7.388	1875	1881	1886	rBV2	357	480	0.03%	0.005%
50	7.501	1912	1916	1920	rVB4	316	270	0.02%	0.003%
51	7.565	1923	1936	1961	rBV	140585	280084	20.06%	2.805%
52	7.710	1979	1981	1986	rVB3	319	254	0.02%	0.003%
53	7.816	2010	2014	2018	rVB3	438	357	0.03%	0.004%
54	7.896	2023	2039	2061	rBV	581403	1060593	75.97%	10.621%
55	7.993	2062	2069	2088	rVB4	6814	15837	1.13%	0.159%
56	8.121	2105	2109	2114	rVB2	391	439	0.03%	0.004%
57	8.182	2114	2128	2151	rBV	92864	185909	13.32%	1.862%
58	8.298	2162	2164	2168	rVB2	415	229	0.02%	0.002%
59	8.343	2173	2178	2180	rVV3	822	709	0.05%	0.007%
60	8.359	2180	2183	2187	rVV2	1270	1162	0.08%	0.012%
61	8.375	2187	2188	2194	rVB3	453	321	0.02%	0.003%
62	8.404	2194	2197	2201	rBV2	315	278	0.02%	0.003%
63	8.552	2233	2243	2259	rVB3	30896	52507	3.76%	0.526%
64	8.665	2259	2278	2314	rBV3	244127	720867	51.64%	7.219%
65	8.957	2366	2369	2371	rBV2	364	229	0.02%	0.002%
66	9.356	2490	2493	2500	rVB2	270	323	0.02%	0.003%
67	9.420	2500	2513	2542	rBV	532019	1018740	72.97%	10.201%
68	9.552	2551	2554	2558	rBV3	267	213	0.02%	0.002%
69	9.809	2631	2634	2638	rBV	253	213	0.02%	0.002%
70	9.941	2671	2675	2677	rBV2	367	318	0.02%	0.003%
71	10.121	2729	2731	2736	rVB2	321	221	0.02%	0.002%
72	10.166	2742	2745	2749	rBV2	305	227	0.02%	0.002%
73	10.259	2770	2774	2780	rVV	236	253	0.02%	0.003%
74	10.610	2880	2883	2887	rVB2	388	298	0.02%	0.003%
75	10.642	2891	2893	2897	rVB2	313	234	0.02%	0.002%
76	10.664	2897	2900	2904	rBV	410	268	0.02%	0.003%

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

77	10.764	2917	2931	2951	rBV	442120	737077	52.80%	7.381%
78	11.121	3034	3042	3048	rVB4	1404	2020	0.14%	0.020%
79	11.407	3129	3131	3136	rVB2	325	210	0.02%	0.002%
80	11.471	3149	3151	3154	rBV2	253	213	0.02%	0.002%
81	11.533	3167	3170	3174	rBV2	303	286	0.02%	0.003%
82	11.751	3236	3238	3243	rVB4	510	460	0.03%	0.005%
83	11.816	3245	3258	3275	rBV	468004	745079	53.37%	7.461%
84	12.198	3363	3377	3397	rBV	478202	786431	56.33%	7.875%
85	12.372	3425	3431	3437	rBV4	488	690	0.05%	0.007%
86	12.407	3439	3442	3447	rVV3	347	300	0.02%	0.003%
87	12.526	3476	3479	3482	rVB2	416	289	0.02%	0.003%
88	12.561	3482	3490	3493	rBV2	669	839	0.06%	0.008%
89	12.922	3599	3602	3605	rBV2	429	279	0.02%	0.003%
90	13.349	3733	3735	3738	rBV2	392	280	0.02%	0.003%
91	13.851	3887	3891	3904	rVB4	1320	1891	0.14%	0.019%
92	13.925	3911	3914	3918	rBV3	507	419	0.03%	0.004%
93	14.185	3992	3995	3998	rVB2	441	280	0.02%	0.003%
94	14.224	4004	4007	4010	rBV3	589	384	0.03%	0.004%
95	14.336	4038	4042	4045	rBV4	931	725	0.05%	0.007%
96	14.655	4139	4141	4145	rVB3	567	286	0.02%	0.003%
97	15.114	4280	4284	4286	rBV4	647	528	0.04%	0.005%
98	15.397	4369	4372	4373	rBV	627	374	0.03%	0.004%
99	15.446	4384	4387	4388	rBV2	641	316	0.02%	0.003%
100	15.632	4442	4445	4448	rBV3	870	590	0.04%	0.006%

