

Data File : H:\VOL1\GCMSDATA\J\120426\BJ000811.D
 Acq On : 26 Apr 2012 23:51
 Sample : D2330-11MSD
 Misc : WATER BNA J HLM
 MS Integration Params: rteint.p
 Quant Time: Apr 27 11:33 2012

Vial: 27
 Operator: HLM
 Inst : BNA J
 Multiplr: 1.00

Quant Results File: BJ042612.RES

Quant Method : H:\VOL1\GCMSDATA\J\METHODS\BJ042612.M (RTE Integrator)
 Title : CWA degradation products by GCMS
 Last Update : Fri Apr 27 11:32:02 2012
 Response via : Initial Calibration
 DataAcq Meth : CWAJ

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	4.75	152	276076	2.00	ug/mL	-0.01
6) Naphthalene-d8	6.05	136	1112809	2.00	ug/mL	-0.01

System Monitoring Compounds

10) Tripropylphosphate	7.12	99	213182	0.56	ug/mL	0.02
Spiked Amount	0.500	Range	70 - 130	Recovery	=	112.00%
12) 2-Bromothioanisole	7.36	204	332014	4.55	ug/mL	0.00
Spiked Amount	5.000	Range	70 - 130	Recovery	=	91.00%

Target Compounds

	R.T.	QIon	Response	Conc	Units	Ovalue
2) Dimethyl Disulfide	2.76	94	301916	2.97	ug/mL#	68
3) DMMP	3.67	79	14498	0.26	ug/mL	98
4) DIMP	5.10	97	502779	2.07	ug/mL	92
5) 1,4-Oxathiane	3.76	46	2525064	25.79	ug/mL#	60
7) 1,4-Dithiane	5.22	46	5649873	76.87	ug/mL	95
8) Thiodiglycol	5.96	61	244335	4.89	ug/mL#	11
9) Benzothiazole	6.35	135	2735806	9.88	ug/mL	98
11) p-Chlorophenylmethyldisulfide	6.60	158	1825287	9.52	ug/mL	97
13) p-Chlorophenylmethyldisulfox	8.03	159	1148807	10.75	ug/mL	99
14) p-Chlorophenylmethyldisulfon	8.23	111	1520386	9.65	ug/mL	98

