

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041122\
 Data File : VU047937.D
 Acq On : 12 Apr 2022 03:37
 Operator : SY/MD
 Sample : N2293-19ME
 Misc : 6.47g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP7ME

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\SFAMULM032422WMA.M
 Title : VOC Analysis

Signal : TIC: VU047937.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.356	3	5	25	rVB	98842	105701	2.68%	0.753%
2	1.482	39	44	49	rBV3	2465	3167	0.08%	0.023%
3	1.597	72	80	113	rVB	70467	154979	3.93%	1.103%
4	2.540	361	373	386	rBV	207687	361573	9.17%	2.574%
5	2.887	478	481	484	rBV2	515	455	0.01%	0.003%
6	2.961	500	504	511	rBV5	1178	1701	0.04%	0.012%
7	3.144	558	561	564	rVB2	468	327	0.01%	0.002%
8	3.195	571	577	580	rBV3	522	566	0.01%	0.004%
9	3.231	583	588	592	rBV2	514	401	0.01%	0.003%
10	3.253	592	595	602	rVB3	498	509	0.01%	0.004%
11	3.408	635	643	644	rBV	227	286	0.01%	0.002%
12	3.424	644	648	653	rVV3	467	513	0.01%	0.004%
13	3.507	671	674	676	rBV	373	306	0.01%	0.002%
14	3.607	699	705	709	rBV2	324	350	0.01%	0.002%
15	3.951	809	812	819	rVB2	390	470	0.01%	0.003%
16	3.986	819	823	826	rBV2	384	376	0.01%	0.003%
17	4.646	1013	1028	1077	rBV	88763	339939	8.62%	2.420%
18	5.064	1141	1158	1187	rBV	209526	488040	12.37%	3.475%
19	5.292	1220	1229	1231	rBV3	574	705	0.02%	0.005%
20	5.375	1250	1255	1259	rVV3	439	474	0.01%	0.003%
21	5.507	1287	1296	1300	rVB2	303	459	0.01%	0.003%
22	5.719	1341	1362	1375	rBV2	481820	1261611	31.98%	8.982%
23	6.038	1459	1461	1468	rVB3	413	380	0.01%	0.003%
24	6.115	1480	1485	1492	rBV3	299	391	0.01%	0.003%
25	6.247	1510	1526	1554	rBV	520601	1043526	26.45%	7.429%
26	6.404	1572	1575	1582	rVB2	465	357	0.01%	0.003%
27	6.690	1648	1664	1684	rBV	272108	566345	14.36%	4.032%
28	6.800	1696	1698	1699	rBV	554	316	0.01%	0.002%
29	6.809	1699	1701	1706	rVV3	910	702	0.02%	0.005%
30	6.832	1706	1708	1713	rVB3	641	393	0.01%	0.003%
31	6.883	1720	1724	1730	rVB3	296	344	0.01%	0.002%
32	6.967	1746	1750	1757	rBV2	325	299	0.01%	0.002%
33	7.051	1769	1776	1777	rBV	470	388	0.01%	0.003%
34	7.198	1811	1822	1823	rBV4	5005	6486	0.16%	0.046%
35	7.498	1905	1915	1923	rBV6	3625	6885	0.17%	0.049%
36	7.568	1925	1937	1957	rVB	128725	254571	6.45%	1.812%

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 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP7ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

Filtering: 5

Sampling : 1

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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\SFAMULM032422WMA.M
 Title : VOC Analysis

