

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071922\
 Data File : VU049790.D
 Acq On : 19 Jul 2022 17:14
 Operator : SY/MD
 Sample : N3721-08ME
 Misc : 6.25g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 16 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5C28ME

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\SFAMULM071122WMA.M
 Title : VOC Analysis

Signal : TIC: VU049790.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.594	71	79	85	rBV	108277	140638	8.61%	1.211%
2	1.870	123	165	173	rBV2	95377	262220	16.05%	2.258%
3	2.237	275	279	282	rBV3	784	670	0.04%	0.006%
4	2.282	291	293	294	rBV2	549	245	0.01%	0.002%
5	2.520	354	367	385	rVB	312966	509448	31.19%	4.388%
6	2.655	399	409	424	rVB5	2057	4545	0.28%	0.039%
7	2.745	433	437	444	rVB4	554	677	0.04%	0.006%
8	2.854	467	471	476	rBV3	281	295	0.02%	0.003%
9	2.899	483	485	489	rBV2	264	223	0.01%	0.002%
10	3.025	514	524	538	rBV2	9177	17757	1.09%	0.153%
11	3.176	556	571	591	rVV	37925	89015	5.45%	0.767%
12	3.295	605	608	615	rBV3	439	469	0.03%	0.004%
13	3.668	718	724	727	rVB3	381	368	0.02%	0.003%
14	3.861	782	784	787	rBV2	191	123	0.01%	0.001%
15	3.938	802	808	811	rBV2	393	350	0.02%	0.003%
16	4.140	868	871	876	rBV2	264	281	0.02%	0.002%
17	4.276	910	913	915	rBV	199	127	0.01%	0.001%
18	4.349	930	936	941	rBV2	224	291	0.02%	0.003%
19	4.456	966	969	974	rBV2	237	207	0.01%	0.002%
20	4.636	1012	1025	1071	rBV	153104	493732	30.23%	4.252%
21	4.880	1097	1101	1104	rVB3	532	470	0.03%	0.004%
22	4.999	1134	1138	1140	rBV	308	245	0.01%	0.002%
23	5.060	1140	1157	1182	rVV	278724	642880	39.36%	5.537%
24	5.285	1220	1227	1233	rBV4	629	948	0.06%	0.008%
25	5.340	1239	1244	1246	rBV3	229	188	0.01%	0.002%
26	5.362	1247	1251	1257	rVB4	639	762	0.05%	0.007%
27	5.433	1271	1273	1279	rVB2	164	126	0.01%	0.001%
28	5.716	1340	1361	1388	rBV2	640542	1633451	100.00%	14.068%
29	5.851	1401	1403	1406	rBV	238	122	0.01%	0.001%
30	5.976	1431	1442	1457	rBV4	8411	18854	1.15%	0.162%
31	6.128	1484	1489	1491	rBV2	160	140	0.01%	0.001%
32	6.173	1500	1503	1505	rBV2	187	120	0.01%	0.001%
33	6.243	1510	1525	1547	rBV	298484	586174	35.89%	5.048%
34	6.375	1563	1566	1568	rBV	335	194	0.01%	0.002%
35	6.401	1568	1574	1575	rBV2	389	390	0.02%	0.003%
36	6.430	1581	1583	1586	rVB	295	168	0.01%	0.001%

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Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
 Title : VOC Analysis