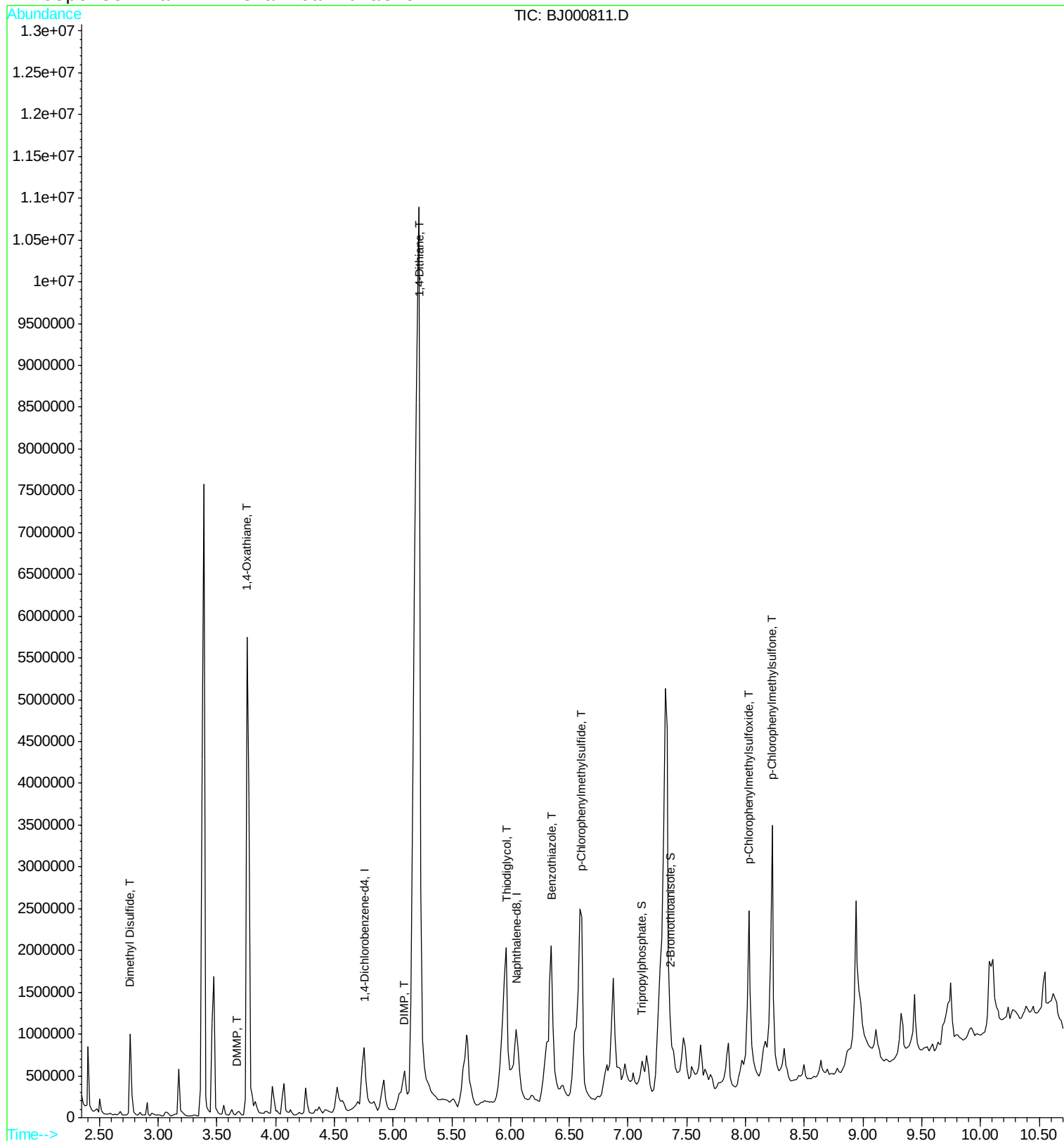
Quantitation Report

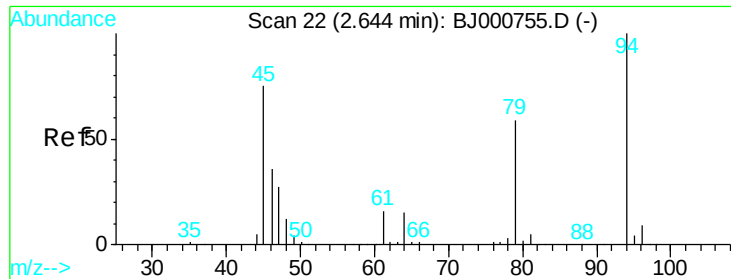
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Vial: 27
Operator: HLM
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Quant Results File: BJ042612.RES

