

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU101023\
 Data File : VU055725.D
 Acq On : 10 Oct 2023 16:48
 Operator : MD/SY
 Sample : 04771-07ME
 Misc : 6.25g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 E05J2ME

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\SFAMULM101023WMA.M
 Title : VOC Analysis

Signal : TIC: VU055725.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	87	95	119	rVB	244036	452161	13.80%	1.986%
2	2.534	374	387	408	rBV	652890	1065568	32.51%	4.680%
3	2.853	483	486	493	rVB4	934	802	0.02%	0.004%
4	2.885	494	496	502	rVV4	840	739	0.02%	0.003%
5	3.029	532	541	557	rBV5	6486	14240	0.43%	0.063%
6	3.171	572	585	605	rBV	27244	61929	1.89%	0.272%
7	3.518	690	693	695	rBV	379	272	0.01%	0.001%
8	3.605	716	720	723	rBV	371	303	0.01%	0.001%
9	3.624	723	726	729	rBV	351	231	0.01%	0.001%
10	3.666	735	739	740	rBV2	1008	707	0.02%	0.003%
11	3.721	754	756	761	rVB2	415	271	0.01%	0.001%
12	3.746	761	764	766	rBV	280	130	0.00%	0.001%
13	3.763	766	769	770	rBV	278	154	0.00%	0.001%
14	3.792	776	778	785	rVB2	521	519	0.02%	0.002%
15	3.830	785	790	793	rBV2	451	486	0.01%	0.002%
16	3.849	793	796	801	rBV	476	407	0.01%	0.002%
17	4.007	843	845	847	rBV	415	178	0.01%	0.001%
18	4.078	865	867	871	rVB	176	116	0.00%	0.001%
19	4.139	885	886	887	rBV	135	42	0.00%	0.000%
20	4.251	917	921	925	rBV3	737	620	0.02%	0.003%
21	4.483	991	993	997	rBV	256	202	0.01%	0.001%
22	4.554	1012	1015	1016	rBV	248	116	0.00%	0.001%
23	4.624	1021	1037	1081	rBV	223747	821956	25.08%	3.610%
24	5.055	1154	1171	1202	rBV	546244	1300100	39.67%	5.710%
25	5.428	1285	1287	1289	rBV	425	215	0.01%	0.001%
26	5.512	1309	1313	1318	rBV2	655	613	0.02%	0.003%
27	5.599	1338	1340	1342	rBV2	394	187	0.01%	0.001%
28	5.714	1355	1376	1402	rBV2	1233291	3277514	100.00%	14.395%
29	6.161	1513	1515	1516	rBV	414	164	0.01%	0.001%
30	6.242	1526	1540	1570	rBV	567523	1166179	35.58%	5.122%
31	6.525	1617	1628	1642	rBV5	19070	41851	1.28%	0.184%
32	6.685	1664	1678	1702	rBV	713412	1478222	45.10%	6.492%
33	7.119	1811	1813	1815	rBV	163	44	0.00%	0.000%
34	7.135	1815	1818	1822	rBV2	373	306	0.01%	0.001%
35	7.190	1827	1835	1841	rBV7	4219	7977	0.24%	0.035%
36	7.396	1896	1899	1901	rBV2	482	271	0.01%	0.001%

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 Title : VOC Analysis

37	7.434	1909	1911	1913	rBV2	290	108	0.00%	0.000%
38	7.447	1913	1915	1919	rVB2	529	355	0.01%	0.002%
39	7.492	1925	1929	1933	rBV2	649	634	0.02%	0.003%
40	7.563	1937	1951	1982	rVV	369283	759656	23.18%	3.336%
41	7.894	2041	2054	2078	rBV	1444915	2639097	80.52%	11.591%
42	8.177	2130	2142	2169	rBV	234701	527054	16.08%	2.315%
43	8.656	2273	2291	2322	rBV2	845947	2051704	62.60%	9.011%
44	9.258	2475	2478	2482	rBV	501	440	0.01%	0.002%
45	9.418	2515	2528	2554	rBV	762684	1533993	46.80%	6.737%
46	9.656	2599	2602	2604	rBV2	476	286	0.01%	0.001%
47	9.666	2604	2605	2608	rVB2	607	189	0.01%	0.001%
48	9.695	2609	2614	2615	rBV2	2093	1455	0.04%	0.006%
49	9.807	2647	2649	2651	rBV2	252	93	0.00%	0.000%
50	9.859	2663	2665	2670	rVB2	752	455	0.01%	0.002%
51	9.955	2694	2695	2696	rBV	352	68	0.00%	0.000%
52	10.097	2737	2739	2740	rBV2	468	186	0.01%	0.001%
53	10.222	2775	2778	2780	rVB	374	203	0.01%	0.001%
54	10.560	2880	2883	2885	rBV	297	212	0.01%	0.001%
55	10.627	2900	2904	2905	rBV	407	194	0.01%	0.001%
56	10.711	2927	2930	2931	rBV	719	380	0.01%	0.002%
57	10.759	2932	2945	2962	rVV	1145641	1887855	57.60%	8.291%
58	10.897	2984	2988	2992	rBV2	754	608	0.02%	0.003%
59	10.955	3003	3006	3008	rVB	427	193	0.01%	0.001%
60	11.347	3124	3128	3130	rBV2	404	350	0.01%	0.002%
61	11.550	3189	3191	3195	rBV2	398	246	0.01%	0.001%
62	11.814	3260	3273	3289	rBV	871059	1386890	42.32%	6.091%
63	12.000	3329	3331	3334	rBV2	639	490	0.01%	0.002%
64	12.193	3374	3391	3416	rBV	1403299	2278856	69.53%	10.009%
65	12.772	3568	3571	3573	rBV2	845	526	0.02%	0.002%

