

Data Path : Z:\voasrv\HPCHEM1\MSVOA_U\Data\VU041422\
 Data File : VU048079.D
 Acq On : 14 Apr 2022 23:26
 Operator : SY/MD
 Sample : N2374-04ME
 Misc : 5.32g/5.0mL/100uL/5.0mL/MSVOA_U/MEOH
 ALS Vial : 38 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BFFD9ME

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: VU048079.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	106	rVB	80236	152882	11.53%	1.617%
2	1.793	120	141	142	rBV5	20529	53302	4.02%	0.564%
3	1.871	161	165	171	rBV	37931	46391	3.50%	0.491%
4	2.346	311	313	317	rBV6	1171	1058	0.08%	0.011%
5	2.539	361	373	386	rBV	209128	364177	27.46%	3.853%
6	2.829	461	463	468	rVB	308	199	0.02%	0.002%
7	2.919	481	491	497	rBV6	916	1699	0.13%	0.018%
8	2.951	498	501	502	rBV3	506	301	0.02%	0.003%
9	3.038	519	528	535	rBV5	1485	2625	0.20%	0.028%
10	3.176	559	571	573	rBV4	5506	7131	0.54%	0.075%
11	3.253	593	595	600	rVB3	633	596	0.04%	0.006%
12	3.288	600	606	609	rBV	616	619	0.05%	0.007%
13	3.507	671	674	676	rBV	313	197	0.01%	0.002%
14	3.584	696	698	702	rBV3	273	203	0.02%	0.002%
15	3.616	706	708	713	rBV2	203	220	0.02%	0.002%
16	3.739	742	746	749	rVB3	277	260	0.02%	0.003%
17	3.896	792	795	802	rVB3	349	424	0.03%	0.004%
18	3.935	802	807	809	rBV2	236	216	0.02%	0.002%
19	3.993	819	825	830	rBV3	360	427	0.03%	0.005%
20	4.227	893	898	903	rBV2	154	211	0.02%	0.002%
21	4.282	910	915	917	rBV2	265	224	0.02%	0.002%
22	4.475	969	975	977	rBV2	294	241	0.02%	0.003%
23	4.632	1010	1024	1077	rBV	119727	393682	29.68%	4.165%
24	5.063	1141	1158	1185	rBV	232401	534616	40.31%	5.656%
25	5.288	1223	1228	1231	rBV3	493	564	0.04%	0.006%
26	5.337	1235	1243	1250	rVV4	1401	2382	0.18%	0.025%
27	5.494	1288	1292	1296	rBV	343	304	0.02%	0.003%
28	5.719	1341	1362	1385	rBV2	509287	1326364	100.00%	14.032%
29	5.976	1429	1442	1459	rBV3	13207	32391	2.44%	0.343%
30	6.247	1510	1526	1547	rBV	183313	358653	27.04%	3.794%
31	6.362	1559	1562	1568	rVB3	567	580	0.04%	0.006%
32	6.523	1602	1612	1623	rBV7	5582	10806	0.81%	0.114%
33	6.597	1626	1635	1649	rVV4	6009	13300	1.00%	0.141%
34	6.690	1649	1664	1686	rVB	303916	611290	46.09%	6.467%
35	6.793	1693	1696	1701	rBV3	561	527	0.04%	0.006%
36	6.938	1738	1741	1746	rBV3	370	299	0.02%	0.003%

