

Data File : H:\VOL1\GCMSDATA\L\120215\BL000558.D

Vial: 2

Acq On : 15 Feb 2012 13:05

Operator: HLM

Sample : CWA-6

Inst : BNA L

Misc : BNA L HLM

Multiplr: 1.00

MS Integration Params: rteint.p

Quant Time: Feb 15 14:57 2012

Quant Results File: BL021512.RES

Quant Method : H:\VOL1\GCMSDATA\L\METHODS\BL021512.M (RTE Integrator)

Title : CWA degradation products by GCMS

Last Update : Wed Feb 15 14:49:38 2012

Response via : Initial Calibration

DataAcq Meth : CWAL

Internal Standards	R.T.	QIon	Response	Conc	Units	Dev(Min)
1) 1,4-Dichlorobenzene-d4	5.83	152	3473095	2.00	ug/mL	0.07
6) Naphthalene-d8	7.10	136	10200933	2.00	ug/mL	0.03

System Monitoring Compounds

10) Tripropylphosphate	8.09	99	13291701	4.28	ug/mL	0.00
Spiked Amount 500.000	Range 70 - 130		Recovery	=	0.86%#	
12) 2-Bromothioanisole	8.41	204	12125072	13.00	ug/mL	0.00
Spiked Amount 5000.000	Range 70 - 130		Recovery	=	0.26%#	

Target Compounds

	R.T.	QIon	Response	Conc	Units	Ovalue
2) Dimethyl Disulfide	3.61	94	16815181m	9.79	ug/mL	
3) DMMP	4.79	79	6782116m	4.97	ug/mL	
4) DIMP	6.00	97	12509406	4.40	ug/mL	81
5) 1,4-Oxathiane	4.98	46	19810114	11.95	ug/mL#	65
7) 1,4-Dithiane	6.29	46	10896866	13.08	ug/mL	96
8) Thiodiglycol	7.05	61	72744329	81.64	ug/mL#	73
9) Benzothiazole	7.38	135	21189863	7.86	ug/mL#	52
11) p-Chlorophenylmethyldisulfide	7.62	158	17030540	10.54	ug/mL#	19
13) p-Chlorophenylmethyldisulfoxide	9.09	159	22769147	24.09	ug/mL	89
14) p-Chlorophenylmethyldisulfonate	9.30	111	20715736	17.34	ug/mL#	55

