

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU090618\
 Data File : VU026575.D
 Acq On : 06 Sep 2018 13:01
 Operator : MD/SY
 Sample : J4694-01
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 4 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BEE18

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	1.392	62	68	82	rVB	48139	52466	1.99%	0.704%
2	1.485	86	97	150	rBV	888529	2642523	100.00%	35.463%
3	1.678	153	157	178	rVB	46456	68736	2.60%	0.922%
4	2.125	289	296	306	rVB	19633	28542	1.08%	0.383%
5	2.209	311	322	332	rBV	66508	140225	5.31%	1.882%
6	2.267	333	340	354	rVB	88363	141840	5.37%	1.904%
7	2.595	439	442	445	rBV3	475	291	0.01%	0.004%
8	2.636	445	455	472	rBV	3871	9631	0.36%	0.129%
9	3.177	620	623	624	rBV	430	276	0.01%	0.004%
10	3.643	757	768	776	rBV2	1148	2974	0.11%	0.040%
11	3.797	812	816	817	rBV2	550	423	0.02%	0.006%
12	3.923	850	855	862	rBV2	125	186	0.01%	0.002%
13	4.009	862	882	888	rBV4	2276	5529	0.21%	0.074%
14	4.122	906	917	921	rBV2	2921	5752	0.22%	0.077%
15	4.212	930	945	982	rBV2	40858	155201	5.87%	2.083%
16	4.649	1066	1081	1101	rVB2	51736	123657	4.68%	1.659%
17	4.878	1147	1152	1153	rBV3	831	599	0.02%	0.008%
18	5.340	1275	1296	1321	rVB2	104479	306300	11.59%	4.111%
19	5.694	1403	1406	1410	rBV3	558	436	0.02%	0.006%
20	5.771	1423	1430	1434	rBV5	860	1171	0.04%	0.016%
21	5.816	1434	1444	1453	rVV5	2034	4927	0.19%	0.066%
22	5.887	1453	1466	1483	rVB	96935	185852	7.03%	2.494%
23	6.006	1497	1503	1505	rBV3	668	572	0.02%	0.008%
24	6.128	1534	1541	1544	rBV4	1038	1455	0.06%	0.020%
25	6.189	1552	1560	1568	rVB5	1563	2611	0.10%	0.035%
26	6.334	1591	1605	1622	rBV	69979	138970	5.26%	1.865%
27	6.440	1633	1638	1640	rBV2	164	125	0.00%	0.002%
28	6.492	1651	1654	1658	rBV3	497	496	0.02%	0.007%
29	6.540	1660	1669	1678	rVB6	2833	5365	0.20%	0.072%
30	6.736	1723	1730	1731	rBV2	964	853	0.03%	0.011%
31	6.961	1790	1800	1801	rBV3	1834	2571	0.10%	0.035%
32	7.231	1872	1884	1899	rVV2	34210	59373	2.25%	0.797%
33	7.324	1910	1913	1915	rBV	154	110	0.00%	0.001%
34	7.363	1923	1925	1931	rVB2	280	144	0.01%	0.002%

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

35	7.405	1935	1938	1939	rBV2	242	139	0.01%	0.002%
36	7.466	1952	1957	1970	rVB2	607	1161	0.04%	0.016%
37	7.565	1976	1988	2005	rBV	123025	210746	7.98%	2.828%
38	7.852	2064	2077	2091	rVB2	21446	36099	1.37%	0.484%
39	7.922	2094	2099	2104	rBV3	616	568	0.02%	0.008%
40	8.054	2135	2140	2141	rBV	147	112	0.00%	0.002%
41	8.183	2166	2180	2183	rBV3	18068	27817	1.05%	0.373%
42	8.228	2183	2194	2207	rVV	655886	1094053	41.40%	14.682%
43	8.315	2211	2221	2237	rVB	176076	302472	11.45%	4.059%
44	8.469	2262	2269	2280	rVB2	5269	9084	0.34%	0.122%
45	8.517	2280	2284	2286	rVV	339	215	0.01%	0.003%
46	8.553	2290	2295	2297	rBV2	232	201	0.01%	0.003%
47	8.627	2315	2318	2319	rBV	191	111	0.00%	0.001%
48	8.646	2319	2324	2329	rBV3	483	577	0.02%	0.008%
49	8.729	2347	2350	2352	rVB2	313	147	0.01%	0.002%
50	8.803	2369	2373	2375	rBV	306	229	0.01%	0.003%
51	8.897	2387	2402	2404	rBV5	2678	6271	0.24%	0.084%
52	9.035	2436	2445	2448	rBV7	1317	2036	0.08%	0.027%
53	9.093	2451	2463	2487	rVB	113123	190487	7.21%	2.556%
54	9.260	2509	2515	2518	rVB2	230	223	0.01%	0.003%
55	9.318	2530	2533	2537	rVB2	262	138	0.01%	0.002%
56	9.382	2549	2553	2556	rBV2	340	294	0.01%	0.004%
57	9.437	2556	2570	2598	rBV2	51275	161421	6.11%	2.166%
58	9.643	2630	2634	2637	rBV2	367	297	0.01%	0.004%
59	9.678	2642	2645	2651	rVB	122	135	0.01%	0.002%
60	9.803	2680	2684	2689	rBV2	188	236	0.01%	0.003%
61	9.916	2716	2719	2721	rBV	245	164	0.01%	0.002%
62	10.032	2745	2755	2762	rVV3	3597	5553	0.21%	0.075%
63	10.118	2776	2782	2784	rBV2	1064	1064	0.04%	0.014%
64	10.218	2810	2813	2822	rVB	115	126	0.00%	0.002%
65	10.434	2869	2880	2896	rBV	97741	158872	6.01%	2.132%
66	10.508	2896	2903	2918	rVB3	2143	4301	0.16%	0.058%
67	10.614	2925	2936	2952	rVB	9187	18587	0.70%	0.249%
68	10.681	2953	2957	2961	rVV2	136	133	0.01%	0.002%
69	10.803	2992	2995	2996	rBV	290	169	0.01%	0.002%
70	10.816	2996	2999	3009	rVB3	651	642	0.02%	0.009%
71	11.028	3062	3065	3069	rBV	254	172	0.01%	0.002%

