

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU083022\
 Data File : VU050529.D
 Acq On : 30 Aug 2022 20:52
 Operator : SY/MD
 Sample : N4345-16ME
 Misc : 6.13g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 DBVT4ME

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: VU050529.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	39	43	49	rBV3	4555	5138	0.29%	0.039%
2	1.511	50	53	59	rVV	3261	3782	0.21%	0.029%
3	1.591	71	78	87	rBV	109535	147276	8.37%	1.114%
4	1.887	165	170	177	rBV	35176	42480	2.41%	0.321%
5	2.523	356	368	386	rVB	345256	563612	32.01%	4.265%
6	2.742	434	436	445	rVB4	1311	1667	0.09%	0.013%
7	2.787	445	450	451	rBV3	357	252	0.01%	0.002%
8	3.028	514	525	553	rVB3	14720	34549	1.96%	0.261%
9	3.179	555	572	611	rBV	77551	234096	13.30%	1.771%
10	3.572	689	694	698	rBV3	363	411	0.02%	0.003%
11	3.626	706	711	716	rBV3	294	357	0.02%	0.003%
12	3.662	716	722	731	rVB5	1201	1924	0.11%	0.015%
13	3.790	756	762	765	rBV2	330	367	0.02%	0.003%
14	4.073	844	850	853	rBV	590	607	0.03%	0.005%
15	4.179	878	883	887	rVB2	287	278	0.02%	0.002%
16	4.649	1014	1029	1079	rBV2	121842	490608	27.87%	3.712%
17	5.060	1139	1157	1187	rBV	284474	662509	37.63%	5.013%
18	5.240	1207	1213	1214	rBV	487	331	0.02%	0.003%
19	5.269	1218	1222	1223	rBV2	579	394	0.02%	0.003%
20	5.289	1225	1228	1235	rVB4	1010	1077	0.06%	0.008%
21	5.337	1240	1243	1246	rVB3	486	350	0.02%	0.003%
22	5.372	1246	1254	1263	rBV5	763	1564	0.09%	0.012%
23	5.440	1272	1275	1280	rBV	364	302	0.02%	0.002%
24	5.507	1293	1296	1300	rBV2	454	280	0.02%	0.002%
25	5.607	1322	1327	1332	rBV2	220	298	0.02%	0.002%
26	5.716	1338	1361	1397	rBV2	705595	1760618	100.00%	13.322%
27	5.983	1433	1444	1467	rBV3	14432	36306	2.06%	0.275%
28	6.118	1483	1486	1494	rVB3	448	466	0.03%	0.004%
29	6.166	1494	1501	1506	rVB2	406	463	0.03%	0.004%
30	6.247	1506	1526	1557	rBV	529847	1079950	61.34%	8.172%
31	6.530	1605	1614	1628	rBV6	5865	12468	0.71%	0.094%
32	6.607	1628	1638	1649	rVV3	6463	15459	0.88%	0.117%
33	6.690	1649	1664	1692	rVV	387852	797717	45.31%	6.036%
34	6.803	1693	1699	1703	rVV6	1083	1128	0.06%	0.009%
35	6.922	1734	1736	1742	rVB2	309	256	0.01%	0.002%
36	6.973	1748	1752	1753	rBV2	447	323	0.02%	0.002%

