

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU090518\
 Data File : VU026551.D
 Acq On : 05 Sep 2018 18:55
 Operator : MD/SY
 Sample : J4694-04
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 25 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BEE22

Integration Parameters: LSCINT.P

Integrator: RTE
 Smoothing : OFF
 Sampling : 1
 Start Thrs: 0.2
 Stop Thrs : 0

Filtering: 5
 Min Area: 0 % of largest Peak
 Max Peaks: 100
 Peak Location: TOP

If leading or trailing edge < 100 prefer < Baseline drop else tangent >
 Peak separation: 5

Method : Z:\VOASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
 Title : VOC Analysis

Signal : TIC

peak #	R.T. min	first scan	max scan	last scan	PK TY	peak height	corr. area	corr. % max.	% of total
1	0.738	42	46	49	rBV	185	197	0.02%	0.004%
2	0.792	61	63	65	rBV	257	135	0.01%	0.002%
3	0.889	90	93	96	rBV	125	135	0.01%	0.002%
4	1.085	137	154	168	rBV	292941	336078	34.47%	6.119%
5	1.265	206	210	225	rVB2	16653	23616	2.42%	0.430%
6	1.397	245	251	267	rBV2	84601	102952	10.56%	1.874%
7	1.471	270	274	287	rVB	25402	30547	3.13%	0.556%
8	1.677	332	338	361	rVB	50913	70357	7.22%	1.281%
9	2.268	512	522	534	rVV	97686	147994	15.18%	2.694%
10	2.326	535	540	549	rVB4	3015	4317	0.44%	0.079%
11	2.378	553	556	560	rBV2	505	383	0.04%	0.007%
12	2.452	570	579	581	rBV2	416	704	0.07%	0.013%
13	2.702	649	657	666	rVB3	2729	4693	0.48%	0.085%
14	2.844	689	701	709	rBV2	1256	2805	0.29%	0.051%
15	2.876	709	711	716	rVB2	200	133	0.01%	0.002%
16	2.940	728	731	734	rVB	138	100	0.01%	0.002%
17	2.982	734	744	755	rVV4	3143	5727	0.59%	0.104%
18	3.037	759	761	765	rBV2	212	124	0.01%	0.002%
19	3.114	783	785	790	rBV2	114	103	0.01%	0.002%
20	3.220	815	818	820	rBV	214	150	0.02%	0.003%
21	3.445	881	888	889	rBV2	452	422	0.04%	0.008%
22	3.805	996	1000	1002	rBV2	287	241	0.02%	0.004%
23	3.895	1025	1028	1033	rBV	92	91	0.01%	0.002%
24	4.034	1068	1071	1080	rVB	209	148	0.02%	0.003%
25	4.098	1080	1091	1102	rBV	986	2323	0.24%	0.042%
26	4.226	1102	1131	1160	rVV2	353464	975105	100.00%	17.753%
27	4.410	1183	1188	1191	rVB2	443	444	0.05%	0.008%
28	4.455	1199	1202	1205	rBV	489	373	0.04%	0.007%
29	4.558	1231	1234	1241	rBV2	215	267	0.03%	0.005%
30	4.648	1242	1262	1282	rBV	85155	202199	20.74%	3.681%
31	5.342	1453	1478	1504	rBV2	163227	490010	50.25%	8.921%
32	5.615	1561	1563	1569	rVB	186	94	0.01%	0.002%
33	5.889	1634	1648	1664	rBV	182463	351426	36.04%	6.398%
34	6.046	1692	1697	1703	rBV	115	166	0.02%	0.003%

