

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU090518\
 Data File : VU026543.D
 Acq On : 05 Sep 2018 14:09
 Operator : MD/SY
 Sample : J4694-14
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BEE32

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	0.699	31	34	36	rBV	133	114	0.002%	0.0002%
2	0.777	56	58	60	rBV	151	100	0.002%	0.0002%
3	0.841	76	78	82	rBB	152	128	0.002%	0.0003%
4	1.018	131	133	136	rBB	140	96	0.002%	0.0002%
5	1.088	137	155	168	rBV	204094	234194	44.46%	4.944%
6	1.182	180	184	193	rBV2	11706	13647	2.59%	0.288%
7	1.355	218	238	241	rBV3	60673	162892	30.92%	3.439%
8	1.680	334	339	355	rVB	57354	77749	14.76%	1.641%
9	2.272	512	523	532	rBV	100809	153795	29.20%	3.247%
10	2.323	533	539	550	rVB	17865	27026	5.13%	0.571%
11	2.477	578	587	597	rBV	6442	10400	1.97%	0.220%
12	3.436	876	885	895	rVB2	1331	2678	0.51%	0.057%
13	3.538	912	917	920	rBV	213	205	0.04%	0.004%
14	3.571	924	927	931	rVV	114	83	0.02%	0.002%
15	4.178	1102	1116	1125	rBV2	47442	117884	22.38%	2.489%
16	4.410	1186	1188	1191	rVB	167	88	0.002%	0.0002%
17	4.651	1246	1263	1284	rBV	89192	206133	39.13%	4.352%
18	4.728	1284	1287	1288	rBV2	155	107	0.002%	0.0002%
19	4.995	1360	1370	1387	rVB5	4610	9937	1.89%	0.210%
20	5.056	1387	1389	1393	rBV	271	213	0.04%	0.004%
21	5.342	1453	1478	1511	rBV2	172599	526752	100.00%	11.121%
22	5.509	1527	1530	1534	rBV	200	107	0.002%	0.0002%
23	5.796	1614	1619	1624	rBV2	190	294	0.06%	0.006%
24	5.889	1631	1648	1668	rBV	199027	382496	72.61%	8.075%
25	6.008	1680	1685	1692	rVB4	718	971	0.18%	0.021%
26	6.191	1729	1742	1757	rBV	26716	49894	9.47%	1.053%
27	6.333	1772	1786	1804	rBV	124528	243775	46.28%	5.147%
28	6.834	1938	1942	1945	rBV2	179	128	0.002%	0.0003%
29	6.857	1945	1949	1950	rVV	208	161	0.003%	0.0003%
30	6.866	1950	1952	1956	rVB	393	249	0.05%	0.005%
31	7.079	2015	2018	2022	rBV	103	83	0.002%	0.0002%
32	7.230	2054	2065	2084	rVB	39778	69005	13.10%	1.457%
33	7.384	2110	2113	2117	rVB	178	90	0.002%	0.0002%
34	7.468	2130	2139	2154	rBV2	2030	2974	0.56%	0.063%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU090518\
 Data File : VU026543.D
 Acq On : 05 Sep 2018 14:09
 Operator : MD/SY
 Sample : J4694-14
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BEE32

