

Data Path : Z:\voasrv\HPCHEM1\MSVOA_X\Data\VX081722\
 Data File : VX030669.D
 Acq On : 17 Aug 2022 18:45
 Operator : JC/MD
 Sample : N4221-01ME
 Misc : 5.01g/5mL/100uL/5.00mL/MSVOA_X/MEOH
 ALS Vial : 18 Sample Multiplier: 1

Instrument :
 MSVOA_X
 ClientSampleId :
 C0KP2ME

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_X\Method\SFAMXML080422WMA.M
 Title : VOC Analysis

Signal : TIC: VX030669.D\data.ms

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	1.258	23	28	41	rBV2	13345	34907	3.58%	0.494%
2	1.368	42	46	56	rVB	108374	144543	14.83%	2.045%
3	1.654	90	93	99	rVB	35355	44844	4.60%	0.634%
4	2.276	189	195	208	rVB	223941	359882	36.92%	5.092%
5	2.587	242	246	250	rVB2	520	789	0.08%	0.011%
6	2.709	264	266	268	rBV3	624	707	0.07%	0.010%
7	2.776	272	277	284	rVB3	6733	13755	1.41%	0.195%
8	2.880	290	294	296	rBV2	636	963	0.10%	0.014%
9	2.947	297	305	320	rVV	15345	42774	4.39%	0.605%
10	3.276	356	359	362	rBV	485	511	0.05%	0.007%
11	3.306	362	364	367	rVB2	530	520	0.05%	0.007%
12	3.398	377	379	380	rBV	585	404	0.04%	0.006%
13	3.416	380	382	385	rVB3	674	704	0.07%	0.010%
14	3.587	408	410	412	rVV3	608	612	0.06%	0.009%
15	3.611	412	414	417	rVB2	508	428	0.04%	0.006%
16	3.709	428	430	433	rVB	545	482	0.05%	0.007%
17	3.812	445	447	453	rBV4	404	711	0.07%	0.010%
18	3.898	458	461	463	rVB2	494	540	0.06%	0.008%
19	3.934	466	467	470	rBV2	355	404	0.04%	0.006%
20	4.117	495	497	500	rVB3	417	540	0.06%	0.008%
21	4.166	503	505	508	rVB	458	408	0.04%	0.006%
22	4.251	518	519	523	rVB2	491	517	0.05%	0.007%
23	4.501	549	560	583	rBV2	49273	207895	21.33%	2.941%
24	4.916	626	628	631	rVB3	528	542	0.06%	0.008%
25	5.068	640	653	671	rBV	118732	383867	39.38%	5.431%
26	5.294	687	690	693	rVB2	473	593	0.06%	0.008%
27	5.385	702	705	707	rBV2	656	930	0.10%	0.013%
28	5.483	716	721	722	rBV	424	475	0.05%	0.007%
29	5.550	728	732	738	rVV4	1200	2775	0.28%	0.039%
30	5.971	788	801	814	rBV2	347125	974660	100.00%	13.790%
31	6.080	817	819	821	rBV2	555	414	0.04%	0.006%
32	6.367	859	866	877	rBV4	8231	24094	2.47%	0.341%
33	6.623	906	908	910	rBV	426	388	0.04%	0.005%
34	6.763	922	931	944	rVV	178350	425437	43.65%	6.019%
35	6.964	960	964	965	rBV2	760	939	0.10%	0.013%
36	6.989	965	968	970	rBV2	426	558	0.06%	0.008%