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72	11.064	3073	3076	3078	rBV2	192	109	0.00%	0.001%
73	11.170	3092	3109	3128	rBV3	4105	13923	0.53%	0.187%
74	11.337	3157	3161	3165	rVV2	208	223	0.01%	0.003%
75	11.372	3165	3172	3181	rVV4	3916	5532	0.21%	0.074%
76	11.421	3185	3187	3191	rVB2	525	360	0.01%	0.005%
77	11.485	3197	3207	3223	rBV	76300	118159	4.47%	1.586%
78	11.597	3239	3242	3245	rVB	179	120	0.00%	0.002%
79	11.749	3281	3289	3295	rBV4	1959	2607	0.10%	0.035%
80	11.816	3304	3310	3314	rBV5	1620	2134	0.08%	0.029%
81	11.874	3314	3328	3380	rBV2	301456	807726	30.57%	10.840%
82	12.569	3535	3544	3556	rVB2	69517	100360	3.80%	1.347%
83	13.015	3681	3683	3687	rVB4	774	459	0.02%	0.006%
84	13.192	3737	3738	3739	rBV	450	166	0.01%	0.002%
85	13.318	3767	3777	3798	rBV2	26457	51412	1.95%	0.690%
86	13.610	3865	3868	3870	rBV2	552	405	0.02%	0.005%
87	13.662	3879	3884	3890	rVB5	2861	3677	0.14%	0.049%
88	13.745	3906	3910	3915	rBV4	1117	979	0.04%	0.013%
89	13.929	3964	3967	3970	rVB3	547	330	0.01%	0.004%
90	13.990	3983	3986	3991	rVB4	679	707	0.03%	0.009%
91	14.051	4001	4005	4011	rBV2	439	428	0.02%	0.006%
92	14.167	4039	4041	4042	rBV2	355	165	0.01%	0.002%
93	14.221	4055	4058	4059	rBV	381	201	0.01%	0.003%
94	14.282	4069	4077	4088	rVB2	2173	3893	0.15%	0.052%
95	14.388	4108	4110	4111	rBV2	344	124	0.00%	0.002%
96	14.675	4193	4199	4202	rBV5	1054	1225	0.05%	0.016%
97	14.726	4213	4215	4218	rVB2	353	186	0.01%	0.002%
98	15.240	4368	4375	4386	rBV6	5230	9345	0.35%	0.125%
99	15.462	4439	4444	4446	rBV3	896	899	0.03%	0.012%
100	16.096	4639	4641	4645	rBV2	498	381	0.01%	0.005%

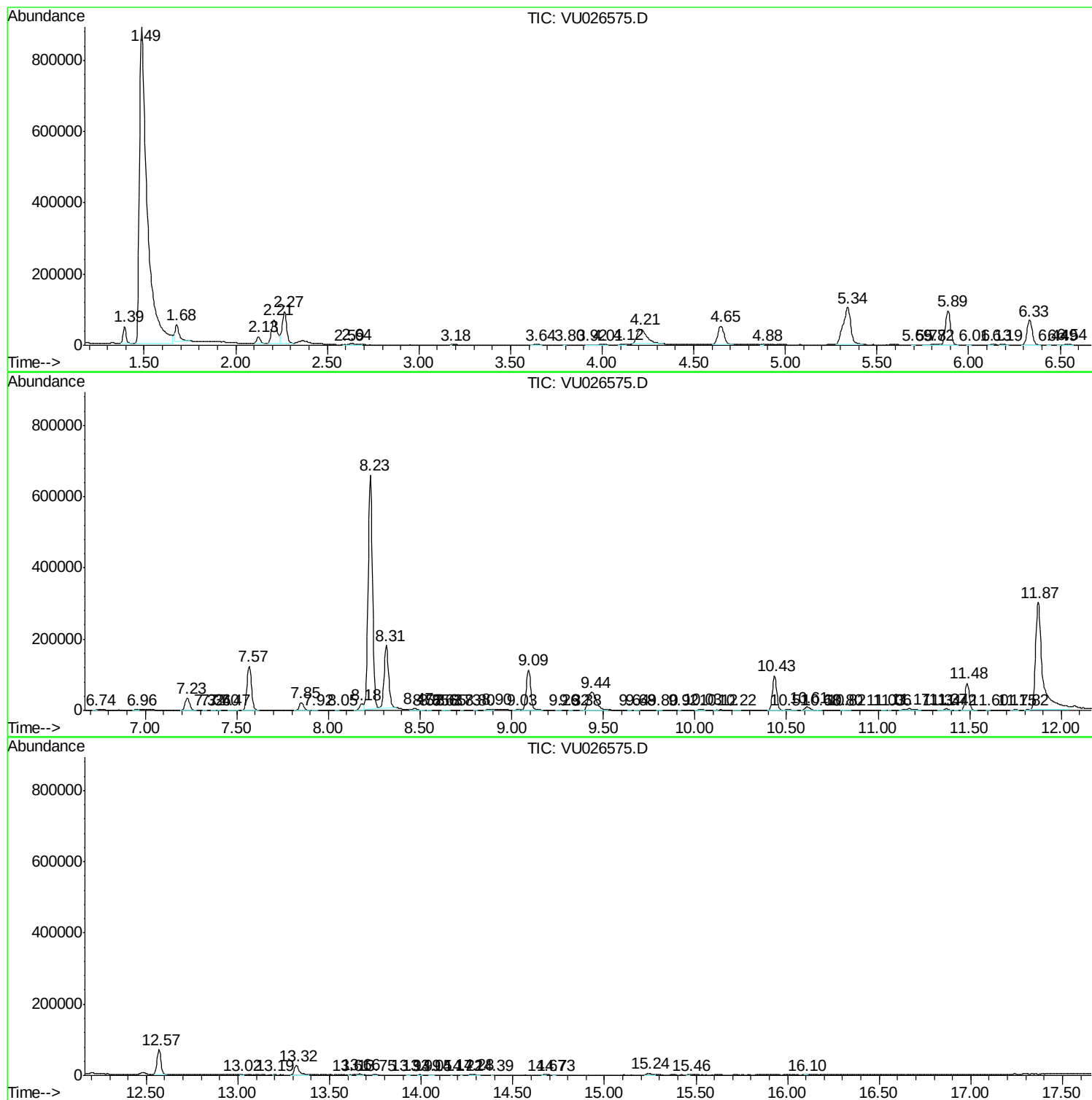
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Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
Quant Title : VOC Analysis