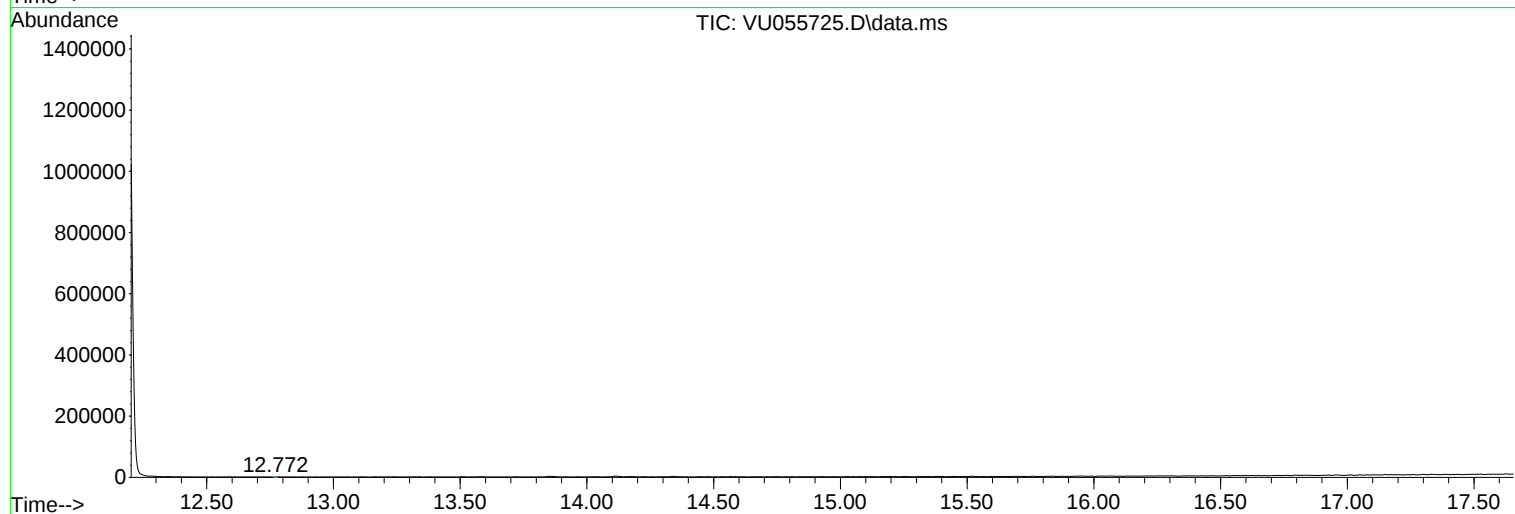
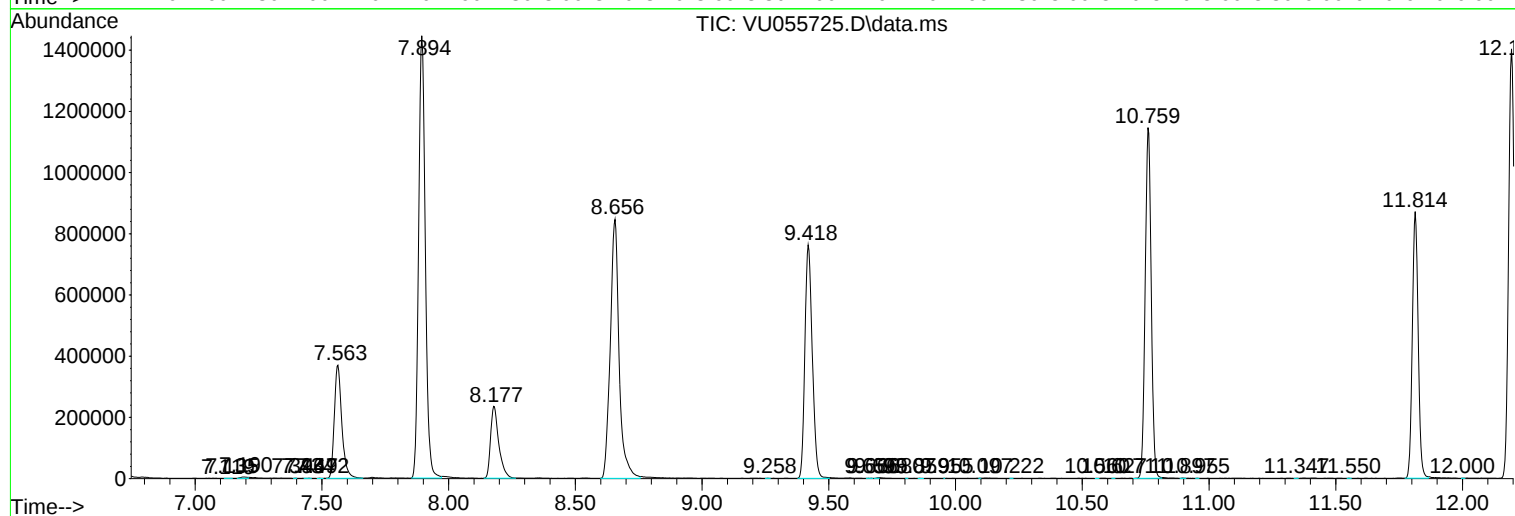
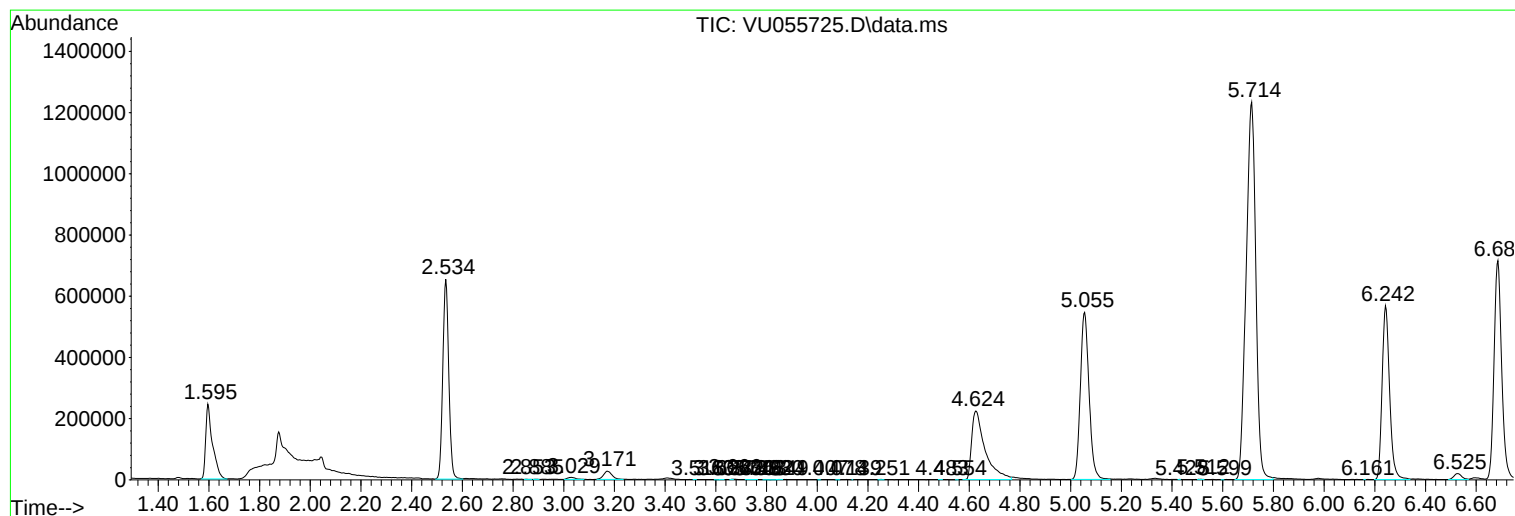
Sum of corrected areas: 22768568

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Quant Title : VOC Analysis

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



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No Library Search Compounds Detected

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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc