

Data File : H:\VOL1\GCMSDATA\J\120720\BJ001043.D
 Acq On : 20 Jul 2012 15:09
 Sample : PB64247BS
 Misc : WATER BNA J HLM
 MS Integration Params: rteint.p
 Quant Time: Jul 20 16:26 2012

Vial: 10
 Operator: HLM
 Inst : BNA J
 Multiplr: 1.00

Quant Results File: BJ072012.RES

Quant Method : H:\VOL1\GCMSDATA\J\METHODS\BJ072012.M (RTE Integrator)
 Title : CWA degradation products by GCMS
 Last Update : Fri Jul 20 14:08:00 2012
 Response via : Initial Calibration
 DataAcq Meth : CWAJ

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	4.65	152	237080	2.00	ug/mL	-0.02
6) Naphthalene-d8	5.95	136	942183	2.00	ug/mL	0.00

System Monitoring Compounds

10) Tripropylphosphate	7.01	99	165684	0.48	ug/mL	0.00
Spiked Amount	0.500	Range	70 - 130	Recovery	=	96.00%
12) 2-Bromothioanisole	7.26	204	323775	4.40	ug/mL	0.00
Spiked Amount	5.000	Range	70 - 130	Recovery	=	88.00%

Target Compounds

	R.T.	QIon	Response	Conc	Units	Ovalue
2) Dimethyl Disulfide	2.70	94	302940	3.41	ug/mL	95
3) DMMP	3.54	79	130884	1.23	ug/mL	95
4) DIMP	4.92	97	790017	3.58	ug/mL#	79
5) 1,4-Oxathiane	3.67	46	494529	4.48	ug/mL	84
7) 1,4-Dithiane	5.09	46	375416	4.24	ug/mL#	86
8) Thiodiglycol	5.89	61	2306508	30.69	ug/mL	98
9) Benzothiazole	6.25	135	2226128	9.17	ug/mL	93
11) p-Chlorophenylmethyldisulfid	6.50	158	1265236	8.51	ug/mL	90
13) p-Chlorophenylmethyldisulfox	7.94	159	748780	8.41	ug/mL	97
14) p-Chlorophenylmethyldisulfon	8.14	111	1052698	7.09	ug/mL	93

Quantitation Report

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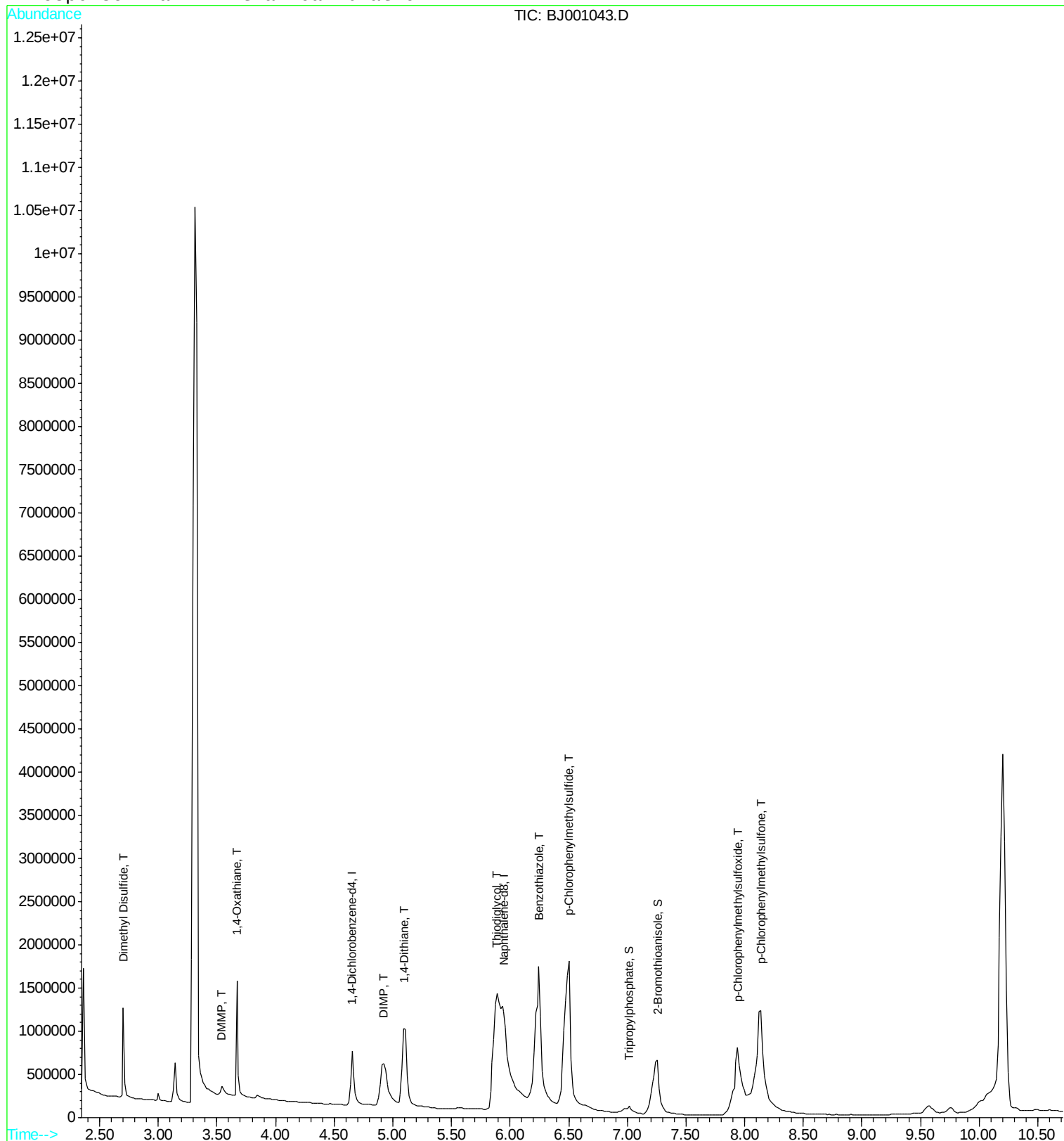
Quant Results File: BJ072012.RES