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

35	7.567	2157	2170	2186	rBV	227973	391604	74.34%	8.268%
36	7.699	2209	2211	2213	rBV2	277	145	0.03%	0.003%
37	7.709	2213	2214	2218	rVB	470	163	0.03%	0.003%
38	7.744	2221	2225	2231	rBV2	319	448	0.09%	0.009%
39	7.853	2245	2259	2272	rBV	28347	47033	8.93%	0.993%
40	7.934	2279	2284	2287	rBV2	399	426	0.08%	0.009%
41	7.963	2291	2293	2297	rVB	274	192	0.04%	0.004%
42	7.988	2297	2301	2304	rBV2	151	164	0.03%	0.003%
43	8.008	2304	2307	2309	rVB2	243	156	0.03%	0.003%
44	8.033	2313	2315	2319	rVB	132	93	0.02%	0.002%
45	8.075	2326	2328	2334	rVB	146	97	0.02%	0.002%
46	8.181	2349	2361	2371	rBV2	17974	36061	6.85%	0.761%
47	8.313	2391	2402	2426	rVB	161101	273973	52.01%	5.784%
48	8.416	2432	2434	2439	rVB2	442	256	0.05%	0.005%
49	8.490	2454	2457	2464	rVB2	269	230	0.04%	0.005%
50	8.522	2464	2467	2470	rBV	217	133	0.03%	0.003%
51	8.599	2488	2491	2493	rBV	201	103	0.02%	0.002%
52	8.779	2544	2547	2551	rBV	146	112	0.02%	0.002%
53	8.876	2575	2577	2584	rVB	170	79	0.01%	0.002%
54	9.091	2632	2644	2661	rBV	284384	456815	86.72%	9.645%
55	9.255	2691	2695	2701	rVV2	340	405	0.08%	0.009%
56	9.394	2726	2738	2772	rBV	60147	121123	22.99%	2.557%
57	9.570	2789	2793	2795	rVB3	252	172	0.03%	0.004%
58	9.583	2795	2797	2802	rVV2	170	112	0.02%	0.002%
59	9.631	2809	2812	2819	rVB	180	120	0.02%	0.003%
60	9.667	2820	2823	2825	rVB	140	80	0.02%	0.002%
61	9.789	2859	2861	2865	rVB	245	144	0.03%	0.003%
62	9.959	2911	2914	2915	rBV	249	89	0.02%	0.002%
63	10.185	2974	2984	3002	rVB3	4010	7925	1.50%	0.167%
64	10.371	3039	3042	3044	rBV2	287	172	0.03%	0.004%
65	10.432	3050	3061	3081	rBV	172285	273655	51.95%	5.778%
66	10.506	3082	3084	3087	rVB	173	91	0.02%	0.002%
67	10.612	3108	3117	3129	rVB2	6104	10957	2.08%	0.231%
68	10.718	3147	3150	3153	rBV	166	90	0.02%	0.002%
69	10.799	3173	3175	3180	rVB	150	95	0.02%	0.002%
70	10.885	3194	3202	3205	rVB	197	288	0.05%	0.006%
71	10.921	3205	3213	3222	rBV2	3266	4232	0.80%	0.089%

Data Path : Z:\VOASRV\HPCHEM1\MSVOA U\DATA\VU090518\
 Data File : VU026543.D
 Acq On : 05 Sep 2018 14:09
 Operator : MD/SY
 Sample : J4694-14
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 17 Sample Multiplier: 1

Instrument :
 MSVOA_U
 ClientSampleId :
 BEE32

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

72	11.088	3263	3265	3268	rBV	215	123	0.02%	0.003%
73	11.123	3274	3276	3281	rBV	176	122	0.02%	0.003%
74	11.178	3291	3293	3295	rBV	154	107	0.02%	0.002%
75	11.229	3305	3309	3311	rBV	161	126	0.02%	0.003%
76	11.294	3322	3329	3341	rVV2	6150	9402	1.78%	0.198%
77	11.487	3377	3389	3408	rVV	252026	395534	75.09%	8.351%
78	11.580	3415	3418	3419	rBV	150	88	0.02%	0.002%
79	11.747	3463	3470	3484	rBV4	1938	2736	0.52%	0.058%
80	11.863	3494	3506	3521	rBV	228203	364034	69.11%	7.686%
81	12.056	3564	3566	3569	rBV	119	92	0.02%	0.002%
82	12.149	3592	3595	3602	rVB	455	455	0.09%	0.010%
83	12.300	3634	3642	3647	rVB4	435	611	0.12%	0.013%
84	12.483	3688	3699	3708	rVB3	1498	2607	0.49%	0.055%
85	12.689	3759	3763	3768	rVB	519	471	0.09%	0.010%
86	12.969	3849	3850	3859	rVB	228	171	0.03%	0.004%
87	13.020	3864	3866	3870	rBV2	154	89	0.02%	0.002%
88	13.053	3874	3876	3881	rBV	161	149	0.03%	0.003%
89	13.104	3891	3892	3895	rVB	184	81	0.02%	0.002%
90	13.381	3976	3978	3986	rBV2	193	163	0.03%	0.003%
91	13.474	4005	4007	4009	rBV	244	115	0.02%	0.002%
92	13.683	4065	4072	4080	rBV3	1966	2558	0.49%	0.054%
93	13.734	4084	4088	4092	rBV2	265	250	0.05%	0.005%
94	13.850	4116	4124	4131	rBV4	2754	3948	0.75%	0.083%
95	13.940	4143	4152	4162	rVV3	16093	24806	4.71%	0.524%
96	13.982	4162	4165	4170	rVB3	471	386	0.07%	0.008%
97	14.091	4196	4199	4200	rBV	207	105	0.02%	0.002%
98	14.281	4249	4258	4266	rBV	1165	1893	0.36%	0.040%
99	15.355	4590	4592	4600	rVB3	485	436	0.08%	0.009%
100	16.567	4963	4969	4976	rBV5	1772	2391	0.45%	0.050%