(#) = qualifier out of range (m) = manual integration

BL000558.D BL021512.M

Fri Feb 17 10:48:01 2012

A

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Vial: 2

Acq On : 15 Feb 2012 13:05

Operator: HLM

Sample : CWA-6

Inst : BNA L

Misc : BNA L HLM

Multiplr: 1.00

MS Integration Params: rteint.p

Quant Time: Feb 15 14:57 2012

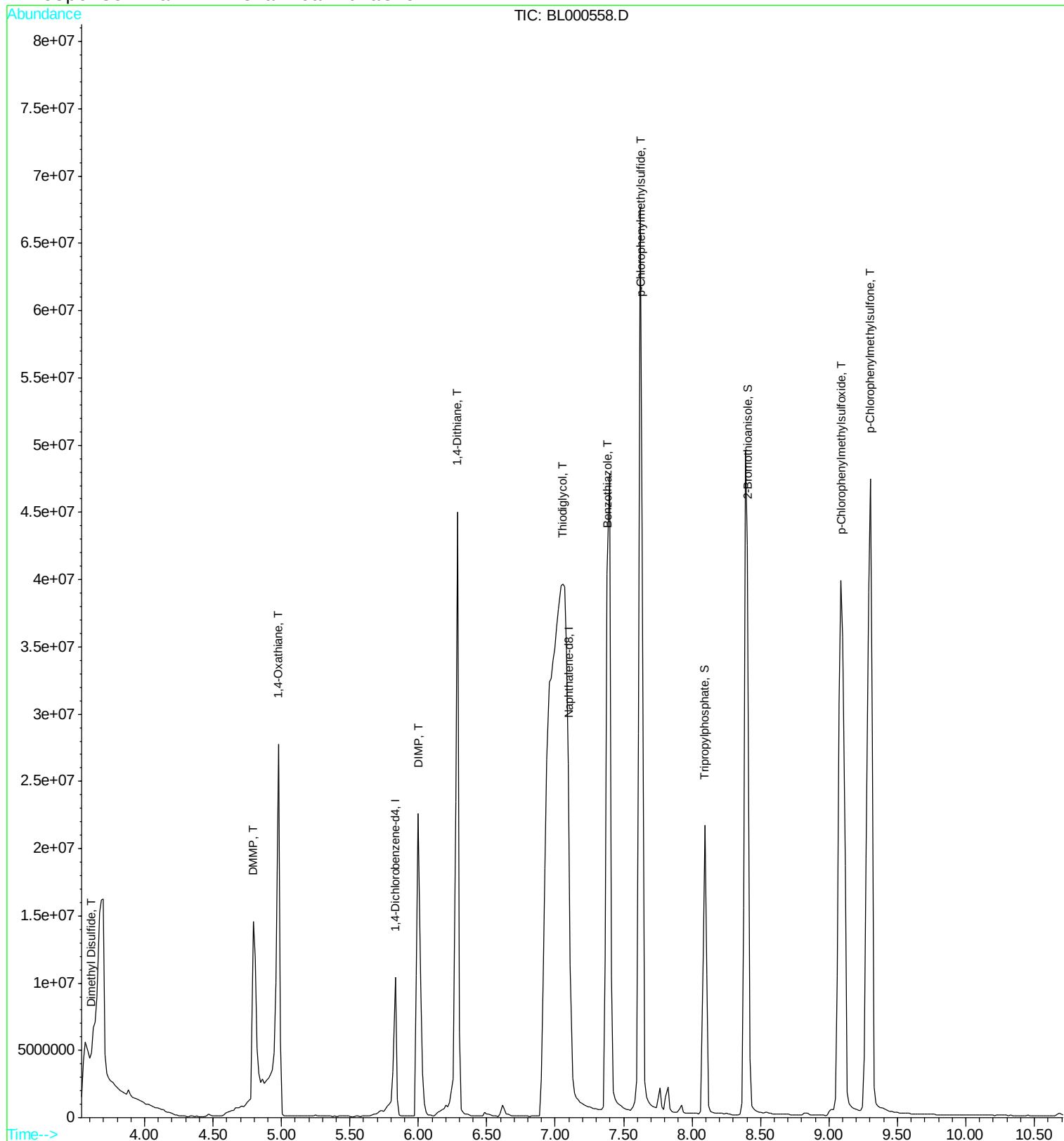
Quant Results File: BL021512.RES

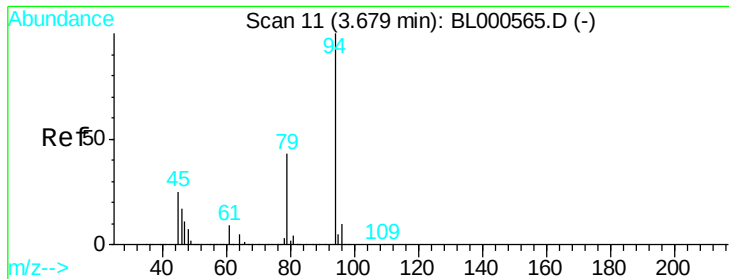
Method : H:\VOL1\GCMSDATA\L\METHODS\BL021512.M (RTE Integrator)

Title : CWA degradation products by GCMS

Last Update : Fri Feb 17 10:16:01 2012

Response via : Initial Calibration

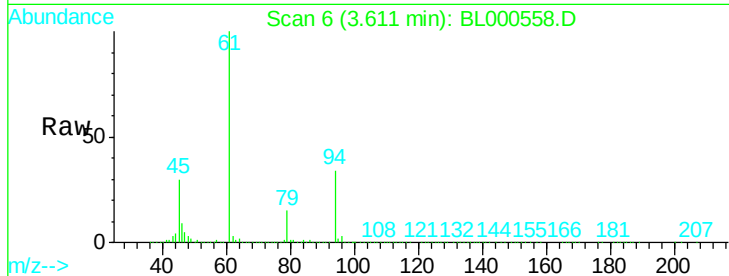




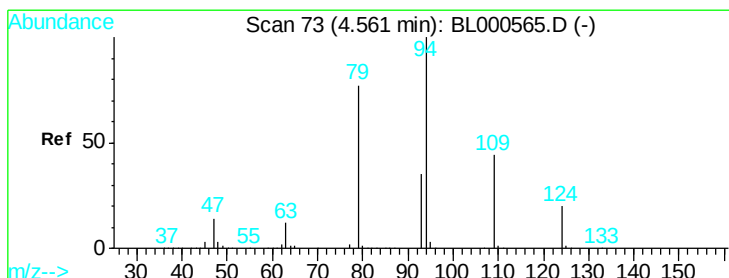
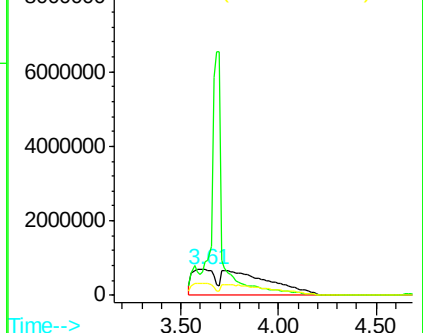
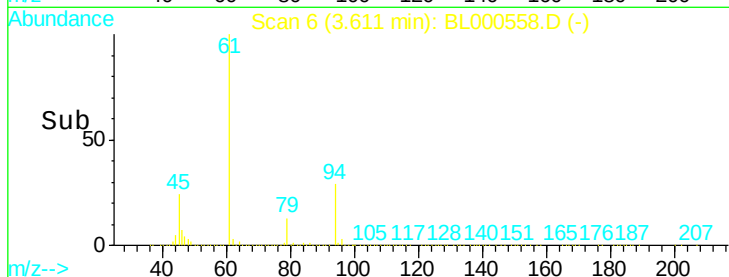
#2