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



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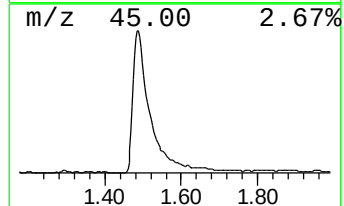
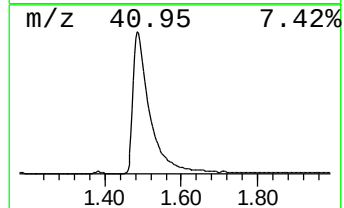
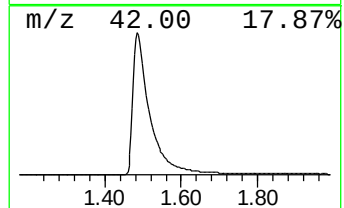
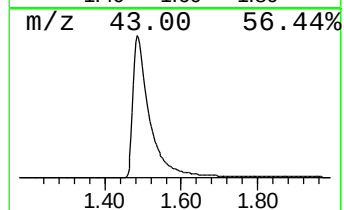
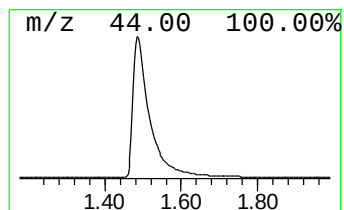
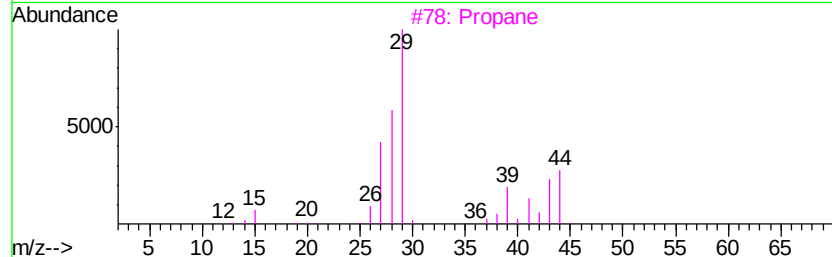
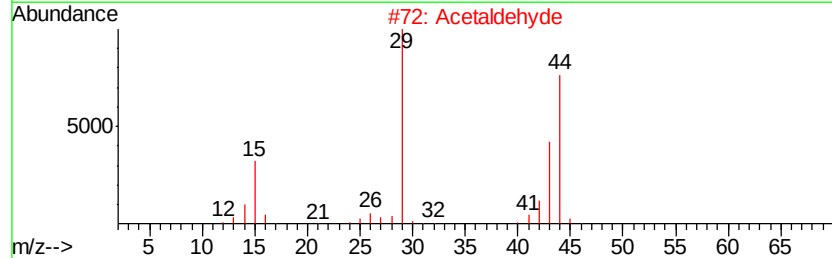
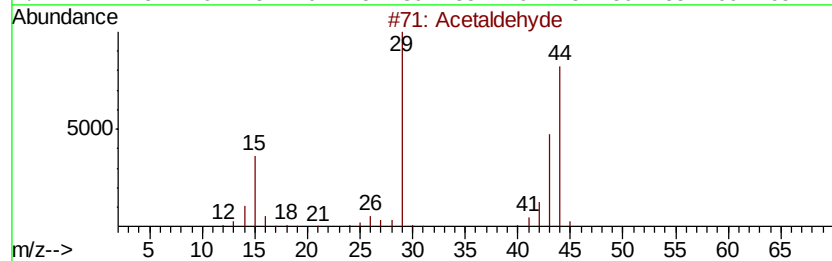
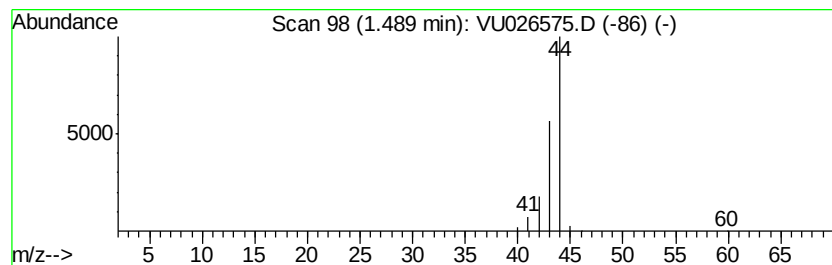
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
Quant Title : VOC Analysis

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

Peak Number 1 Acetaldehyde Concentration Rank 1

R.T.	EstConc	Area	Relative to ISTD	R.T.
1.49	710.92 ug/L	2642520	1,4-Difluorobenzene	5.89

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Acetaldehyd		44	C2H4O	000075-07-0	74
2	Acetaldehyd		44	C2H4O	000075-07-0	74
3	Propane		44	C3H8	000074-98-6	5
4	Ethylene oxide		44	C2H4O	000075-21-8	5
5	Ethylene oxide		44	C2H4O	000075-21-8	5



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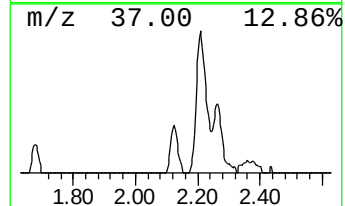
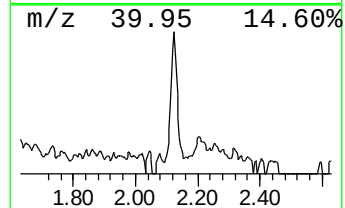
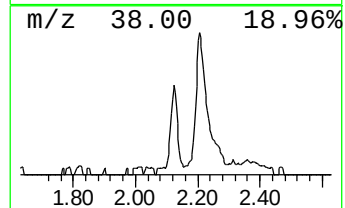
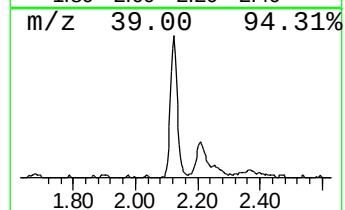
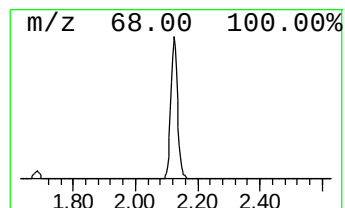
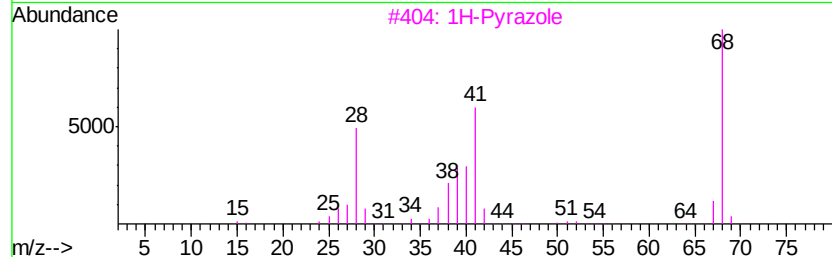
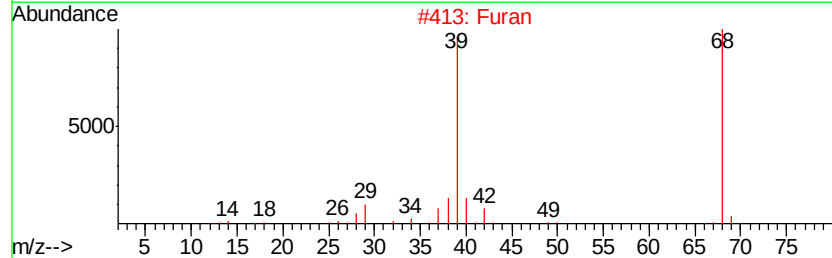
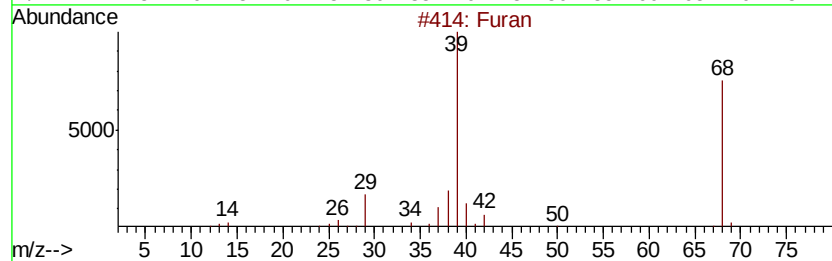
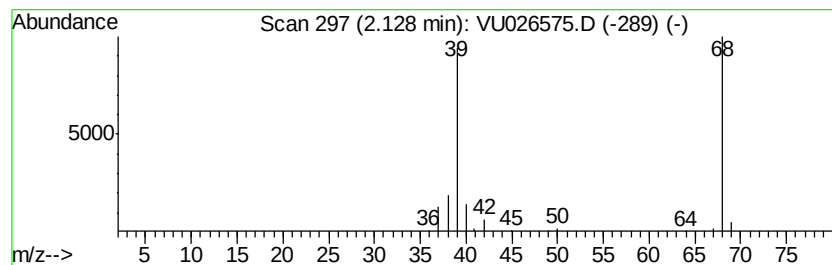
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Furan Concentration Rank 8