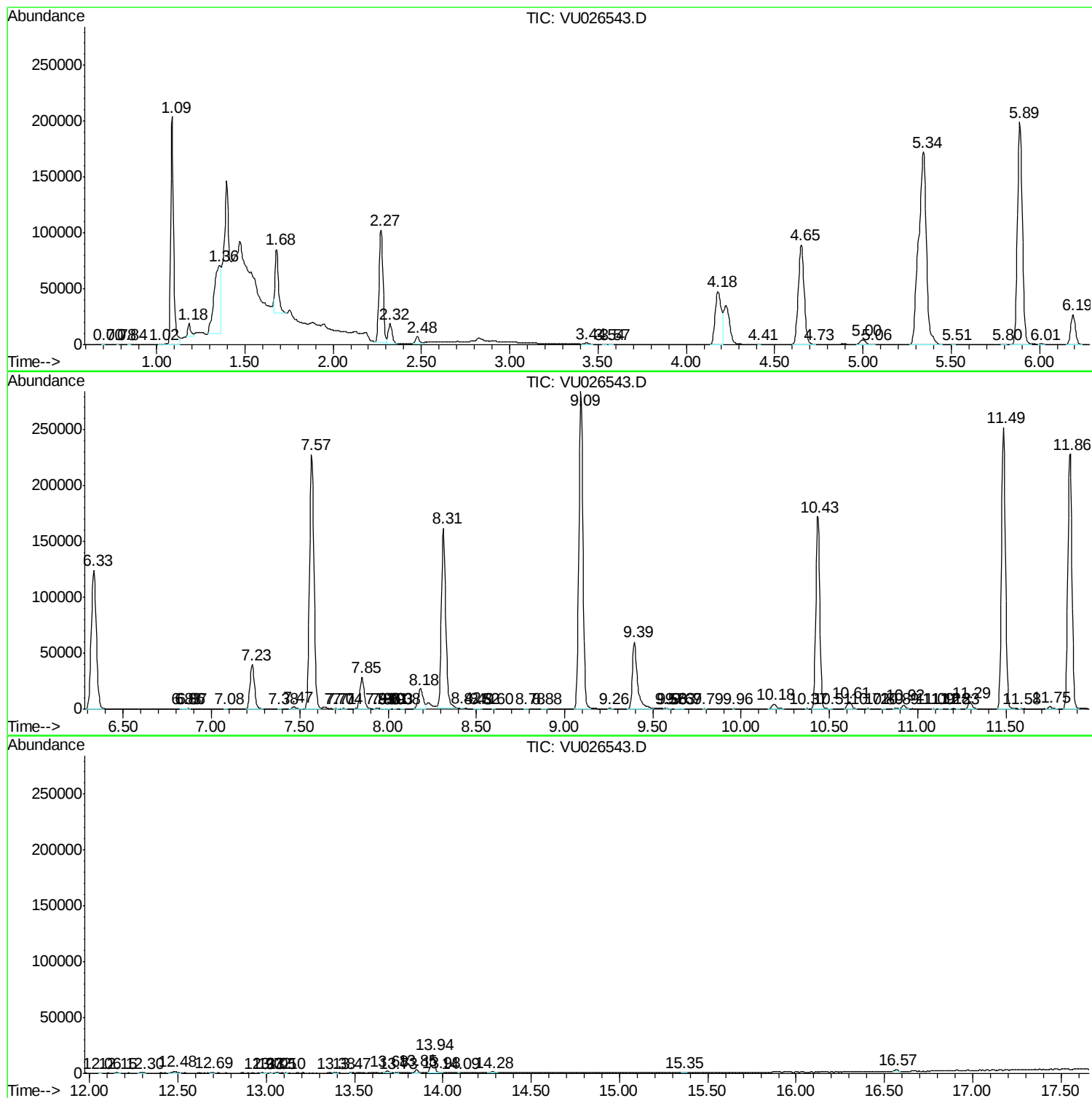
Sum of corrected areas: 4736530

Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU090518\
Data File : VU026543.D
Acq On : 05 Sep 2018 14:09
Operator : MD/SY
Sample : J4694-14
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampled :
BEE32

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



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU090518\
Data File : VU026543.D
Acq On : 05 Sep 2018 14:09
Operator : MD/SY
Sample : J4694-14
