

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041522\
 Data File : VU048097.D
 Acq On : 15 Apr 2022 13:03
 Operator : SY/MD
 Sample : N2373-02ME
 Misc : 5.54g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 5 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFD3ME

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: VU048097.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.597	73	80	108	rVB	30787	69419	7.98%	0.935%
2	1.810	123	146	147	rBV	26570	72406	8.32%	0.976%
3	2.536	361	372	384	rBV	89241	157275	18.07%	2.119%
4	2.851	466	470	473	rBV4	520	420	0.05%	0.006%
5	2.877	476	478	481	rVB3	426	222	0.03%	0.003%
6	3.028	519	525	538	rVB6	2297	4007	0.46%	0.054%
7	3.179	555	572	596	rBV	46888	116891	13.43%	1.575%
8	3.372	628	632	633	rBV2	747	579	0.07%	0.008%
9	3.703	730	735	739	rVV2	290	309	0.04%	0.004%
10	3.739	743	746	750	rVB3	292	223	0.03%	0.003%
11	3.822	769	772	774	rBV	273	211	0.02%	0.003%
12	3.983	817	822	825	rBV2	358	344	0.04%	0.005%
13	4.080	849	852	857	rVB	278	209	0.02%	0.003%
14	4.311	919	924	928	rBV	290	311	0.04%	0.004%
15	4.401	946	952	954	rBV	309	240	0.03%	0.003%
16	4.633	1012	1024	1069	rBV	85298	297296	34.17%	4.006%
17	5.060	1141	1157	1183	rVV	140904	329570	37.88%	4.441%
18	5.160	1186	1188	1192	rVB3	436	254	0.03%	0.003%
19	5.282	1222	1226	1229	rBV2	828	666	0.08%	0.009%
20	5.337	1234	1243	1249	rBV2	2244	3786	0.44%	0.051%
21	5.424	1267	1270	1274	rVB	332	244	0.03%	0.003%
22	5.472	1281	1285	1290	rBV2	220	217	0.02%	0.003%
23	5.546	1301	1308	1312	rBV2	331	473	0.05%	0.006%
24	5.716	1341	1361	1397	rVV2	301529	806950	92.74%	10.873%
25	5.973	1429	1441	1459	rBV4	12878	31423	3.61%	0.423%
26	6.137	1489	1492	1497	rVB2	287	220	0.03%	0.003%
27	6.247	1511	1526	1545	rBV	314450	623201	71.62%	8.397%
28	6.526	1602	1613	1625	rBV7	4791	9419	1.08%	0.127%
29	6.600	1625	1636	1649	rVV3	6459	14078	1.62%	0.190%
30	6.690	1650	1664	1688	rVV	185253	382102	43.91%	5.148%
31	6.970	1748	1751	1753	rBV2	387	227	0.03%	0.003%
32	6.983	1753	1755	1762	rVB3	375	268	0.03%	0.004%
33	7.057	1771	1778	1787	rBV5	825	1635	0.19%	0.022%
34	7.150	1803	1807	1809	rBV2	374	319	0.04%	0.004%
35	7.189	1809	1819	1826	rBV2	9384	19231	2.21%	0.259%
36	7.330	1860	1863	1869	rVB4	671	557	0.06%	0.008%

