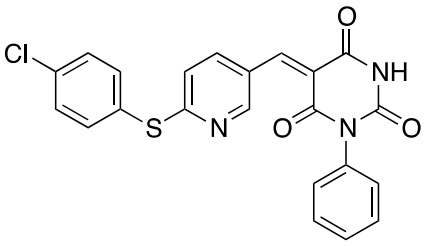
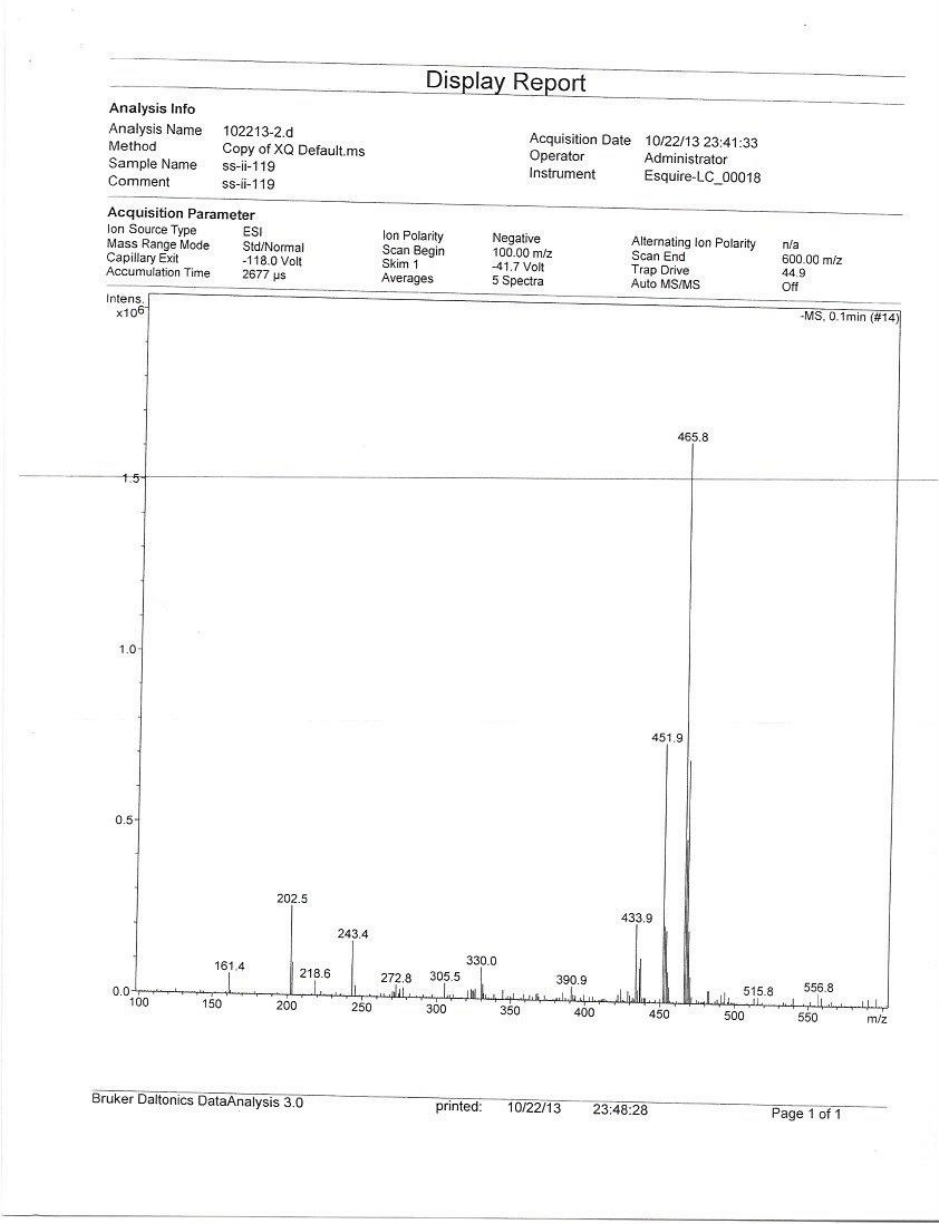