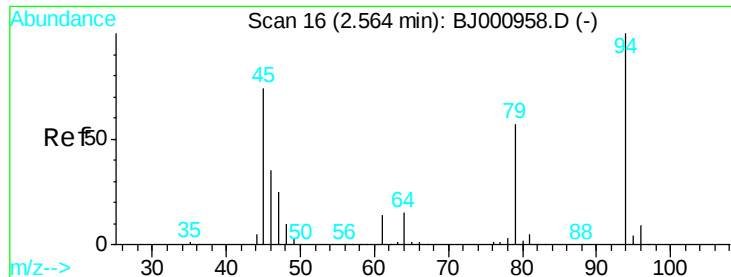
Method : H:\VOL1\GCMSDATA\J\METHODS\BJ072012.M (RTE Integrator)

Title : CWA degradation products by GCMS

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#2

Dimethyl Disulfide

Concen: 3.41 ug/mL

RT: 2.70 min Scan# 26

Delta R.T. 0.12 min

Lab File: BJ001043.D

Acq: 20 Jul 2012 15:09

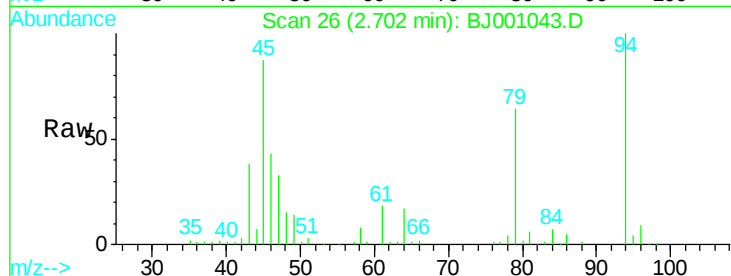
Tgt Ion: 94 Resp: 302940

Ion Ratio Lower Upper

94 100

45 86.9 75.2 115.2

79 63.6 43.1 83.1

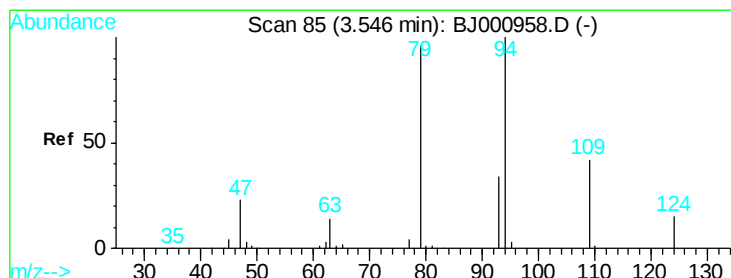
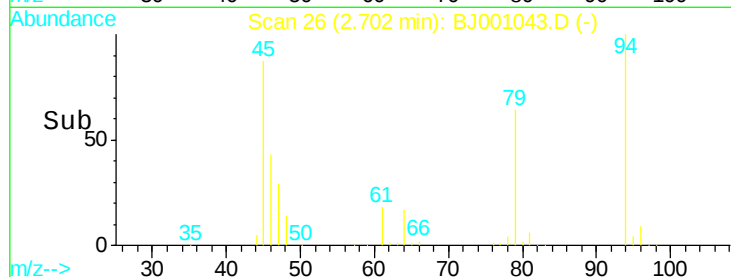
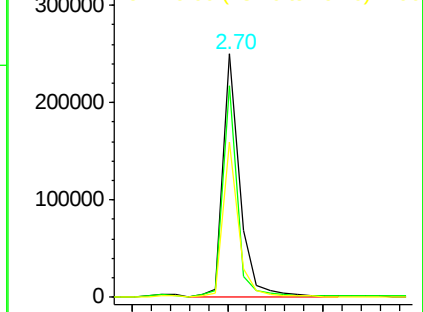


Abundance

Ion 94.00 (93.70 to 94.70): BJ0

Ion 45.00 (44.70 to 45.70): BJ0

Ion 79.00 (78.70 to 79.70): BJ0



#3

DMMP

Concen: 1.23 ug/mL

RT: 3.54 min Scan# 85

Delta R.T. -0.00 min

Lab File: BJ001043.D

Acq: 20 Jul 2012 15:09

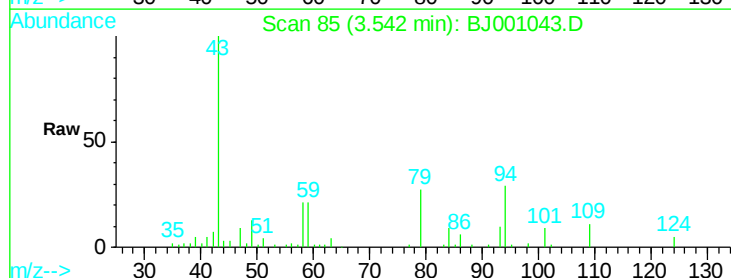
Tgt Ion: 79 Resp: 130884

Ion Ratio Lower Upper

79 100

94 108.0 83.0 123.0

109 42.4 20.0 60.0

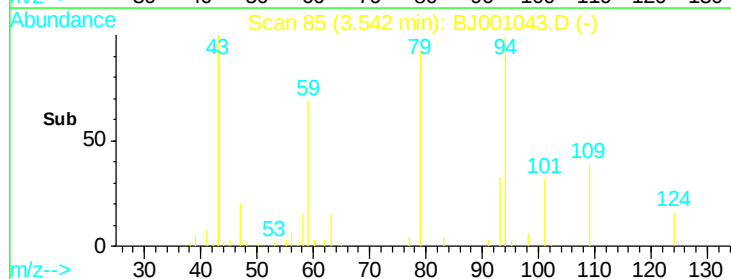
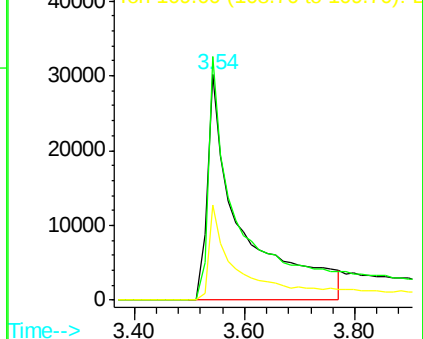