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Instrument :
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 ClientSampleId :
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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	7.565	1924	1936	1956	rBV	79966	157244	18.07%	2.119%
38	7.636	1956	1958	1962	rVB2	362	243	0.03%	0.003%
39	7.687	1969	1974	1977	rBV3	1601	1664	0.19%	0.022%
40	7.790	1994	2006	2026	rBV4	9401	23201	2.67%	0.313%
41	7.899	2026	2040	2056	rBV	266186	487329	56.01%	6.566%
42	8.063	2089	2091	2096	rVB3	511	379	0.04%	0.005%
43	8.112	2100	2106	2109	rBV2	435	400	0.05%	0.005%
44	8.182	2117	2128	2146	rBV2	51369	112039	12.88%	1.510%
45	8.285	2157	2160	2164	rVB2	361	239	0.03%	0.003%
46	8.304	2164	2166	2169	rBV3	277	237	0.03%	0.003%
47	8.356	2175	2182	2188	rBV7	1025	1453	0.17%	0.020%
48	8.446	2206	2210	2211	rBV	397	251	0.03%	0.003%
49	8.481	2219	2221	2225	rVB2	439	256	0.03%	0.003%
50	8.507	2225	2229	2232	rVB3	316	230	0.03%	0.003%
51	8.530	2232	2236	2239	rBV2	357	341	0.04%	0.005%
52	8.655	2255	2275	2307	rBV	321644	698264	80.25%	9.408%
53	8.800	2314	2320	2332	rVB6	3620	6738	0.77%	0.091%
54	9.041	2390	2395	2398	rBV3	306	328	0.04%	0.004%
55	9.423	2499	2514	2540	rBV	427352	870144	100.00%	11.724%
56	9.636	2575	2580	2589	rBV2	402	579	0.07%	0.008%
57	9.681	2591	2594	2597	rBV	480	413	0.05%	0.006%
58	9.828	2636	2640	2645	rVB2	252	253	0.03%	0.003%
59	9.941	2672	2675	2681	rVV	293	307	0.04%	0.004%
60	10.047	2705	2708	2711	rBV3	354	228	0.03%	0.003%
61	10.211	2755	2759	2765	rVV3	351	376	0.04%	0.005%
62	10.391	2813	2815	2819	rVB2	489	321	0.04%	0.004%
63	10.423	2819	2825	2828	rBV	304	391	0.04%	0.005%
64	10.607	2878	2882	2884	rBV3	308	215	0.02%	0.003%
65	10.632	2885	2890	2892	rBV4	463	416	0.05%	0.006%
66	10.655	2892	2897	2898	rBV5	766	696	0.08%	0.009%
67	10.764	2918	2931	2951	rVV	384805	623755	71.68%	8.404%
68	10.835	2951	2953	2957	rVB3	406	223	0.03%	0.003%
69	10.861	2958	2961	2964	rBV3	251	227	0.03%	0.003%
70	10.896	2967	2972	2978	rVB2	926	907	0.10%	0.012%
71	10.983	2996	2999	3005	rVB2	270	282	0.03%	0.004%
72	11.057	3018	3022	3024	rVB2	343	260	0.03%	0.004%
73	11.082	3024	3030	3032	rBV2	465	411	0.05%	0.006%
74	11.118	3035	3041	3047	rVB5	1380	1957	0.22%	0.026%
75	11.378	3117	3122	3123	rBV2	510	464	0.05%	0.006%
76	11.465	3140	3149	3153	rBV5	1293	1978	0.23%	0.027%

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Instrument :
 MSVOA_U
 ClientSampleId :
 BFFD3ME

Integration Parameters: LSCINT.P

Integrator: RTE

Smoothing : OFF

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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	11.520	3161	3166	3167	rBV2	370	257	0.03%	0.003%
78	11.578	3181	3184	3189	rBV3	485	465	0.05%	0.006%
79	11.697	3218	3221	3229	rVB4	759	674	0.08%	0.009%
80	11.751	3229	3238	3245	rBV2	1854	2597	0.30%	0.035%
81	11.816	3245	3258	3278	rBV	517740	861034	98.95%	11.601%
82	11.918	3285	3290	3296	rBV5	2662	3067	0.35%	0.041%
83	11.970	3304	3306	3308	rBV3	465	296	0.03%	0.004%
84	12.050	3329	3331	3336	rBV2	241	227	0.03%	0.003%
85	12.108	3347	3349	3354	rBV	394	314	0.04%	0.004%
86	12.198	3361	3377	3398	rVV	346265	580396	66.70%	7.820%
87	12.330	3415	3418	3422	rBV4	284	213	0.02%	0.003%
88	12.410	3438	3443	3447	rBV	487	585	0.07%	0.008%
89	12.603	3499	3503	3505	rBV2	401	349	0.04%	0.005%
90	12.735	3541	3544	3546	rBV2	340	256	0.03%	0.003%
91	12.770	3549	3555	3564	rVV2	1207	2091	0.24%	0.028%
92	12.922	3598	3602	3604	rBV2	368	296	0.03%	0.004%
93	13.227	3694	3697	3698	rBV2	610	311	0.04%	0.004%
94	13.848	3881	3890	3901	rBV4	9580	14641	1.68%	0.197%
95	14.089	3960	3965	3978	rBV	2232	3997	0.46%	0.054%
96	14.336	4034	4042	4053	rVB6	3165	5194	0.60%	0.070%
97	14.577	4108	4117	4127	rVB2	1342	2220	0.26%	0.030%
98	15.012	4247	4252	4253	rBV2	605	543	0.06%	0.007%
99	15.249	4323	4326	4329	rBV2	688	668	0.08%	0.009%
100	15.500	4402	4404	4405	rBV	624	293	0.03%	0.004%

