

Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050718\
 Data File : VU023721.D
 Acq On : 07 May 2018 18:36
 Operator : MD/SY
 Sample : J2725-09
 Misc : 5.0mL/MSVOA U/WATER
 ALS Vial : 19 Sample Multiplier: 1

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 : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.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	1.089	137	155	174	rBV	1226247	1386998	100.00%	10.159%
2	1.185	180	185	195	rVB2	9446	9402	0.68%	0.069%
3	1.294	209	219	231	rBV2	18440	48022	3.46%	0.352%
4	1.400	245	252	283	rVB	152455	182285	13.14%	1.335%
5	1.680	332	339	353	rVB	119209	148073	10.68%	1.085%
6	2.272	513	523	536	rBV	247725	371099	26.76%	2.718%
7	2.445	568	577	594	rVB4	3423	7551	0.54%	0.055%
8	2.616	624	630	642	rVB2	442	899	0.06%	0.007%
9	2.786	678	683	693	rBV5	1247	1965	0.14%	0.014%
10	3.105	775	782	789	rBV	307	538	0.04%	0.004%
11	3.391	868	871	875	rBV2	207	203	0.01%	0.001%
12	3.445	884	888	891	rBV	208	170	0.01%	0.001%
13	3.609	935	939	949	rBV2	532	816	0.06%	0.006%
14	3.725	970	975	978	rBV2	197	196	0.01%	0.001%
15	3.761	982	986	990	rVV2	185	168	0.01%	0.001%
16	3.812	998	1002	1008	rBV2	172	177	0.01%	0.001%
17	4.182	1100	1117	1156	rBV	127601	338710	24.42%	2.481%
18	4.381	1176	1179	1180	rBV2	319	198	0.01%	0.001%
19	4.651	1246	1263	1288	rBV	198790	471720	34.01%	3.455%
20	4.960	1353	1359	1362	rBV	200	220	0.02%	0.002%
21	4.998	1368	1371	1380	rVB4	686	799	0.06%	0.006%
22	5.156	1416	1420	1424	rBV	195	194	0.01%	0.001%
23	5.342	1452	1478	1520	rBV2	411231	1252592	90.31%	9.174%
24	5.786	1612	1616	1618	rBV3	354	264	0.02%	0.002%
25	5.889	1633	1648	1692	rBV	338408	689256	49.69%	5.048%
26	6.156	1728	1731	1735	rVB2	360	288	0.02%	0.002%
27	6.336	1772	1787	1820	rBV	277210	570983	41.17%	4.182%
28	6.500	1835	1838	1840	rVB2	337	185	0.01%	0.001%
29	6.860	1943	1950	1958	rBV2	882	1415	0.10%	0.010%
30	7.233	2052	2066	2089	rBV	151904	273549	19.72%	2.004%
31	7.384	2105	2113	2115	rBV4	537	700	0.05%	0.005%
32	7.567	2154	2170	2189	rBV	565114	990897	71.44%	7.258%
33	7.854	2247	2259	2283	rBV	103370	180050	12.98%	1.319%
34	8.175	2355	2359	2360	rBV2	432	234	0.02%	0.002%

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 Title : VOC Analysis

35	8.313	2390	2402	2433	rBV	439167	750800	54.13%	5.499%
36	8.464	2442	2449	2462	rVB4	9028	15983	1.15%	0.117%
37	8.844	2564	2567	2571	rVB2	376	264	0.02%	0.002%
38	9.091	2631	2644	2671	rBV	503640	828374	59.72%	6.067%
39	9.259	2688	2696	2702	rBV4	1314	2373	0.17%	0.017%
40	9.384	2727	2735	2744	rVB	2558	3699	0.27%	0.027%
41	9.503	2765	2772	2783	rBV5	4567	7124	0.51%	0.052%
42	9.564	2784	2791	2799	rVB2	1275	2229	0.16%	0.016%
43	9.654	2813	2819	2821	rBV	240	257	0.02%	0.002%
44	9.786	2856	2860	2867	rVB4	896	991	0.07%	0.007%
45	10.014	2928	2931	2937	rBV4	354	354	0.03%	0.003%
46	10.172	2970	2980	2988	rBV	6772	10345	0.75%	0.076%
47	10.435	3049	3062	3087	rVB	416668	655633	47.27%	4.802%
48	10.612	3113	3117	3121	rVB3	443	430	0.03%	0.003%
49	10.776	3165	3168	3170	rVB	295	177	0.01%	0.001%
50	10.857	3184	3193	3203	rBV4	2844	4558	0.33%	0.033%
51	10.976	3222	3230	3238	rBV2	1998	2863	0.21%	0.021%
52	11.043	3247	3251	3254	rBV2	342	338	0.02%	0.002%
53	11.104	3263	3270	3278	rVB3	3398	5031	0.36%	0.037%
54	11.140	3278	3281	3284	rBV2	836	797	0.06%	0.006%
55	11.284	3321	3326	3328	rBV3	686	615	0.04%	0.005%
56	11.329	3331	3340	3357	rVB2	6371	10004	0.72%	0.073%
57	11.406	3361	3364	3367	rBV3	403	247	0.02%	0.002%
58	11.487	3377	3389	3408	rBV	544730	856069	61.72%	6.270%
59	11.609	3424	3427	3429	rBV	269	195	0.01%	0.001%
60	11.693	3445	3453	3461	rVB	6509	9111	0.66%	0.067%
61	11.779	3469	3480	3490	rBV5	6183	12083	0.87%	0.088%
62	11.863	3494	3506	3524	rBV	627285	997425	71.91%	7.305%
63	11.988	3538	3545	3553	rVB3	2021	2937	0.21%	0.022%
64	12.178	3601	3604	3610	rVB	627	513	0.04%	0.004%
65	12.255	3624	3628	3634	rVB2	974	942	0.07%	0.007%
66	12.358	3650	3660	3674	rBV	73108	111728	8.06%	0.818%
67	12.477	3687	3697	3711	rBV2	40237	63677	4.59%	0.466%
68	12.545	3711	3718	3722	rBV6	2102	2522	0.18%	0.018%
69	12.596	3723	3734	3748	rBV	171632	270767	19.52%	1.983%
70	12.696	3757	3765	3769	rBV4	7921	11540	0.83%	0.085%
71	12.779	3785	3791	3804	rVB	107202	171167	12.34%	1.254%

