

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU020724\
 Data File : VU057844.D
 Acq On : 07 Feb 2024 16:47
 Operator : MD/SY
 Sample : P1329-14ME
 Misc : 5.36g/5.0ml/100uL//5.0mL/MSVOA_U/MEOH
 ALS Vial : 19 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 C0FR5ME

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\SFAMULM020724WMA.M
 Title : VOC Analysis

Signal : TIC: VU057844.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.595	88	95	116	rVB	81613	145900	15.97%	2.002%
2	2.534	376	387	405	rVB	192350	311564	34.10%	4.275%
3	2.692	432	436	439	rBV3	769	748	0.08%	0.010%
4	2.840	479	482	486	rBV	251	222	0.02%	0.003%
5	2.891	496	498	500	rVB2	163	47	0.01%	0.001%
6	3.251	608	610	614	rVB2	211	79	0.01%	0.001%
7	3.335	634	636	642	rVB	292	208	0.02%	0.003%
8	3.441	665	669	672	rBV2	408	324	0.04%	0.004%
9	3.480	678	681	684	rBV	199	147	0.02%	0.002%
10	3.682	736	744	751	rVB6	724	997	0.11%	0.014%
11	3.875	801	804	807	rBV	234	161	0.02%	0.002%
12	3.917	812	817	819	rBV2	198	185	0.02%	0.003%
13	4.335	943	947	952	rVB2	210	155	0.02%	0.002%
14	4.460	983	986	991	rVB2	269	219	0.02%	0.003%
15	4.486	991	994	996	rBV	270	200	0.02%	0.003%
16	4.624	1024	1037	1086	rBV2	49683	177376	19.41%	2.434%
17	5.049	1153	1169	1198	rBV	158110	354259	38.77%	4.861%
18	5.197	1213	1215	1218	rBV3	422	288	0.03%	0.004%
19	5.328	1247	1256	1269	rVB4	893	2050	0.22%	0.028%
20	5.576	1330	1333	1336	rVB2	138	83	0.01%	0.001%
21	5.621	1346	1347	1348	rVB2	96	18	0.00%	0.000%
22	5.711	1356	1375	1407	rBV2	346346	913761	100.00%	12.538%
23	5.978	1449	1458	1467	rBV5	2161	4251	0.47%	0.058%
24	6.107	1496	1498	1500	rBV2	201	99	0.01%	0.001%
25	6.164	1512	1516	1519	rVB2	191	142	0.02%	0.002%
26	6.238	1526	1539	1566	rBV	312444	601166	65.79%	8.249%
27	6.521	1617	1627	1637	rBV6	2887	5102	0.56%	0.070%
28	6.589	1643	1648	1663	rVB4	2571	5111	0.56%	0.070%
29	6.679	1663	1676	1702	rVB	201790	402923	44.10%	5.529%
30	6.901	1741	1745	1748	rBV	212	146	0.02%	0.002%
31	7.010	1776	1779	1780	rBV2	90	51	0.01%	0.001%
32	7.084	1798	1802	1807	rBV	258	214	0.02%	0.003%
33	7.106	1807	1809	1811	rBV	131	78	0.01%	0.001%
34	7.196	1824	1837	1840	rBV7	2482	4075	0.45%	0.056%
35	7.325	1876	1877	1880	rVB2	153	67	0.01%	0.001%
36	7.377	1888	1893	1900	rBV2	278	386	0.04%	0.005%

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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\SFAMULM020724WMA.M
 Title : VOC Analysis