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.13	7.68 ug/L	28542	1,4-Difluorobenzene	5.89

Hit#	of	5	Tentative ID	MW	MolForm	CAS#	Qual
1	Furan			68	C4H4O	000110-00-9	90
2	Furan			68	C4H4O	000110-00-9	80
3	1H-Pyrazole			68	C3H4N2	000288-13-1	27
4	Methylenecyclopropane			54	C4H6	006142-73-0	9
5	2-Propyn-1-amine, N-methyl-			69	C4H7N	035161-71-8	4



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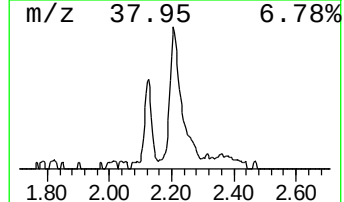
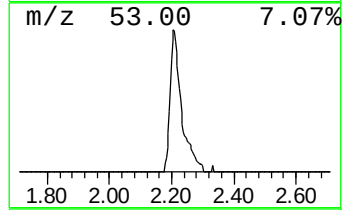
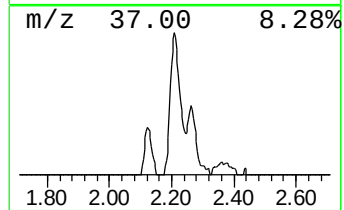
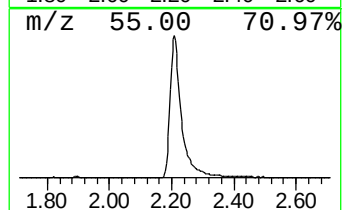
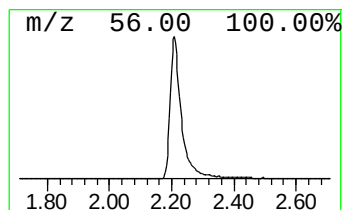
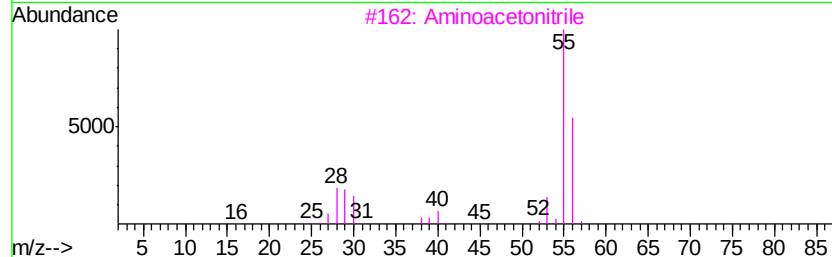
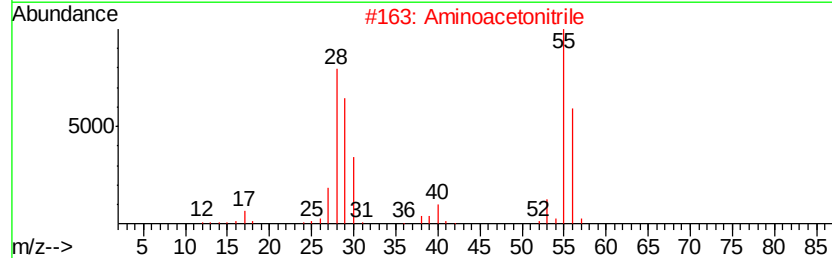
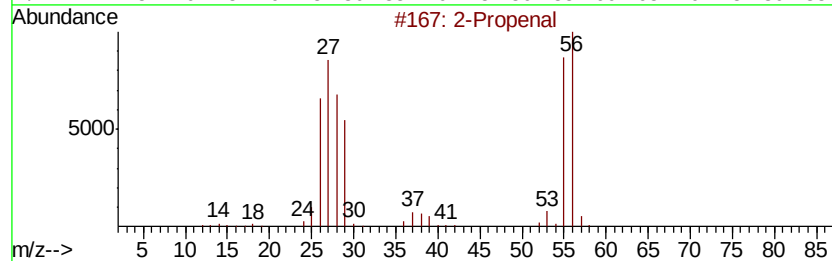
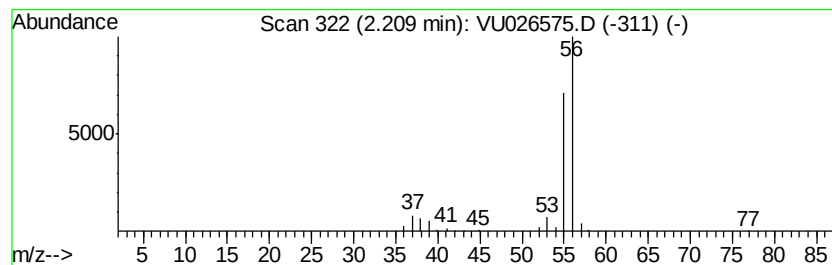
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Quant Title : VOC Analysis