Dimethyl Disulfide
 Concen: 9.79 ug/mL m
 RT: 3.61 min Scan# 6
 Delta R.T. -0.14 min
 Lab File: BL000558.D
 Acq: 15 Feb 2012 13:05

Tgt Ion: 94 Resp:16815181
 Ion Ratio Lower Upper
 94 100
 45 89.3 37.9 77.9#
 79 44.4 36.3 76.3



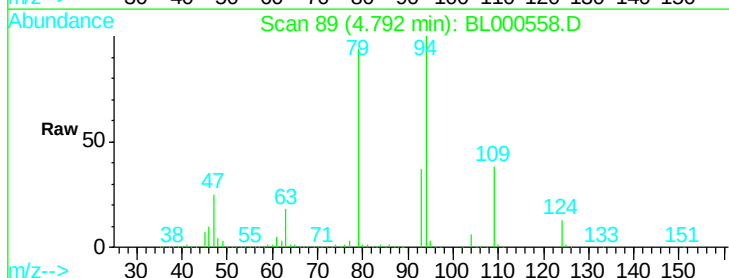
Abundance Ion 94.00 (93.70 to 94.70): BL0
 Ion 45.00 (44.70 to 45.70): BL0
 Ion 79.00 (78.70 to 79.70): BL0



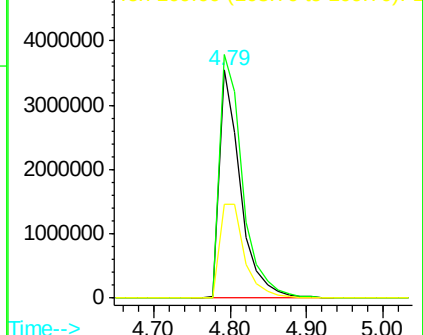
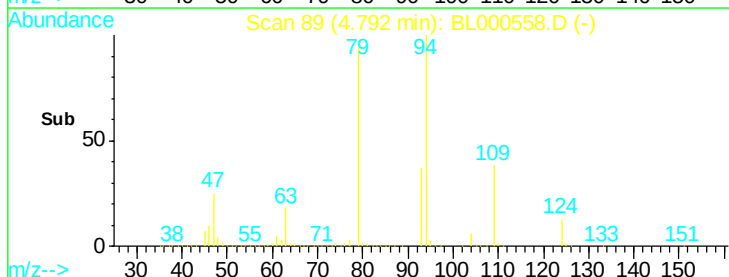
#3

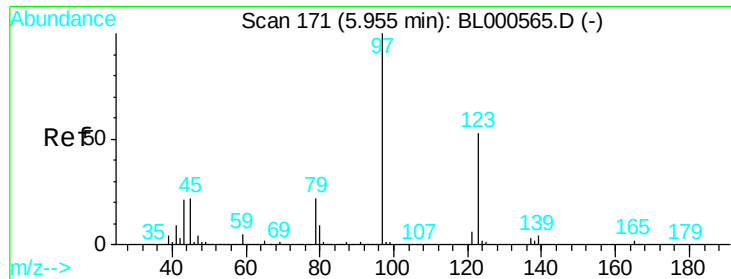
DMMP
 Concen: 4.97 ug/mL m
 RT: 4.79 min Scan# 89
 Delta R.T. 0.21 min
 Lab File: BL000558.D
 Acq: 15 Feb 2012 13:05

Tgt Ion: 79 Resp: 6782116
 Ion Ratio Lower Upper
 79 100
 94 106.9 98.3 138.3
 109 41.0 26.6 66.6



Abundance Ion 79.00 (78.70 to 79.70): BL0
 Ion 94.00 (93.70 to 94.70): BL0
 Ion 109.00 (108.70 to 109.70): BL0