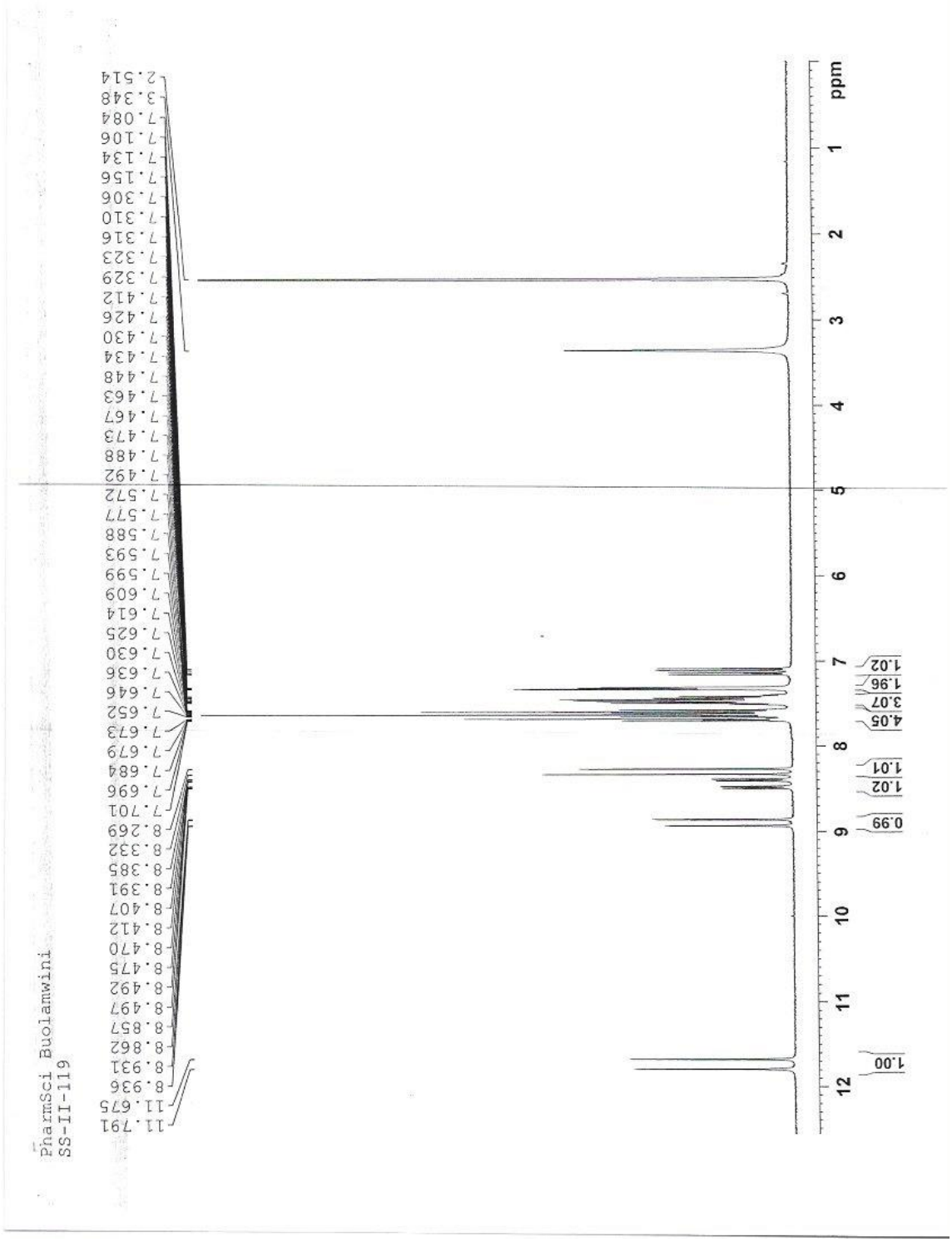
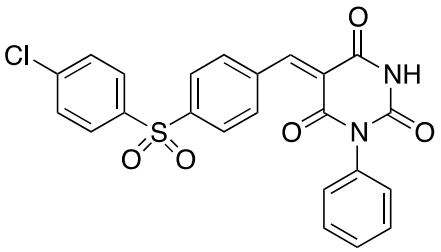