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Integrator: RTE

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Peak Location: TOP

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

37	7.038	1768	1772	1773	rBV	804	554	0.04%	0.006%
38	7.185	1807	1818	1847	rVB6	9181	30229	2.28%	0.320%
39	7.311	1851	1857	1863	rVV5	702	1029	0.08%	0.011%
40	7.337	1863	1865	1868	rVB3	549	284	0.02%	0.003%
41	7.568	1924	1937	1956	rBV	138867	268658	20.26%	2.842%
42	7.690	1968	1975	1993	rVB4	2825	5993	0.45%	0.063%
43	7.812	2008	2013	2016	rBV2	548	584	0.04%	0.006%
44	7.899	2025	2040	2056	rBV	572209	1020941	76.97%	10.801%
45	8.182	2116	2128	2146	rBV	94288	187861	14.16%	1.987%
46	8.320	2168	2171	2174	rBV3	264	253	0.02%	0.003%
47	8.349	2174	2180	2192	rVB6	1912	3008	0.23%	0.032%
48	8.398	2192	2195	2199	rBV3	235	200	0.02%	0.002%
49	8.475	2216	2219	2227	rVB3	600	667	0.05%	0.007%
50	8.652	2256	2274	2301	rBV	447069	902971	68.08%	9.553%
51	8.796	2311	2319	2330	rVB5	4679	9178	0.69%	0.097%
52	8.938	2361	2363	2369	rVB3	333	253	0.02%	0.003%
53	9.282	2467	2470	2477	rVB3	224	215	0.02%	0.002%
54	9.423	2500	2514	2539	rBV	260012	482982	36.41%	5.110%
55	9.574	2557	2561	2564	rBV2	472	454	0.03%	0.005%
56	9.587	2564	2565	2571	rVB2	546	224	0.02%	0.002%
57	9.684	2590	2595	2596	rBV	480	321	0.02%	0.003%
58	9.700	2596	2600	2608	rVB4	731	882	0.07%	0.009%
59	9.787	2620	2627	2629	rVV3	240	301	0.02%	0.003%
60	9.803	2629	2632	2636	rVB2	309	224	0.02%	0.002%
61	9.951	2674	2678	2682	rBV	187	207	0.02%	0.002%
62	10.005	2691	2695	2700	rBV2	238	244	0.02%	0.003%
63	10.034	2700	2704	2707	rBV2	334	264	0.02%	0.003%
64	10.099	2720	2724	2729	rBV3	512	528	0.04%	0.006%
65	10.150	2737	2740	2743	rVB	476	296	0.02%	0.003%
66	10.176	2743	2748	2751	rBV2	378	433	0.03%	0.005%
67	10.272	2775	2778	2783	rVB3	273	261	0.02%	0.003%
68	10.295	2783	2785	2791	rBV2	242	198	0.01%	0.002%
69	10.468	2830	2839	2847	rBV3	7528	11937	0.90%	0.126%
70	10.549	2861	2864	2865	rBV2	504	325	0.02%	0.003%
71	10.616	2877	2885	2887	rBV4	1469	1758	0.13%	0.019%
72	10.671	2892	2902	2912	rVB7	3621	7388	0.56%	0.078%
73	10.764	2917	2931	2949	rBV	567865	906886	68.37%	9.594%
74	10.835	2951	2953	2956	rVB2	990	470	0.04%	0.005%
75	10.877	2956	2966	2967	rBV5	1226	1525	0.11%	0.016%
76	11.015	3005	3009	3013	rVB4	305	290	0.02%	0.003%

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Integrator: RTE

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

77	11.115	3029	3040	3048	rBV6	4685	7947	0.60%	0.084%
78	11.208	3063	3069	3073	rVB2	579	658	0.05%	0.007%
79	11.311	3094	3101	3110	rBV4	1401	2033	0.15%	0.022%
80	11.378	3114	3122	3128	rVV3	1093	1660	0.13%	0.018%
81	11.417	3130	3134	3139	rVV5	1004	1300	0.10%	0.014%
82	11.462	3139	3148	3161	rVB5	2194	4912	0.37%	0.052%
83	11.578	3178	3184	3187	rBV5	761	873	0.07%	0.009%
84	11.623	3195	3198	3199	rBV2	334	212	0.02%	0.002%
85	11.700	3215	3222	3229	rVB4	2007	2703	0.20%	0.029%
86	11.748	3229	3237	3245	rBV6	5709	7686	0.58%	0.081%
87	11.815	3246	3258	3276	rBV	336300	538573	40.61%	5.698%
88	11.944	3292	3298	3303	rBV5	1497	2227	0.17%	0.024%
89	11.976	3303	3308	3318	rVB5	2862	4012	0.30%	0.042%
90	12.198	3362	3377	3400	rBV	671412	1095688	82.61%	11.592%
91	12.475	3458	3463	3464	rBV2	376	270	0.02%	0.003%
92	12.671	3521	3524	3530	rBV3	444	565	0.04%	0.006%
93	12.815	3564	3569	3572	rBV3	530	527	0.04%	0.006%
94	13.330	3726	3729	3732	rBV	332	239	0.02%	0.003%
95	13.851	3885	3891	3899	rBV5	1144	1743	0.13%	0.018%
96	14.571	4112	4115	4118	rBV3	645	385	0.03%	0.004%
97	14.780	4177	4180	4182	rBV	338	227	0.02%	0.002%
98	15.240	4320	4323	4325	rBV3	559	395	0.03%	0.004%
99	15.404	4368	4374	4385	rVB6	4094	5170	0.39%	0.055%
100	15.561	4418	4423	4428	rBV5	1251	1520	0.11%	0.016%

