

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU071522\
 Data File : VU049743.D
 Acq On : 15 Jul 2022 17:46
 Operator : SY/MD
 Sample : N3698-04ME
 Misc : 5.23g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 21 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 F5B69ME

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: VU049743.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	87	rBV	72021	102533	7.24%	0.983%
2	1.871	160	165	174	rBV	50217	63544	4.49%	0.609%
3	2.523	355	368	385	rVB	209333	341391	24.12%	3.274%
4	2.652	401	408	419	rVB4	1167	2160	0.15%	0.021%
5	2.845	463	468	472	rBV	357	435	0.03%	0.004%
6	2.906	483	487	490	rBV2	329	287	0.02%	0.003%
7	3.031	507	526	539	rVB5	6850	16657	1.18%	0.160%
8	3.173	561	570	584	rVB5	1724	4089	0.29%	0.039%
9	3.327	607	618	628	rBV8	2253	4353	0.31%	0.042%
10	3.526	676	680	683	rVB2	223	174	0.01%	0.002%
11	3.661	715	722	723	rBV3	783	750	0.05%	0.007%
12	3.890	790	793	799	rVB2	194	205	0.01%	0.002%
13	4.041	836	840	844	rBV2	213	191	0.01%	0.002%
14	4.337	928	932	936	rBV2	195	197	0.01%	0.002%
15	4.395	942	950	952	rBV2	1163	1232	0.09%	0.012%
16	4.504	974	984	994	rBV5	1945	3614	0.26%	0.035%
17	4.636	1010	1025	1058	rBV	173216	551569	38.97%	5.289%
18	5.057	1139	1156	1180	rBV	266615	612012	43.24%	5.869%
19	5.285	1220	1227	1236	rBV2	622	1005	0.07%	0.010%
20	5.353	1242	1248	1249	rBV3	1721	1296	0.09%	0.012%
21	5.446	1264	1277	1291	rVB5	8029	17891	1.26%	0.172%
22	5.581	1310	1319	1328	rBV5	2144	3500	0.25%	0.034%
23	5.716	1340	1361	1391	rBV2	545754	1415227	100.00%	13.571%
24	5.838	1391	1399	1400	rVV3	1321	1528	0.11%	0.015%
25	5.886	1403	1414	1429	rVB4	10385	25577	1.81%	0.245%
26	5.976	1430	1442	1460	rBV5	7845	19216	1.36%	0.184%
27	6.137	1489	1492	1493	rBV2	276	179	0.01%	0.002%
28	6.157	1493	1498	1502	rVB	287	358	0.03%	0.003%
29	6.243	1511	1525	1547	rBV	234586	457160	32.30%	4.384%
30	6.366	1559	1563	1566	rBV2	370	282	0.02%	0.003%
31	6.436	1582	1585	1588	rBV2	186	187	0.01%	0.002%
32	6.523	1603	1612	1625	rBV10	8161	16214	1.15%	0.155%
33	6.594	1626	1634	1645	rBV4	3536	6761	0.48%	0.065%
34	6.687	1649	1663	1693	rVB	349676	720184	50.89%	6.906%
35	6.800	1693	1698	1701	rBV6	1240	1311	0.09%	0.013%
36	6.857	1710	1716	1730	rVB6	1390	2430	0.17%	0.023%