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

37	7.067	1777	1781	1784	rBV	354	277	0.02%	0.002%
38	7.115	1789	1796	1805	rBV	296	333	0.02%	0.003%
39	7.231	1816	1832	1847	rBV9	5396	15179	0.86%	0.115%
40	7.321	1853	1860	1863	rBV5	844	1128	0.06%	0.009%
41	7.346	1866	1868	1872	rVB2	743	455	0.03%	0.003%
42	7.501	1915	1916	1923	rVV3	471	357	0.02%	0.003%
43	7.568	1923	1937	1961	rVV	159104	309731	17.59%	2.344%
44	7.652	1961	1963	1968	rVV2	609	547	0.03%	0.004%
45	7.684	1970	1973	1975	rVV2	451	292	0.02%	0.002%
46	7.713	1977	1982	1985	rVV3	703	610	0.03%	0.005%
47	7.732	1985	1988	1994	rVB3	584	600	0.03%	0.005%
48	7.764	1994	1998	1999	rBV2	374	258	0.01%	0.002%
49	7.896	2025	2039	2059	rBV	748000	1361698	77.34%	10.304%
50	8.182	2116	2128	2156	rBV2	102400	204050	11.59%	1.544%
51	8.353	2175	2181	2188	rVV8	1386	1760	0.10%	0.013%
52	8.385	2189	2191	2196	rVB	831	486	0.03%	0.004%
53	8.404	2196	2197	2202	rBV3	308	277	0.02%	0.002%
54	8.552	2230	2243	2258	rBV	106750	185169	10.52%	1.401%
55	8.661	2259	2277	2306	rBV2	351335	958055	54.42%	7.250%
56	8.893	2346	2349	2353	rVB4	606	472	0.03%	0.004%
57	8.938	2355	2363	2366	rBV5	696	954	0.05%	0.007%
58	8.996	2378	2381	2382	rVV	413	258	0.01%	0.002%
59	9.018	2386	2388	2395	rVB2	293	287	0.02%	0.002%
60	9.166	2432	2434	2438	rVB3	425	283	0.02%	0.002%
61	9.192	2438	2442	2445	rBV2	405	327	0.02%	0.002%
62	9.237	2451	2456	2458	rBV	257	270	0.02%	0.002%
63	9.420	2496	2513	2534	rBV	696676	1283917	72.92%	9.715%
64	9.575	2557	2561	2563	rBV3	562	438	0.02%	0.003%
65	9.796	2624	2630	2635	rBV2	412	514	0.03%	0.004%
66	9.919	2662	2668	2671	rBV3	268	300	0.02%	0.002%
67	10.057	2705	2711	2717	rVB2	256	343	0.02%	0.003%
68	10.263	2773	2775	2784	rVB2	288	352	0.02%	0.003%
69	10.346	2798	2801	2806	rVB2	332	334	0.02%	0.003%
70	10.488	2839	2845	2851	rVB2	422	487	0.03%	0.004%
71	10.546	2860	2863	2866	rBV	358	269	0.02%	0.002%
72	10.626	2879	2888	2890	rBV3	737	759	0.04%	0.006%
73	10.764	2917	2931	2956	rVV	540653	914200	51.92%	6.918%
74	11.086	3025	3031	3035	rBV3	482	583	0.03%	0.004%
75	11.118	3035	3041	3049	rVV6	2583	3421	0.19%	0.026%
76	11.182	3056	3061	3064	rBV2	302	315	0.02%	0.002%

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 Title : VOC Analysis

77	11.314	3097	3102	3106	rVB4	524	449	0.03%	0.003%
78	11.349	3110	3113	3118	rBV	231	276	0.02%	0.002%
79	11.378	3118	3122	3126	rVB3	495	416	0.02%	0.003%
80	11.414	3130	3133	3134	rVV	481	298	0.02%	0.002%
81	11.475	3146	3152	3158	rVB4	743	1009	0.06%	0.008%
82	11.507	3158	3162	3167	rBV2	318	274	0.02%	0.002%
83	11.671	3209	3213	3220	rBV3	382	422	0.02%	0.003%
84	11.751	3233	3238	3244	rVB3	1145	1110	0.06%	0.008%
85	11.816	3245	3258	3279	rBV	618523	994160	56.47%	7.523%
86	11.989	3308	3312	3314	rBV2	479	376	0.02%	0.003%
87	12.198	3363	3377	3398	rBV	654448	1059383	60.17%	8.016%
88	12.446	3451	3454	3458	rBV2	313	287	0.02%	0.002%
89	12.565	3487	3491	3497	rBV4	461	420	0.02%	0.003%
90	12.806	3564	3566	3570	rVB	443	279	0.02%	0.002%
91	12.835	3570	3575	3576	rBV	517	350	0.02%	0.003%
92	13.356	3734	3737	3739	rBV	464	283	0.02%	0.002%
93	13.394	3747	3749	3752	rBV2	380	317	0.02%	0.002%
94	13.668	3832	3834	3840	rVB	462	360	0.02%	0.003%
95	13.922	3909	3913	3919	rBV	642	622	0.04%	0.005%
96	14.050	3951	3953	3957	rBV	395	252	0.01%	0.002%
97	14.098	3960	3968	3976	rBV4	1649	2900	0.16%	0.022%
98	14.330	4038	4040	4043	rBV4	598	450	0.03%	0.003%
99	14.815	4188	4191	4193	rBV	539	293	0.02%	0.002%
100	14.976	4239	4241	4247	rVB2	615	441	0.03%	0.003%