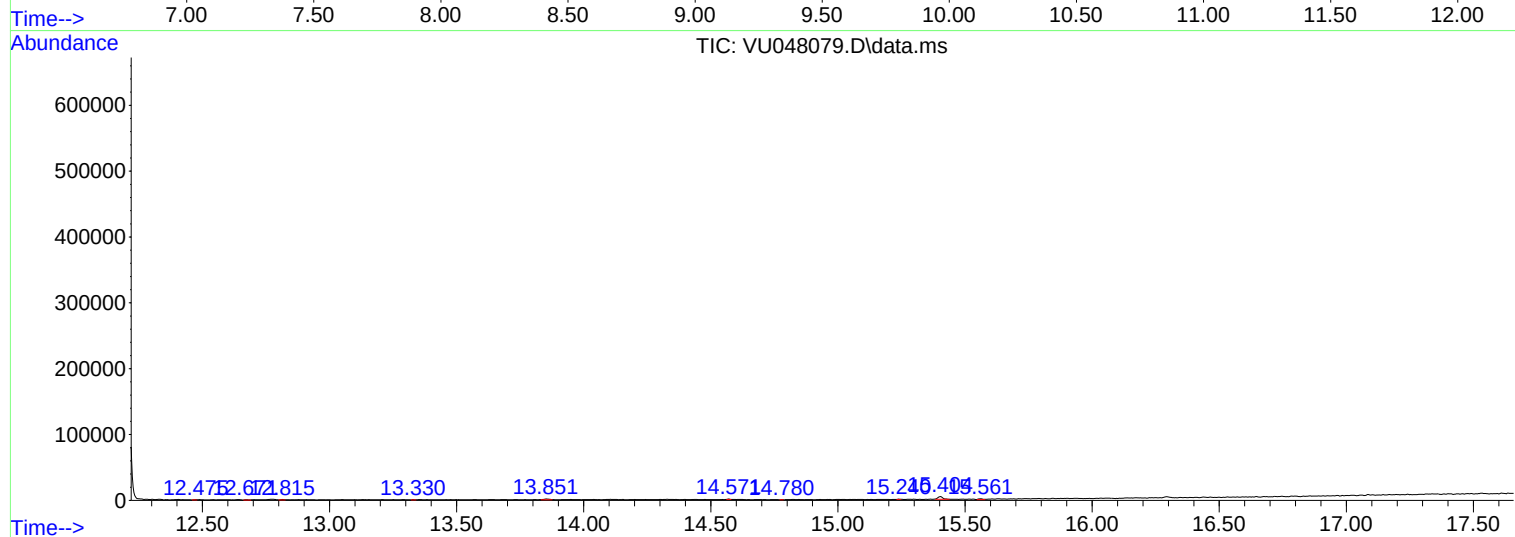
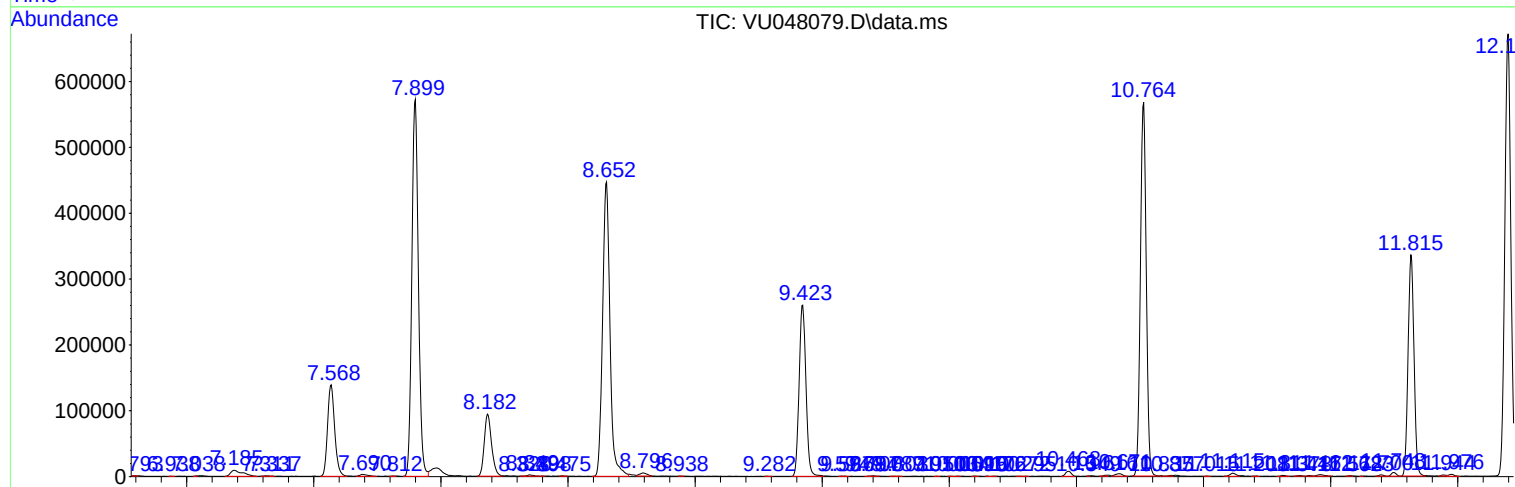