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Integrator: RTE

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37	7.129	981	991	1000	rBV5	84739	204619	20.99%	2.895%
38	7.312	1012	1021	1034	rVB	193970	424902	43.59%	6.012%
39	7.458	1043	1045	1048	rBV2	427	450	0.05%	0.006%
40	7.489	1048	1050	1056	rVB4	917	1095	0.11%	0.015%
41	7.635	1071	1074	1077	rBV2	440	728	0.07%	0.010%
42	7.708	1082	1086	1088	rBV3	721	1001	0.10%	0.014%
43	7.781	1095	1098	1099	rBV2	368	394	0.04%	0.006%
44	7.860	1110	1111	1114	rVB	796	414	0.04%	0.006%
45	7.964	1120	1128	1136	rVB10	4409	11266	1.16%	0.159%
46	8.031	1138	1139	1141	rBV2	437	428	0.04%	0.006%
47	8.056	1141	1143	1145	rBV2	833	812	0.08%	0.011%
48	8.104	1149	1151	1154	rVB2	931	882	0.09%	0.012%
49	8.251	1170	1175	1177	rBV2	993	1322	0.14%	0.019%
50	8.330	1181	1188	1198	rBV	122140	200624	20.58%	2.838%
51	8.488	1209	1214	1215	rBV2	770	1211	0.12%	0.017%
52	8.519	1217	1219	1221	rVB	575	465	0.05%	0.007%
53	8.653	1231	1241	1253	rBV	484671	776667	79.69%	10.988%
54	8.757	1254	1258	1269	rVB3	6884	15444	1.58%	0.219%
55	8.860	1273	1275	1281	rVB4	587	990	0.10%	0.014%
56	8.952	1285	1290	1301	rBV	82422	132666	13.61%	1.877%
57	9.116	1313	1317	1322	rBV5	2146	3674	0.38%	0.052%
58	9.214	1330	1333	1335	rVB2	416	397	0.04%	0.006%
59	9.275	1337	1343	1351	rVB	109395	161554	16.58%	2.286%
60	9.403	1357	1364	1376	rBV	216941	415367	42.62%	5.877%
61	9.537	1382	1386	1393	rVB	5349	8747	0.90%	0.124%
62	9.720	1413	1416	1424	rVB7	4302	7608	0.78%	0.108%
63	9.982	1457	1459	1461	rBV	678	552	0.06%	0.008%
64	10.055	1465	1471	1484	rVV	355126	489322	50.20%	6.923%
65	10.195	1491	1494	1495	rBV2	736	655	0.07%	0.009%
66	10.299	1507	1511	1515	rVV3	807	1238	0.13%	0.018%
67	10.732	1578	1582	1584	rBV2	284	450	0.05%	0.006%
68	10.890	1606	1608	1611	rVB	386	463	0.05%	0.007%
69	11.067	1635	1637	1638	rBV2	685	534	0.05%	0.008%
70	11.201	1653	1659	1666	rBV	302215	413426	42.42%	5.849%
71	11.311	1672	1677	1680	rBV3	836	1163	0.12%	0.016%
72	11.433	1695	1697	1698	rVV2	493	434	0.04%	0.006%
73	11.482	1701	1705	1709	rVV3	3379	4777	0.49%	0.068%
74	11.518	1709	1711	1714	rVB	582	473	0.05%	0.007%
75	11.561	1714	1718	1719	rVB2	408	494	0.05%	0.007%
76	11.634	1728	1730	1735	rVB3	1392	1800	0.18%	0.025%

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Integrator: RTE

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 Title : VOC Analysis

77	11.683	1735	1738	1741	rBV3	967	1504	0.15%	0.021%
78	11.713	1741	1743	1746	rVB3	979	1068	0.11%	0.015%
79	11.762	1746	1751	1753	rBV4	665	1042	0.11%	0.015%
80	11.841	1762	1764	1767	rVB3	516	544	0.06%	0.008%
81	12.024	1789	1794	1802	rBV	348259	439191	45.06%	6.214%
82	12.262	1830	1833	1835	rBV3	499	737	0.08%	0.010%
83	12.323	1838	1843	1852	rVB	505501	648613	66.55%	9.177%
84	12.634	1892	1894	1897	rVB2	504	407	0.04%	0.006%
85	12.768	1913	1916	1918	rBV2	876	1014	0.10%	0.014%
86	12.866	1928	1932	1935	rVV3	717	941	0.10%	0.013%
87	12.902	1935	1938	1941	rVB3	449	558	0.06%	0.008%
88	13.036	1958	1960	1962	rVV	508	486	0.05%	0.007%
89	13.146	1976	1978	1981	rBV2	430	395	0.04%	0.006%
90	13.250	1993	1995	1997	rBV2	722	656	0.07%	0.009%
91	13.451	2027	2028	2030	rBV	565	502	0.05%	0.007%
92	13.518	2038	2039	2046	rBV2	518	874	0.09%	0.012%
93	13.780	2080	2082	2086	rBV3	595	987	0.10%	0.014%
94	13.920	2104	2105	2108	rBV	438	578	0.06%	0.008%
95	14.000	2117	2118	2120	rBV	784	491	0.05%	0.007%
96	14.061	2126	2128	2129	rBV	405	410	0.04%	0.006%
97	14.365	2175	2178	2179	rBV	732	749	0.08%	0.011%
98	14.445	2189	2191	2193	rVB2	540	401	0.04%	0.006%
99	14.524	2198	2204	2207	rBV2	843	2153	0.22%	0.030%
100	15.182	2311	2312	2316	rVB3	962	685	0.07%	0.010%