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 Title : VOC Analysis

35	6.188	1728	1741	1760	rBV	110338	207723	21.30%	3.782%
36	6.332	1772	1786	1808	rVB	117541	231372	23.73%	4.213%
37	6.461	1821	1826	1829	rBV2	358	327	0.03%	0.006%
38	6.599	1867	1869	1875	rVB2	168	118	0.01%	0.002%
39	6.834	1938	1942	1944	rBV	166	124	0.01%	0.002%
40	7.230	2052	2065	2081	rBV	53006	93135	9.55%	1.696%
41	7.336	2094	2098	2104	rBB	107	101	0.01%	0.002%
42	7.365	2104	2107	2110	rBV2	188	164	0.02%	0.003%
43	7.567	2157	2170	2189	rBV	197817	341549	35.03%	6.218%
44	7.850	2247	2258	2272	rBV2	38921	63669	6.53%	1.159%
45	8.037	2314	2316	2318	rBV	153	93	0.01%	0.002%
46	8.181	2349	2361	2368	rBV2	15978	30305	3.11%	0.552%
47	8.229	2368	2376	2391	rVV2	35015	66175	6.79%	1.205%
48	8.313	2391	2402	2429	rVB	174678	301386	30.91%	5.487%
49	8.480	2450	2454	2459	rVB3	454	487	0.05%	0.009%
50	8.506	2459	2462	2468	rVB	186	136	0.01%	0.002%
51	8.593	2485	2489	2494	rBV2	344	335	0.03%	0.006%
52	8.615	2494	2496	2498	rVB	259	104	0.01%	0.002%
53	8.680	2511	2516	2519	rBV	93	102	0.01%	0.002%
54	9.091	2631	2644	2662	rBV	246213	401309	41.16%	7.306%
55	9.397	2730	2739	2755	rBV2	17888	35870	3.68%	0.653%
56	9.548	2783	2786	2790	rBV2	215	180	0.02%	0.003%
57	9.676	2823	2826	2831	rBV	119	97	0.01%	0.002%
58	10.104	2954	2959	2962	rBV3	269	228	0.02%	0.004%
59	10.133	2966	2968	2970	rBV	238	137	0.01%	0.002%
60	10.233	2996	2999	3002	rBV	130	114	0.01%	0.002%
61	10.371	3038	3042	3047	rBV2	221	173	0.02%	0.003%
62	10.432	3050	3061	3081	rVV	169549	269559	27.64%	4.908%
63	10.612	3107	3117	3130	rBV2	9480	17109	1.75%	0.311%
64	10.856	3190	3193	3194	rBV	200	109	0.01%	0.002%
65	10.882	3197	3201	3204	rVB3	553	470	0.05%	0.009%
66	10.959	3222	3225	3228	rBV	99	98	0.01%	0.002%
67	11.188	3294	3296	3299	rVB	267	112	0.01%	0.002%
68	11.204	3299	3301	3303	rVV	154	95	0.01%	0.002%
69	11.220	3303	3306	3310	rVB2	321	226	0.02%	0.004%
70	11.377	3353	3355	3363	rVB	239	137	0.01%	0.002%
71	11.487	3377	3389	3408	rVV	217555	337232	34.58%	6.140%

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72	11.718	3458	3461	3463	rBV	197	128	0.01%	0.002%
73	11.747	3464	3470	3478	rVB4	1419	1882	0.19%	0.034%
74	11.863	3494	3506	3524	rBV	201232	316124	32.42%	5.756%
75	11.985	3541	3544	3545	rBV	245	118	0.01%	0.002%
76	12.130	3587	3589	3592	rBV	154	97	0.01%	0.002%
77	12.197	3608	3610	3614	rVB	261	130	0.01%	0.002%
78	12.220	3614	3617	3620	rVB2	244	198	0.02%	0.004%
79	12.239	3620	3623	3626	rBV2	256	192	0.02%	0.003%
80	12.400	3670	3673	3675	rBV	173	118	0.01%	0.002%
81	12.480	3690	3698	3708	rVB	4308	6670	0.68%	0.121%
82	12.570	3720	3726	3733	rVB3	3429	3785	0.39%	0.069%
83	12.795	3793	3796	3797	rBV	186	110	0.01%	0.002%
84	12.837	3807	3809	3812	rBV	184	129	0.01%	0.002%
85	12.898	3825	3828	3831	rBV3	279	238	0.02%	0.004%
86	13.024	3863	3867	3872	rBV2	300	372	0.04%	0.007%
87	13.181	3913	3916	3918	rBV	189	113	0.01%	0.002%
88	13.245	3933	3936	3938	rVV	242	157	0.02%	0.003%
89	13.329	3957	3962	3966	rBV2	822	741	0.08%	0.013%
90	13.348	3966	3968	3973	rVB2	618	492	0.05%	0.009%
91	13.548	4028	4030	4033	rVB	268	149	0.02%	0.003%
92	13.798	4105	4108	4110	rBV	235	139	0.01%	0.003%
93	13.921	4143	4146	4149	rBV	259	214	0.02%	0.004%
94	14.133	4209	4212	4214	rBV	368	192	0.02%	0.003%
95	14.146	4214	4216	4219	rVV	206	115	0.01%	0.002%
96	14.197	4230	4232	4235	rBV2	180	117	0.01%	0.002%
97	14.281	4246	4258	4268	rBV	2356	3890	0.40%	0.071%
98	14.551	4339	4342	4346	rVB2	237	190	0.02%	0.003%
99	14.577	4348	4350	4353	rBV2	280	232	0.02%	0.004%
100	14.763	4406	4408	4414	rBV	280	242	0.02%	0.004%