37	7.899	2021	2040	2055	rVV	533647	975467	24.73%	6.945%
38	7.970	2056	2062	2087	rVB2	21376	46758	1.19%	0.333%
39	8.182	2116	2128	2155	rBV2	82768	175102	4.44%	1.247%
40	8.472	2215	2218	2226	rVB3	660	563	0.01%	0.004%
41	8.507	2226	2229	2236	rVB4	525	537	0.01%	0.004%
42	8.546	2236	2241	2244	rBV3	425	275	0.01%	0.002%
43	8.575	2244	2250	2252	rBV4	1302	1185	0.03%	0.008%
44	8.665	2260	2278	2301	rBV	357135	781337	19.81%	5.563%
45	8.864	2337	2340	2346	rVB5	660	488	0.01%	0.003%
46	8.948	2362	2366	2371	rVB4	377	339	0.01%	0.002%
47	9.031	2388	2392	2394	rBV3	554	427	0.01%	0.003%
48	9.369	2491	2497	2499	rVV3	842	700	0.02%	0.005%
49	9.449	2499	2522	2555	rVV2	1390464	3944699	100.00%	28.084%
50	9.575	2558	2561	2570	rVB6	1632	2028	0.05%	0.014%
51	9.697	2590	2599	2611	rBV3	2985	5291	0.13%	0.038%
52	9.832	2637	2641	2648	rBV2	238	304	0.01%	0.002%
53	9.935	2667	2673	2679	rVV3	405	642	0.02%	0.005%
54	9.964	2679	2682	2685	rVV2	347	355	0.01%	0.003%
55	10.073	2713	2716	2720	rVV3	378	289	0.01%	0.002%
56	10.108	2720	2727	2736	rVB5	2032	2907	0.07%	0.021%
57	10.202	2753	2756	2760	rBV2	338	330	0.01%	0.002%
58	10.298	2780	2786	2788	rBV3	300	322	0.01%	0.002%
59	10.481	2840	2843	2845	rBV	393	279	0.01%	0.002%
60	10.665	2890	2900	2911	rVB10	3491	7190	0.18%	0.051%
61	10.767	2915	2932	2947	rBV	447447	734033	18.61%	5.226%
62	10.896	2969	2972	2980	rVB4	1139	1349	0.03%	0.010%
63	10.980	2989	2998	3009	rBV7	1580	3459	0.09%	0.025%
64	11.063	3019	3024	3027	rBV5	584	616	0.02%	0.004%
65	11.105	3032	3037	3041	rBV4	1139	1211	0.03%	0.009%
66	11.282	3088	3092	3093	rBV	656	458	0.01%	0.003%
67	11.366	3116	3118	3121	rBV	478	376	0.01%	0.003%
68	11.417	3127	3134	3141	rBV4	3085	3845	0.10%	0.027%
69	11.472	3141	3151	3159	rVB7	2704	5108	0.13%	0.036%
70	11.584	3176	3186	3190	rBV6	1336	2239	0.06%	0.016%
71	11.610	3190	3194	3197	rVV4	321	271	0.01%	0.002%
72	11.639	3199	3203	3208	rVB5	1011	1006	0.03%	0.007%
73	11.710	3214	3225	3232	rBV9	3066	6102	0.15%	0.043%
74	11.751	3232	3238	3246	rBV8	3934	4978	0.13%	0.035%
75	11.819	3246	3259	3274	rBV	943795	1495717	37.92%	10.649%
76	12.002	3314	3316	3324	rVB6	2869	3156	0.08%	0.022%

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 ALS Vial : 45 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 ETNP7ME

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

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Peak separation: 5

Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
 Title : VOC Analysis

77	12.034	3324	3326	3332	rVB4	644	495	0.01%	0.004%
78	12.198	3358	3377	3394	rBV	620984	1020559	25.87%	7.266%
79	12.382	3432	3434	3437	rBV3	1217	913	0.02%	0.007%
80	12.529	3476	3480	3481	rBV3	1262	1008	0.03%	0.007%
81	12.600	3498	3502	3509	rVB6	979	985	0.02%	0.007%
82	12.668	3518	3523	3531	rVB5	2672	3577	0.09%	0.025%
83	12.777	3549	3557	3561	rBV7	1786	2599	0.07%	0.019%
84	12.841	3570	3577	3584	rVB8	3367	4580	0.12%	0.033%
85	12.928	3592	3604	3609	rBV5	5233	10767	0.27%	0.077%
86	13.050	3637	3642	3652	rVB5	4910	7445	0.19%	0.053%
87	13.137	3661	3669	3678	rVB9	2288	3964	0.10%	0.028%
88	13.256	3701	3706	3709	rBV6	964	1040	0.03%	0.007%
89	13.333	3725	3730	3737	rBV6	3579	5581	0.14%	0.040%
90	13.378	3739	3744	3755	rVB5	8085	11568	0.29%	0.082%
91	13.587	3803	3809	3815	rBV2	6158	7785	0.20%	0.055%
92	13.845	3884	3889	3890	rBV5	2244	1933	0.05%	0.014%
93	14.095	3960	3967	3973	rBV	4097	5735	0.15%	0.041%
94	14.362	4045	4050	4058	rBV7	2980	3621	0.09%	0.026%
95	14.497	4084	4092	4107	rVB7	11331	20037	0.51%	0.143%
96	14.578	4110	4117	4123	rBV6	2969	4533	0.11%	0.032%
97	14.661	4136	4143	4151	rVB6	5618	8348	0.21%	0.059%
98	15.050	4260	4264	4266	rBV5	2589	2302	0.06%	0.016%
99	15.545	4411	4418	4430	rVB3	33854	53429	1.35%	0.380%
100	16.391	4673	4681	4692	rBV3	31053	47200	1.20%	0.336%