Sum of corrected areas: 7068006

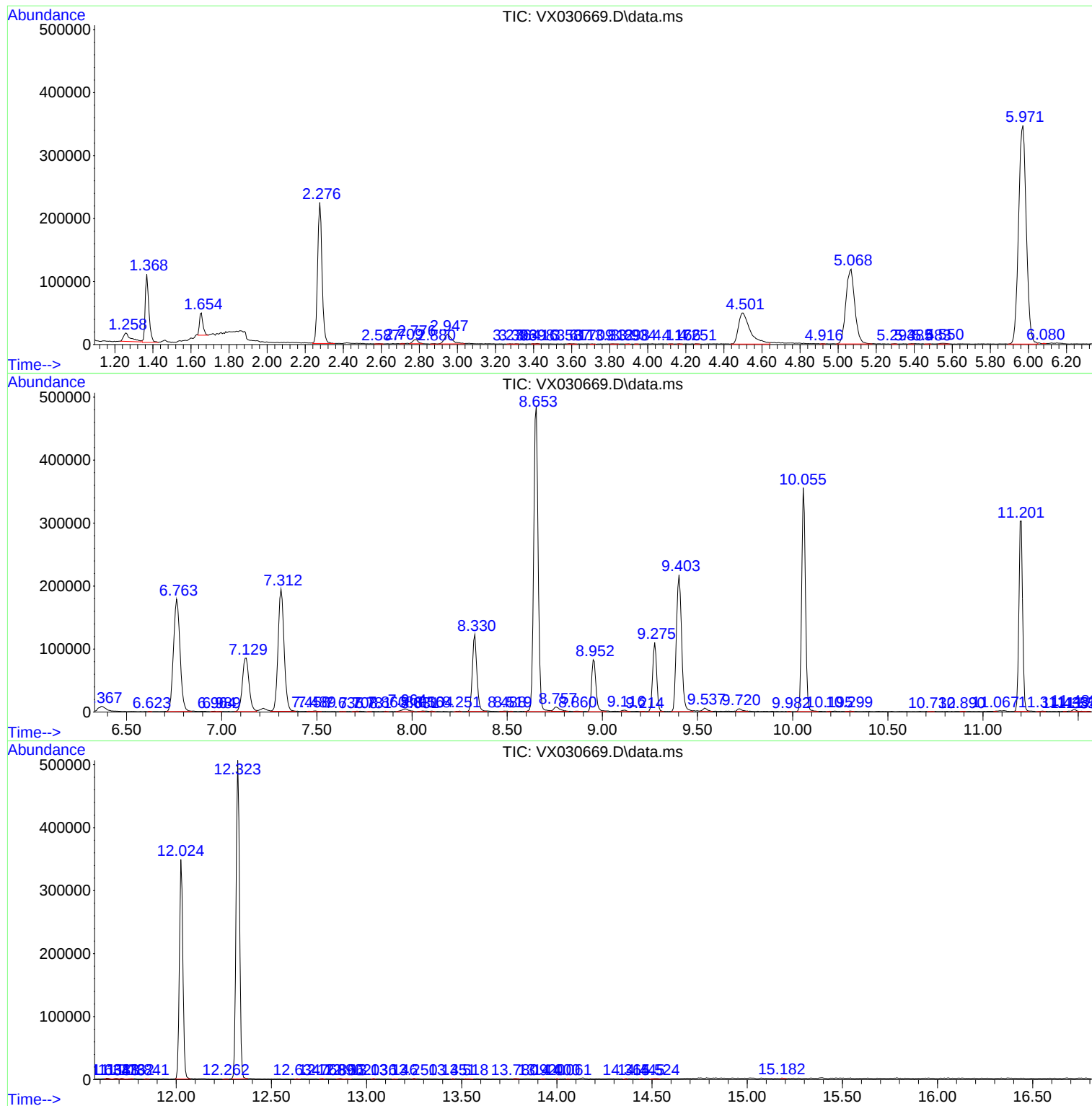
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ALS Vial : 18 Sample Multiplier: 1

Instrument :
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ClientSampleId :
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Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