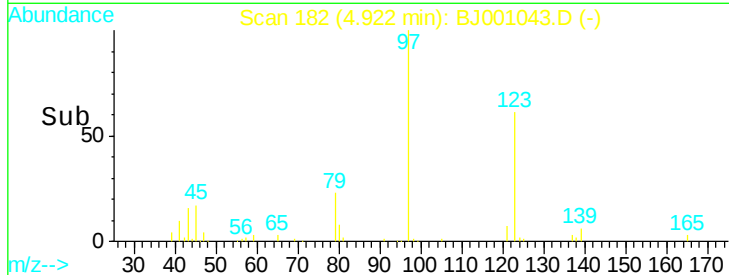
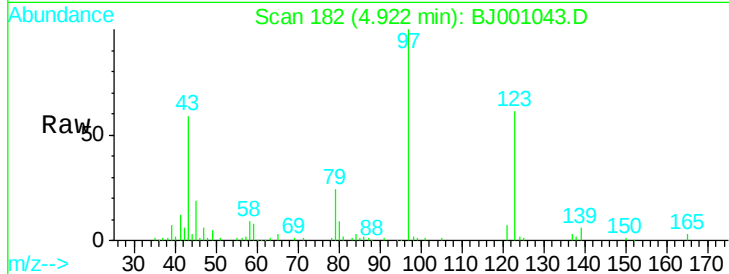
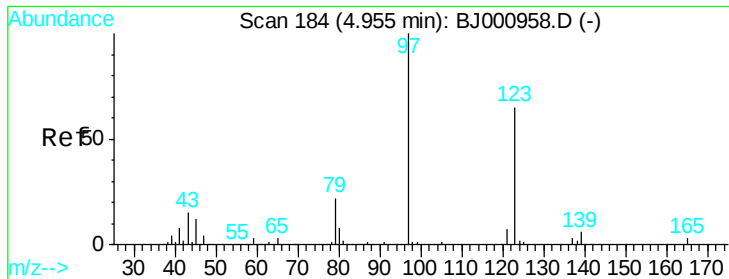
Abundance

Ion 79.00 (78.70 to 79.70): BJ0

Ion 94.00 (93.70 to 94.70): BJ0

Ion 109.00 (108.70 to 109.70): BJ0





#4

DIMP

Concen: 3.58 ug/mL

RT: 4.92 min Scan# 182

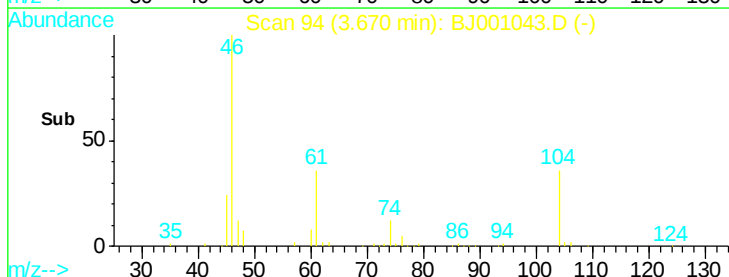
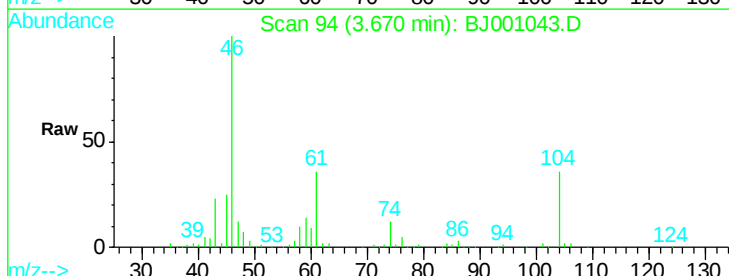
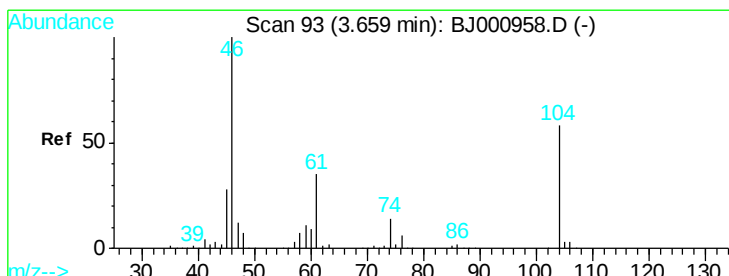
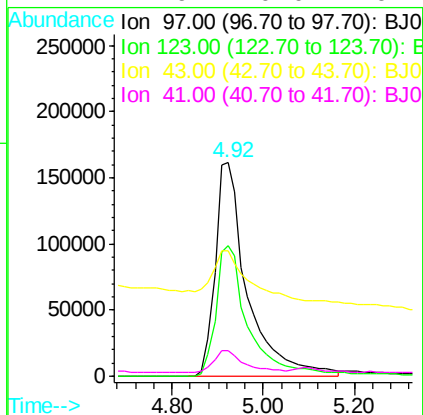
Delta R.T. -0.02 min

Lab File: BJ001043.D

Acq: 20 Jul 2012 15:09

Tgt Ion: 97 Resp: 790017

Ion	Ratio	Lower	Upper
97	100		
123	61.0	43.8	83.8
43	58.6	0.0	38.6
41	11.9	0.0	29.1