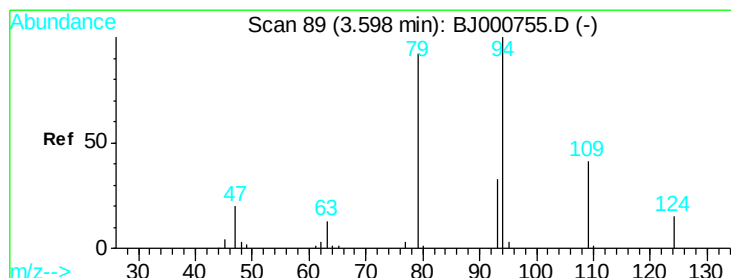
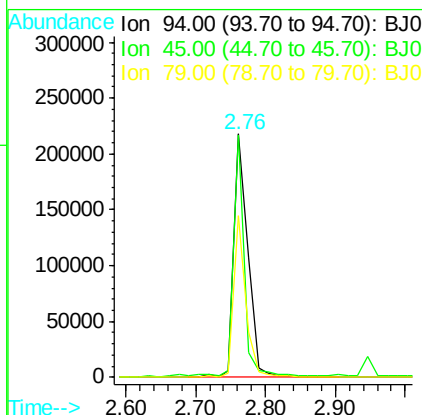
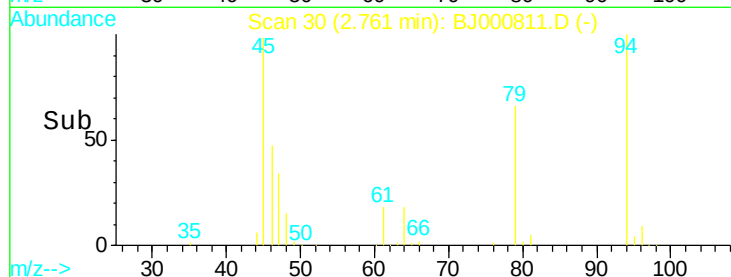
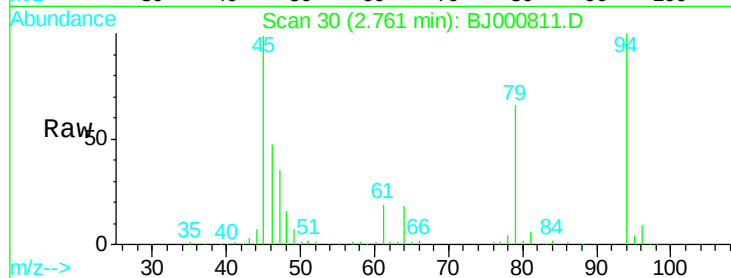
Method : H:\VOL1\GCMSDATA\J\METHODS\BJ042612.M (RTE Integrator)
Title : CWA degradation products by GCMS
Last Update : Fri Apr 27 11:32:02 2012
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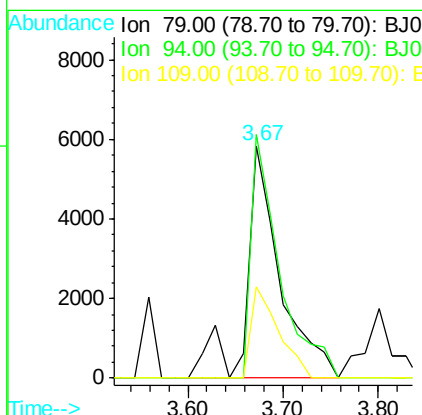
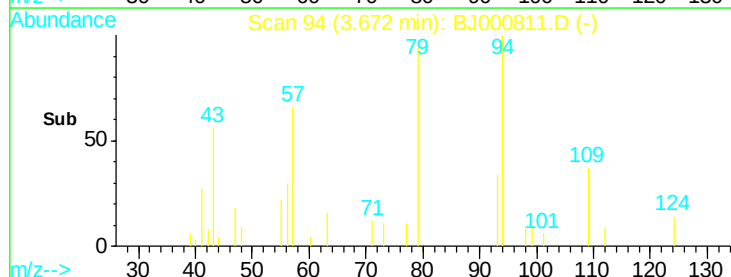
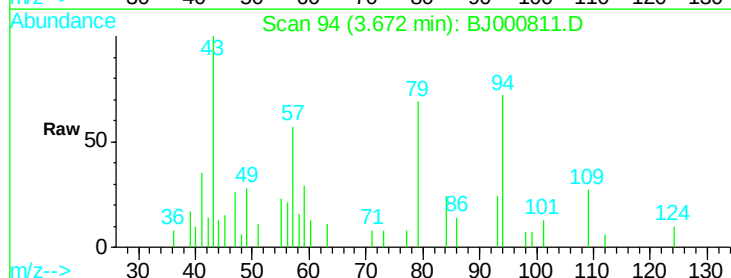
#2
 Dimethyl Disulfide
 Concen: 2.97 ug/mL
 RT: 2.76 min Scan# 30
 Delta R.T. 0.09 min
 Lab File: BJ000811.D
 Acq: 26 Apr 2012 23:51

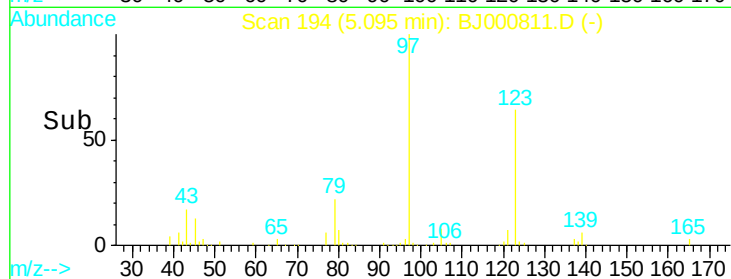
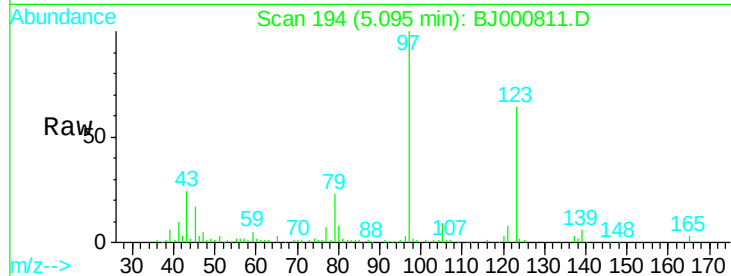
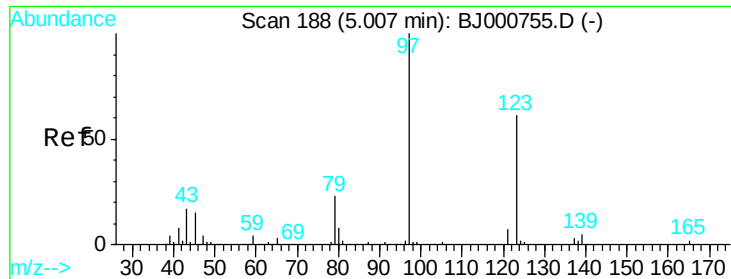
Tgt Ion: 94 Resp: 301916
 Ion Ratio Lower Upper
 94 100
 45 99.3 42.7 82.7#
 79 66.4 35.3 75.3