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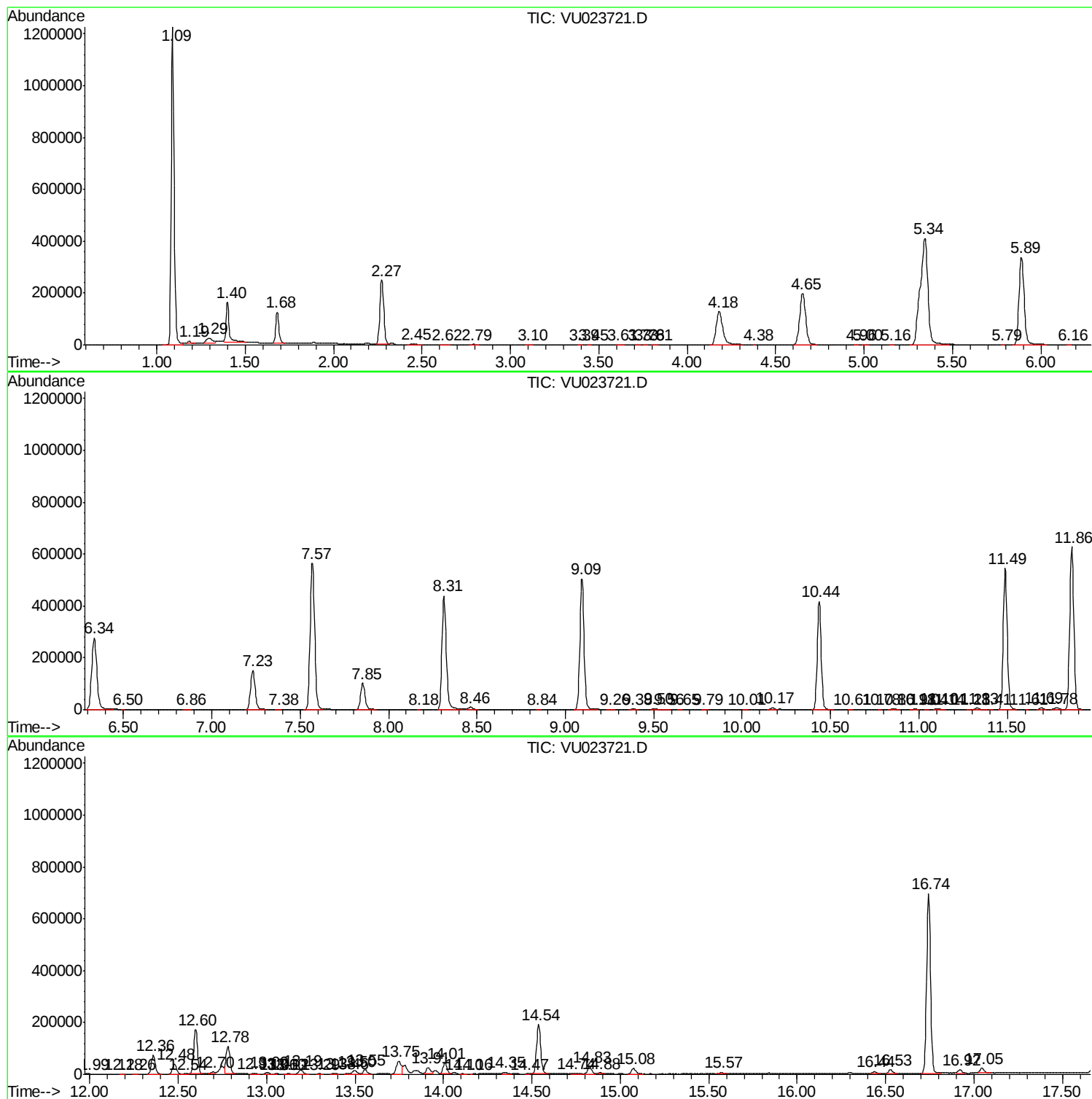
72	12.927	3830	3837	3846	rBV2	4043	5120	0.37%	0.038%
73	13.005	3853	3861	3869	rVB3	7287	10153	0.73%	0.074%
74	13.056	3871	3877	3878	rBV3	1507	1366	0.10%	0.010%
75	13.101	3889	3891	3893	rBV	424	269	0.02%	0.002%
76	13.120	3893	3897	3907	rVV3	1277	1637	0.12%	0.012%
77	13.191	3910	3919	3933	rVB3	16544	27620	1.99%	0.202%
78	13.294	3946	3951	3958	rVB4	1453	1838	0.13%	0.013%
79	13.381	3971	3978	3986	rBV4	3373	4886	0.35%	0.036%
80	13.458	3996	4002	4005	rBV4	2278	2815	0.20%	0.021%
81	13.500	4006	4015	4024	rVV4	12230	24658	1.78%	0.181%
82	13.554	4025	4032	4044	rVB	17729	26658	1.92%	0.195%
83	13.747	4079	4092	4098	rBV	49825	95441	6.88%	0.699%
84	13.914	4135	4144	4151	rBV5	22892	38730	2.79%	0.284%
85	14.008	4165	4173	4183	rVB2	41652	61878	4.46%	0.453%
86	14.104	4200	4203	4211	rBV4	1049	902	0.07%	0.007%
87	14.159	4217	4220	4221	rBV2	540	336	0.02%	0.002%
88	14.345	4274	4278	4290	rVB6	6480	9846	0.71%	0.072%
89	14.474	4314	4318	4322	rBV4	834	845	0.06%	0.006%
90	14.538	4326	4338	4354	rVV	191064	316264	22.80%	2.316%
91	14.741	4395	4401	4414	rVB4	2307	4229	0.30%	0.031%
92	14.828	4417	4428	4438	rBV	28649	46697	3.37%	0.342%
93	14.882	4441	4445	4452	rVB3	4306	5193	0.37%	0.038%
94	15.075	4495	4505	4521	rVB2	22247	37913	2.73%	0.278%
95	15.574	4651	4660	4667	rBV2	5402	8058	0.58%	0.059%
96	16.435	4922	4928	4938	rVB3	7856	11316	0.82%	0.083%
97	16.528	4949	4957	4967	rVB2	14869	23418	1.69%	0.172%
98	16.744	5011	5024	5046	rBV	695317	1089641	78.56%	7.981%
99	16.921	5072	5079	5088	rVB2	12891	18836	1.36%	0.138%
100	17.046	5111	5118	5133	rVB	18169	31615	2.28%	0.232%