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

37	6.912	1730	1733	1735	rBV	339	195	0.01%	0.002%
38	6.970	1748	1751	1753	rBV	745	443	0.03%	0.004%
39	7.066	1776	1781	1784	rBV	472	368	0.03%	0.004%
40	7.111	1792	1795	1802	rVB	390	398	0.03%	0.004%
41	7.185	1804	1818	1826	rBV7	6373	12911	0.91%	0.124%
42	7.304	1850	1855	1859	rBV3	387	407	0.03%	0.004%
43	7.330	1859	1863	1866	rVV2	428	436	0.03%	0.004%
44	7.372	1866	1876	1885	rVV5	3193	5844	0.41%	0.056%
45	7.423	1885	1892	1898	rVB3	1487	2026	0.14%	0.019%
46	7.565	1922	1936	1960	rVV2	163737	314521	22.22%	3.016%
47	7.693	1966	1976	1987	rBV3	3061	5867	0.41%	0.056%
48	7.806	2007	2011	2014	rBV	302	215	0.02%	0.002%
49	7.828	2014	2018	2019	rBV2	505	399	0.03%	0.004%
50	7.896	2025	2039	2060	rBV	563907	988893	69.88%	9.482%
51	7.989	2060	2068	2083	rVB4	4941	10853	0.77%	0.104%
52	8.066	2088	2092	2103	rVB3	797	996	0.07%	0.010%
53	8.115	2103	2107	2114	rVB2	211	215	0.02%	0.002%
54	8.179	2114	2127	2145	rBV	109176	213030	15.05%	2.043%
55	8.269	2153	2155	2158	rVB	297	173	0.01%	0.002%
56	8.285	2158	2160	2163	rVB2	287	171	0.01%	0.002%
57	8.304	2163	2166	2170	rBV	349	244	0.02%	0.002%
58	8.581	2249	2252	2256	rBV2	192	220	0.02%	0.002%
59	8.648	2257	2273	2303	rBV2	517335	1210198	85.51%	11.605%
60	8.796	2313	2319	2328	rVB6	2600	4316	0.30%	0.041%
61	8.857	2336	2338	2346	rVB2	579	436	0.03%	0.004%
62	8.912	2352	2355	2357	rVV	269	191	0.01%	0.002%
63	8.941	2361	2364	2369	rVB3	479	373	0.03%	0.004%
64	9.073	2401	2405	2410	rBV2	205	234	0.02%	0.002%
65	9.420	2499	2513	2531	rBV	316067	570745	40.33%	5.473%
66	9.568	2556	2559	2561	rBV2	338	184	0.01%	0.002%
67	10.433	2824	2828	2830	rBV	279	207	0.01%	0.002%
68	10.600	2874	2880	2883	rBV2	316	316	0.02%	0.003%
69	10.623	2883	2887	2891	rVB4	636	544	0.04%	0.005%
70	10.645	2891	2894	2895	rBV	498	231	0.02%	0.002%
71	10.761	2916	2930	2954	rBV	622944	1017634	71.91%	9.758%
72	10.906	2972	2975	2980	rVB2	269	216	0.02%	0.002%
73	11.115	3034	3040	3047	rBV3	1078	1433	0.10%	0.014%
74	11.150	3049	3051	3056	rVB2	316	227	0.02%	0.002%
75	11.179	3057	3060	3064	rVV2	229	169	0.01%	0.002%
76	11.259	3082	3085	3090	rVB	324	263	0.02%	0.003%

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Peak Location: TOP

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

77	11.375	3119	3121	3128	rVB2	425	301	0.02%	0.003%
78	11.410	3129	3132	3137	rVV2	230	223	0.02%	0.002%
79	11.655	3204	3208	3211	rBV2	397	300	0.02%	0.003%
80	11.815	3245	3258	3283	rBV	341932	537479	37.98%	5.154%
81	11.918	3287	3290	3294	rVB2	584	356	0.03%	0.003%
82	12.005	3314	3317	3323	rVB2	237	219	0.02%	0.002%
83	12.195	3363	3376	3397	rBV	695077	1122012	79.28%	10.759%
84	12.568	3484	3492	3493	rBV2	386	357	0.03%	0.003%
85	12.751	3547	3549	3553	rBV2	325	215	0.02%	0.002%
86	12.857	3578	3582	3583	rBV	310	231	0.02%	0.002%
87	13.095	3653	3656	3659	rBV2	362	272	0.02%	0.003%
88	13.667	3830	3834	3837	rBV2	377	358	0.03%	0.003%
89	13.831	3882	3885	3889	rBV3	249	217	0.02%	0.002%
90	14.018	3940	3943	3948	rBV3	349	415	0.03%	0.004%
91	14.082	3960	3963	3964	rBV2	338	203	0.01%	0.002%
92	14.192	3994	3997	3998	rBV	373	234	0.02%	0.002%
93	14.311	4031	4034	4037	rBV	350	250	0.02%	0.002%
94	14.433	4066	4072	4073	rBV2	365	388	0.03%	0.004%
95	14.478	4084	4086	4089	rBV3	367	199	0.01%	0.002%
96	14.568	4112	4114	4126	rVB3	486	796	0.06%	0.008%
97	14.761	4170	4174	4176	rBV2	281	257	0.02%	0.002%
98	14.854	4201	4203	4207	rBV3	394	380	0.03%	0.004%
99	14.909	4217	4220	4224	rBV2	307	243	0.02%	0.002%
100	16.108	4590	4593	4595	rBV2	505	329	0.02%	0.003%