#3
 DMMP
 Concen: 0.26 ug/mL
 RT: 3.67 min Scan# 94
 Delta R.T. 0.06 min
 Lab File: BJ000811.D
 Acq: 26 Apr 2012 23:51

Tgt Ion: 79 Resp: 14498
 Ion Ratio Lower Upper
 79 100
 94 104.6 85.9 125.9
 109 39.0 20.8 60.8





#4

DIMP

Concen: 2.07 ug/mL

RT: 5.10 min Scan# 194

Delta R.T. 0.07 min

Lab File: BJ000811.D

Acq: 26 Apr 2012 23:51

Tgt Ion: 97 Resp: 502779

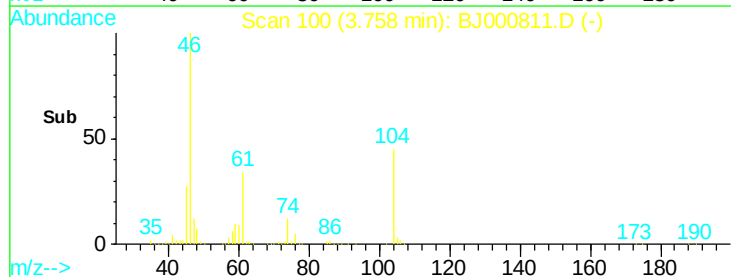
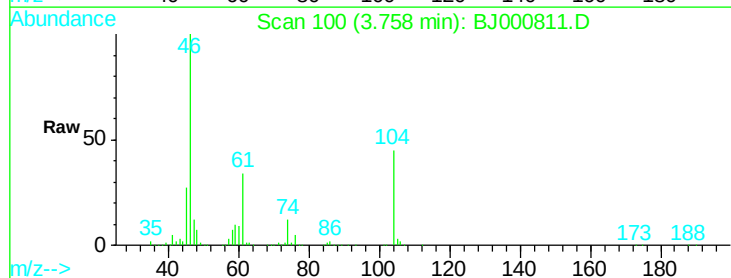
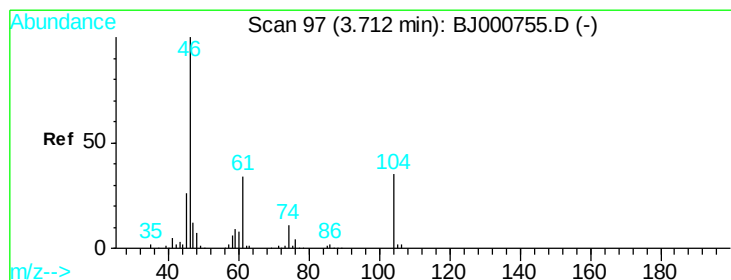
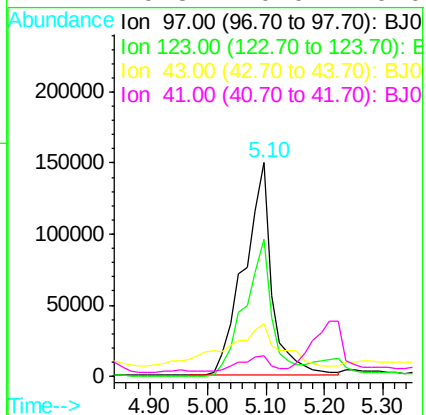
Ion Ratio Lower Upper