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

Peak Number 3 2-Propenal Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
2.21	37.72 ug/L	140225	1,4-Difluorobenzene	5.89

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2-Propenal	56	C3H4O	000107-02-8	90
2		Aminoacetonitrile	56	C2H4N2	000540-61-4	9
3		Aminoacetonitrile	56	C2H4N2	000540-61-4	7
4		2-Propenal	56	C3H4O	000107-02-8	7
5		2-Propenal	56	C3H4O	000107-02-8	5



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ClientSampleId :
BEE18

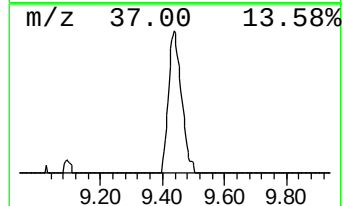
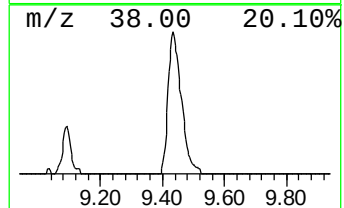
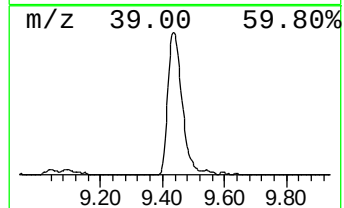
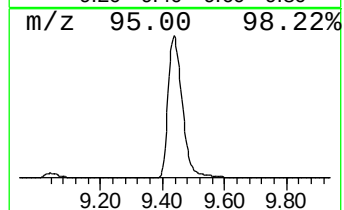
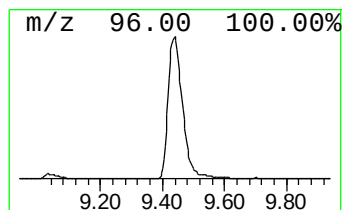
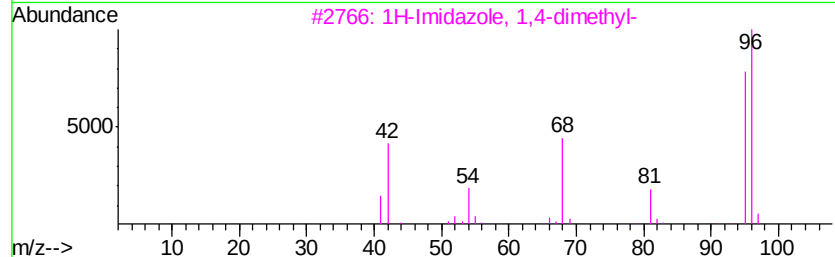
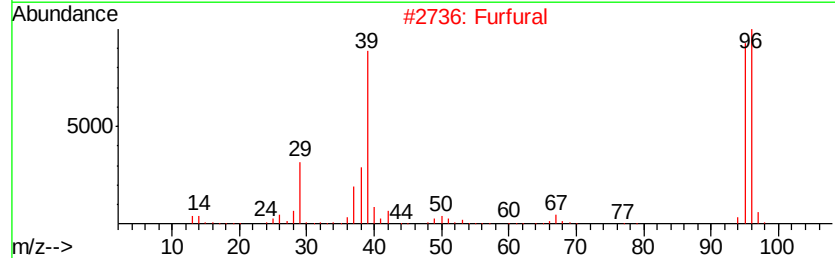
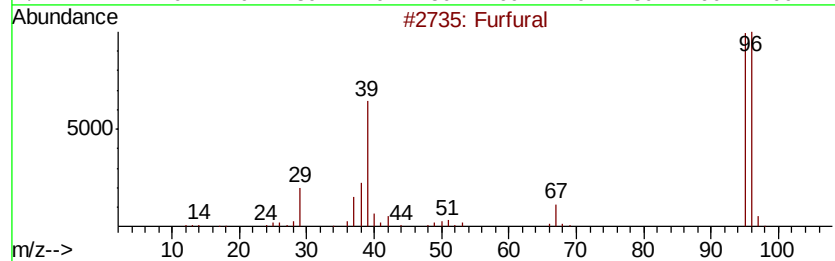
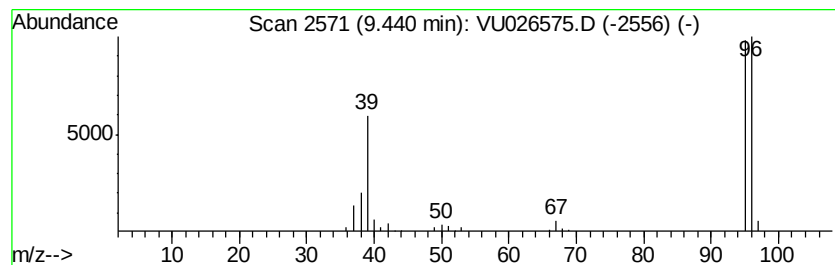
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Quant Title : VOC Analysis

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

Peak Number 6 Furfural Concentration Rank 3

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.44	42.37 ug/L	161421	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Furfural	96	C5H4O2	000098-01-1	94
2		Furfural	96	C5H4O2	000098-01-1	87
3		1H-Imidazole, 1,4-dimethyl-	96	C5H8N2	006338-45-0	86
4		Furfural	96	C5H4O2	000098-01-1	76
5		3-Furaldehyde	96	C5H4O2	000498-60-2	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU090618\
Data File : VU026575.D
Acq On : 06 Sep 2018 13:01
Operator : MD/SY
Sample : J4694-01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BEE18