37	6.523	1603	1612	1624	rBV5	5540	10744	0.66%	0.093%
38	6.600	1624	1636	1647	rVV3	3788	8277	0.51%	0.071%
39	6.690	1649	1664	1688	rVB	373253	764948	46.83%	6.588%
40	6.803	1696	1699	1700	rBV2	356	168	0.01%	0.001%
41	6.967	1747	1750	1756	rBV2	192	213	0.01%	0.002%
42	7.041	1769	1773	1776	rBV2	201	153	0.01%	0.001%
43	7.073	1781	1783	1791	rVB2	298	270	0.02%	0.002%
44	7.140	1800	1804	1809	rVB2	216	171	0.01%	0.001%
45	7.198	1809	1822	1824	rBV6	3268	5759	0.35%	0.050%
46	7.298	1851	1853	1858	rVB2	558	374	0.02%	0.003%
47	7.324	1858	1861	1863	rBV	251	140	0.01%	0.001%
48	7.340	1863	1866	1869	rBV2	274	211	0.01%	0.002%
49	7.497	1912	1915	1916	rBV2	302	122	0.01%	0.001%
50	7.565	1923	1936	1955	rBV	190304	359267	21.99%	3.094%
51	7.687	1968	1974	1977	rBV3	1216	1318	0.08%	0.011%
52	7.787	1999	2005	2010	rBV3	1091	1317	0.08%	0.011%
53	7.896	2025	2039	2060	rBV	700524	1225033	75.00%	10.551%
54	7.989	2062	2068	2084	rVB5	5260	11138	0.68%	0.096%
55	8.179	2115	2127	2148	rBV	125364	242796	14.86%	2.091%
56	8.356	2176	2182	2189	rVB4	734	1022	0.06%	0.009%
57	8.552	2241	2243	2248	rVB2	329	293	0.02%	0.003%
58	8.648	2257	2273	2306	rBV	459860	1085686	66.47%	9.351%
59	8.796	2315	2319	2330	rVB4	2972	4101	0.25%	0.035%
60	8.934	2359	2362	2365	rBV2	651	409	0.03%	0.004%
61	9.037	2391	2394	2398	rBV2	188	120	0.01%	0.001%
62	9.160	2428	2432	2434	rBV	325	238	0.01%	0.002%
63	9.288	2469	2472	2477	rVV	251	205	0.01%	0.002%
64	9.343	2485	2489	2493	rVB2	325	274	0.02%	0.002%
65	9.369	2493	2497	2499	rBV	322	272	0.02%	0.002%
66	9.420	2499	2513	2534	rBV	406029	729439	44.66%	6.282%
67	9.584	2560	2564	2567	rBV2	224	172	0.01%	0.001%
68	9.616	2571	2574	2579	rBV	144	157	0.01%	0.001%
69	9.742	2610	2613	2617	rBV	254	214	0.01%	0.002%
70	10.108	2724	2727	2729	rBV2	183	125	0.01%	0.001%
71	10.147	2736	2739	2746	rVB2	256	257	0.02%	0.002%
72	10.340	2793	2799	2802	rBV	255	331	0.02%	0.003%
73	10.578	2870	2873	2879	rBV2	190	167	0.01%	0.001%
74	10.603	2879	2881	2884	rBV2	167	121	0.01%	0.001%
75	10.648	2893	2895	2896	rBV	275	117	0.01%	0.001%
76	10.761	2916	2930	2956	rBV	559279	928227	56.83%	7.994%

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 Title : VOC Analysis

77	11.037	3013	3016	3021	rVB	299	206	0.01%	0.002%
78	11.118	3036	3041	3047	rVB5	1126	1357	0.08%	0.012%
79	11.311	3097	3101	3106	rBV4	407	479	0.03%	0.004%
80	11.375	3118	3121	3125	rBV2	419	363	0.02%	0.003%
81	11.526	3166	3168	3171	rVB2	243	141	0.01%	0.001%
82	11.549	3171	3175	3177	rBV2	236	204	0.01%	0.002%
83	11.690	3216	3219	3222	rBV2	253	203	0.01%	0.002%
84	11.815	3246	3258	3274	rBV	444103	694933	42.54%	5.985%
85	11.973	3304	3307	3310	rBV	217	119	0.01%	0.001%
86	12.063	3333	3335	3339	rVB2	334	197	0.01%	0.002%
87	12.086	3339	3342	3348	rBV2	311	388	0.02%	0.003%
88	12.195	3363	3376	3402	rBV	674421	1116651	68.36%	9.617%
89	12.401	3437	3440	3448	rVB3	313	362	0.02%	0.003%
90	12.532	3475	3481	3484	rBV	352	463	0.03%	0.004%
91	12.674	3522	3525	3529	rBV2	258	174	0.01%	0.001%
92	12.770	3552	3555	3558	rBV	401	290	0.02%	0.002%
93	12.848	3577	3579	3585	rVB2	305	290	0.02%	0.002%
94	12.954	3610	3612	3618	rVB2	433	265	0.02%	0.002%
95	13.346	3731	3734	3737	rBV	295	207	0.01%	0.002%
96	13.491	3776	3779	3785	rVB3	382	365	0.02%	0.003%
97	14.571	4108	4115	4117	rBV4	828	1015	0.06%	0.009%
98	14.645	4135	4138	4140	rBV2	359	232	0.01%	0.002%
99	14.732	4161	4165	4167	rBV2	484	407	0.02%	0.004%
100	16.053	4573	4576	4578	rBV4	580	403	0.02%	0.003%