97 100

123 64.3 38.9 78.9

43 24.4 0.0 38.8

41 9.8 0.0 29.0



#5

1,4-Oxathiane

Concen: 25.79 ug/mL

RT: 3.76 min Scan# 100

Delta R.T. 0.02 min

Lab File: BJ000811.D

Acq: 26 Apr 2012 23:51

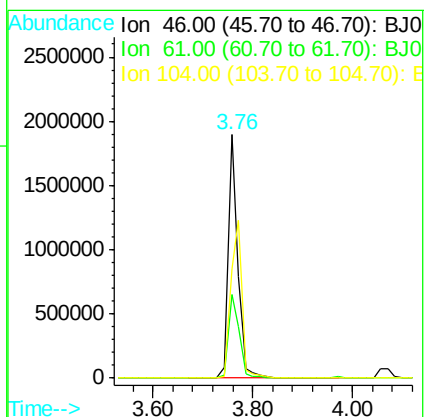
Tgt Ion: 46 Resp: 2525064

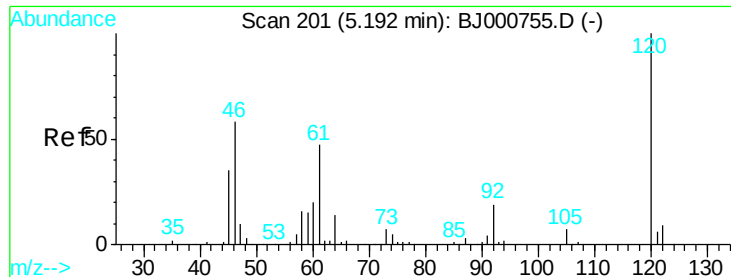
Ion Ratio Lower Upper

46 100

61 34.5 23.6 63.6

104 45.1 76.3 116.3#





#7

1,4-Dithiane

Concen: 76.87 ug/mL

RT: 5.22 min Scan# 203

Delta R.T. 0.02 min

Lab File: BJ000811.D

Acq: 26 Apr 2012 23:51

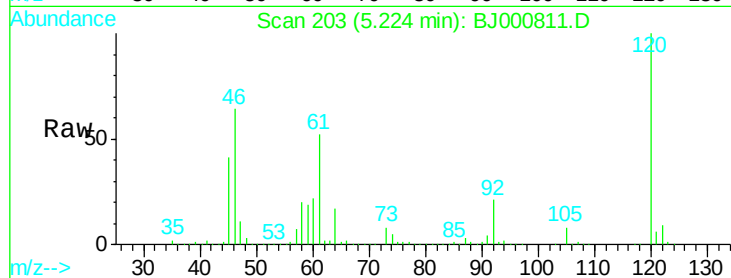
Tgt Ion: 46 Resp: 5649873

Ion Ratio Lower Upper

46 100

61 82.2 60.3 100.3

120 157.3 146.0 186.0

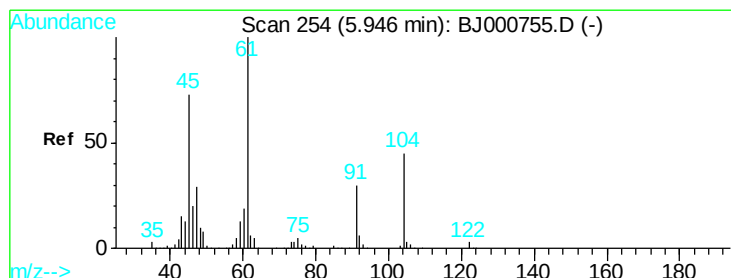
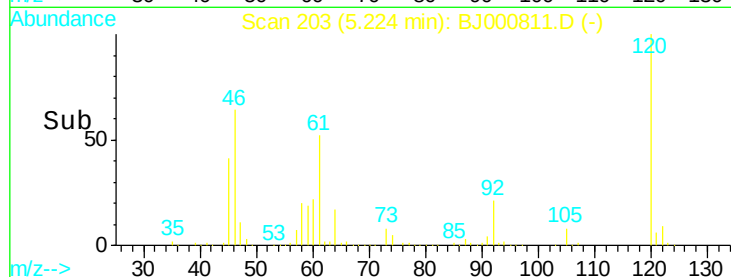
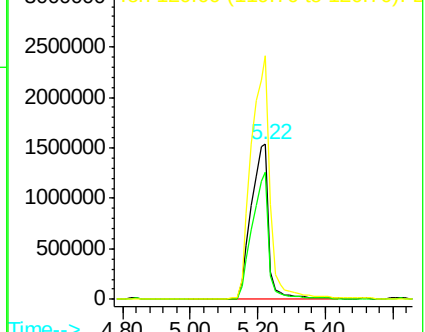