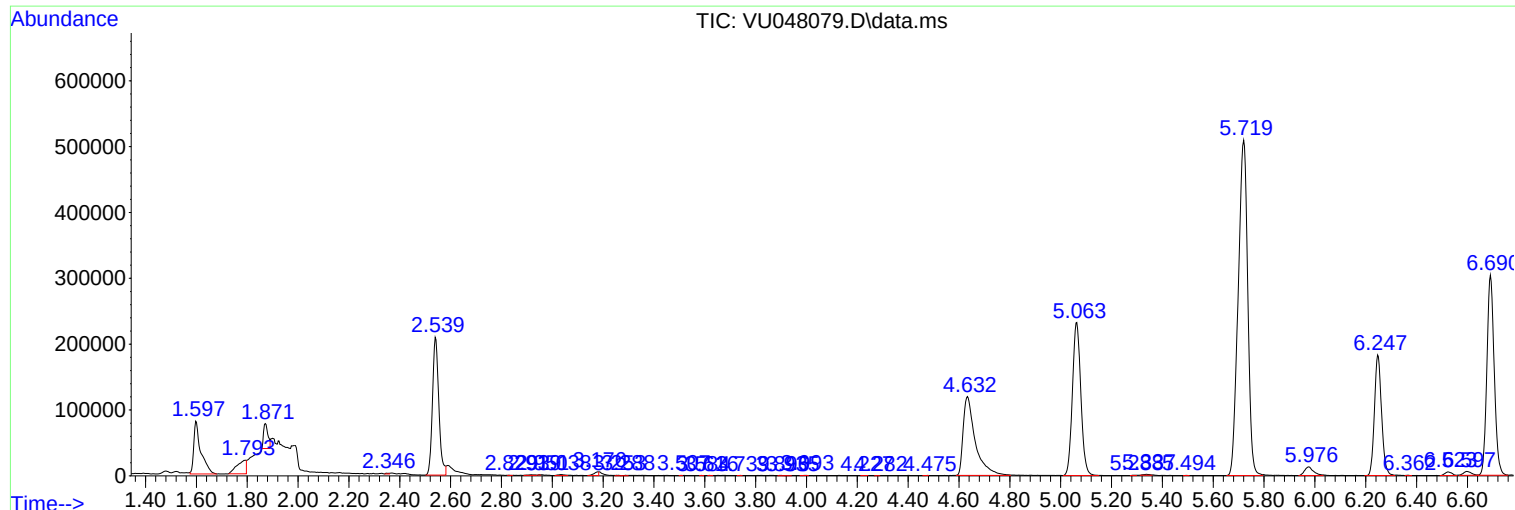
Sum of corrected areas: 9452162