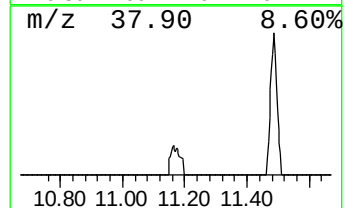
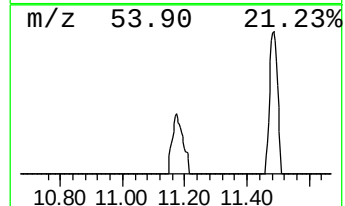
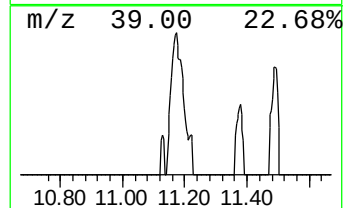
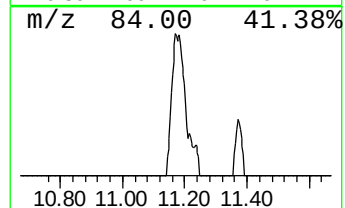
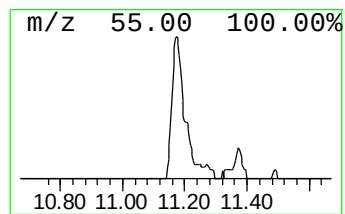
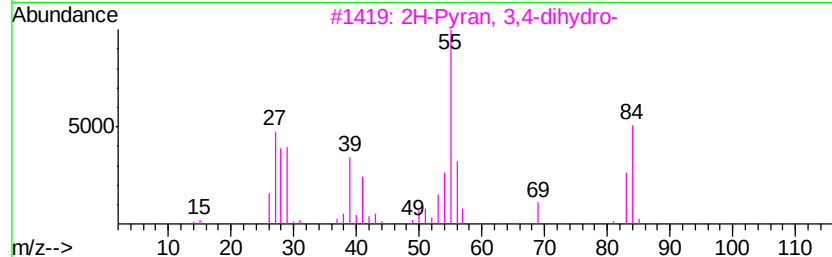
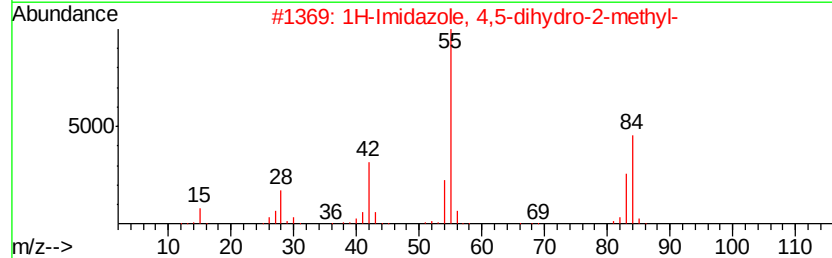
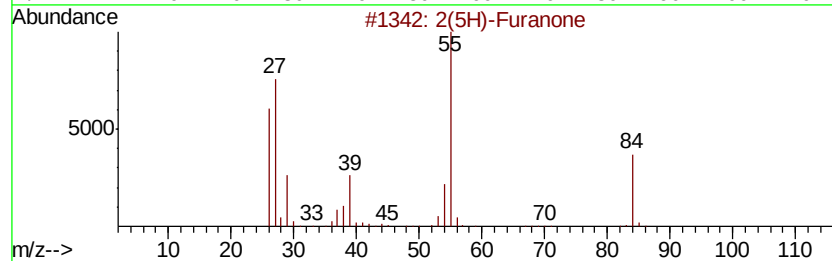
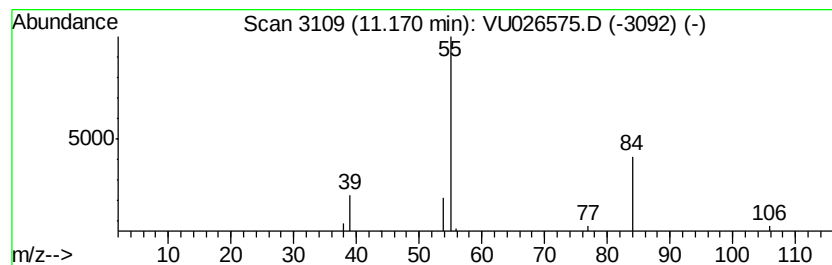
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Quant Title : VOC Analysis

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

Peak Number 8 2(5H)-Furanone Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
11.17	5.89 ug/L	13923	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	2(5H)-Furanone	84	C4H4O2	000497-23-4	86
2		1H-Imidazole, 4,5-dihydro-2-methyl-	84	C4H8N2	000534-26-9	64
3		2H-Pyran, 3,4-dihydro-	84	C5H8O	000110-87-2	9
4		Cyclopentanone	84	C5H8O	000120-92-3	7
5		2-Butenal, 2-methyl-	84	C5H8O	001115-11-3	7



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU090618\
Data File : VU026575.D
Acq On : 06 Sep 2018 13:01
Operator : MD/SY
Sample : J4694-01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

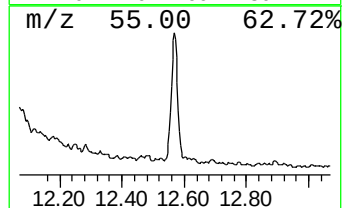
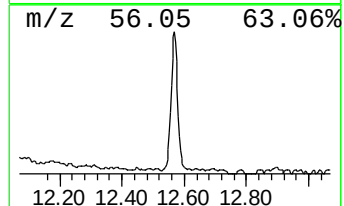
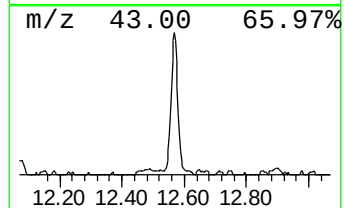
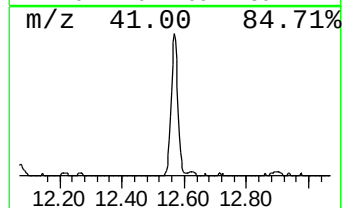
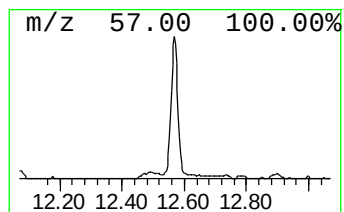
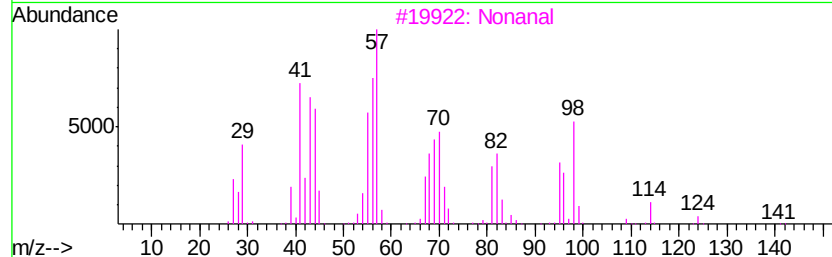
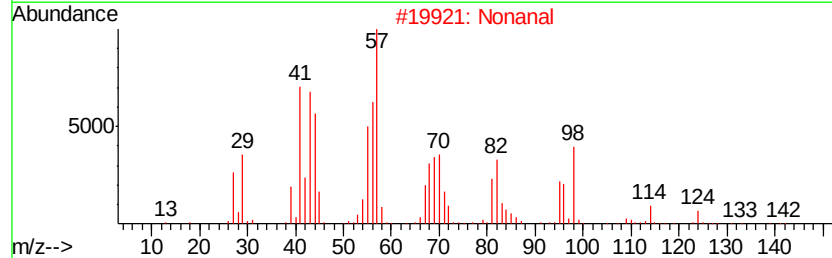
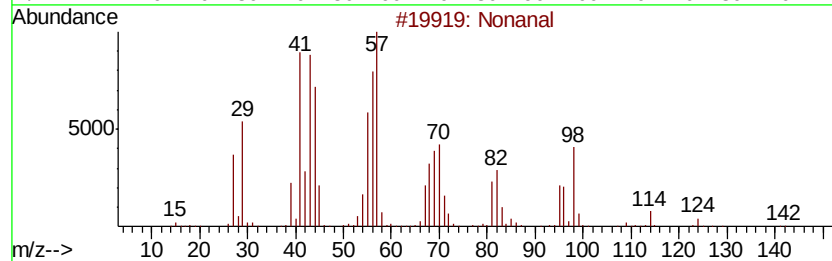
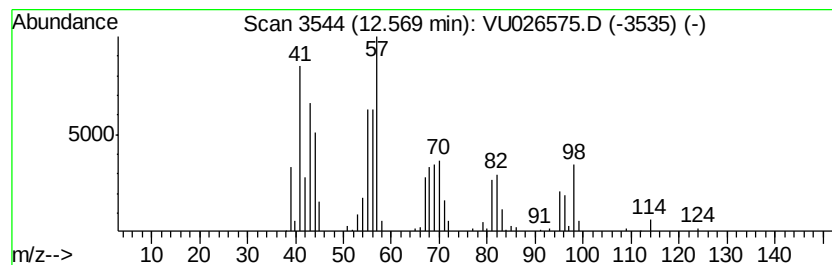
Instrument :
MSVOA_U
ClientSampleId :
BEE18