Abundance

Ion 46.00 (45.70 to 46.70): BJ0

Ion 61.00 (60.70 to 61.70): BJ0

Ion 120.00 (119.70 to 120.70): BJ0



#8

Thiodiglycol

Concen: 4.89 ug/mL

RT: 5.96 min Scan# 255

Delta R.T. -0.01 min

Lab File: BJ000811.D

Acq: 26 Apr 2012 23:51

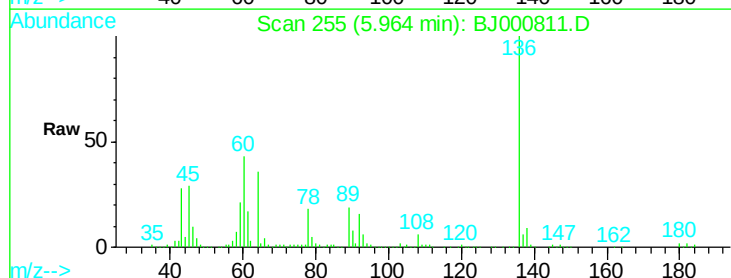
Tgt Ion: 61 Resp: 244335

Ion Ratio Lower Upper

61 100

45 171.5 50.6 90.6#

47 24.6 8.3 48.3

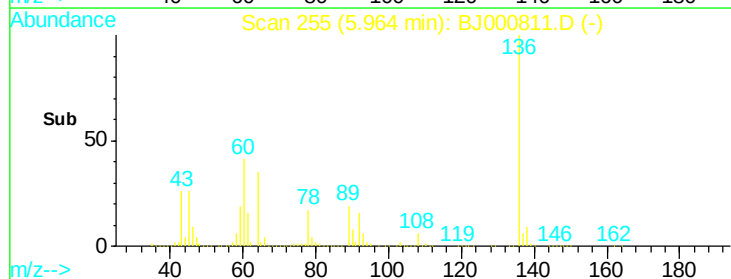
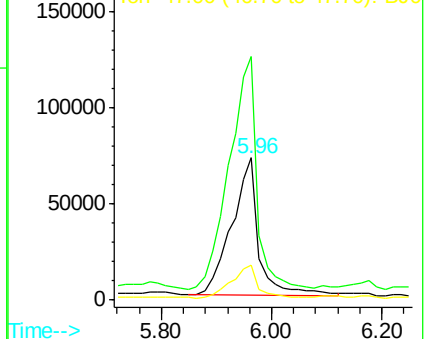