#5

1,4-Oxathiane

Concen: 4.48 ug/mL

RT: 3.67 min Scan# 94

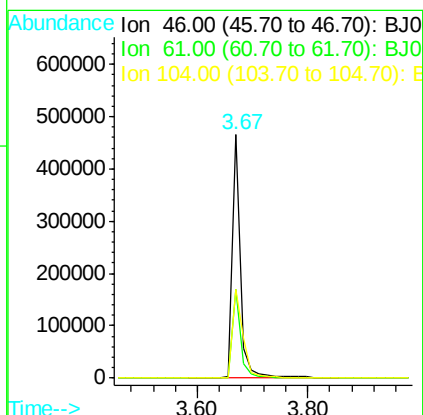
Delta R.T. 0.02 min

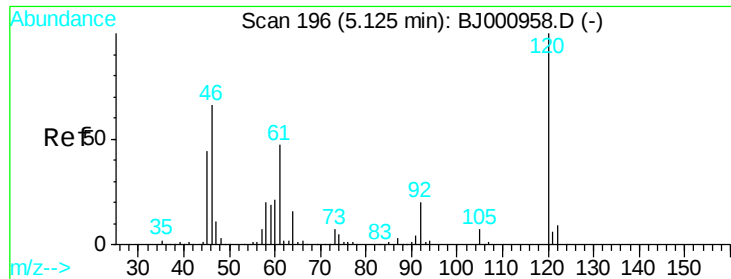
Lab File: BJ001043.D

Acq: 20 Jul 2012 15:09

Tgt Ion: 46 Resp: 494529

Ion	Ratio	Lower	Upper
46	100		
61	36.4	19.4	59.4
104	36.4	34.1	74.1





#7

1,4-Dithiane

Concen: 4.24 ug/mL

RT: 5.09 min Scan# 194

Delta R.T. -0.02 min

Lab File: BJ001043.D

Acq: 20 Jul 2012 15:09

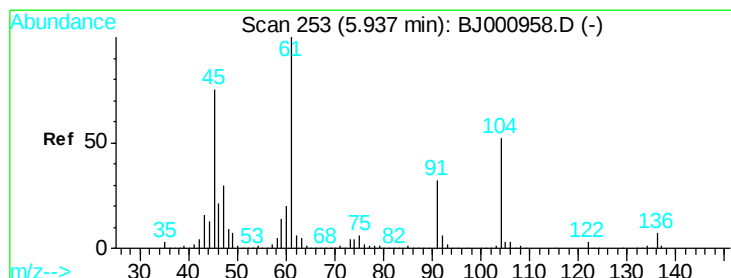
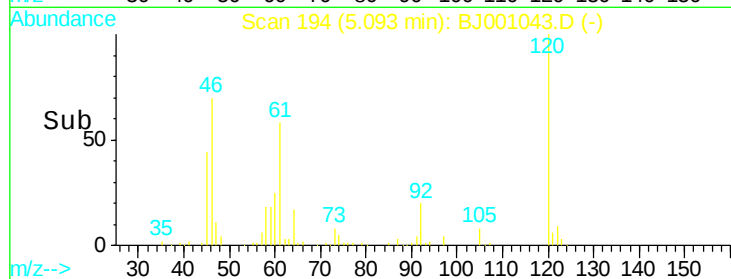
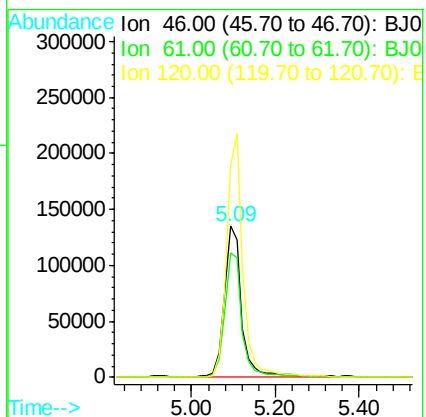
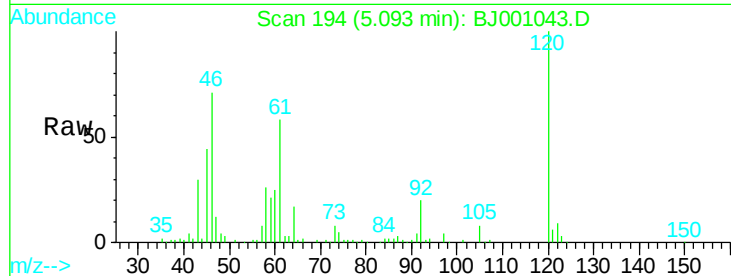
Tgt Ion: 46 Resp: 375416