#4

DIMP

Concen: 4.40 ug/mL

RT: 6.00 min Scan# 174

Delta R.T. 0.04 min

Lab File: BL000558.D

Acq: 15 Feb 2012 13:05

Tgt Ion: 97 Resp:12509406

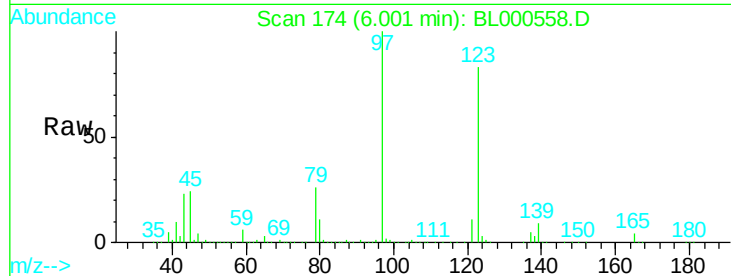
Ion Ratio Lower Upper

97 100

123 83.2 48.8 88.8

43 22.6 0.0 32.3

41 9.5 0.0 25.6



Abundance

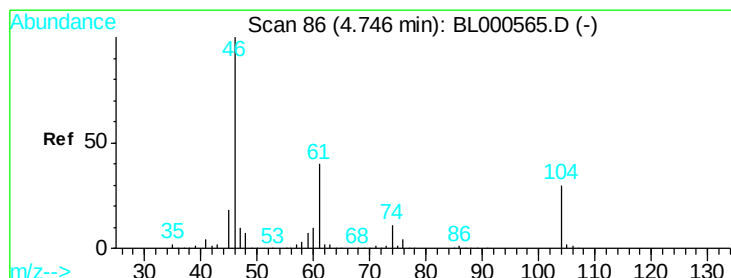
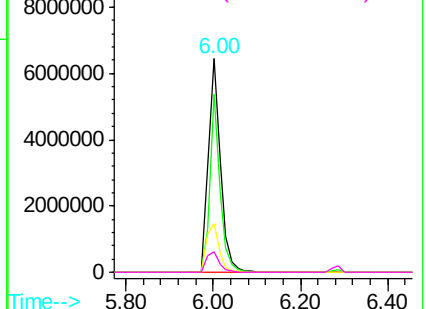
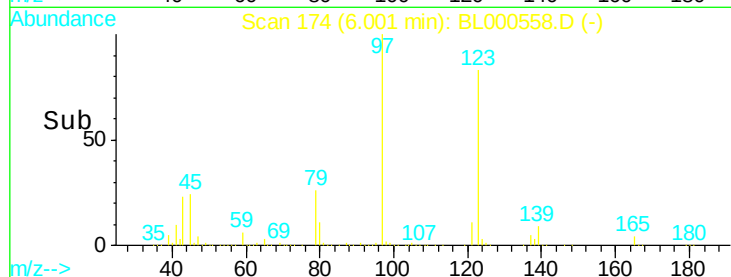
Ion 97.00 (96.70 to 97.70): BL0