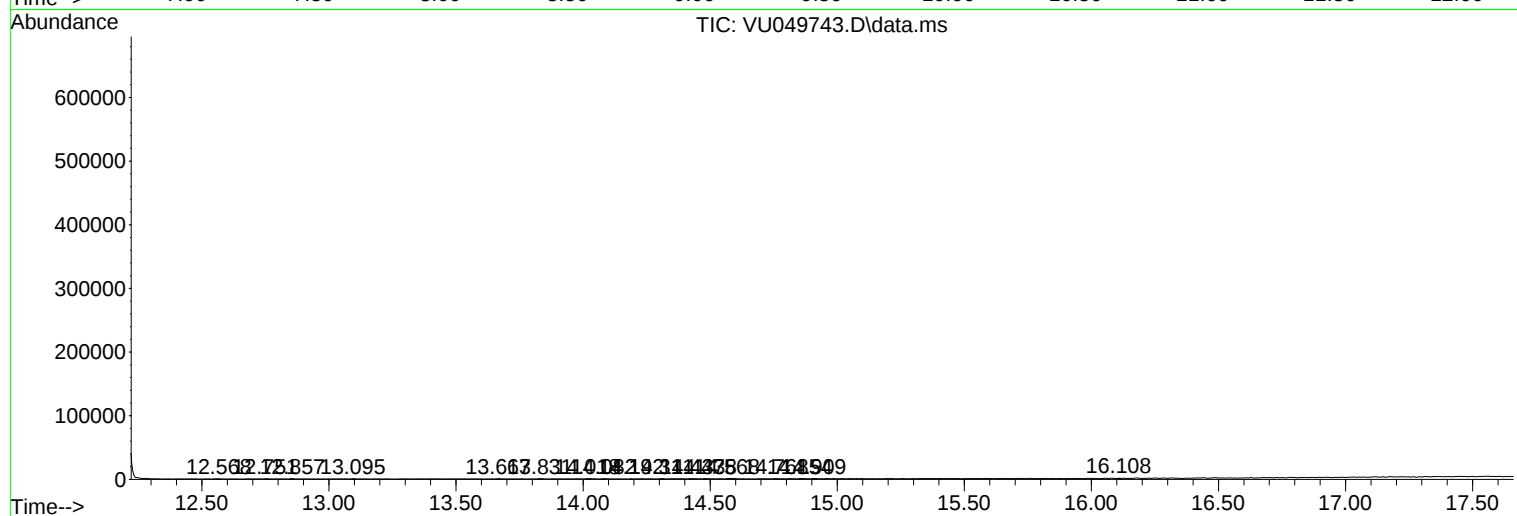
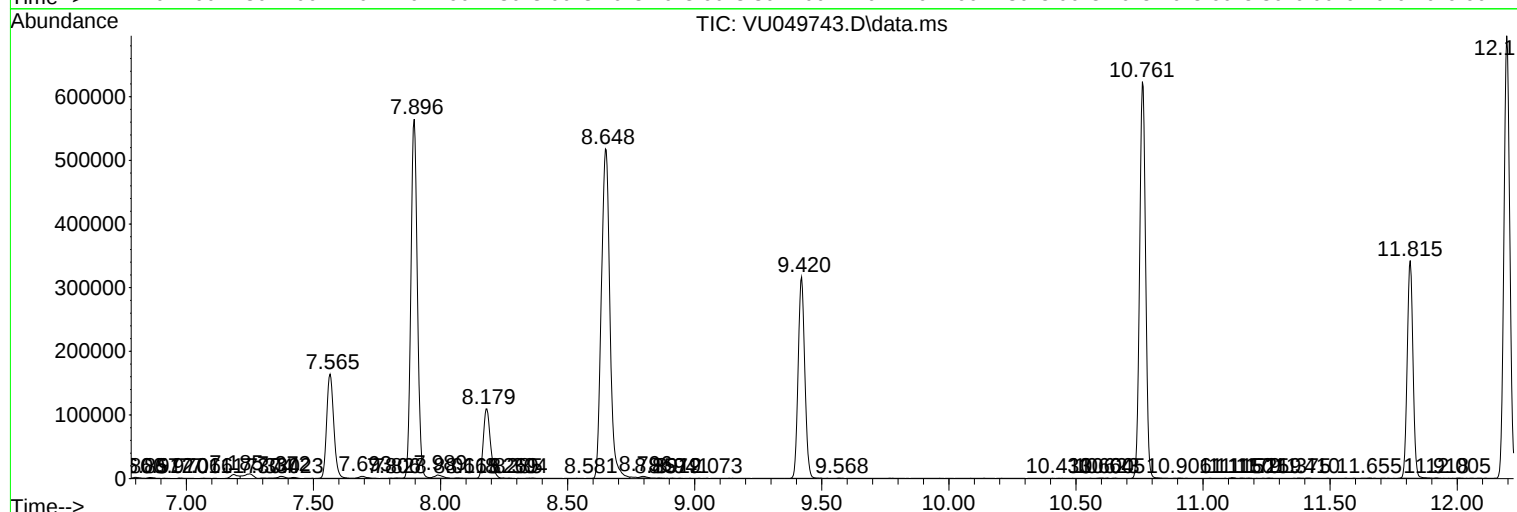