37	7.451	1913	1916	1920	rBV2	131	102	0.01%	0.001%
38	7.512	1932	1935	1937	rBV	72	49	0.01%	0.001%
39	7.560	1937	1950	1977	rVV	111241	212675	23.27%	2.918%
40	7.717	1996	1999	2000	rBV	181	91	0.01%	0.001%
41	7.830	2032	2034	2037	rBV	166	87	0.01%	0.001%
42	7.891	2039	2053	2073	rBV	414832	730705	79.97%	10.026%
43	8.177	2131	2142	2169	rBV2	68021	145945	15.97%	2.003%
44	8.328	2186	2189	2191	rBV2	212	115	0.01%	0.002%
45	8.338	2191	2192	2194	rBV2	343	161	0.02%	0.002%
46	8.589	2264	2270	2272	rBV	246	227	0.02%	0.003%
47	8.643	2273	2287	2323	rVV	216342	485104	53.09%	6.656%
48	8.910	2367	2370	2371	rBV2	215	143	0.02%	0.002%
49	9.000	2395	2398	2402	rVB	187	140	0.02%	0.002%
50	9.032	2402	2408	2411	rBV2	200	223	0.02%	0.003%
51	9.200	2458	2460	2461	rBV2	164	67	0.01%	0.001%
52	9.222	2464	2467	2469	rBV	109	60	0.01%	0.001%
53	9.303	2489	2492	2493	rBV	131	77	0.01%	0.001%
54	9.415	2514	2527	2551	rBV	413200	770275	84.30%	10.569%
55	9.698	2607	2615	2623	rBV2	937	1503	0.16%	0.021%
56	9.782	2637	2641	2644	rBV	281	208	0.02%	0.003%
57	10.074	2725	2732	2735	rBV2	287	331	0.04%	0.005%
58	10.261	2786	2790	2793	rBV2	241	185	0.02%	0.003%
59	10.389	2825	2830	2836	rBV2	229	325	0.04%	0.004%
60	10.576	2885	2888	2890	rBV2	198	126	0.01%	0.002%
61	10.756	2930	2944	2962	rBV	293389	489155	53.53%	6.712%
62	10.891	2978	2986	2993	rBV	1385	1823	0.20%	0.025%
63	11.110	3049	3054	3065	rVB6	2551	3676	0.40%	0.050%
64	11.245	3093	3096	3098	rBV2	229	127	0.01%	0.002%
65	11.309	3112	3116	3117	rBV3	471	322	0.04%	0.004%
66	11.466	3162	3165	3166	rBV	338	186	0.02%	0.003%
67	11.589	3200	3203	3208	rVB2	222	173	0.02%	0.002%
68	11.614	3208	3211	3214	rBV	224	147	0.02%	0.002%
69	11.749	3248	3253	3260	rBV3	819	873	0.10%	0.012%
70	11.810	3260	3272	3295	rBV	498763	797350	87.26%	10.940%
71	12.010	3331	3334	3337	rBV2	342	225	0.02%	0.003%
72	12.190	3378	3390	3419	rBV	428238	711250	77.84%	9.759%
73	12.399	3452	3455	3458	rBV3	279	187	0.02%	0.003%
74	13.524	3802	3805	3812	rVB2	357	351	0.04%	0.005%
75	13.556	3812	3815	3818	rBV	211	172	0.02%	0.002%
76	13.852	3904	3907	3910	rBV2	502	360	0.04%	0.005%

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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\SFAMULM020724WMA.M
Title : VOC Analysis

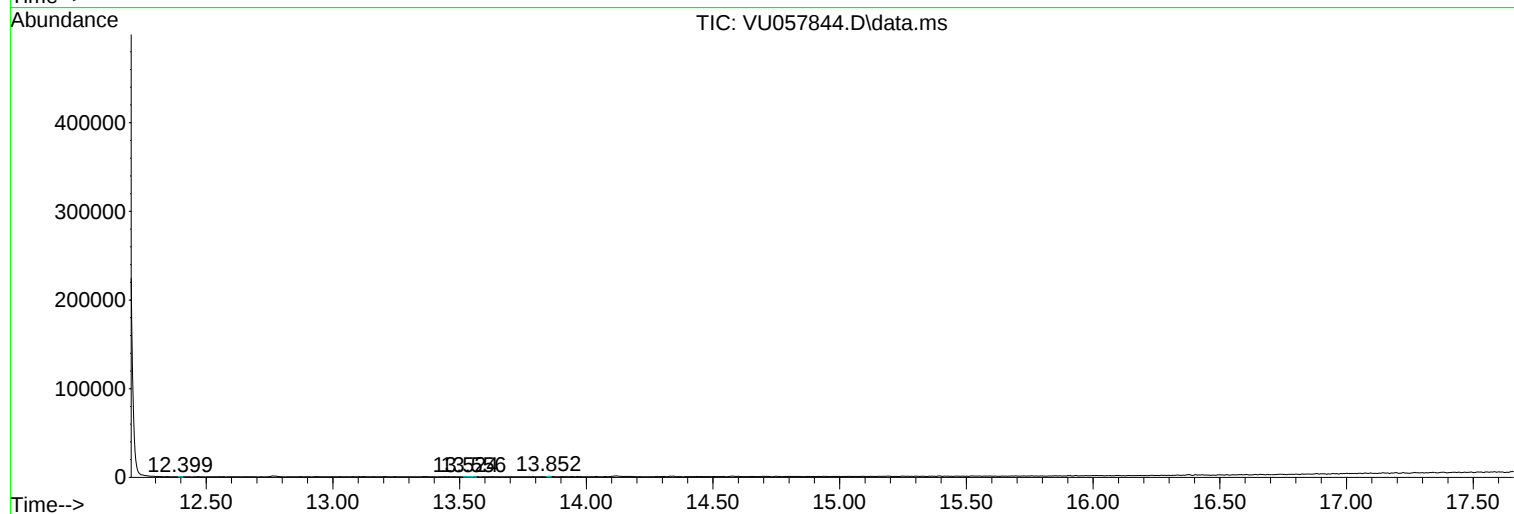
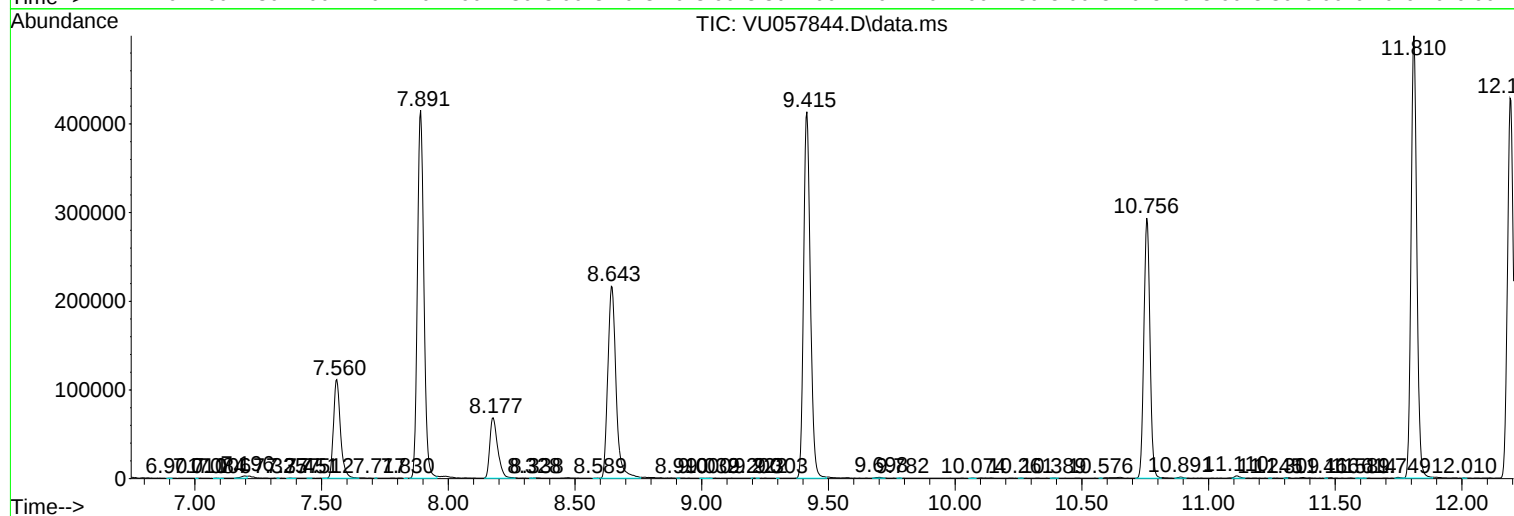
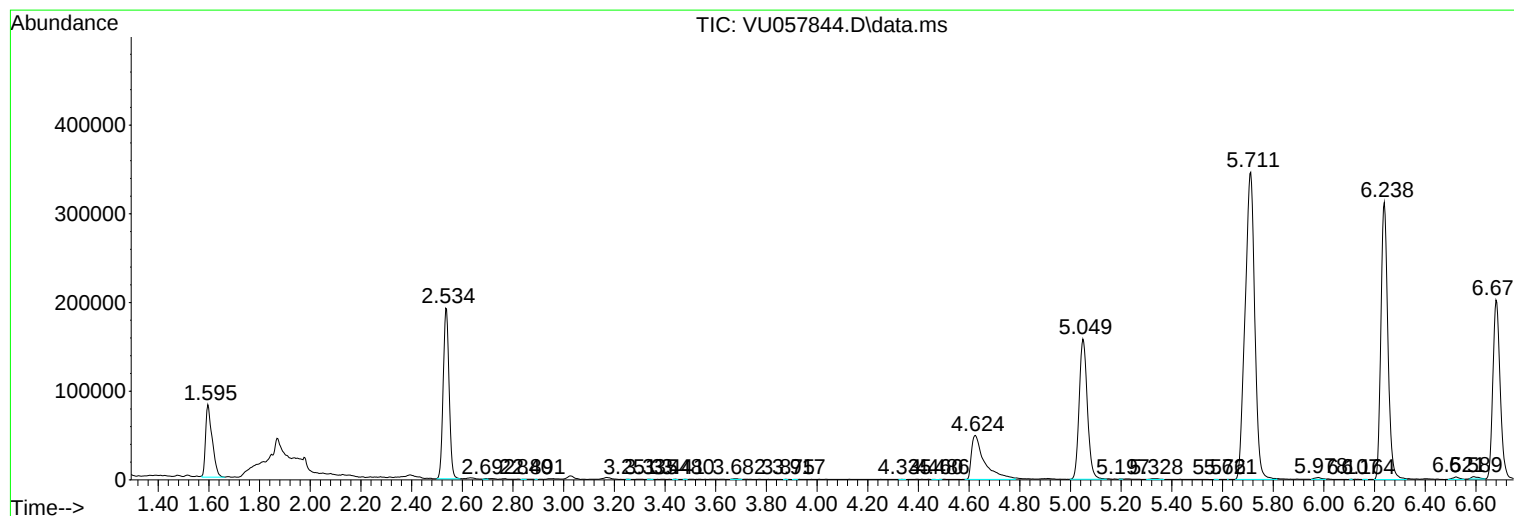
Sum of corrected areas: 7288103

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Instrument :
MSVOA_U
ClientSampleId :
C0FR5ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM020724WMA.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\SFAMULM020724WMA.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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Quant Title : VOC Analysis

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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