TIC Library : C:\Database\NIST20.L

TIC Integration Parameters: LSCINT.P



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Instrument :
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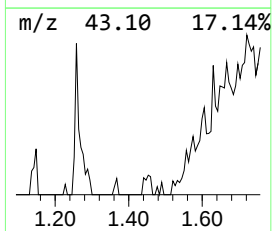
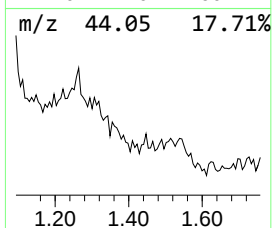
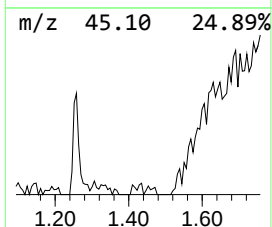
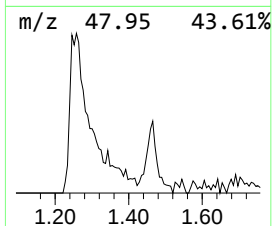
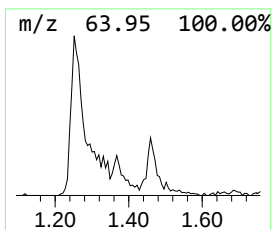
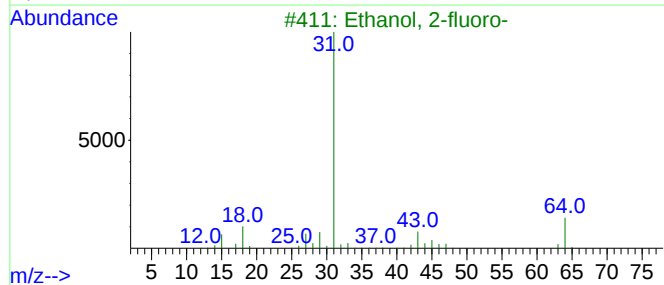
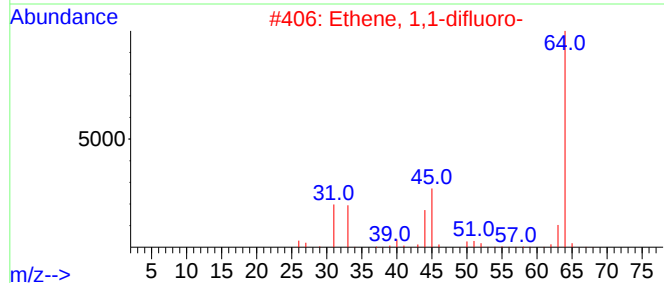
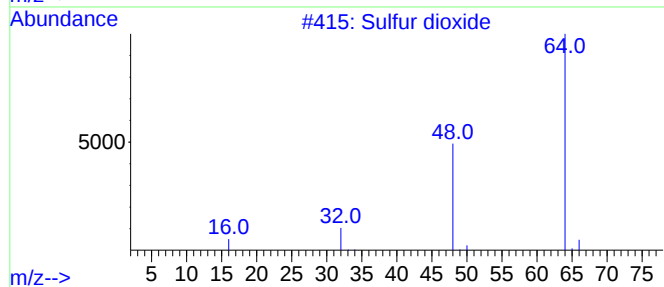
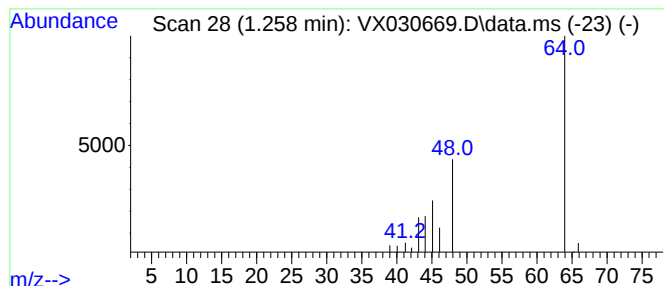
Quant Method : Z:\voasrv\HPCHEM1\MSVOA_X\Method\SFAMXML080422WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Sulfur dioxide Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.258	4.10 ug/L	34907	1,4-Difluorobenzene	6.763

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1			Sulfur dioxide	64	O2S	007446-09-5	64
2			Ethene, 1,1-difluoro-	64	C2H2F2	000075-38-7	9
3			Ethanol, 2-fluoro-	64	C2H5FO	000371-62-0	9
4			L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
5			Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9