Sum of corrected areas: 13653156

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Quant Title : VOC Analysis

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



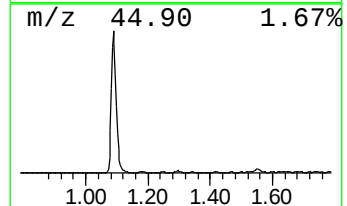
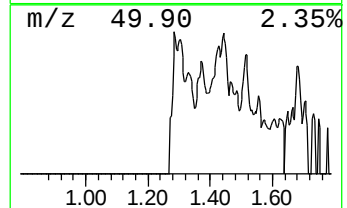
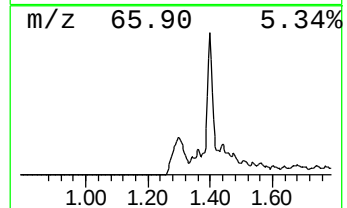
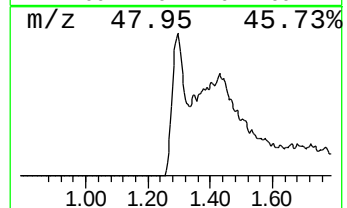
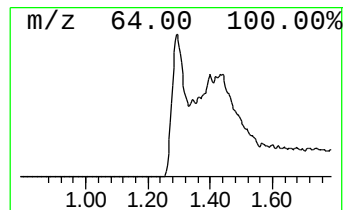
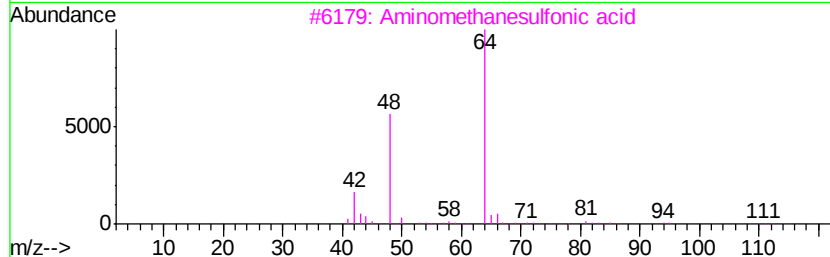
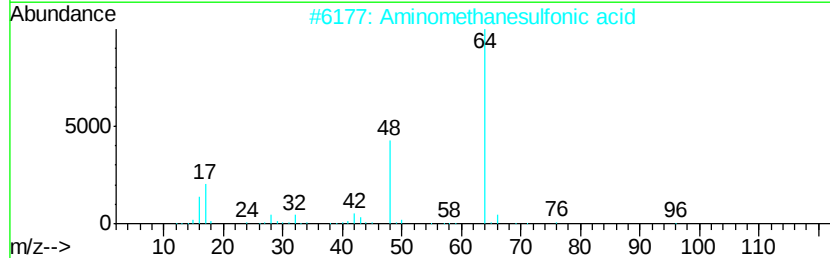
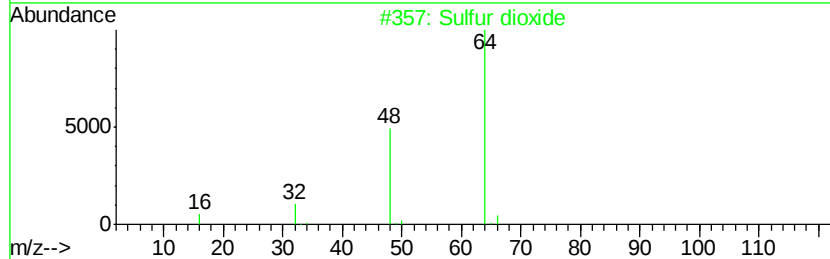
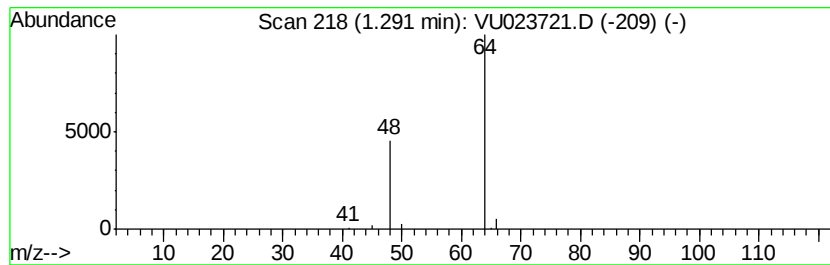
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ALS Vial : 19 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Quant Title : VOC Analysis

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

Peak Number 2 Sulfur dioxide Concentration Rank 11

R.T.	EstConc	Area	Relative to ISTD	R.T.		
1.29	3.48 ug/L	48022	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	74
3	Aminomethanesulfonic acid		111	CH5NO3S	013881-91-9	64
4	L-Alanine, 3-sulfo-		169	C3H7NO5S	000498-40-8	9
5	Sulfur dioxide		64	O2S	007446-09-5	5