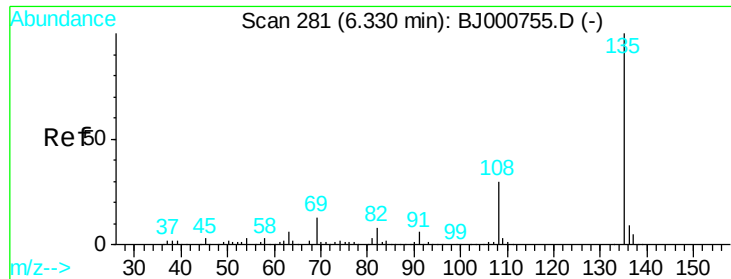
Abundance

Ion 61.00 (60.70 to 61.70): BJ0

Ion 45.00 (44.70 to 45.70): BJ0

Ion 47.00 (46.70 to 47.70): BJ0





#9

Benzothiazole

Concen: 9.88 ug/mL

RT: 6.35 min Scan# 282

Delta R.T. 0.00 min

Lab File: BJ000811.D

Acq: 26 Apr 2012 23:51

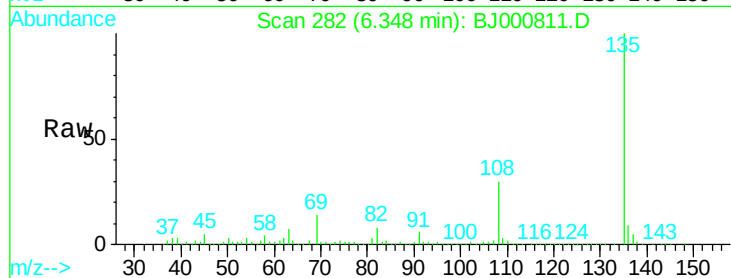
Tgt Ion:135 Resp: 2735806

Ion Ratio Lower Upper

135 100

108 29.8 11.1 51.1

69 13.7 0.0 34.6

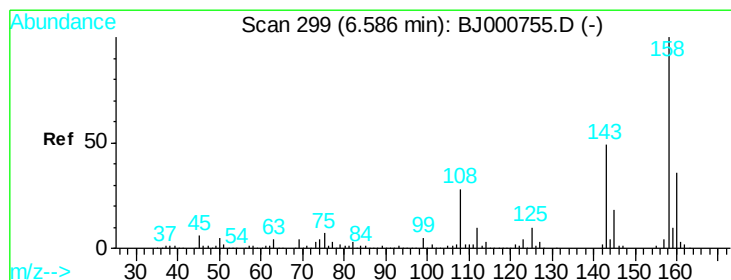
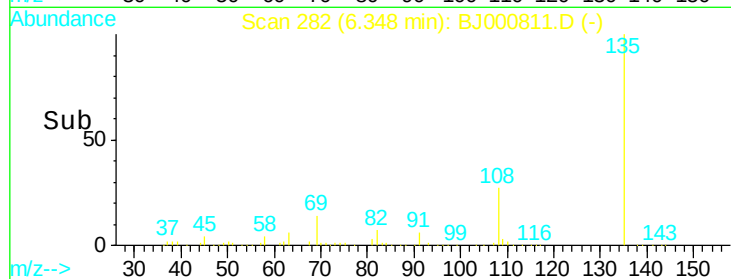
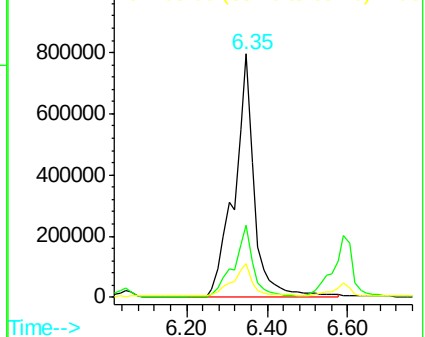


Abundance

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: 9.52 ug/mL

RT: 6.60 min Scan# 300

Delta R.T. 0.00 min

Lab File: BJ000811.D

Acq: 26 Apr 2012 23:51

Tgt Ion:158 Resp: 1825287

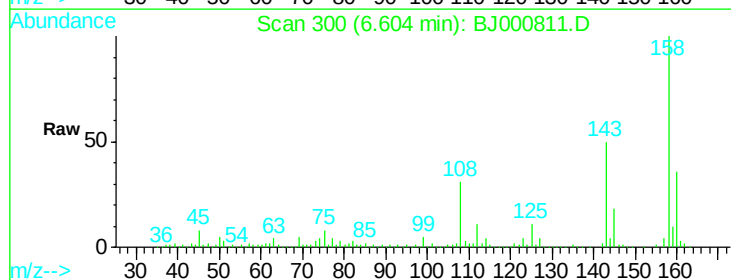
Ion Ratio Lower Upper

158 100

143 50.1 30.8 70.8

108 30.8 14.1 54.1

45 7.9 0.0 29.1



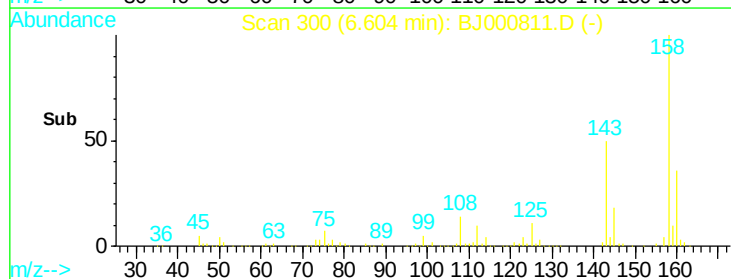
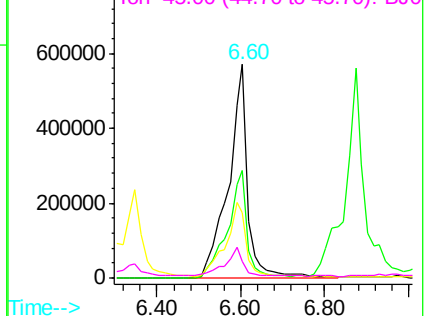
Abundance

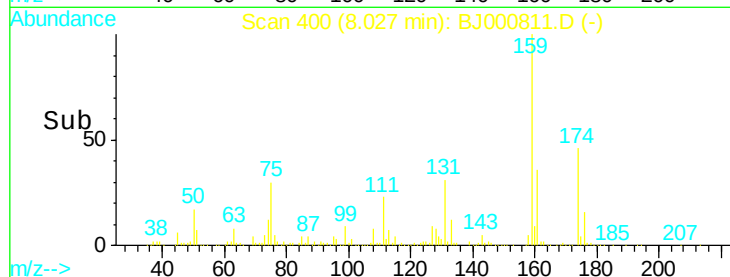
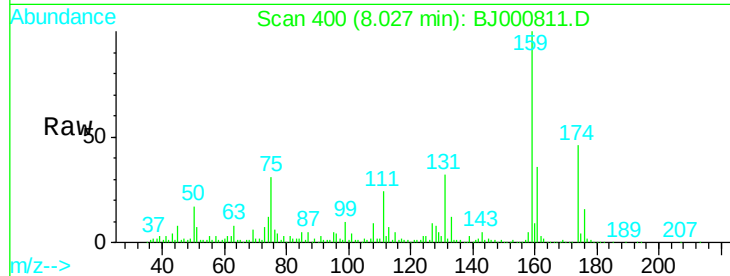
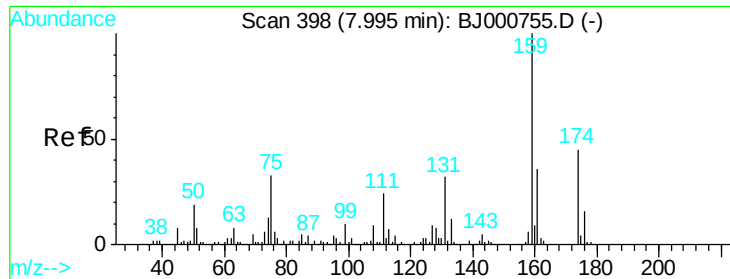
Ion 158.00 (157.70 to 158.70): E