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ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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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



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ALS Vial : 38 Sample Multiplier: 1

Instrument :
MSVOA_U
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BFFD9ME

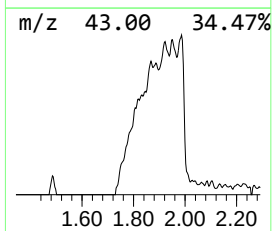
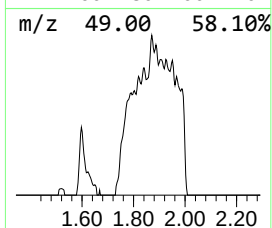
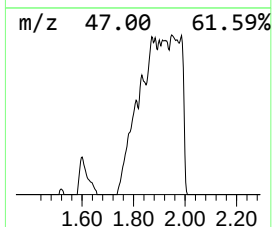
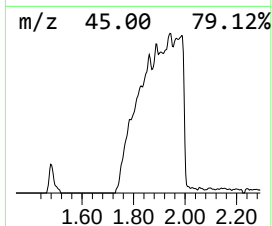
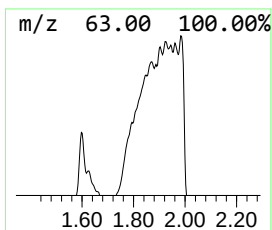
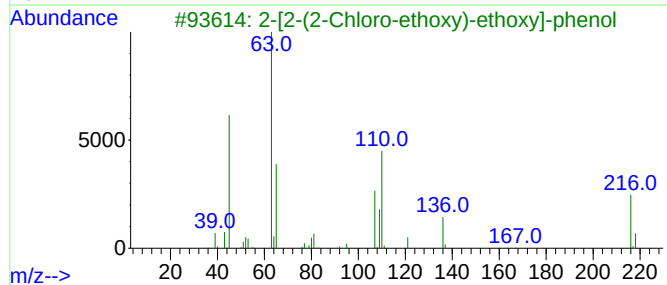
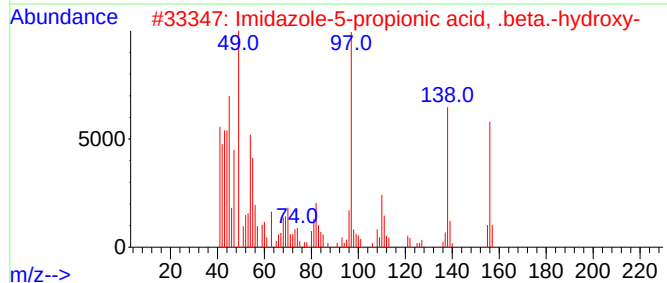
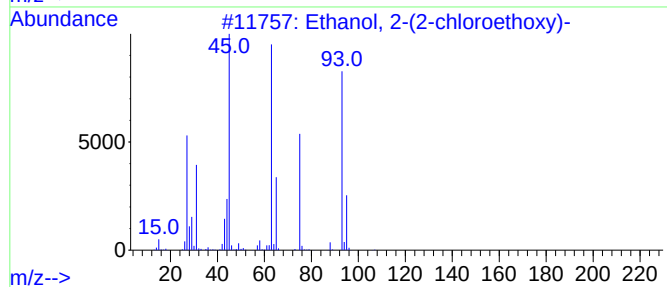
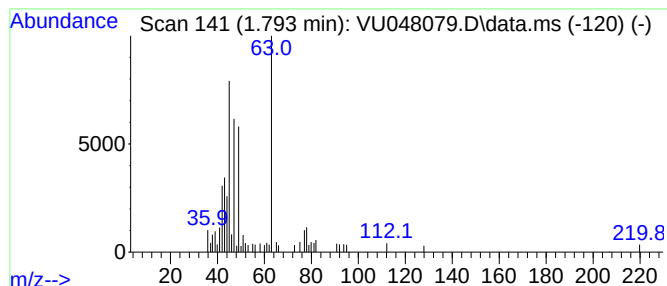
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 unknown-01 Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.793	7.43 ug/L	53302	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Ethanol, 2-(2-chloroethoxy)-	124	C4H9ClO2	000628-89-7	33
2			Imidazole-5-propionic acid, .bet...	156	C6H8N2O3	1000129-47-8	10
3			2-[2-(2-Chloro-ethoxy)-ethoxy]-p...	216	C10H13ClO3	1000317-46-1	9
4			Chloromethyl thiocyanate	107	C2H2ClNS	003268-79-9	9
5			Methanesulfinothioic acid, S-1-p...	138	C4H10OS2	1000322-32-0	9