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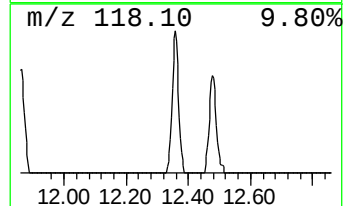
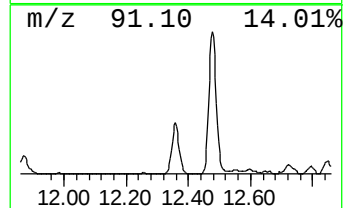
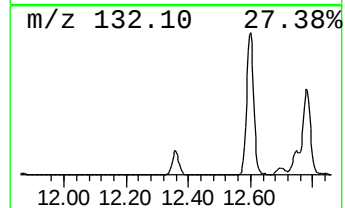
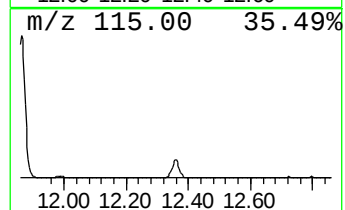
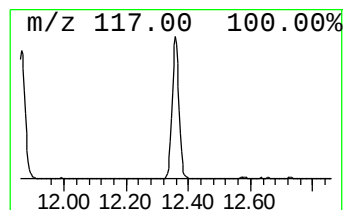
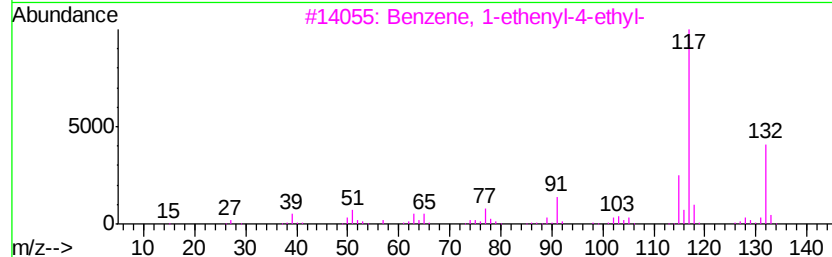
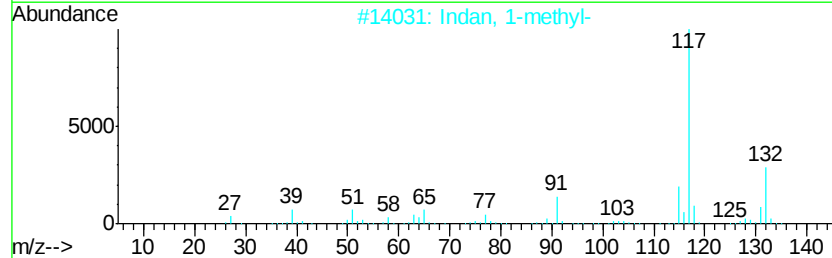
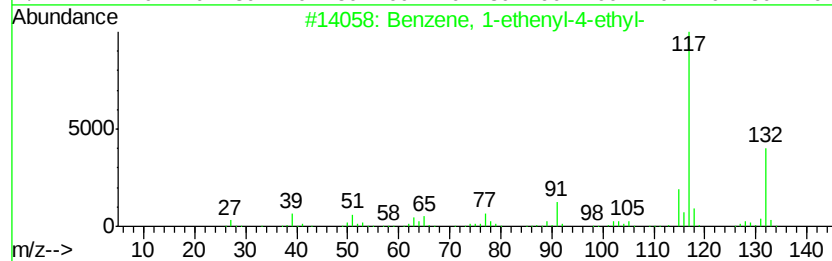
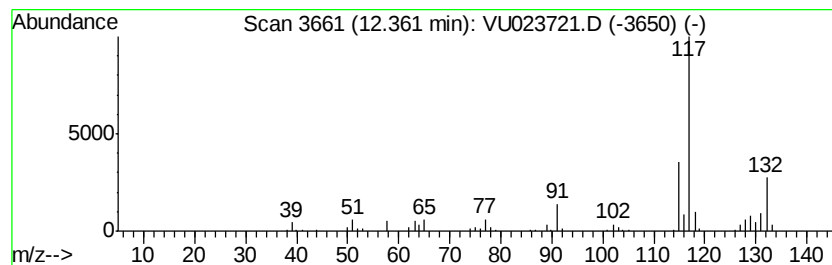
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TIC Library : C:\DATABASE\NIST11.L
TIC Integration Parameters: LSCINT.P

Peak Number 4 Benzene, 1-ethenyl-4-ethyl- Concentration Rank 7

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.36	6.53 ug/L	111728	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	87
2		Indan, 1-methyl-	132	C10H12	000767-58-8	87
3		Benzene, 1-ethenyl-4-ethyl-	132	C10H12	003454-07-7	86
4		Benzene, 1-methyl-4-(2-propenyl)-	132	C10H12	003333-13-9	83
5		Indan, 1-methyl-	132	C10H12	000767-58-8	81