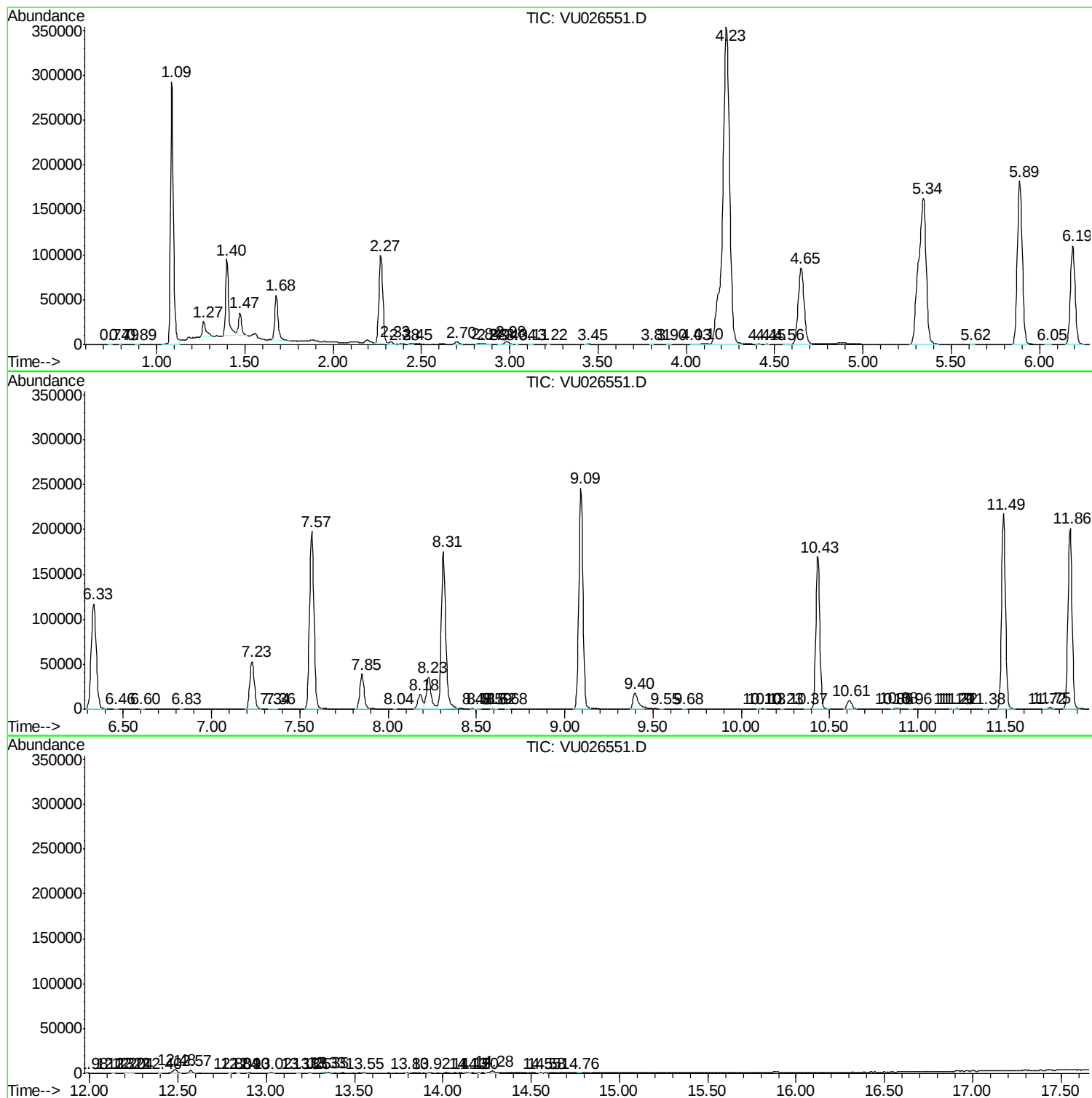
Sum of corrected areas: 5492493

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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
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TIC Library : C:\DATABASE\NIST11.L
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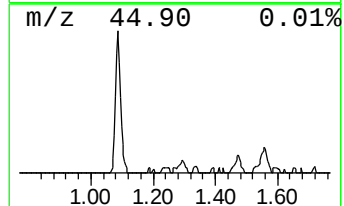
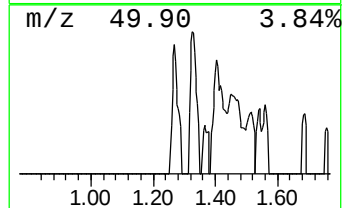
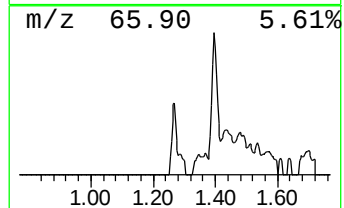
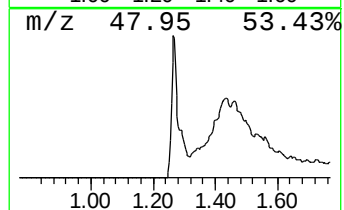
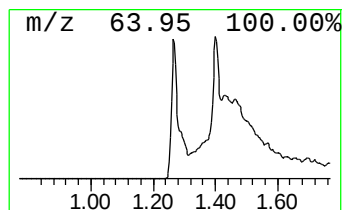
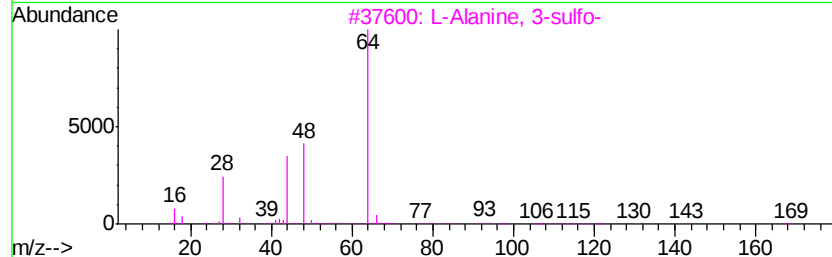