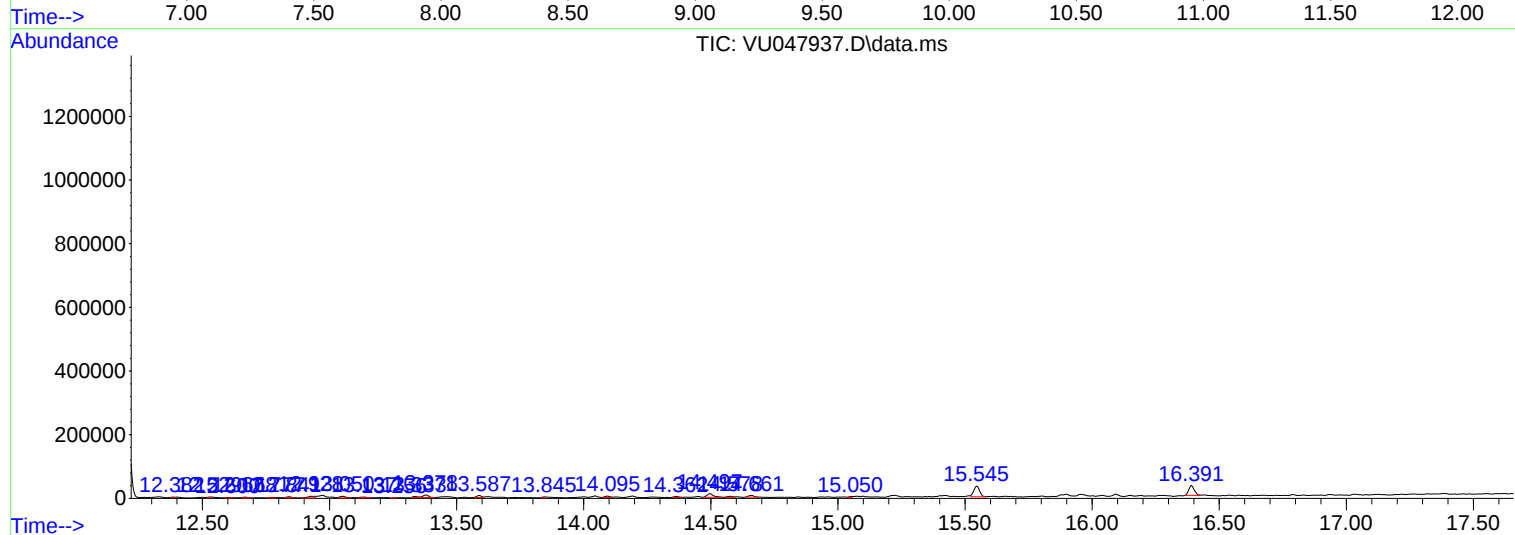
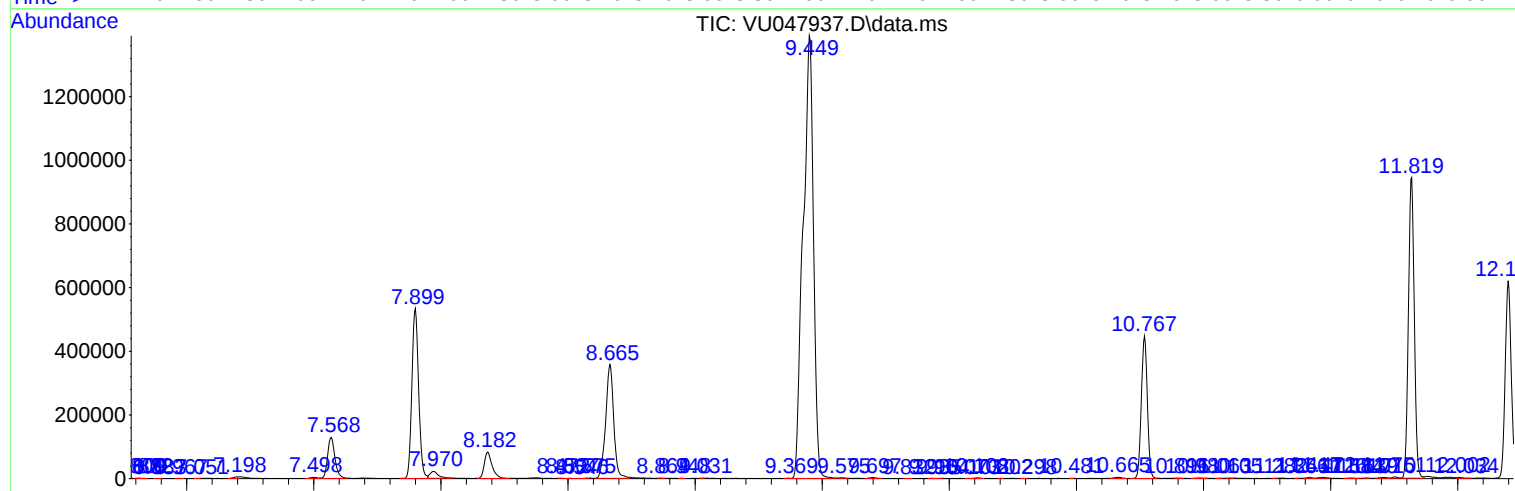