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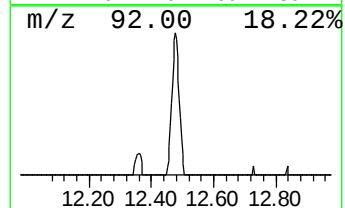
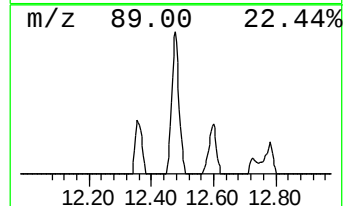
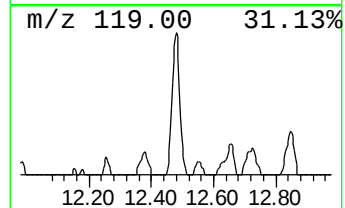
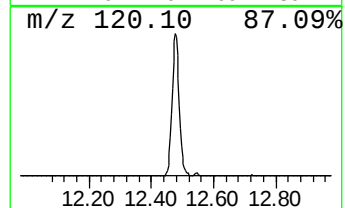
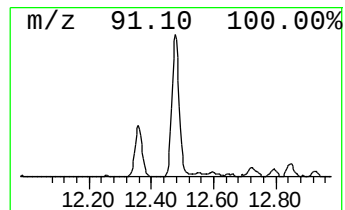
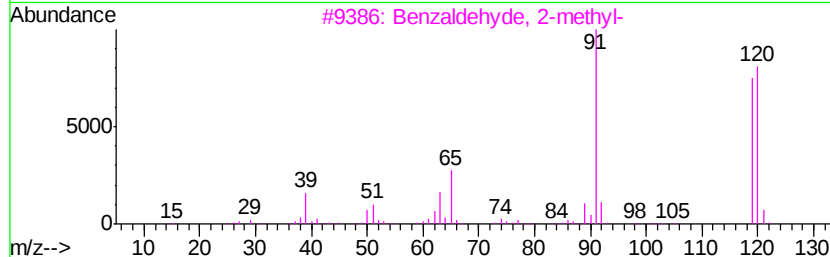
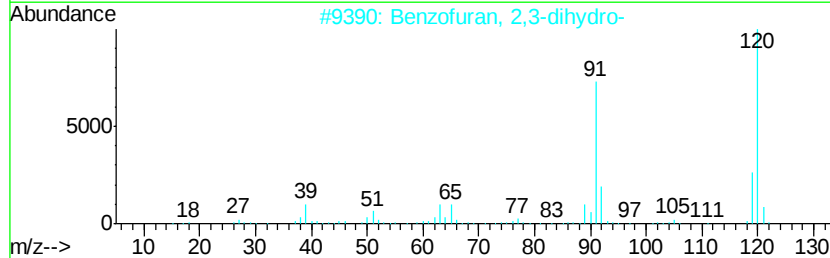
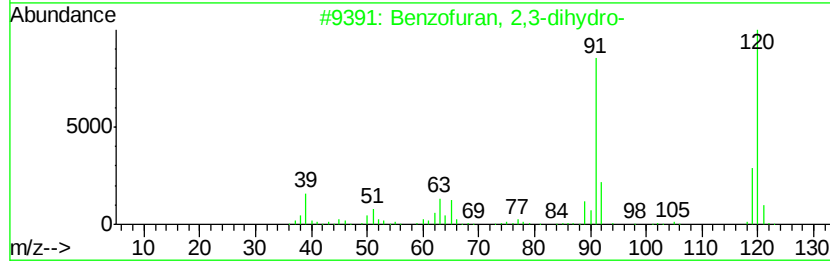
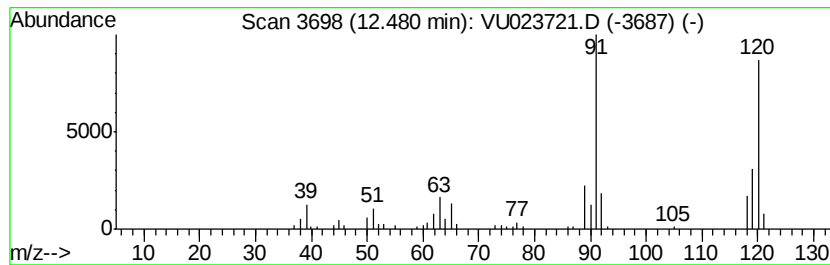
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Quant Title : VOC Analysis

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

Peak Number 5 Benzofuran, 2,3-dihydro- Concentration Rank 9

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.48	3.72 ug/L	63677	1,4-Dichlorobenzene-d4	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		Benzofuran, 2,3-dihydro-	120	C8H8O	000496-16-2	87
2		Benzofuran, 2,3-dihydro-	120	C8H8O	000496-16-2	87
3		Benzaldehyde, 2-methyl-	120	C8H8O	000529-20-4	58
4		Phthalan	120	C8H8O	000496-14-0	58
5		Benzaldehyde, 4-methyl-	120	C8H8O	000104-87-0	53



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Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

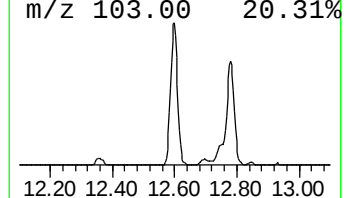
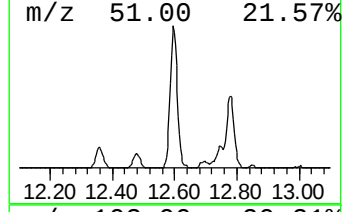
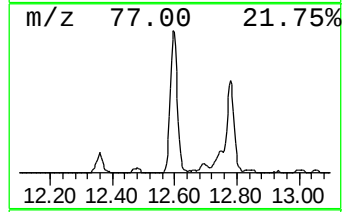
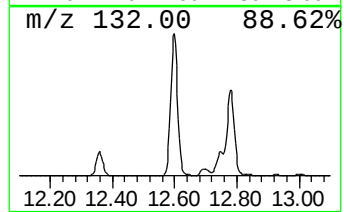
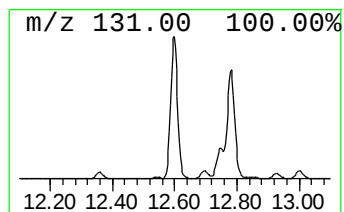
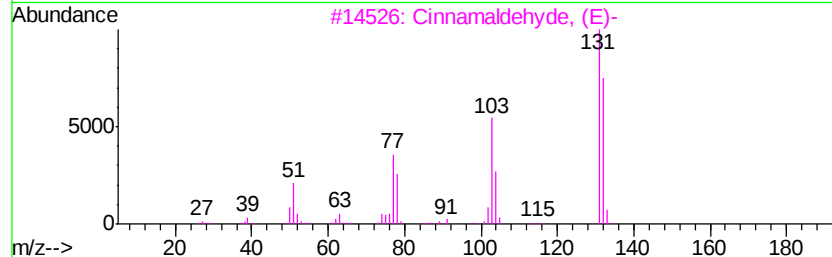
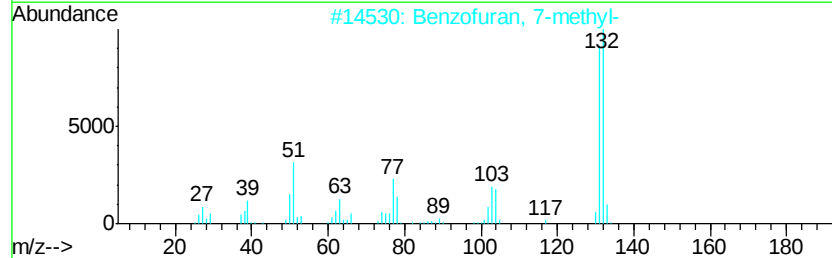
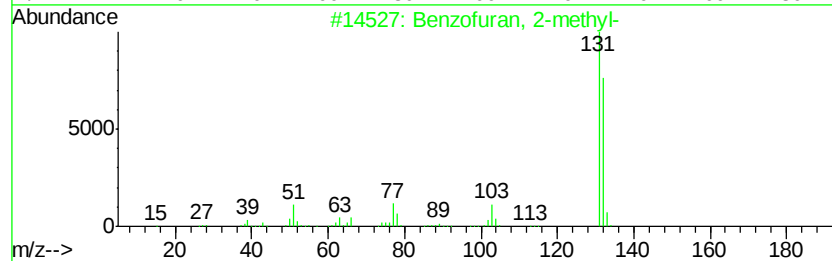
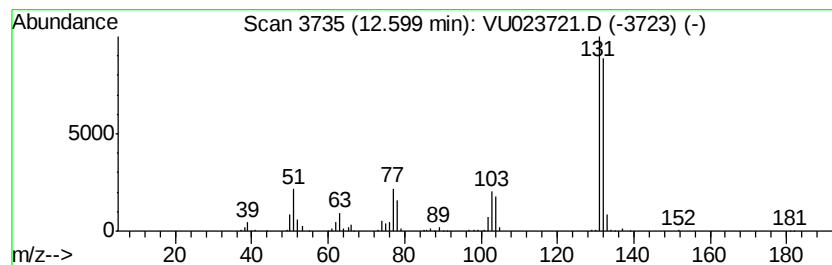
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Quant Title : VOC Analysis