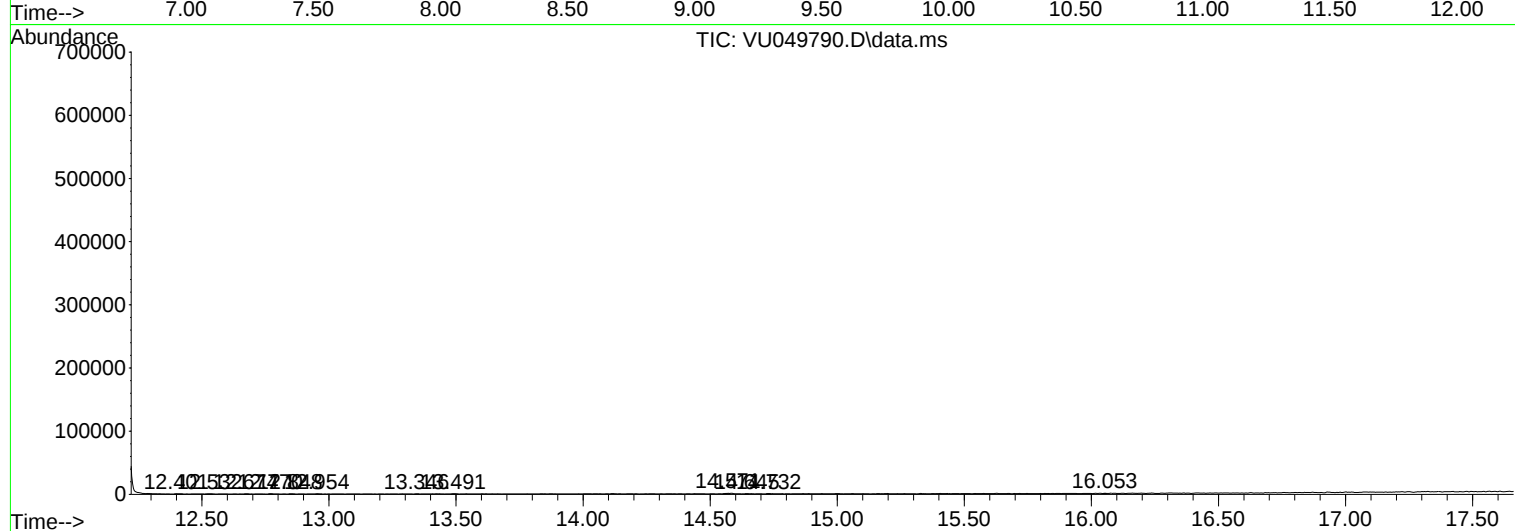
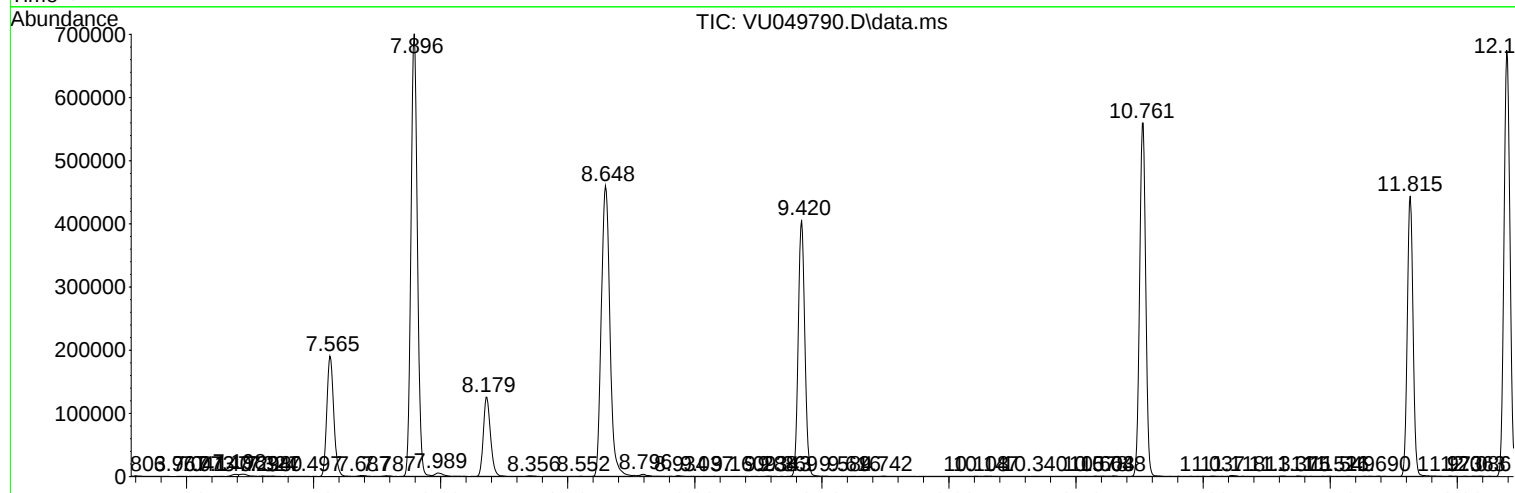
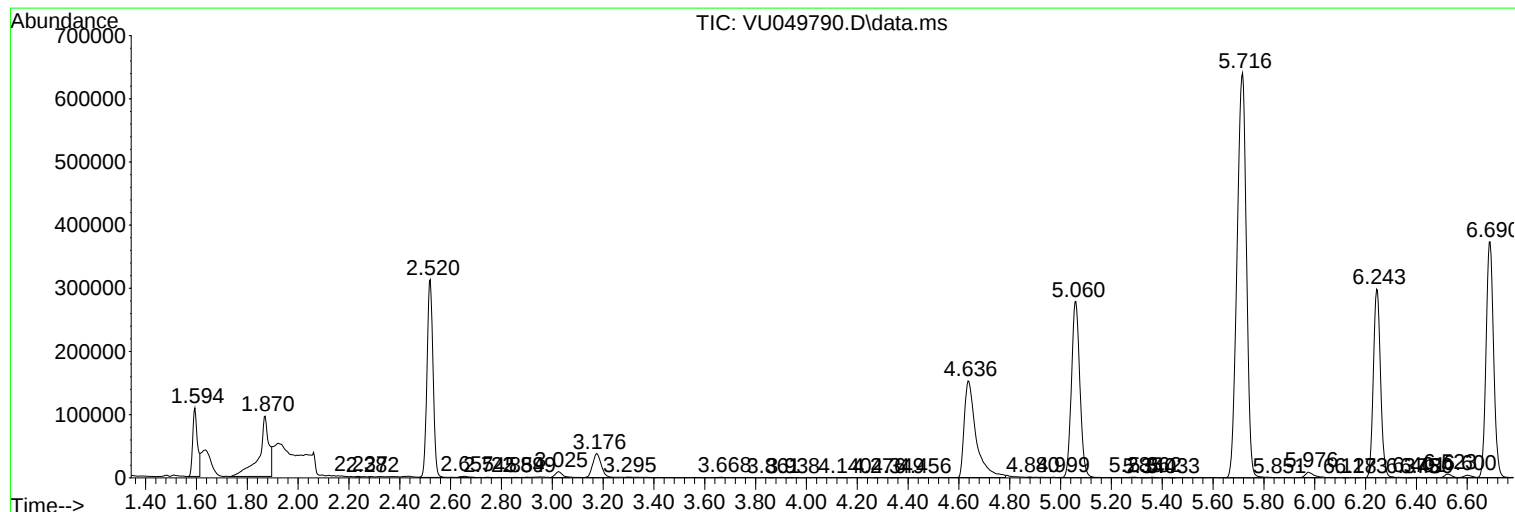
Sum of corrected areas: 11610993

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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.M
Quant Title : VOC Analysis

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



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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM071122WMA.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 Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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