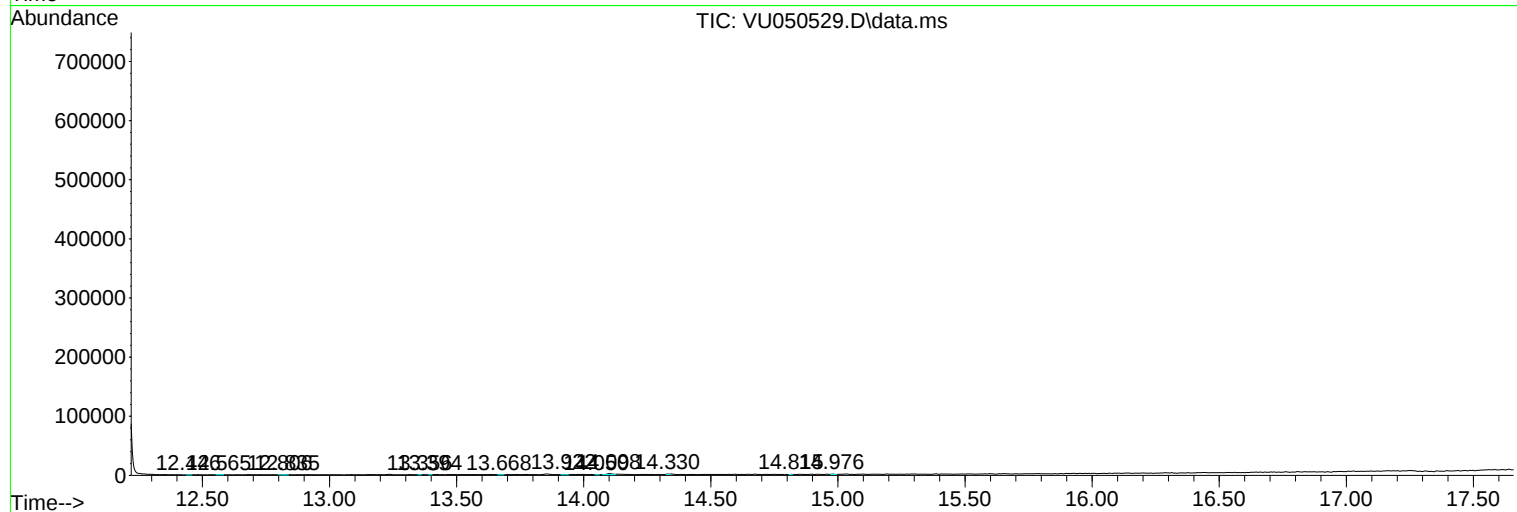
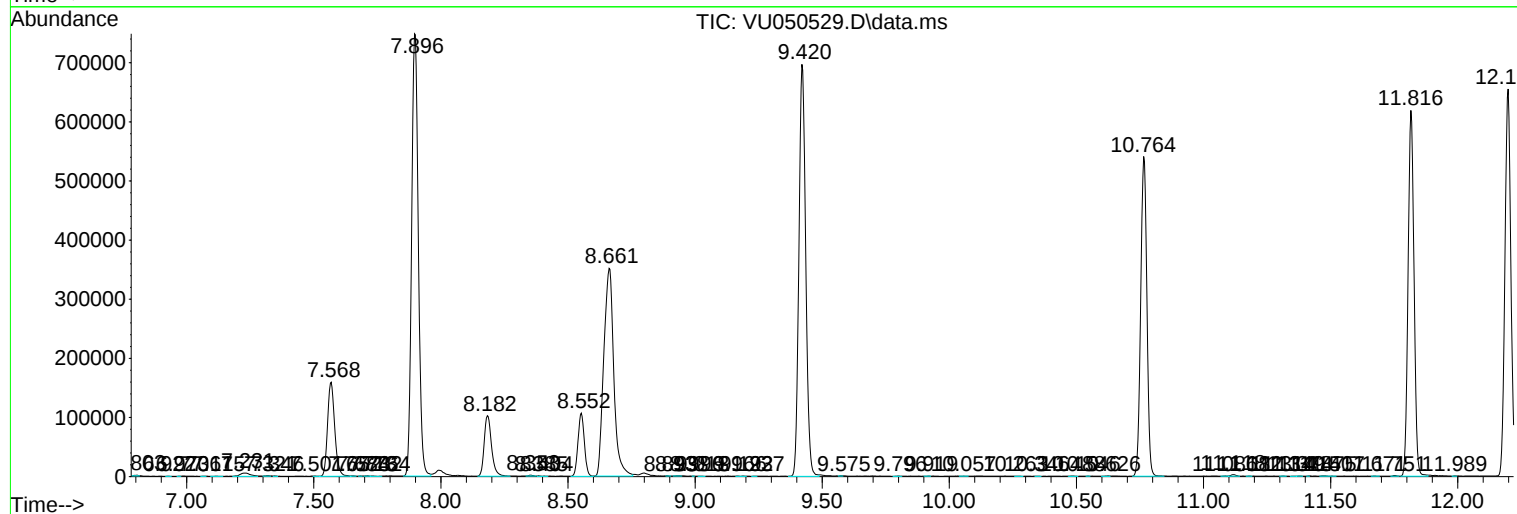
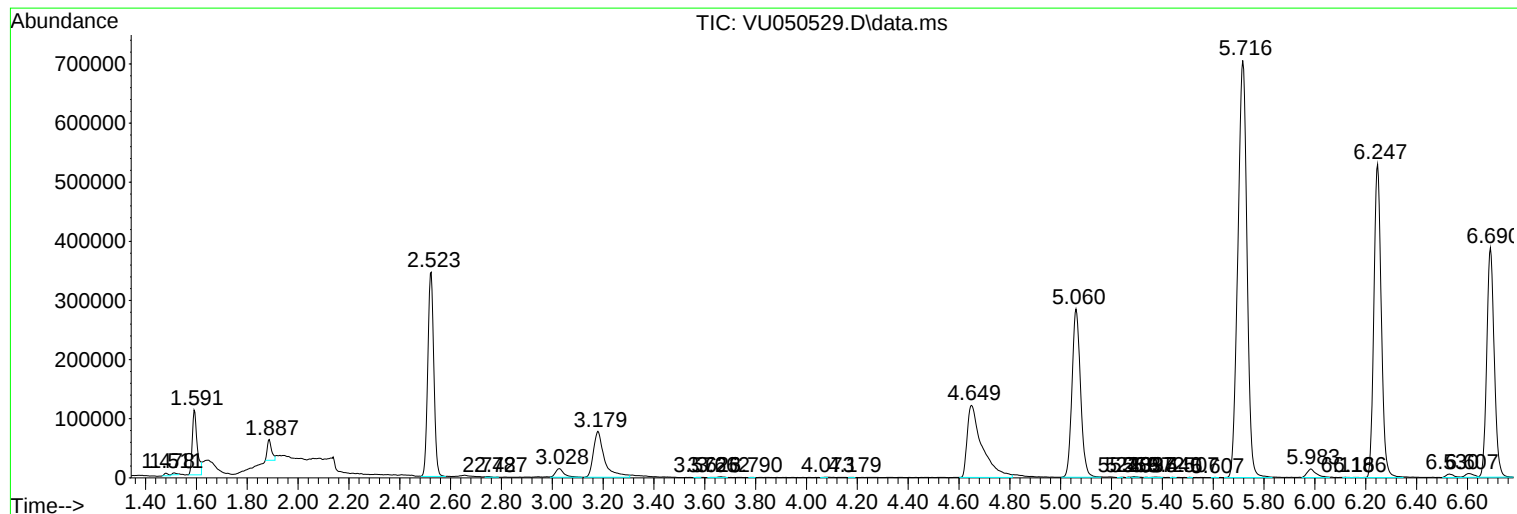
Sum of corrected areas: 13215435

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ClientSampleId :
DBVT4ME

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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