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 9 Nonanal Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.57	42.47 ug/L	100360	1,4-Dichlorobenzene-d4	11.48
Hit# of	5	Tentative ID	MW MolForm	CAS# Qual
1	Nonanal		142 C9H18O	000124-19-6 91
2	Nonanal		142 C9H18O	000124-19-6 90
3	Nonanal		142 C9H18O	000124-19-6 80
4	6-Hepten-1-ol, 3-methyl-		128 C8H16O	004048-32-2 27
5	Cycloheptane		98 C7H14	000291-64-5 27



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU090618\
Data File : VU026575.D
Acq On : 06 Sep 2018 13:01
Operator : MD/SY
Sample : J4694-01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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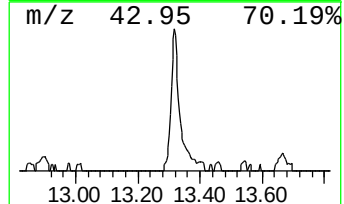
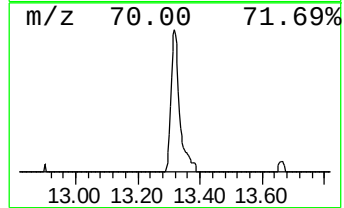
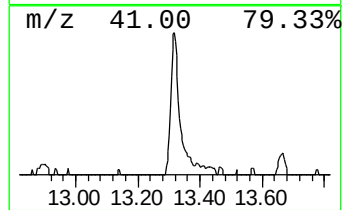
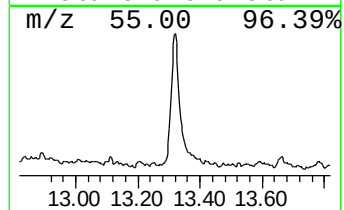
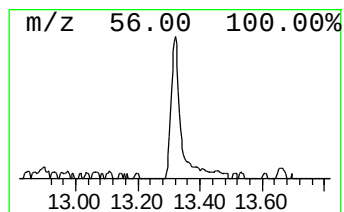
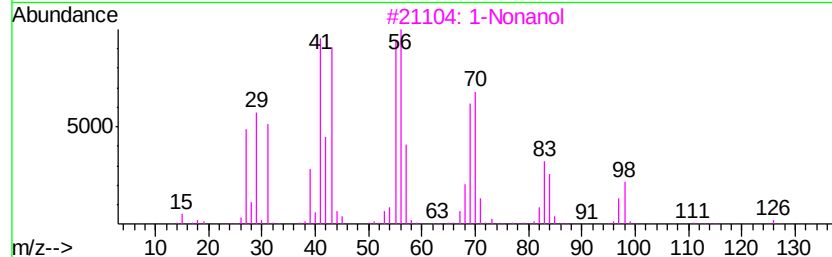
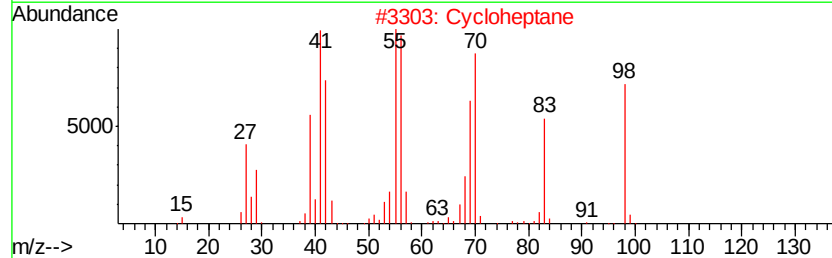
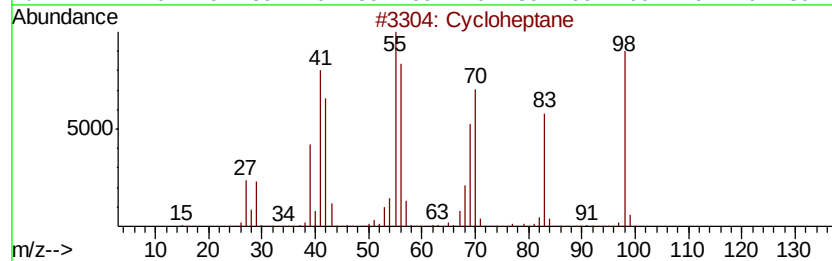
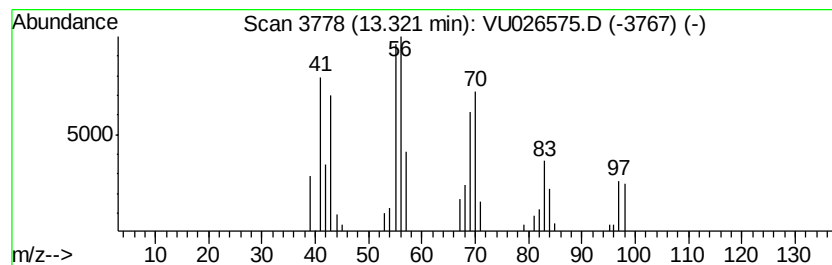
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Quant Title : VOC Analysis