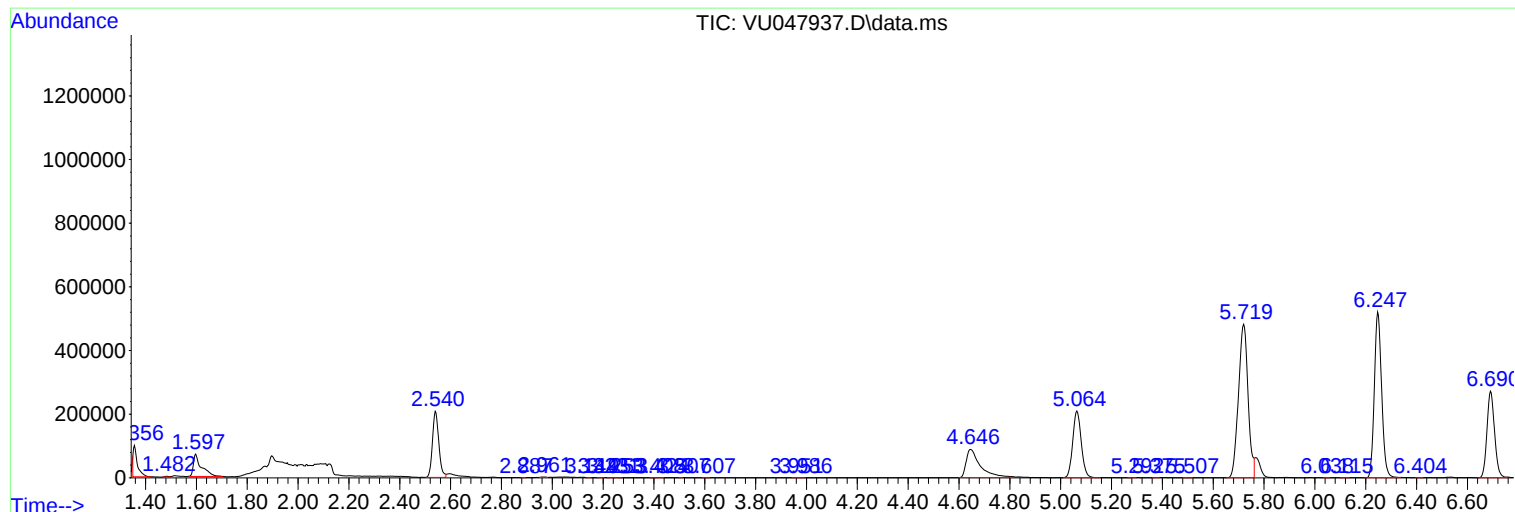
Sum of corrected areas: 14046033