Ion Ratio Lower Upper

46 100

61 82.5 63.7 103.7

120 141.3 148.0 188.0#



#8

Thiodiglycol

Concen: 30.69 ug/mL

RT: 5.89 min Scan# 250

Delta R.T. -0.03 min

Lab File: BJ001043.D

Acq: 20 Jul 2012 15:09

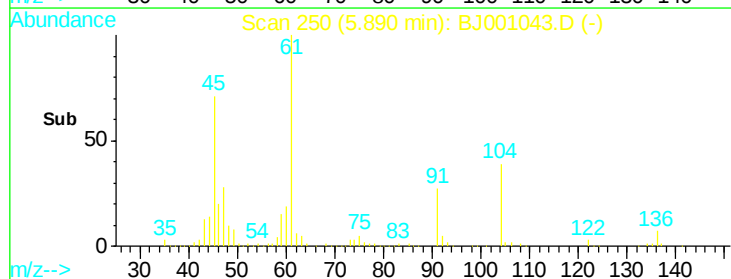
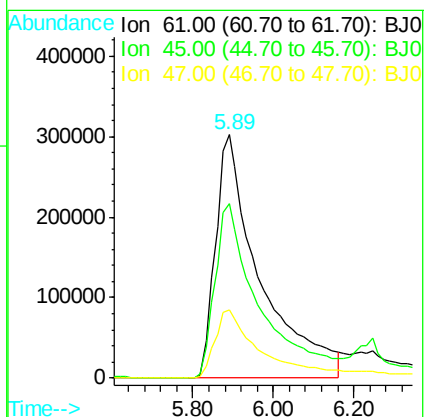
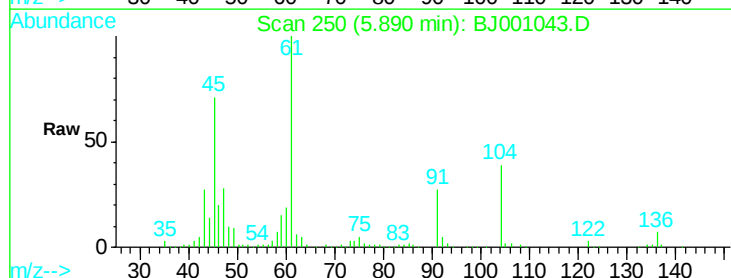
Tgt Ion: 61 Resp: 2306508