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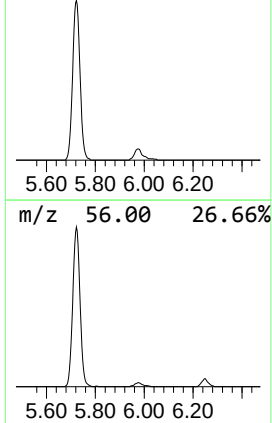
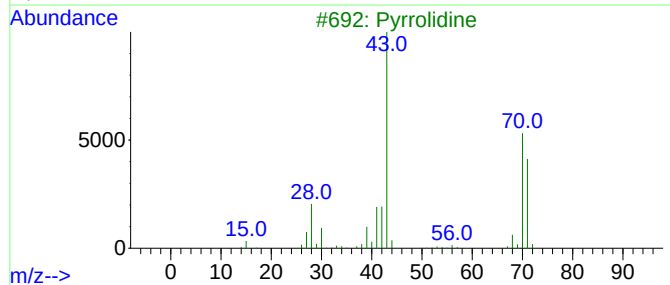
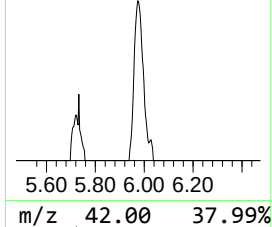
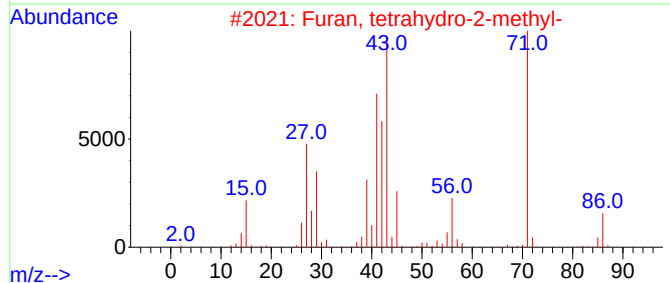
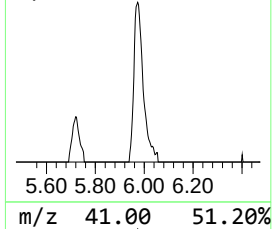
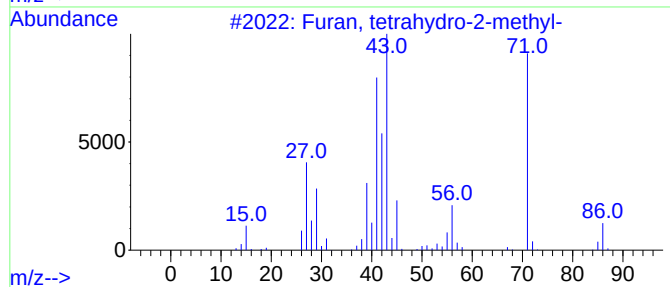
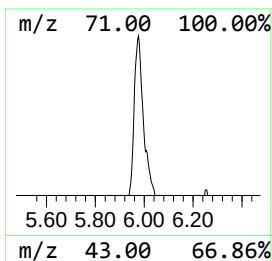
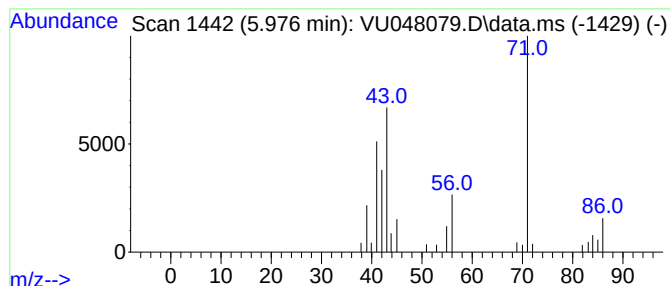
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_U\Method\SFAMULM032422WMA.M
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
5.976	4.52 ug/L	32391	1,4-Difluorobenzene	6.247

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	80
2			Furan, tetrahydro-2-methyl-	86	C5H10O	000096-47-9	72
3			Pyrrolidine	71	C4H9N	000123-75-1	50
4			trans-3-Penten-2-ol	86	C5H10O	003899-34-1	50
5			Tetrahydrofurfuryl chloride	120	C5H9ClO	003003-84-7	47



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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	1.793	7.4	ug/L	53302	1	6.247	358653	50.0
Furan, tetrahyd...	5.976	4.5	ug/L	32391	1	6.247	358653	50.0