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ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP7ME

Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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



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ALS Vial : 45 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
ETNP7ME

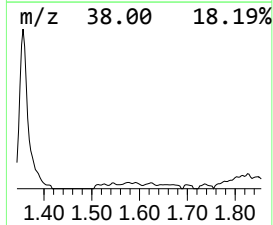
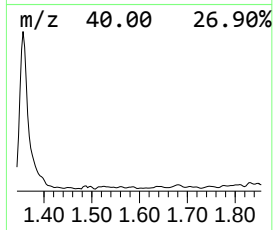
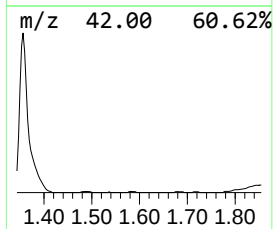
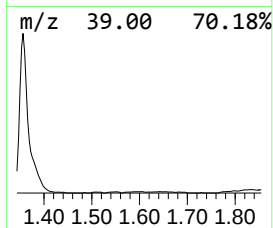
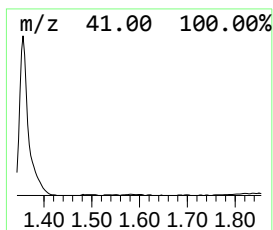
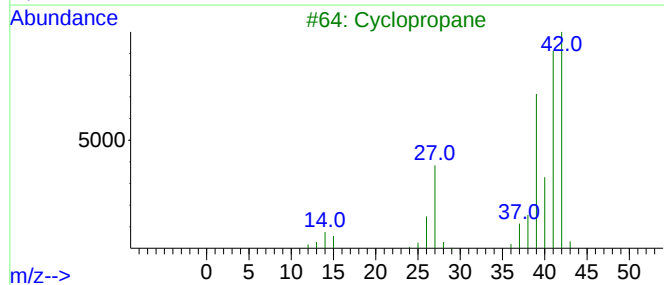
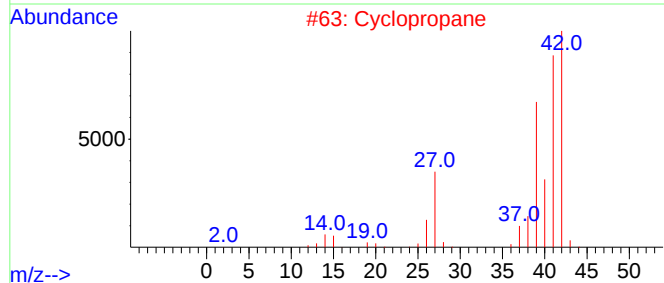
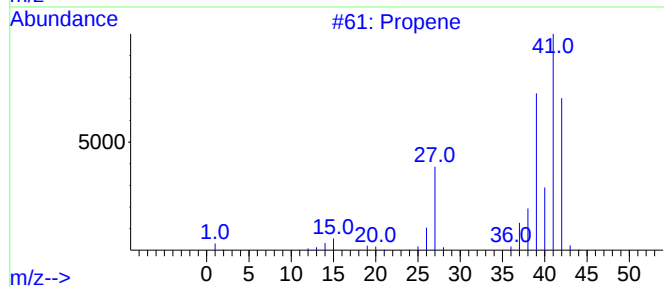
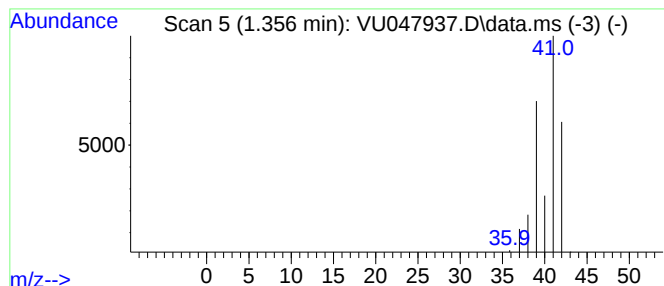
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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.
1.356	5.06 ug/L	105701	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Propene	42	C3H6	000115-07-1	90
2			Cyclopropane	42	C3H6	000075-19-4	78
3			Cyclopropane	42	C3H6	000075-19-4	64
4			Cyclopropene	40	C3H4	002781-85-3	40
5			Propene	42	C3H6	000115-07-1	40



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
(DEL) Alkane: S...	1.356	5.1	ug/L	105701	1	6.247	1043530	50.0