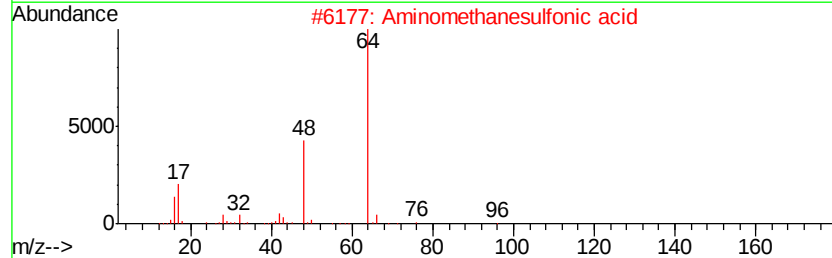
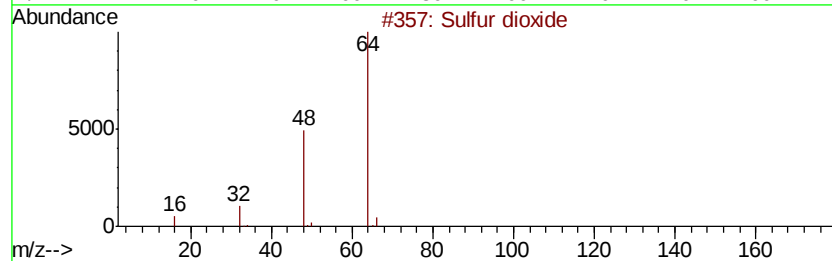
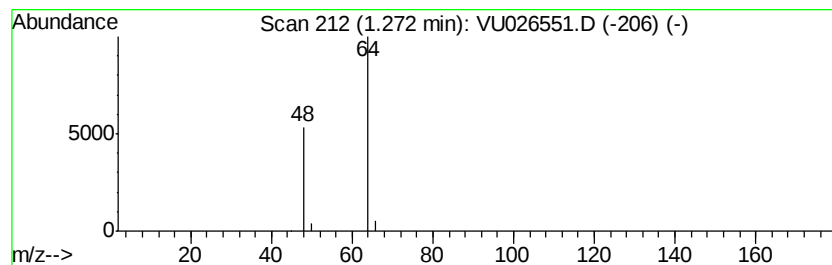
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 2 Sulfur dioxide Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.27	3.36 ug/L	23616	1,4-Difluorobenzene	5.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Sulfur dioxide	64	O2S	007446-09-5	90
2		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	64
3		L-Alanine, 3-sulfo-	169	C3H7NO5S	000498-40-8	9
4		Aminomethanesulfonic acid	111	CH5NO3S	013881-91-9	9
5		Sulfur dioxide	64	O2S	007446-09-5	5