1e+07

Ion 123.00 (122.70 to 123.70): BL0

Ion 43.00 (42.70 to 43.70): BL0

Ion 41.00 (40.70 to 41.70): BL0



#5

1,4-Oxathiane

Concen: 11.95 ug/mL

RT: 4.98 min Scan# 102

Delta R.T. 0.20 min

Lab File: BL000558.D

Acq: 15 Feb 2012 13:05

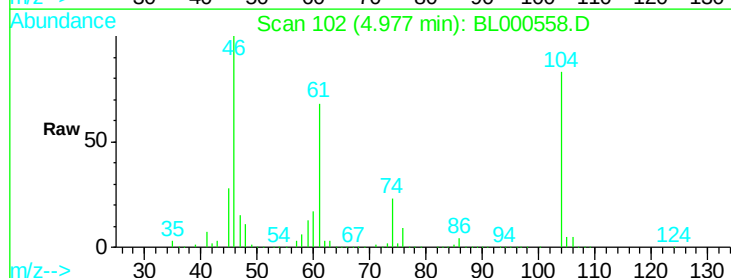
Tgt Ion: 46 Resp:19810114

Ion Ratio Lower Upper

46 100

61 68.0 29.6 69.6

104 83.4 32.6 72.6#

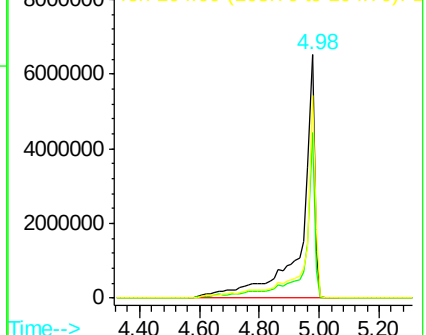
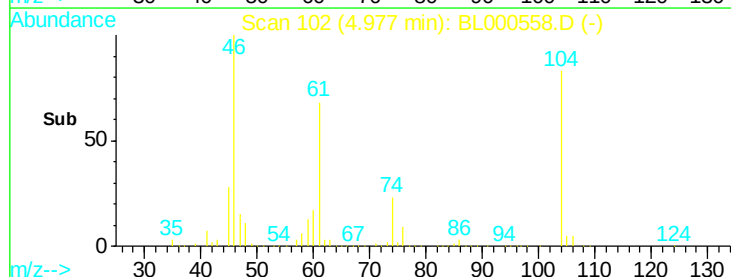


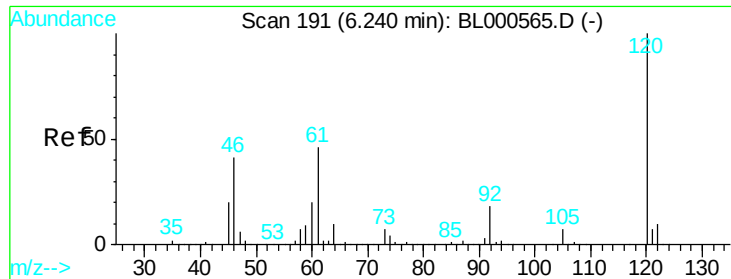
Abundance

Ion 46.00 (45.70 to 46.70): BL0

Ion 61.00 (60.70 to 61.70): BL0

Ion 104.00 (103.70 to 104.70): BL0





#7

1,4-Dithiane

Concen: 13.08 ug/mL

RT: 6.29 min Scan# 194

Delta R.T. 0.06 min

Lab File: BL000558.D

Acq: 15 Feb 2012 13:05

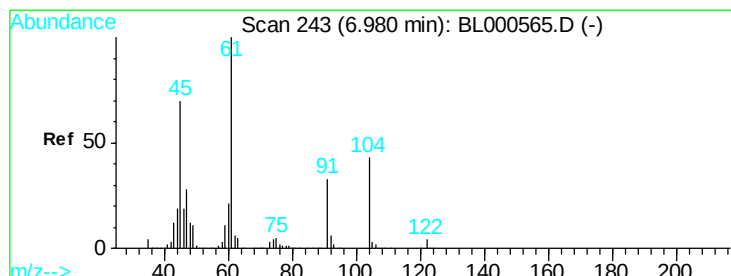
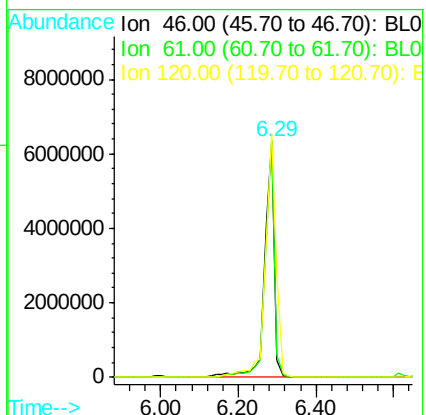
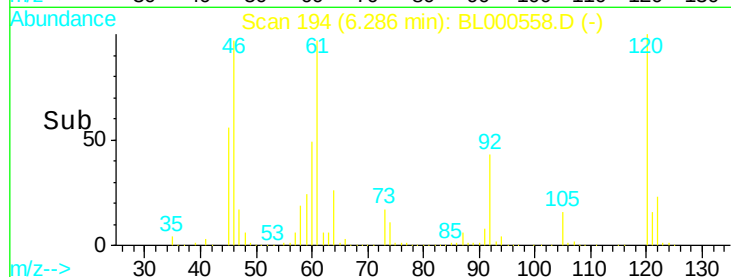
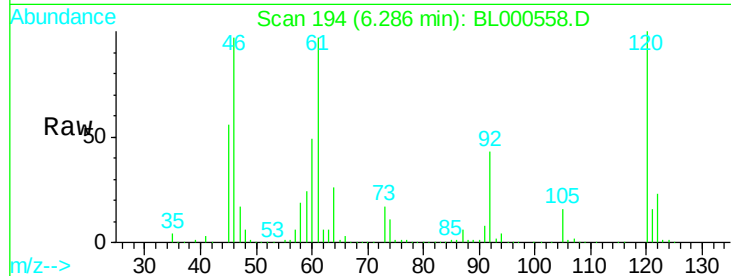
Tgt Ion: 46 Resp:10896866