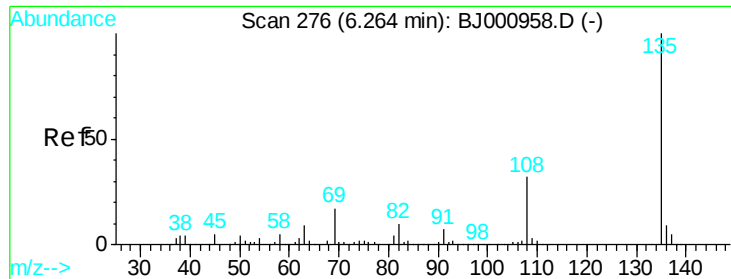
Ion Ratio Lower Upper

61 100

45 71.5 49.0 89.0

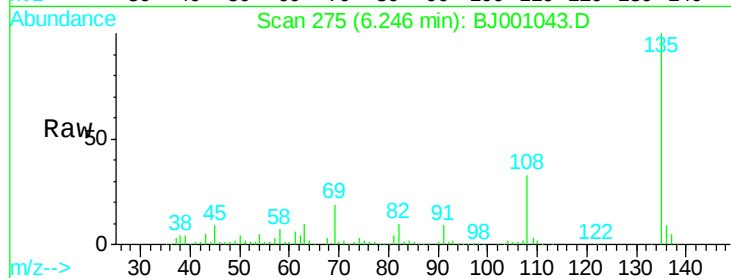
47 28.2 7.6 47.6



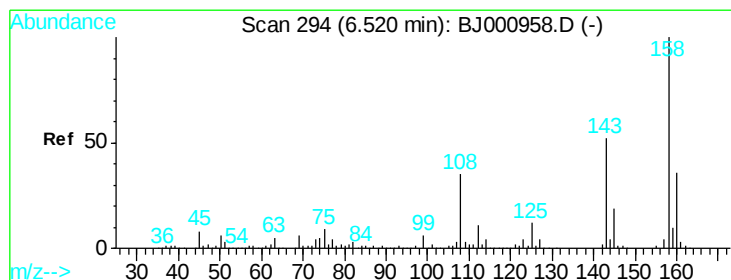
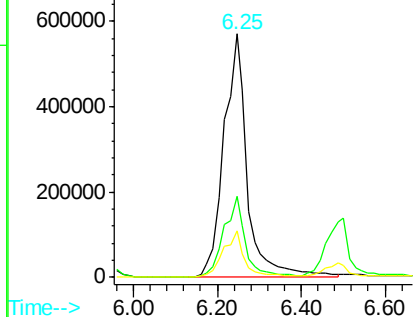
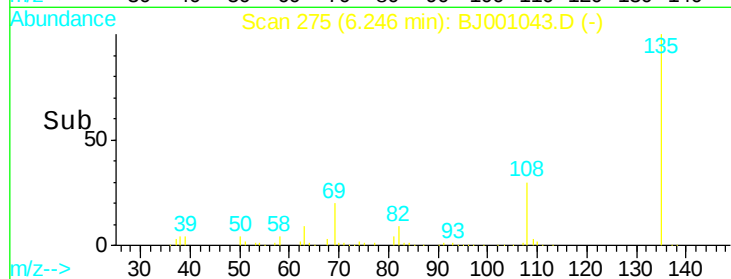


#9
Benzothiazole
Concen: 9.17 ug/mL
RT: 6.25 min Scan# 275
Delta R.T. -0.00 min
Lab File: BJ001043.D
Acq: 20 Jul 2012 15:09

Tgt Ion:135 Resp: 2226128
Ion Ratio Lower Upper
135 100