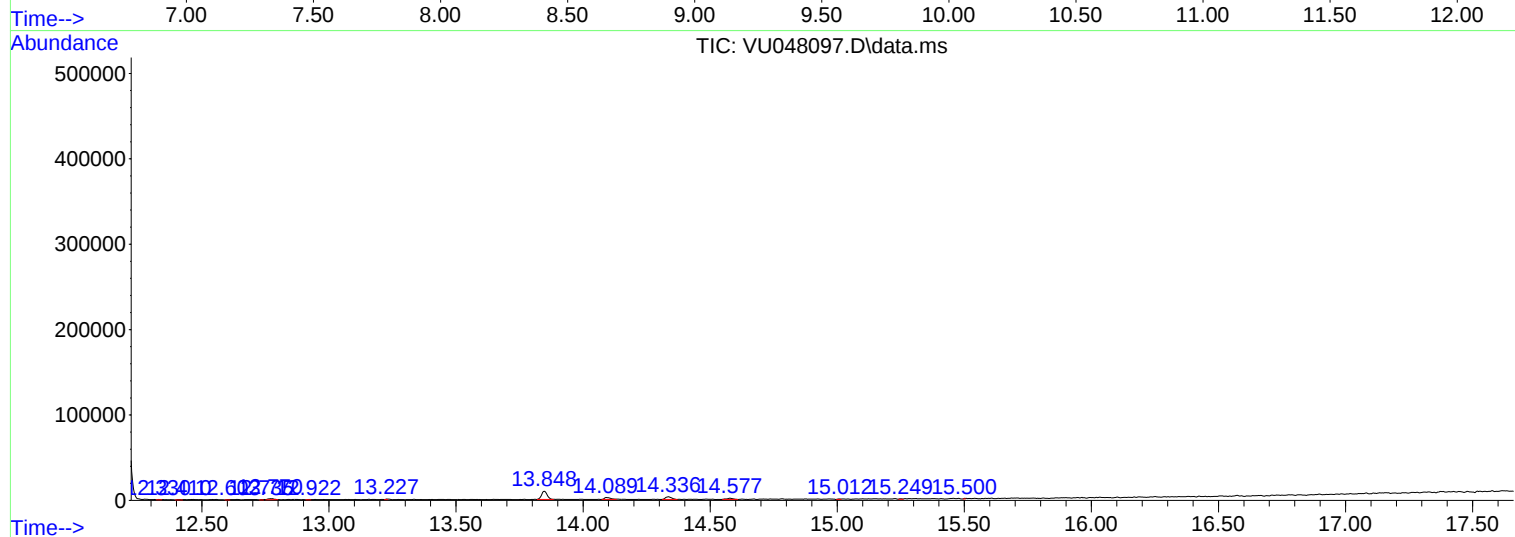
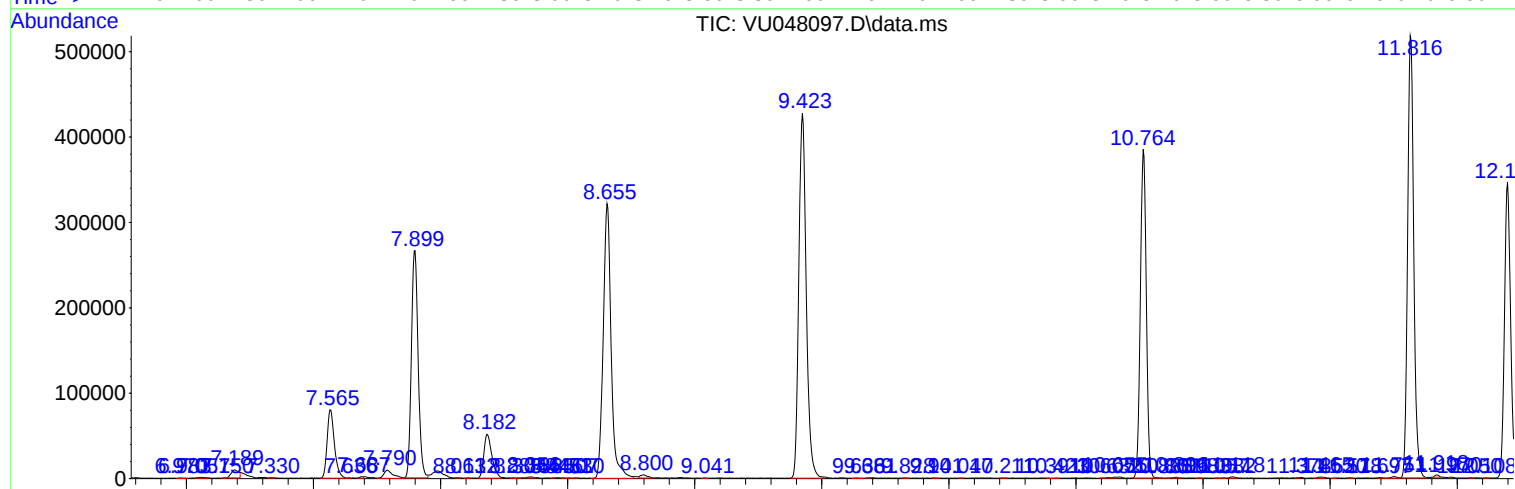