Ion Ratio Lower Upper

46 100

61 100.6 74.1 114.1

120 103.3 81.1 121.1



#8

Thiodiglycol

Concen: 81.64 ug/mL

RT: 7.05 min Scan# 248

Delta R.T. 0.10 min

Lab File: BL000558.D

Acq: 15 Feb 2012 13:05

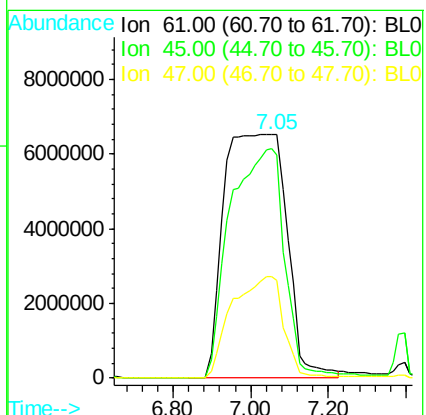
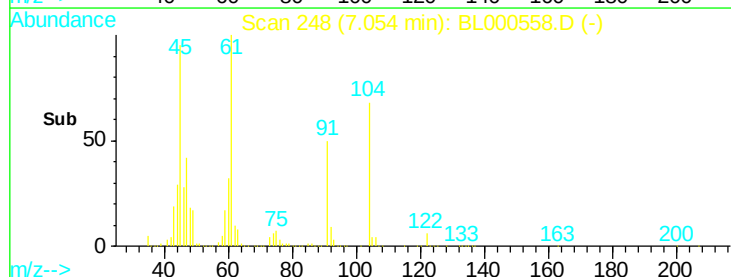
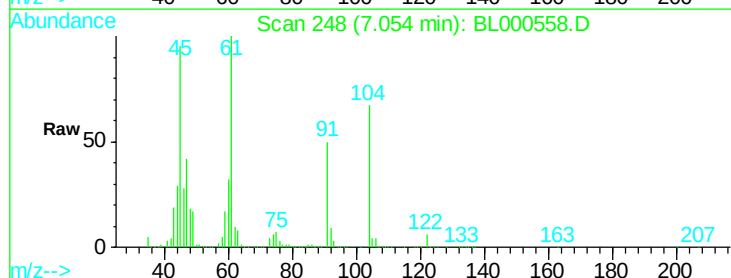
Tgt Ion: 61 Resp:72744329