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

Peak Number 10 (DEL) Alkane: Cyclic13.32 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.32	21.76 ug/L	51412	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Cycloheptane	98	C7H14	000291-64-5	93
2		Cycloheptane	98	C7H14	000291-64-5	91
3		1-Nonanol	144	C9H20O	000143-08-8	91
4		1-Nonanol	144	C9H20O	000143-08-8	91
5		1-Nonanol	144	C9H20O	000143-08-8	86



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU090618\
Data File : VU026575.D
Acq On : 06 Sep 2018 13:01
Operator : MD/SY
Sample : J4694-01
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
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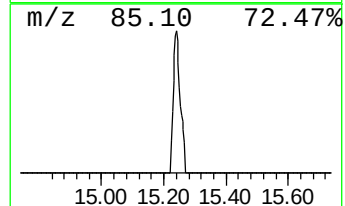
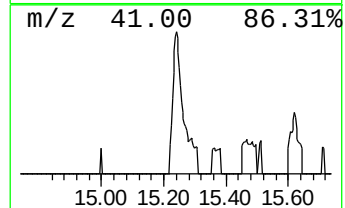
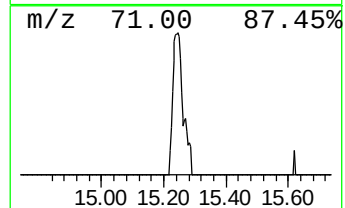
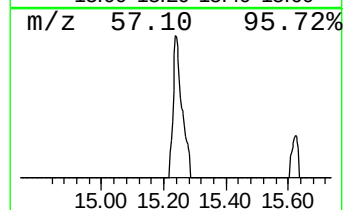
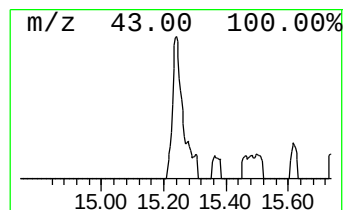
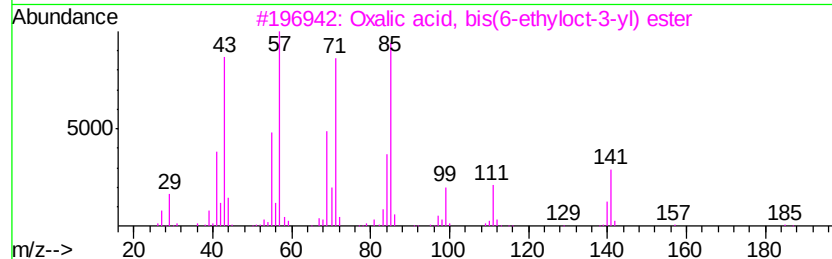
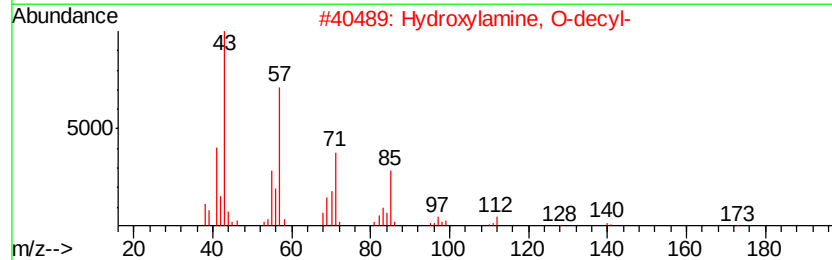
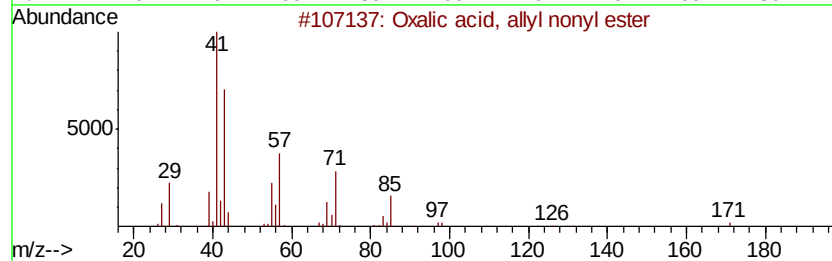
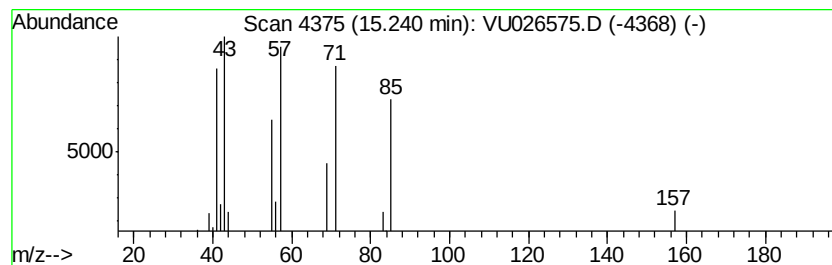
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Quant Title : VOC Analysis

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

Peak Number 11 Oxalic acid, allyl nonyl ester Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
15.24	3.95 ug/L	9345	1,4-Dichlorobenzene-d4	11.48

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Oxalic acid, allyl nonyl ester	256	C14H24O4	1000309-23-7	72
2		Hydroxylamine, O-decyl-	173	C10H23NO	029812-79-1	59
3		Oxalic acid, bis(6-ethyloct-3-yl...)	370	C22H42O4	1000309-34-6	53
4		Sulfurous acid, dodecyl 2-propyl...	292	C15H32O3S	1000309-12-3	53
5		Oxalic acid, allyl octyl ester	242	C13H22O4	1000309-23-6	50



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU090618\
Data File : VU026575.D
Acq On : 06 Sep 2018 13:01
Operator : MD/SY
Sample : J4694-01
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 4 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BEE18

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

TIC Top Hit name	RT	EstConc	Units	Response	--Internal Standard--			
					#	RT	Resp	Conc
Acetaldehyde	1.49	710.9	ug/L	2642520	1	5.89	185852	50.0
Furan	2.13	7.7	ug/L	28542	1	5.89	185852	50.0
2-Propenal	2.21	37.7	ug/L	140225	1	5.89	185852	50.0
Furfural	9.44	42.4	ug/L	161421	2	9.09	190487	50.0
2(5H)-Furanone	11.17	5.9	ug/L	13923	3	11.48	118159	50.0
Nonanal	12.57	42.5	ug/L	100360	3	11.48	118159	50.0
(DEL) Alkane: Cyc...	13.32	21.8	ug/L	51412	3	11.48	118159	50.0
Oxalic acid, ally...	15.24	4.0	ug/L	9345	3	11.48	118159	50.0