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

Peak Number 6 Benzofuran, 2-methyl- Concentration Rank 5

R.T.	EstConc	Area	Relative to ISTD	R.T.
12.60	15.81 ug/L	270767	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzofuran, 2-methyl-	132	C9H8O	004265-25-2	94
2		Benzofuran, 7-methyl-	132	C9H8O	017059-52-8	94
3		Cinnamaldehyde, (E)-	132	C9H8O	014371-10-9	91
4		3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	91
5		3-Phenyl-2-propyn-1-ol	132	C9H8O	001504-58-1	91



Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050718\
Data File : VU023721.D
Acq On : 07 May 2018 18:36
Operator : MD/SY
Sample : J2725-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

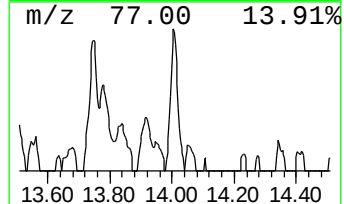
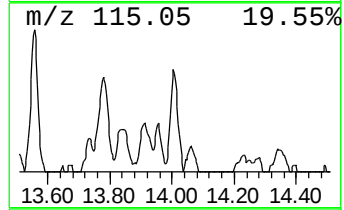
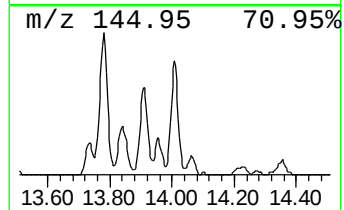
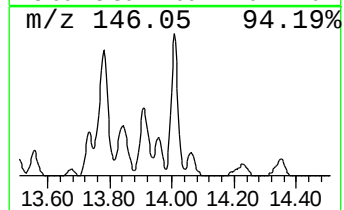
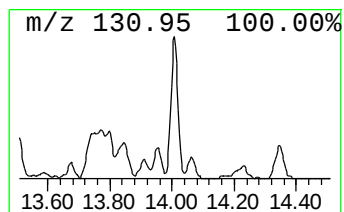
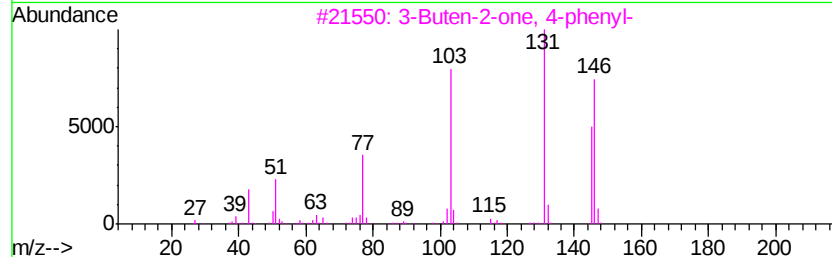
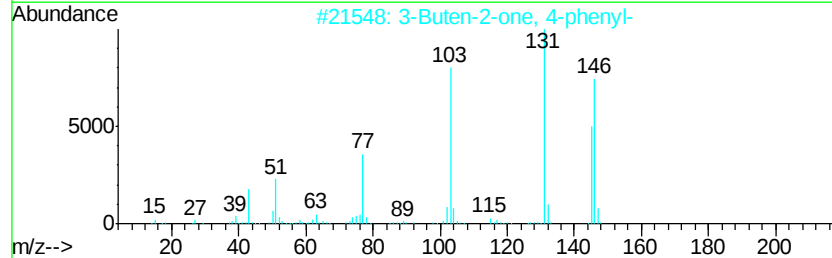
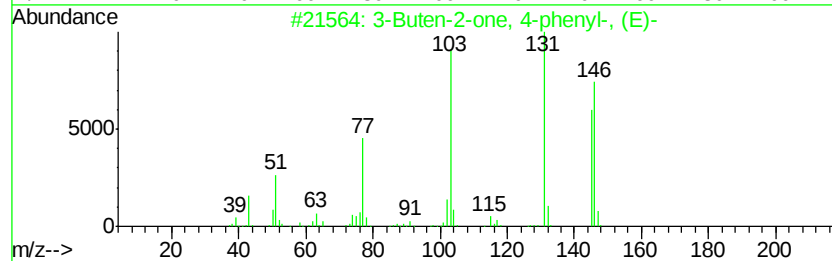
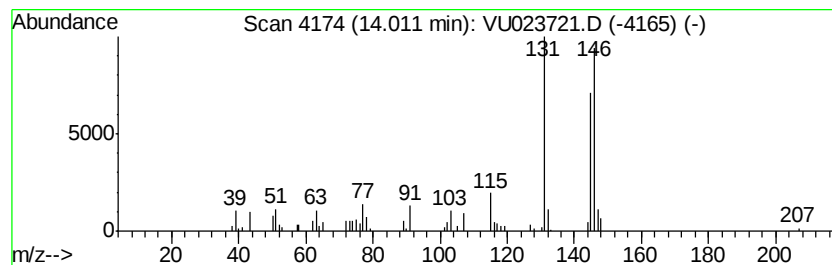
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Quant Title : VOC Analysis

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

Peak Number 9 3-Buten-2-one, 4-phenyl-, (E)- Concentration Rank 10

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.01	3.61 ug/L	61878	1,4-Dichlorobenzene-d4	11.49