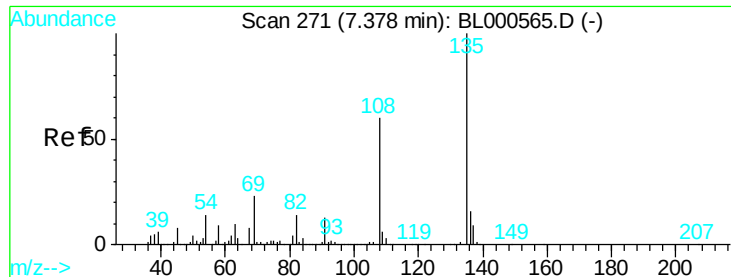
Ion Ratio Lower Upper

61 100

45 94.5 50.8 90.8#

47 41.8 9.0 49.0





#9

Benzothiazole

Concen: 7.86 ug/mL

RT: 7.38 min Scan# 271

Delta R.T. 0.02 min

Lab File: BL000558.D

Acq: 15 Feb 2012 13:05

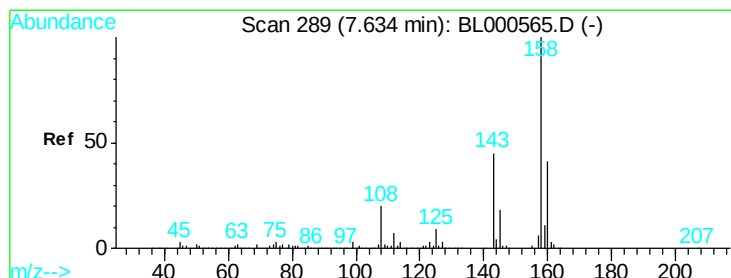
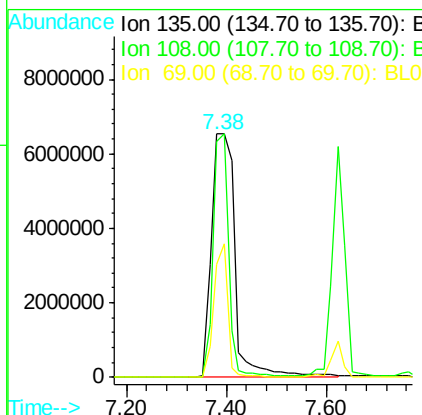
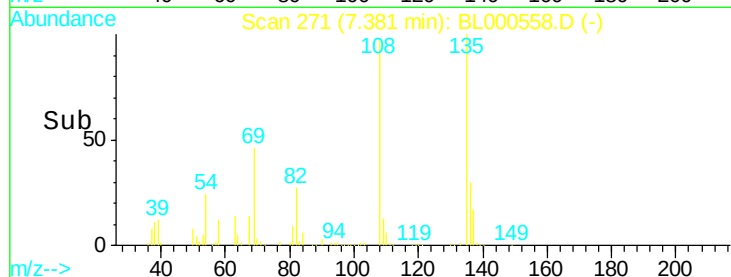
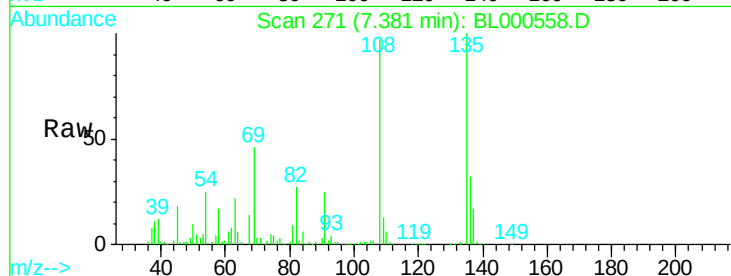
Tgt Ion:135 Resp:21189863

Ion Ratio Lower Upper

135 100

108 97.1 38.8 78.8#

69 46.2 5.9 45.9#



#11

p-Chlorophenylmethylsulfide

Concen: 10.54 ug/mL

RT: 7.62 min Scan# 288

Delta R.T. 0.00 min

Lab File: BL000558.D

Acq: 15 Feb 2012 13:05

Tgt Ion:158 Resp:17030540

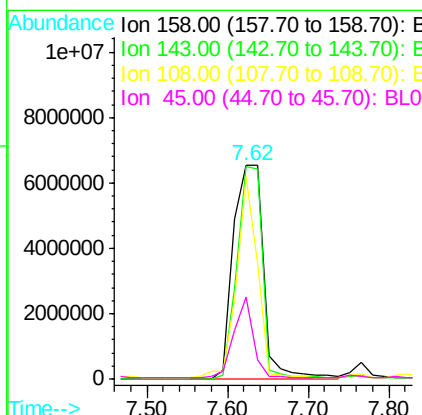
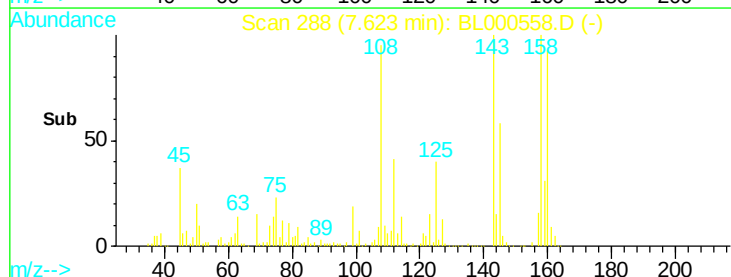
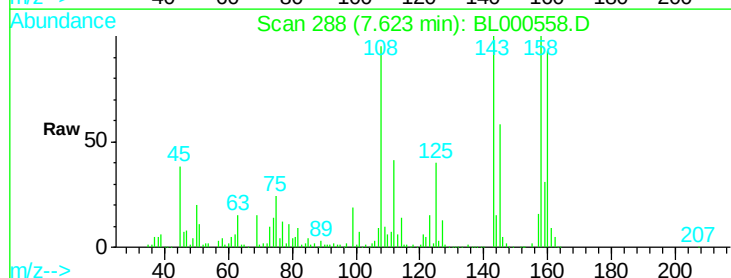
Ion Ratio Lower Upper