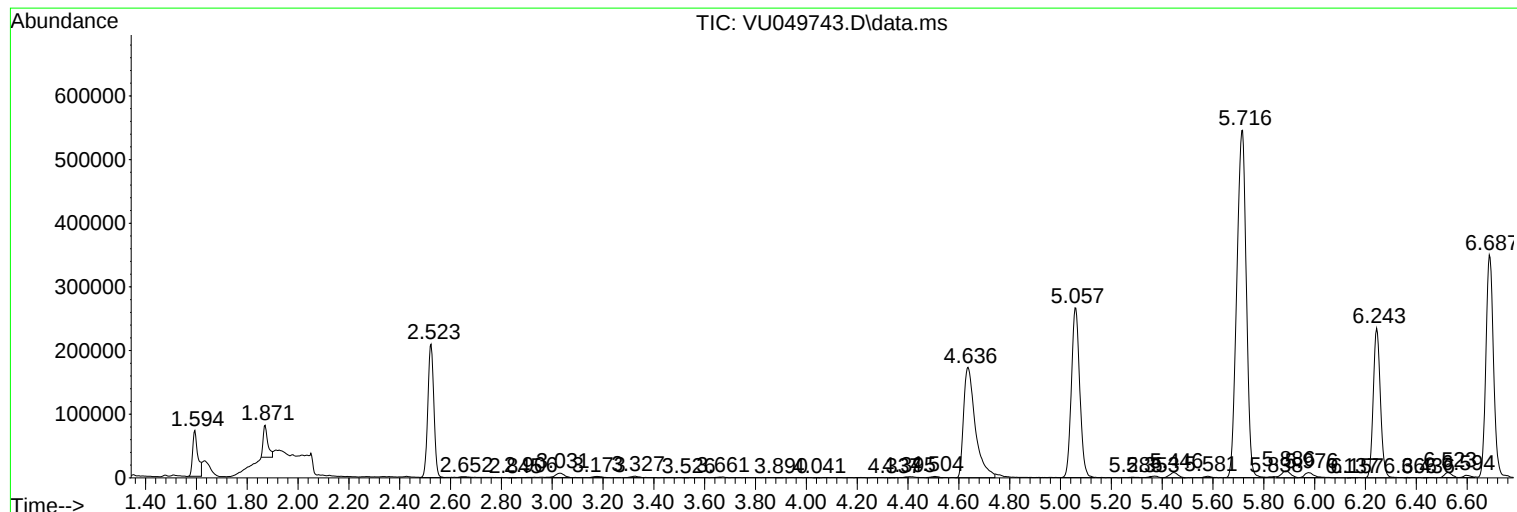
Sum of corrected areas: 10428675