Hit# of	5	Tentative ID	MW	MolForm	CAS#	Qual
1		3-Buten-2-one, 4-phenyl-, (E)-	146	C10H10O	001896-62-4	80
2		3-Buten-2-one, 4-phenyl-	146	C10H10O	000122-57-6	74
3		3-Buten-2-one, 4-phenyl-	146	C10H10O	000122-57-6	74
4		1H-Inden-1-one, 2,3-dihydro-3-me...	146	C10H10O	006072-57-7	72
5		Benzene, (3-methyl-2-butenyl)-	146	C11H14	004489-84-3	64



Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050718\
Data File : VU023721.D
Acq On : 07 May 2018 18:36
Operator : MD/SY
Sample : J2725-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

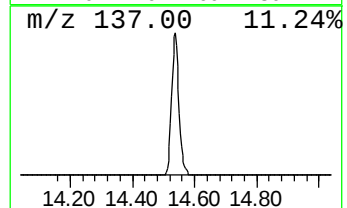
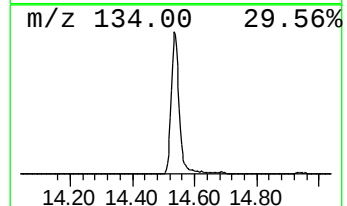
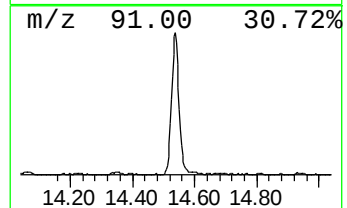
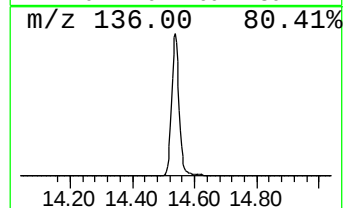
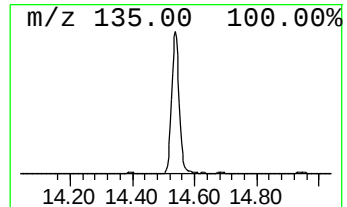
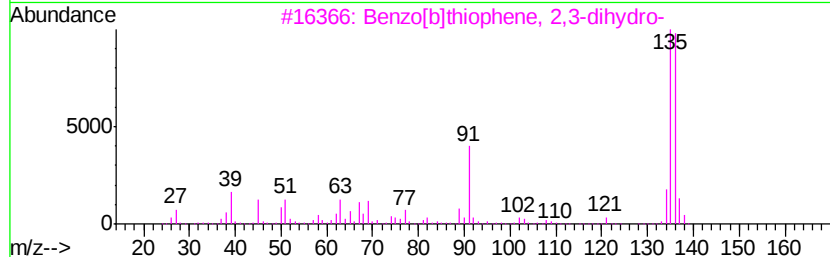
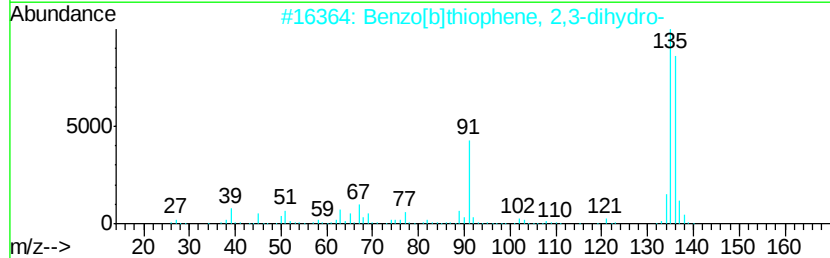
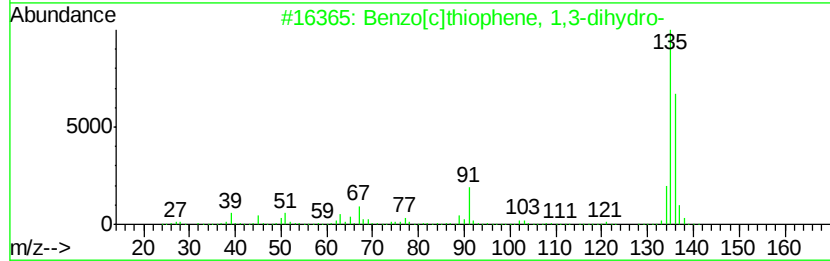
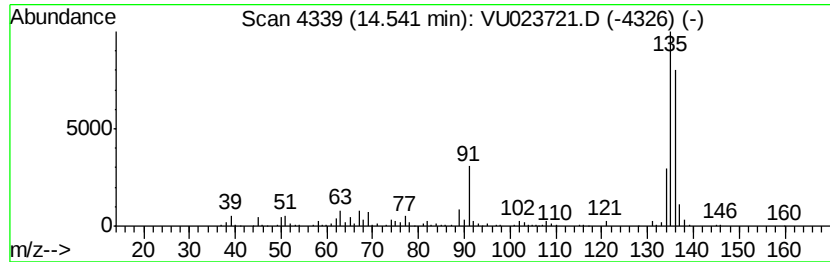
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Quant Title : VOC Analysis

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

Peak Number 10 Benzo[c]thiophene, 1,3-dihy... Concentration Rank 4

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.54	18.47 ug/L	316264	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[c]thiophene, 1,3-dihydro-	136	C8H8S	002471-92-3	93
2		Benzo[b]thiophene, 2,3-dihydro-	136	C8H8S	004565-32-6	93
3		Benzo[b]thiophene, 2,3-dihydro-	136	C8H8S	004565-32-6	76
4		4-Hydroxy-2-methylbenzaldehyde	136	C8H8O2	041438-18-0	72
5		3-Hydroxy-4-methylbenzaldehyde	136	C8H8O2	057295-30-4	72



Data Path : W:\HPCHEM1\MSVOA U\DATA\VU050718\
Data File : VU023721.D
Acq On : 07 May 2018 18:36
Operator : MD/SY
Sample : J2725-09
Misc : 5.0mL/MSVOA U/WATER
ALS Vial : 19 Sample Multiplier: 1