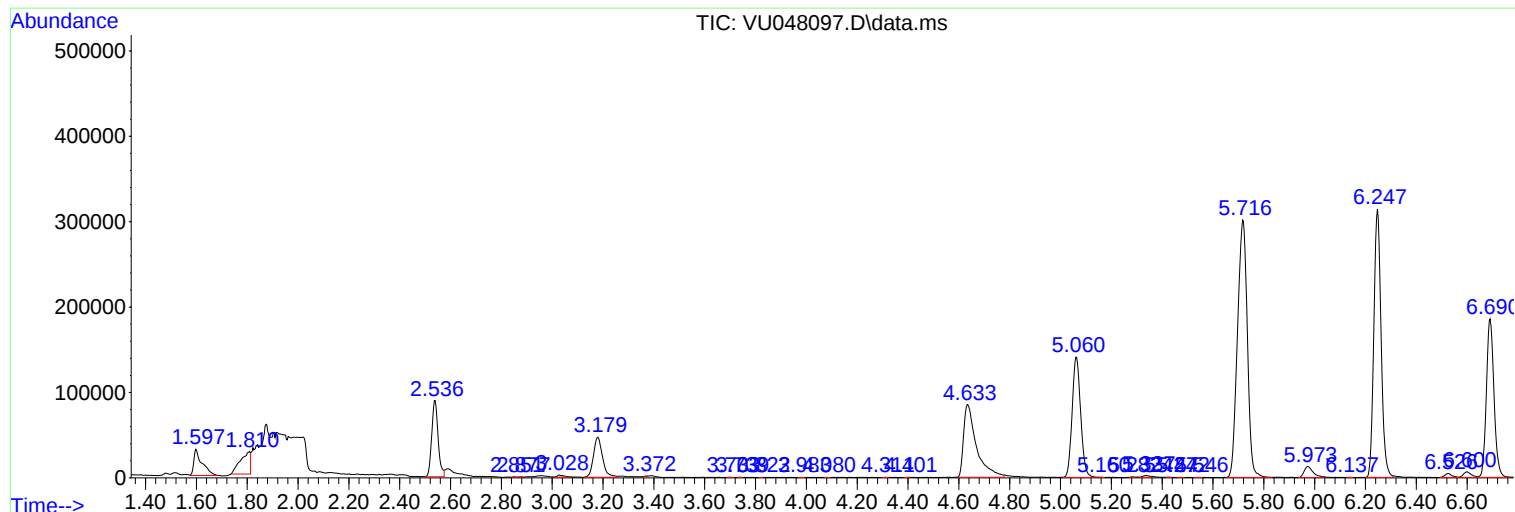
Sum of corrected areas: 7421825