Ion 143.00 (142.70 to 143.70): E

Ion 108.00 (107.70 to 108.70): E

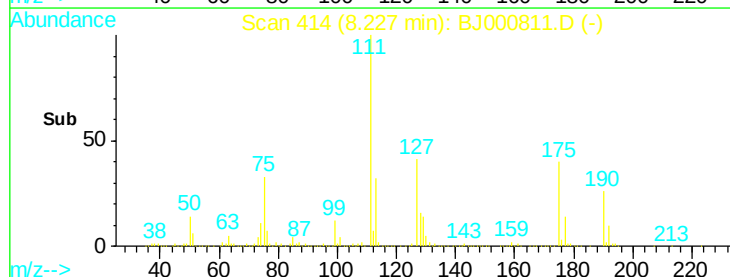
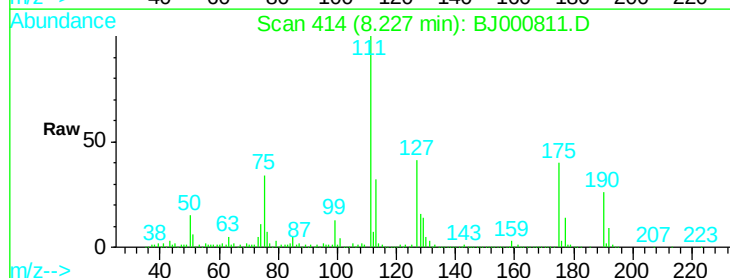
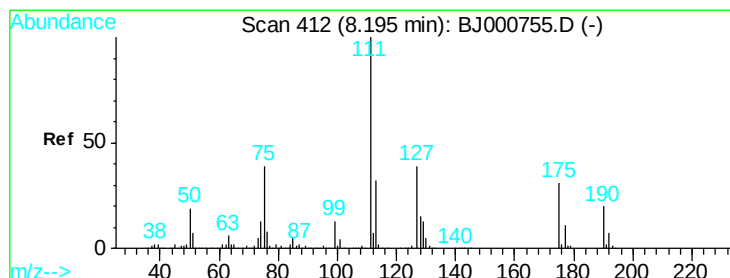
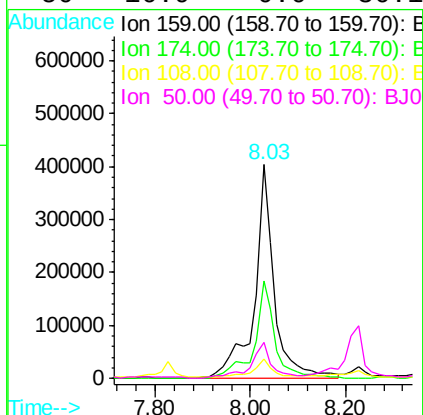
Ion 45.00 (44.70 to 45.70): BJ0





#13
p-Chlorophenylmethylsulfoxide
Concen: 10.75 ug/mL
RT: 8.03 min Scan# 400
Delta R.T. 0.00 min
Lab File: BJ000811.D
Acq: 26 Apr 2012 23:51

Tgt Ion:159 Resp: 1148807
Ion Ratio Lower Upper
159 100
174 48.0 28.6 68.6
108 8.4 0.0 28.2
50 16.9 0.0 36.1



#14
p-Chlorophenylmethylsulfone
Concen: 9.65 ug/mL
RT: 8.23 min Scan# 414
Delta R.T. 0.00 min
Lab File: BJ000811.D
Acq: 26 Apr 2012 23:51

Tgt Ion:111 Resp: 1520386
Ion Ratio Lower Upper
111 100
75 33.8 12.8 52.8
127 40.6 21.9 61.9
190 26.2 7.7 47.7