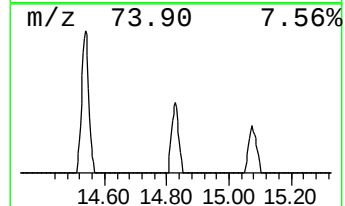
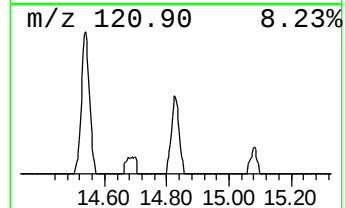
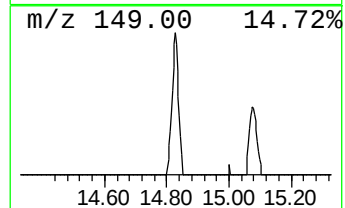
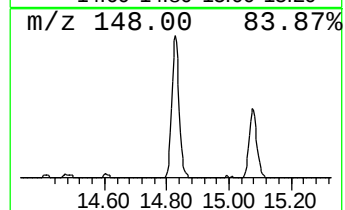
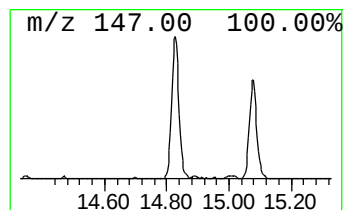
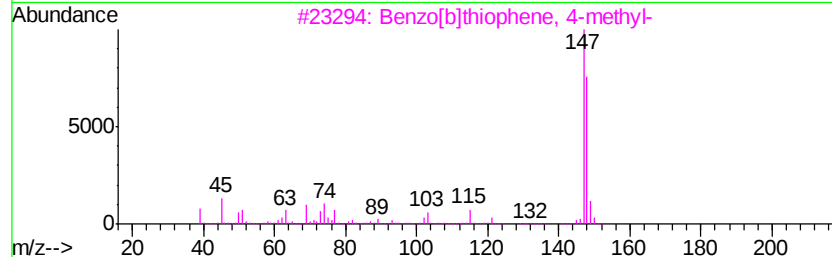
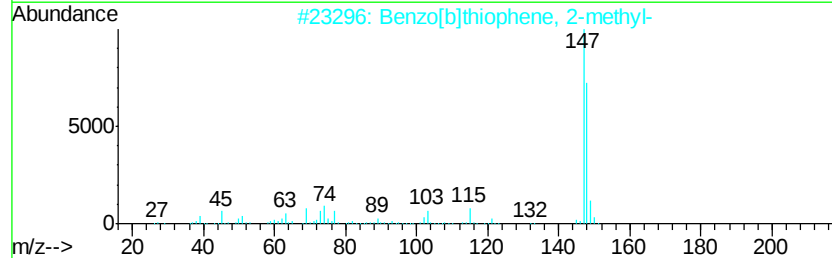
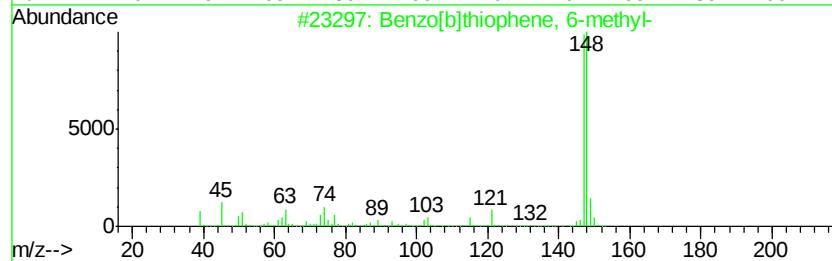
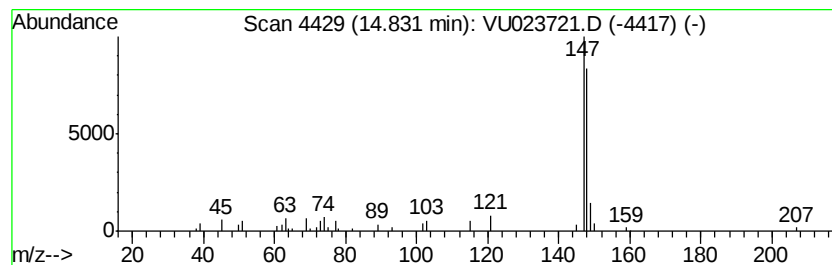
Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.M
Quant Title : VOC Analysis

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

Peak Number 11 Benzo[b]thiophene, 6-methyl- Concentration Rank 12

R.T.	EstConc	Area	Relative to ISTD	R.T.
14.83	2.73 ug/L	46697	1,4-Dichlorobenzene-d4	11.49

Hit#	of	Tentative ID	MW	MolForm	CAS#	Qual
1	5	Benzo[b]thiophene, 6-methyl-	148	C9H8S	016587-47-6	94
2		Benzo[b]thiophene, 2-methyl-	148	C9H8S	001195-14-8	91
3		Benzo[b]thiophene, 4-methyl-	148	C9H8S	014315-11-8	91
4		Benzo[b]thiophene, 2-methyl-	148	C9H8S	001195-14-8	91
5		Benzo[b]thiophene, 5-methyl-	148	C9H8S	014315-14-1	91



Data Path : W:\HPCHEM1\MSVOA_U\DATA\VU050718\
Data File : VU023721.D
Acq On : 07 May 2018 18:36
Operator : MD/SY
Sample : J2725-09
Misc : 5.0mL/MSVOA_U/WATER
ALS Vial : 19 Sample Multiplier: 1

Quant Method : W:\HPCHEM1\MSVOA_U\METHOD\SOMULM050118WMA.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
Sulfur dioxide	1.29	3.5	ug/L	48022	1	5.89	689256	50.0
Benzene, 1-etheny...	12.36	6.5	ug/L	111728	3	11.49	856069	50.0
Benzofuran, 2,3-d...	12.48	3.7	ug/L	63677	3	11.49	856069	50.0
Benzofuran, 2-met...	12.60	15.8	ug/L	270767	3	11.49	856069	50.0
3-Buten-2-one, 4-...	14.01	3.6	ug/L	61878	3	11.49	856069	50.0
Benzo[c]thiophene...	14.54	18.5	ug/L	316264	3	11.49	856069	50.0
Benzo[b]thiophene...	14.83	2.7	ug/L	46697	3	11.49	856069	50.0