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ALS Vial : 5 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BFFD3ME

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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Instrument :
MSVOA_U
ClientSampleId :
BFFD3ME

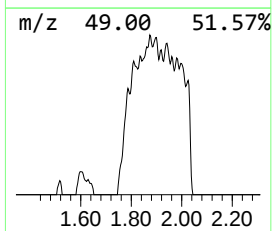
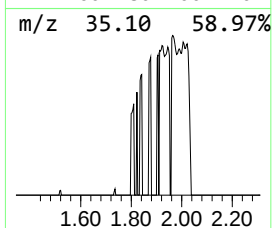
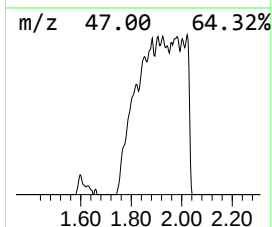
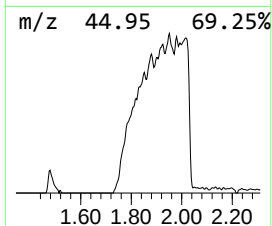
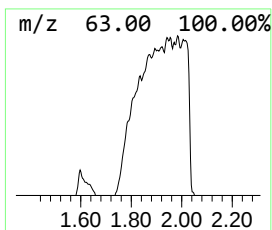
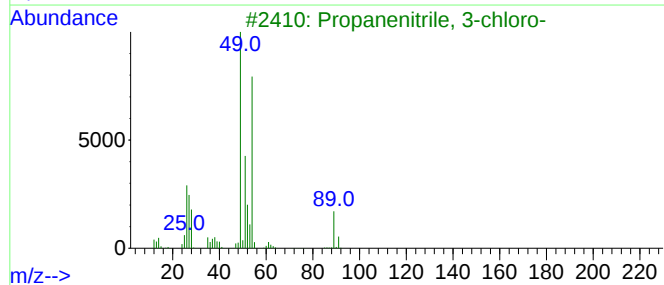
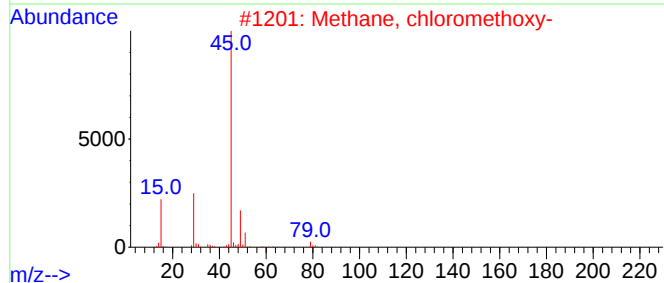
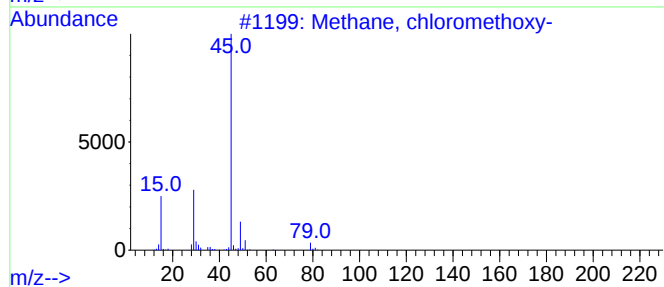
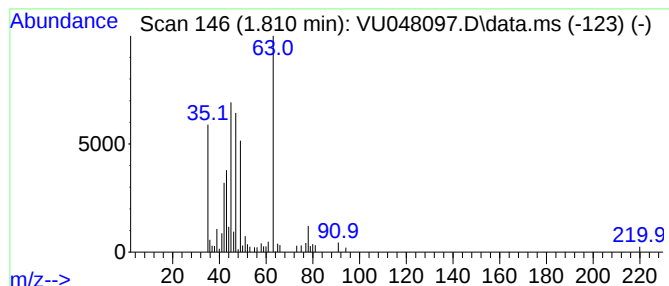
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.810	5.81 ug/L	72406	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	9
2			Methane, chloromethoxy-	80	C2H5ClO	000107-30-2	9
3			Propanenitrile, 3-chloro-	89	C3H4ClN	000542-76-7	9
4			2-Chloropropionyl chloride	126	C3H4Cl2O	007623-09-8	9
5			Silane, bis(fluoromethyl)dimethyl-	124	C4H10F2Si	065864-63-3	9