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BEE32

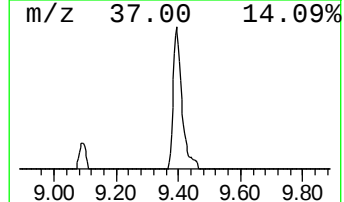
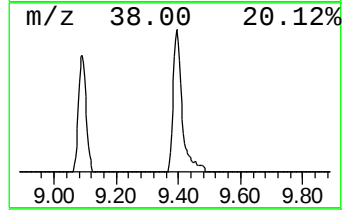
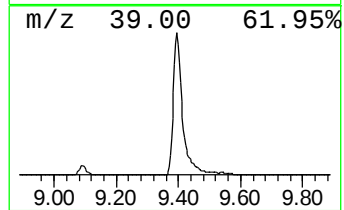
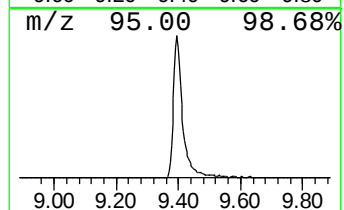
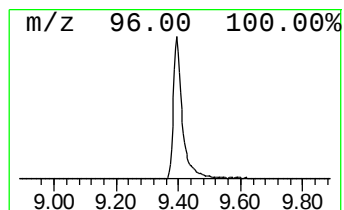
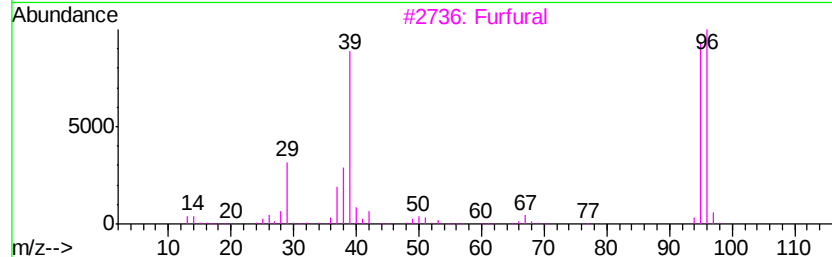
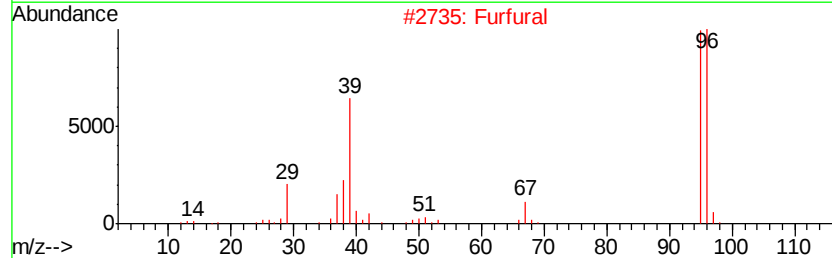
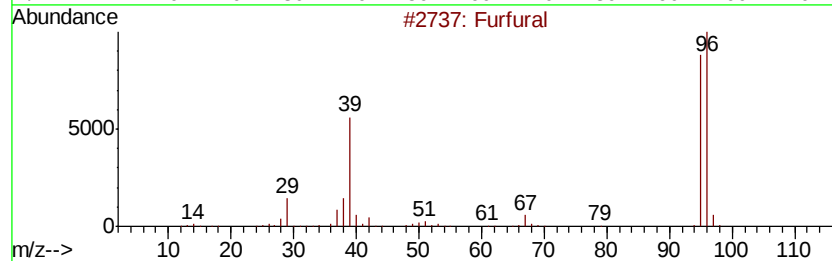
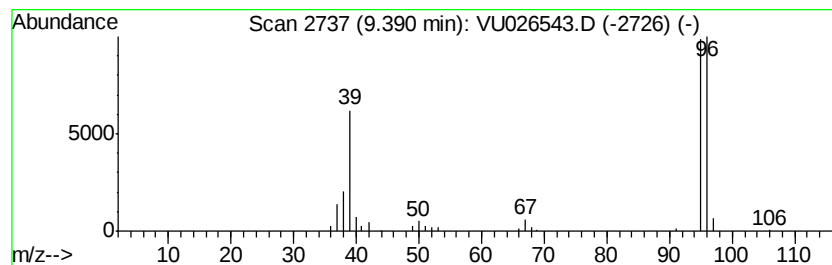
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
Quant Title : VOC Analysis