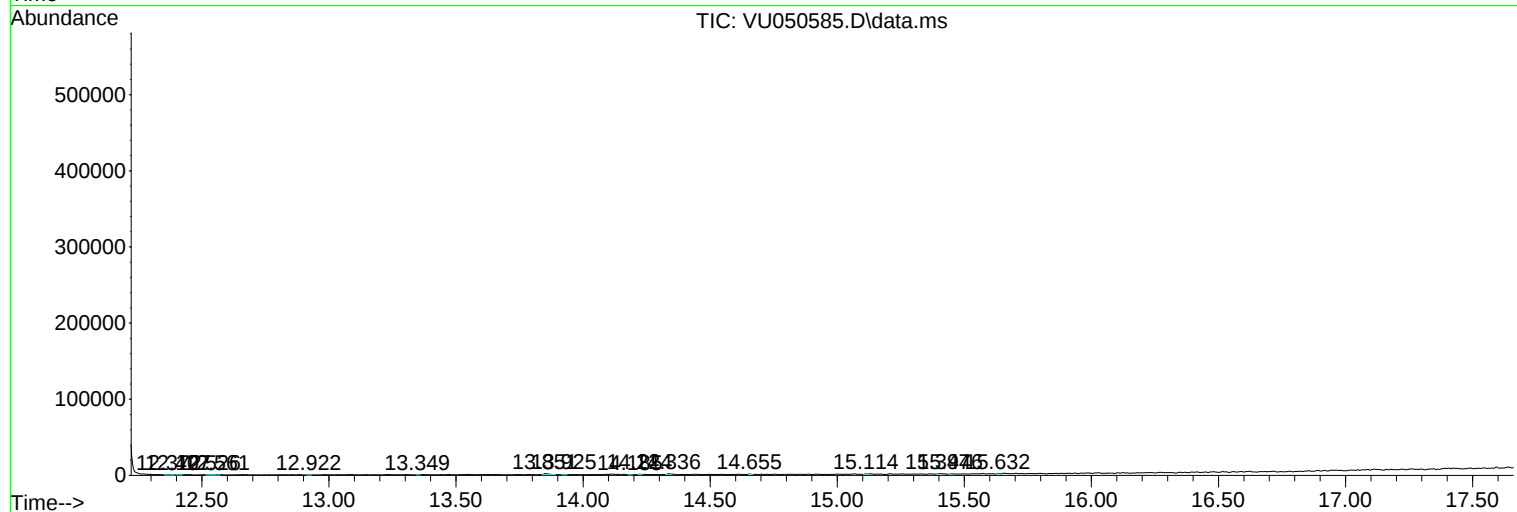
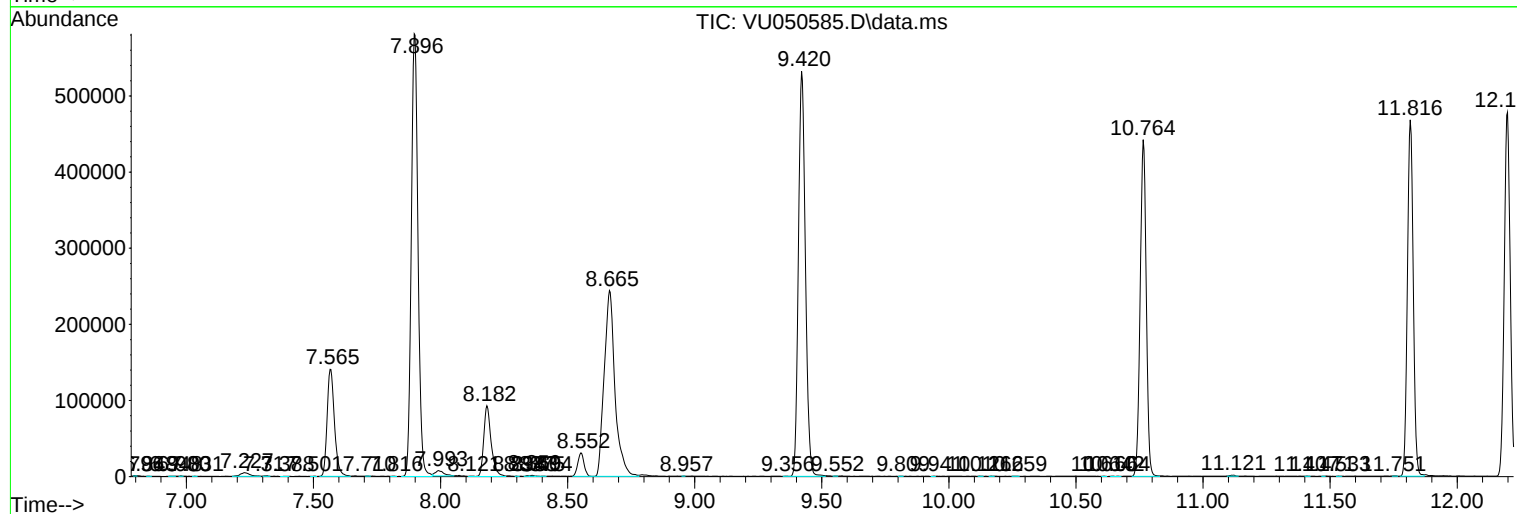
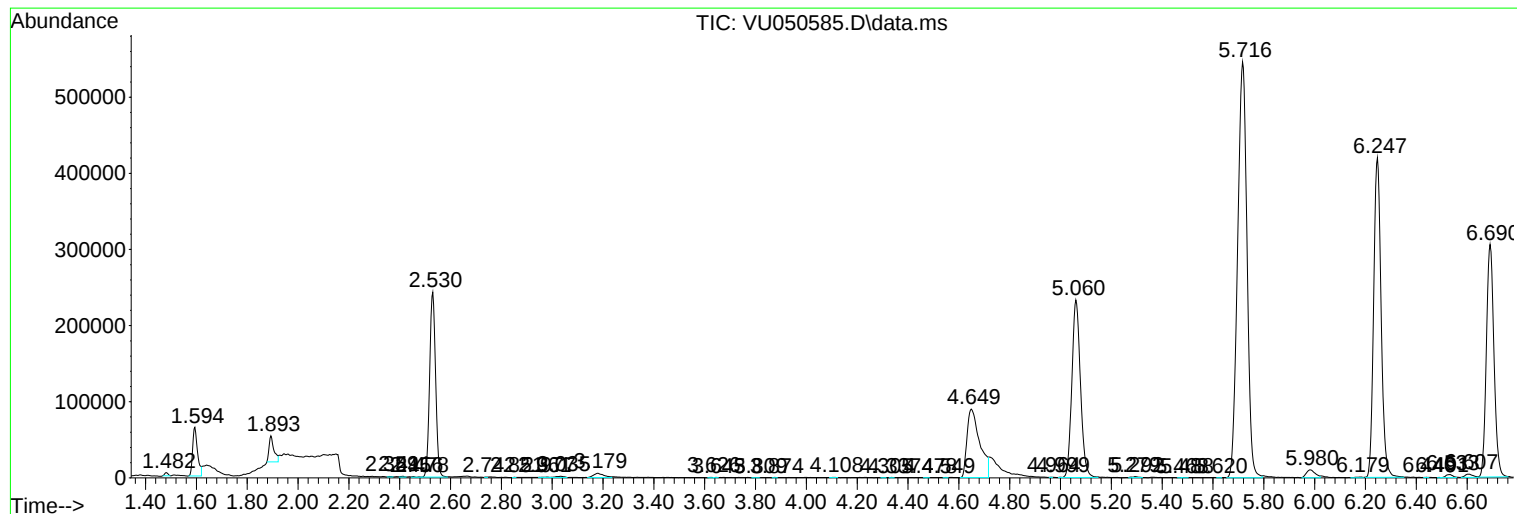
Sum of corrected areas: 9986209

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ClientSampleId :
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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



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Instrument :
MSVOA_U
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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

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TIC Top Hit name	RT	EstConc	Units	Response	#	RT	Resp	Conc
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