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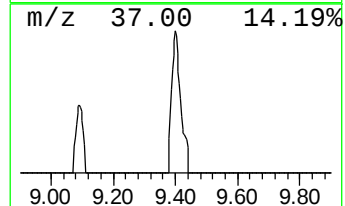
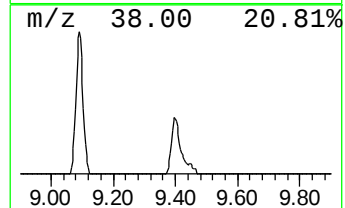
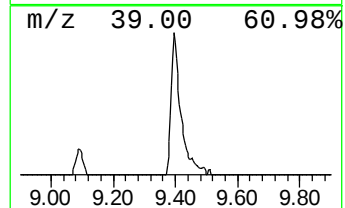
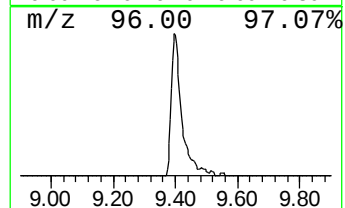
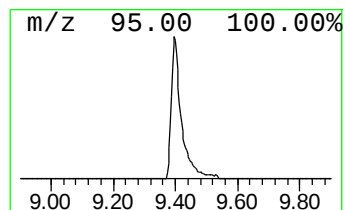
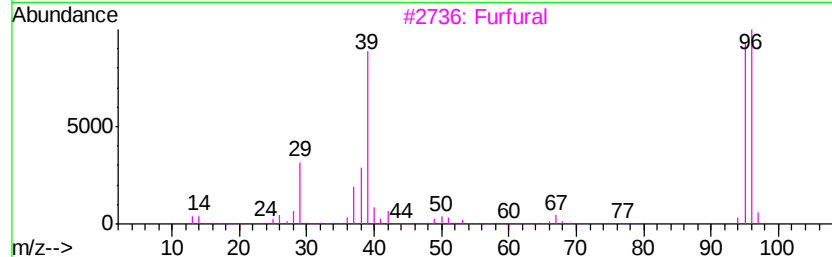
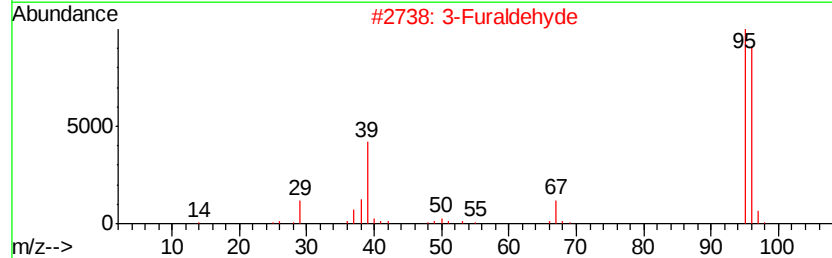
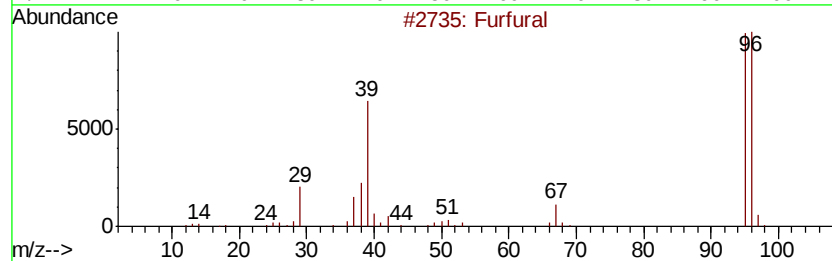
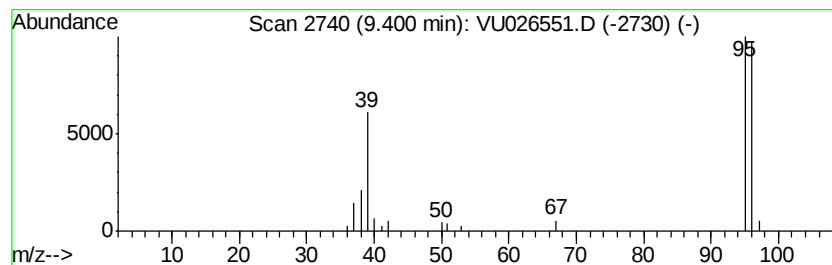
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Quant Title : VOC Analysis

TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 5 Furfural Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.40	4.47 ug/L	35870	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Furfural	96	C5H4O2	000098-01-1	91
2		3-Furaldehyde	96	C5H4O2	000498-60-2	91
3		Furfural	96	C5H4O2	000098-01-1	87
4		Furfural	96	C5H4O2	000098-01-1	68
5		1H-Imidazole, 1,5-dimethyl-	96	C5H8N2	010447-93-5	64



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TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Sulfur dioxide	1.27	3.4	ug/L	23616	1	5.89	351426	50.0
Furfural	9.40	4.5	ug/L	35870	2	9.09	401309	50.0