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ALS Vial : 21 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
F5B69ME

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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ALS Vial : 21 Sample Multiplier: 1

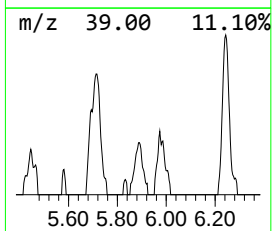
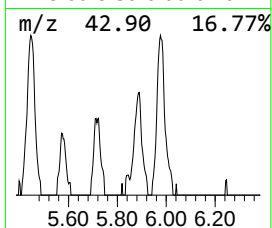
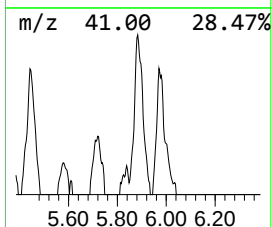
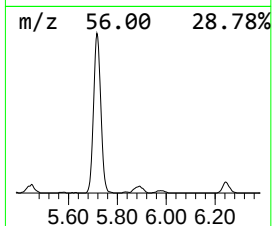
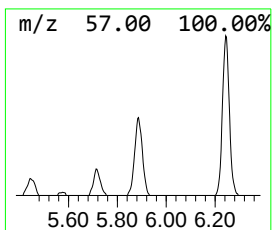
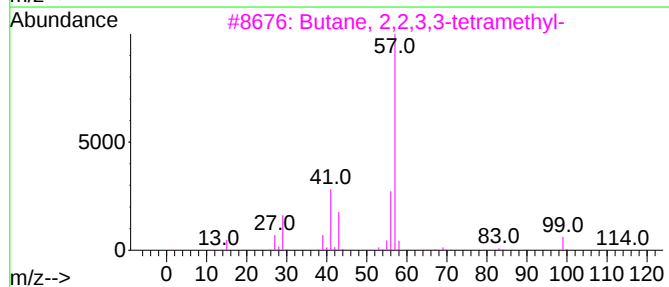
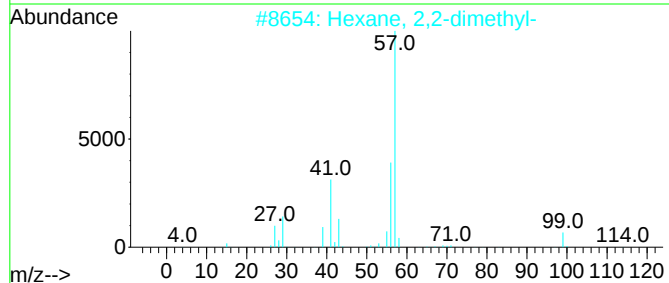
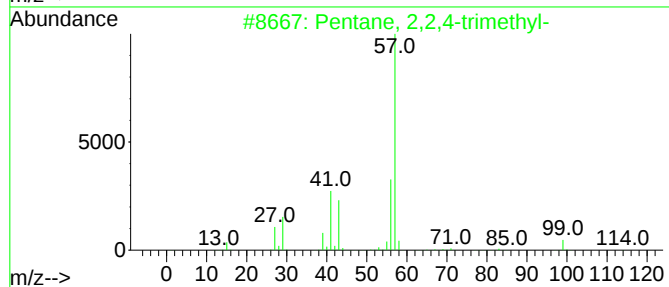
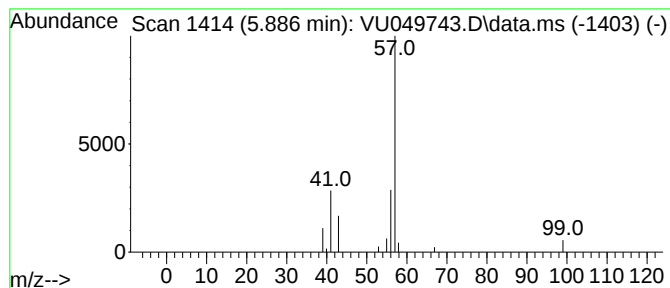
Instrument :
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F5B69ME

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

Peak Number 1 (DEL) Alkane: Straight-Chai... Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.	
5.886	2.80 ug/L	25577	1,4-Difluorobenzene	6.243	
Hit# of 5	Tentative ID	MW	MolForm	CAS#	Qual
1	Pentane, 2,2,4-trimethyl-	114	C8H18	000540-84-1	78
2	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	74
3	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	74
4	Hexane, 2,2-dimethyl-	114	C8H18	000590-73-8	74
5	Butane, 2,2,3,3-tetramethyl-	114	C8H18	000594-82-1	74



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	5.886	2.8	ug/L	25577	1	6.243	457160	50.0