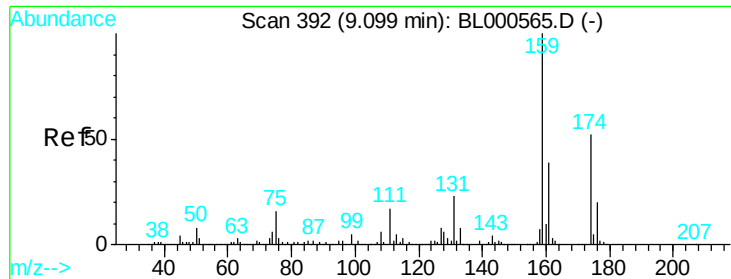
158 100

143 99.6 36.0 76.0#

108 95.0 10.7 50.7#

45 38.1 0.0 26.7#

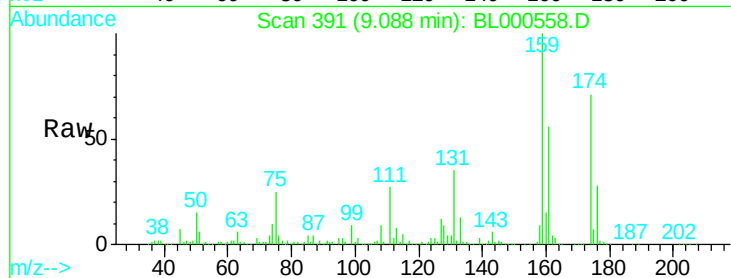




#13
p-Chlorophenylmethylsulfoxide
Concen: 24.09 ug/mL
RT: 9.09 min Scan# 391
Delta R.T. 0.00 min
Lab File: BL000558.D
Acq: 15 Feb 2012 13:05

Tgt Ion:159 Resp:22769147

Ion	Ratio	Lower	Upper
159	100		
174	60.5	30.4	70.4
108	7.2	0.0	27.6
50	13.5	0.0	33.2



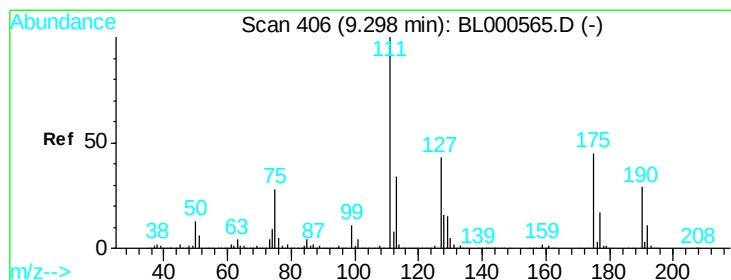
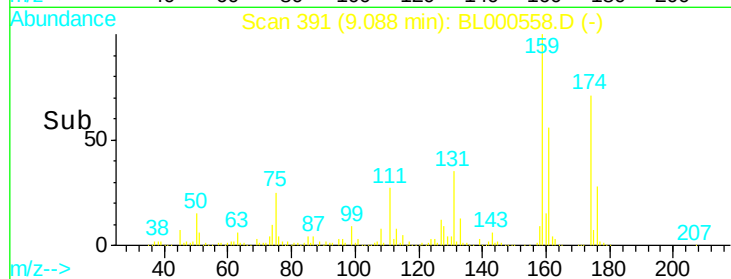
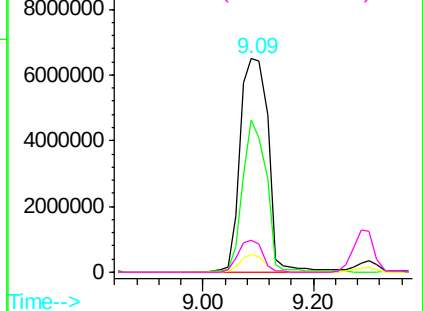
Abundance

Ion 159.00 (158.70 to 159.70): E

Ion 174.00 (173.70 to 174.70): E

Ion 108.00 (107.70 to 108.70): E

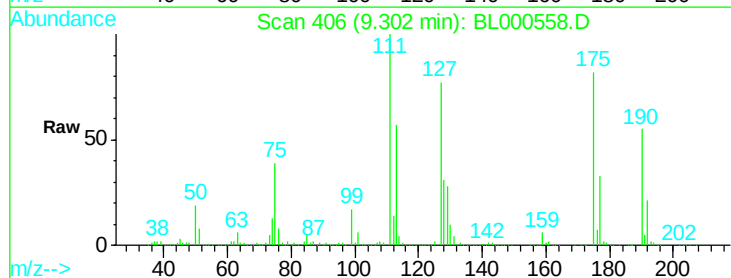
Ion 50.00 (49.70 to 50.70): BL0



#14
p-Chlorophenylmethylsulfone
Concen: 17.34 ug/mL
RT: 9.30 min Scan# 406
Delta R.T. 0.02 min
Lab File: BL000558.D
Acq: 15 Feb 2012 13:05

Tgt Ion:111 Resp:20715736

Ion	Ratio	Lower	Upper
111	100		
75	39.2	9.9	49.9
127	76.8	21.9	61.9#
190	55.4	5.3	45.3#



Abundance

Ion 111.00 (110.70 to 111.70): E

Ion 75.00 (74.70 to 75.70): BL0

Ion 127.00 (126.70 to 127.70): E

Ion 190.00 (189.70 to 190.70): E