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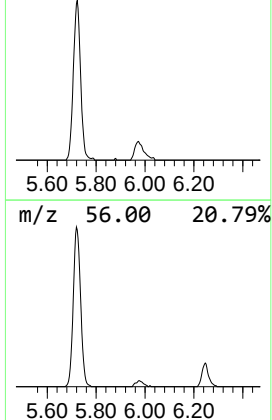
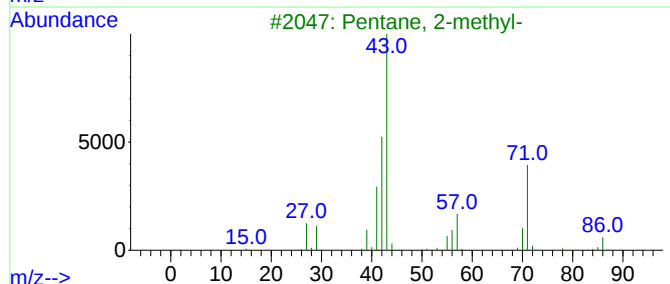
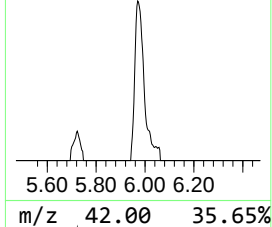
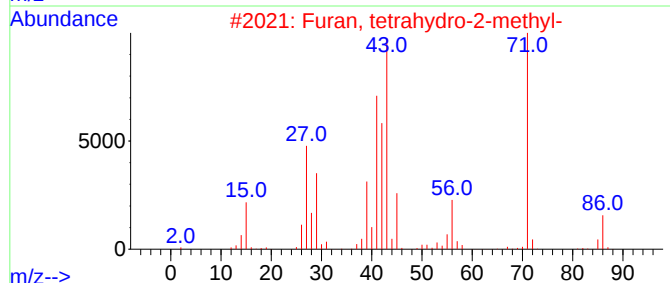
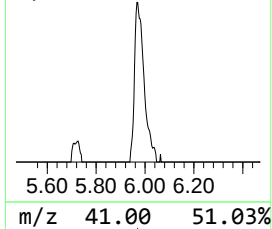
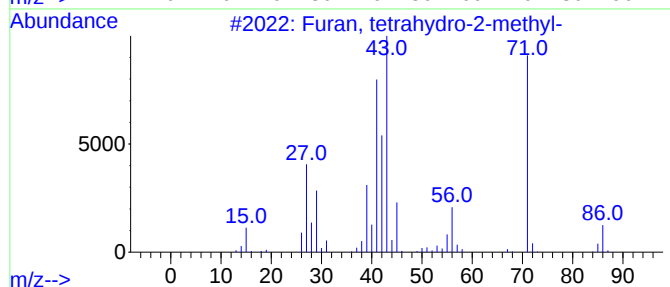
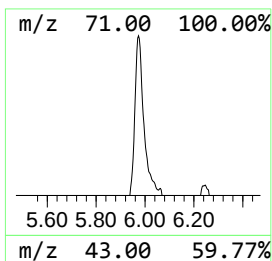
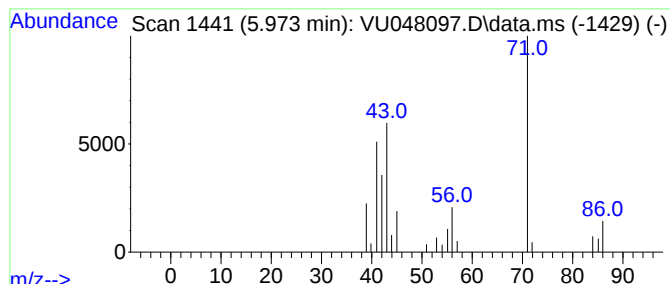
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 3 Furan, tetrahydro-2-methyl- Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.973	2.52 ug/L	31423	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	87
2			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	87
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	59
4			Tetrahydrofurfuryl chloride	120	C5H9ClO	003003-84-7	50
5			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	47



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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	--Internal Standard--			
					#	RT	Resp	Conc
unknown-01	1.810	5.8	ug/L	72406	1	6.247	623201	50.0
Furan, tetrahyd...	5.973	2.5	ug/L	31423	1	6.247	623201	50.0