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

Peak Number 4 Furfural Concentration Rank 2

R.T.	EstConc	Area	Relative to ISTD	R.T.
9.39	13.26 ug/L	121123	Chlorobenzene-d5	9.09

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Furfural	96	C5H4O2	000098-01-1	95
2		Furfural	96	C5H4O2	000098-01-1	95
3		Furfural	96	C5H4O2	000098-01-1	94
4		3-Furaldehyde	96	C5H4O2	000498-60-2	64
5		2(1H)-Pyridinone	95	C5H5NO	000142-08-5	64



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA U\DATA\VU090518\
Data File : VU026543.D
Acq On : 05 Sep 2018 14:09
Operator : MD/SY
Sample : J4694-14
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BEE32

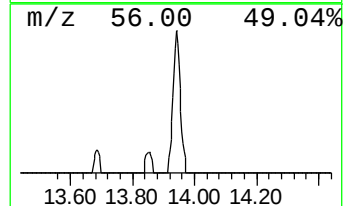
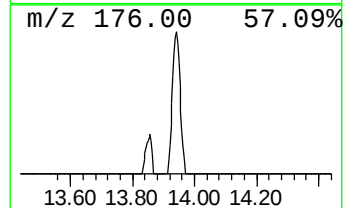
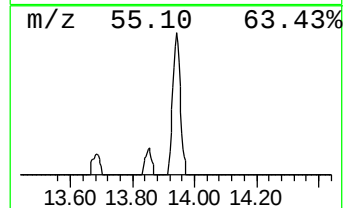
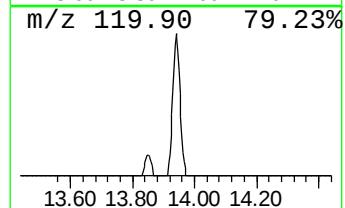
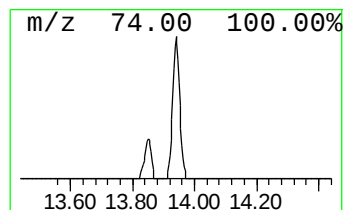
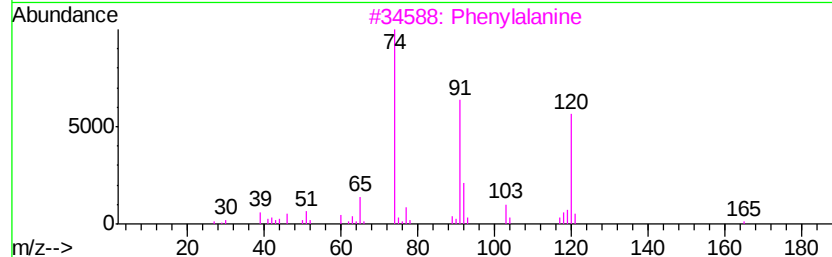
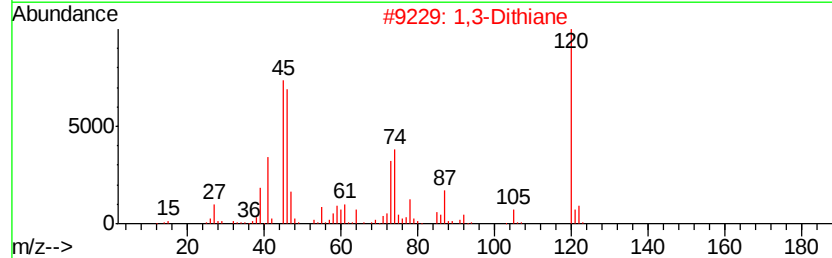
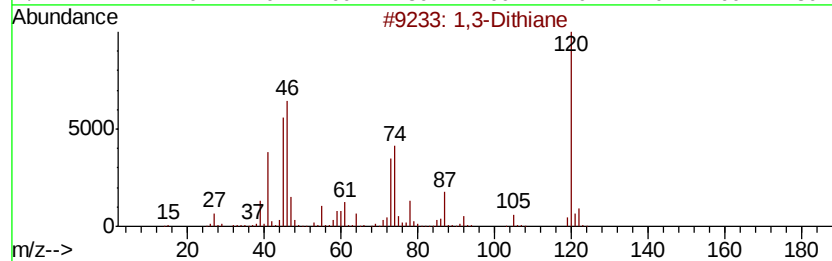