108 33.2 9.9 49.9
69 19.2 0.0 35.1

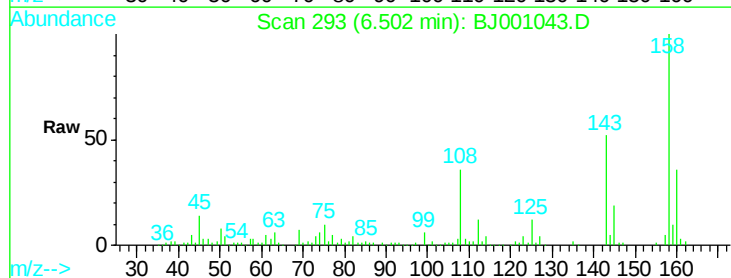


Abundance Ion 135.00 (134.70 to 135.70): E
Ion 108.00 (107.70 to 108.70): E
Ion 69.00 (68.70 to 69.70): BJ0

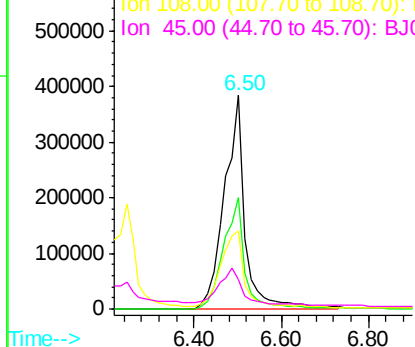
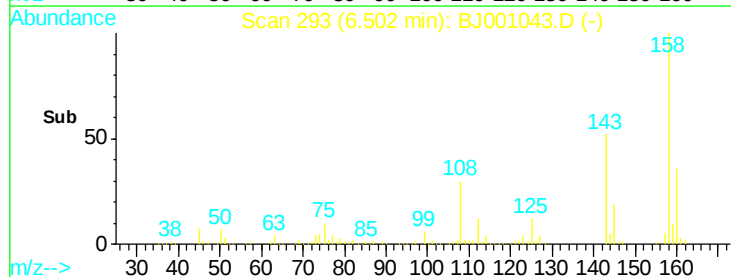


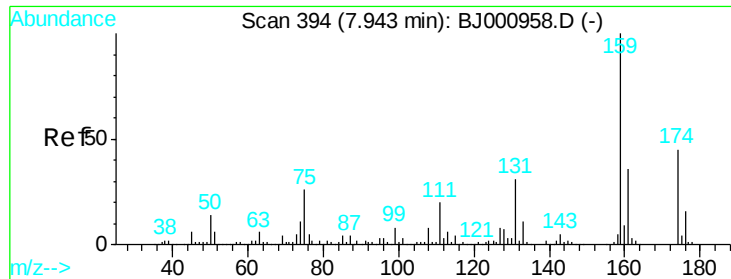
#11
p-Chlorophenylmethylsulfide
Concen: 8.51 ug/mL
RT: 6.50 min Scan# 293
Delta R.T. 0.01 min
Lab File: BJ001043.D
Acq: 20 Jul 2012 15:09