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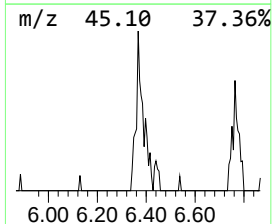
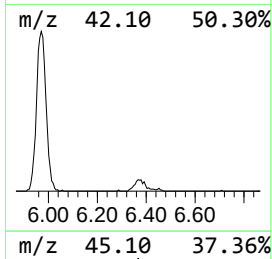
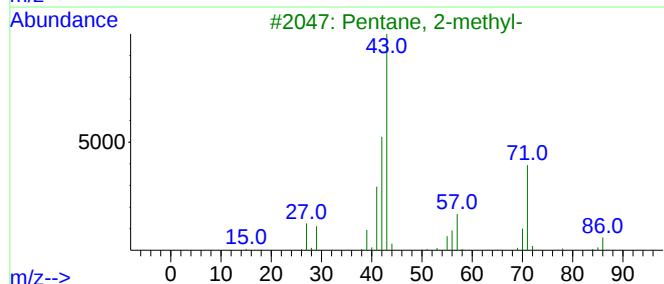
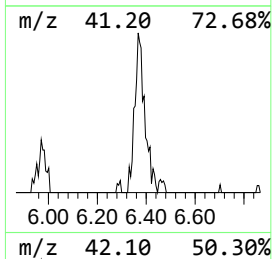
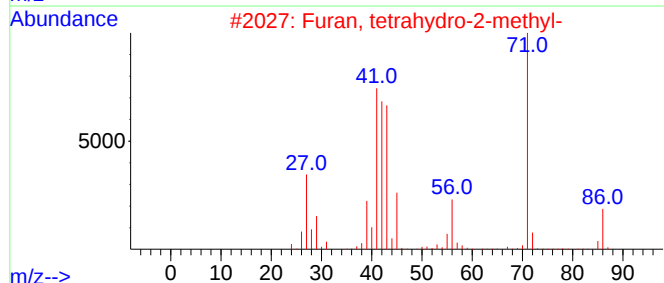
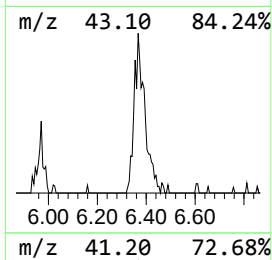
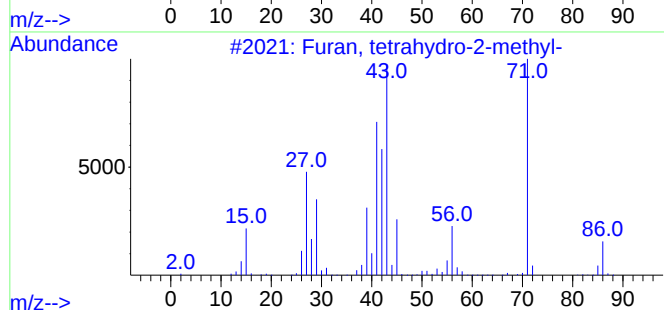
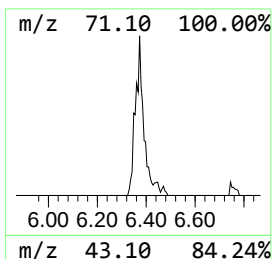
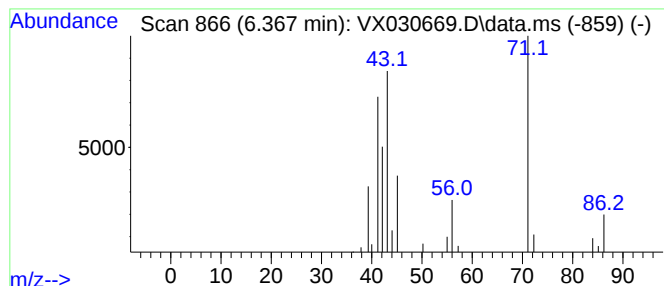
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TIC Library : C:\Database\NIST20.L
TIC Integration Parameters: LSCINT.P

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

R.T.	EstConc	Area	Relative to ISTD	R.T.
6.367	2.83 ug/L	24094	1,4-Difluorobenzene	6.763

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	68
3			Pentane, 2-methyl-	86	C6H14	000107-83-5	47
4			1-Propene, 3-methoxy-2-methyl-	86	C5H10O	022418-49-1	47
5			2-Butene, 1-methoxy-, (E)-	86	C5H10O	010034-14-7	43



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.258	4.1	ug/L	34907	1	6.763	425437	50.0
Furan, tetrahyd...	6.367	2.8	ug/L	24094	1	6.763	425437	50.0