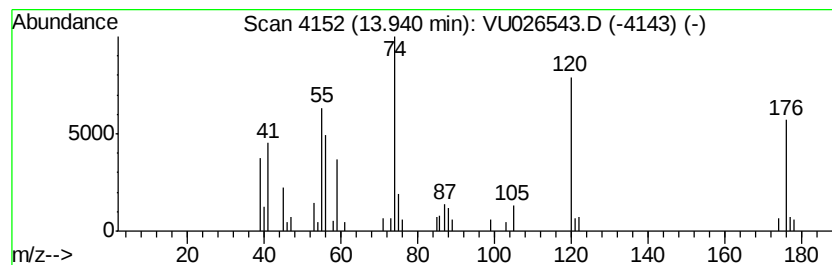
Quant Method : Z:\V0ASRV\HPCHEM1\MSVOA_U\METHOD\SOMULM082918WMA.M
Quant Title : VOC Analysis

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

Peak Number 5 unknown-01 Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
13.94	3.14 ug/L	24806	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	1,3-Dithiane	120	C4H8S2	000505-23-7	27
2		1,3-Dithiane	120	C4H8S2	000505-23-7	27
3		Phenvlalanine	165	C9H11N02	000063-91-2	23
4		D-Ribo-Hexose, 2,6-dideoxy-3-O-m...	162	C7H14O4	013089-76-4	22
5		7-Methoxy-1-tetralone	176	C11H12O2	006836-19-7	22



Data Path : Z:\V0ASRV\HPCHEM1\MSVOA_U\DATA\VU090518\
Data File : VU026543.D
Acq On : 05 Sep 2018 14:09
Operator : MD/SY
Sample : J4694-14
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 17 Sample Multiplier: 1

Instrument :
MSVOA_U
ClientSampleId :
BEE32

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
Furfural	9.39	13.3	ug/L	121123	2	9.09	456815	50.0
unknown-01	13.94	3.1	ug/L	24806	3	11.49	395534	50.0