Tgt Ion:158 Resp: 1265236
Ion Ratio Lower Upper
158 100
143 52.2 36.2 76.2
108 36.4 25.5 65.5
45 13.7 0.7 40.7



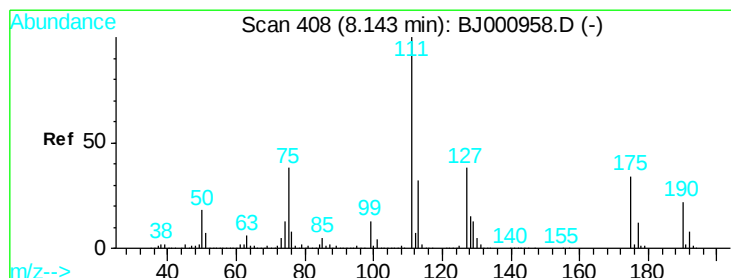
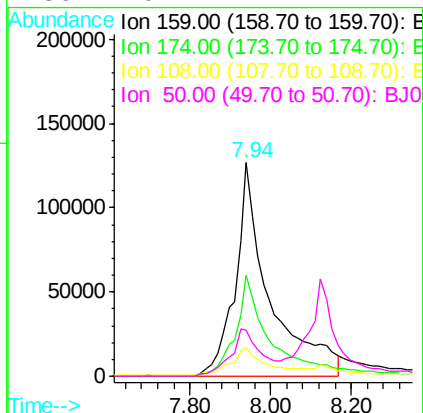
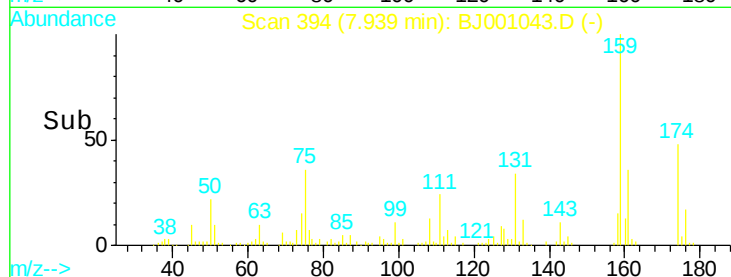
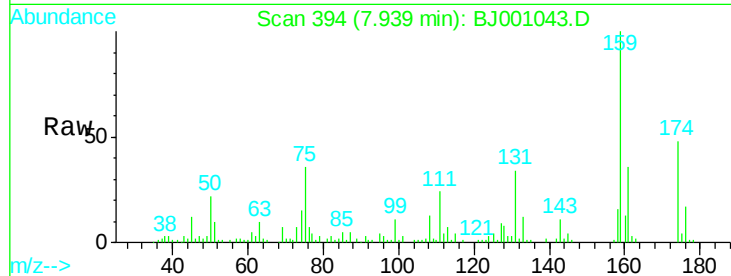
Abundance Ion 158.00 (157.70 to 158.70): E
Ion 143.00 (142.70 to 143.70): E
Ion 108.00 (107.70 to 108.70): E
Ion 45.00 (44.70 to 45.70): BJ0





#13
p-Chlorophenylmethylsulfoxide
Concen: 8.41 ug/mL
RT: 7.94 min Scan# 394
Delta R.T. 0.01 min
Lab File: BJ001043.D
Acq: 20 Jul 2012 15:09

Tgt Ion:	159	Resp:	748780
Ion	Ratio	Lower	Upper
159	100		
174	46.5	27.6	67.6
108	12.7	0.0	31.8
50	19.1	2.7	42.7



#14
p-Chlorophenylmethylsulfone
Concen: 7.09 ug/mL
RT: 8.14 min Scan# 408
Delta R.T. 0.01 min
Lab File: BJ001043.D
Acq: 20 Jul 2012 15:09

Tgt Ion:	111	Resp:	1052698
Ion	Ratio	Lower	Upper
111	100		
75	40.3	22.6	62.6
127	39.6	17.2	57.2
190	30.3	2.0	42.0