Suppl. Mass spectrum and ^{1}H NMR Spectrum of **46**

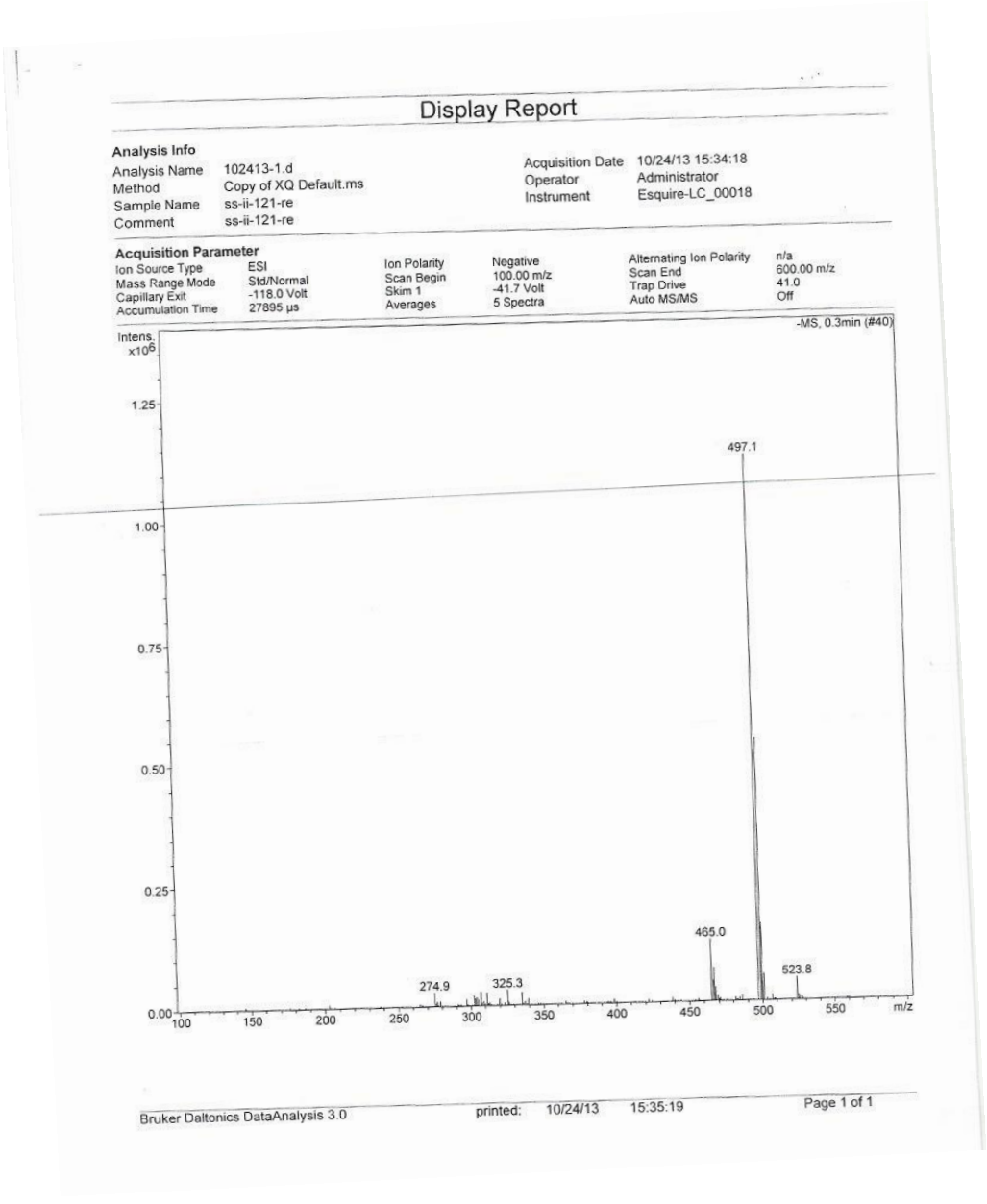


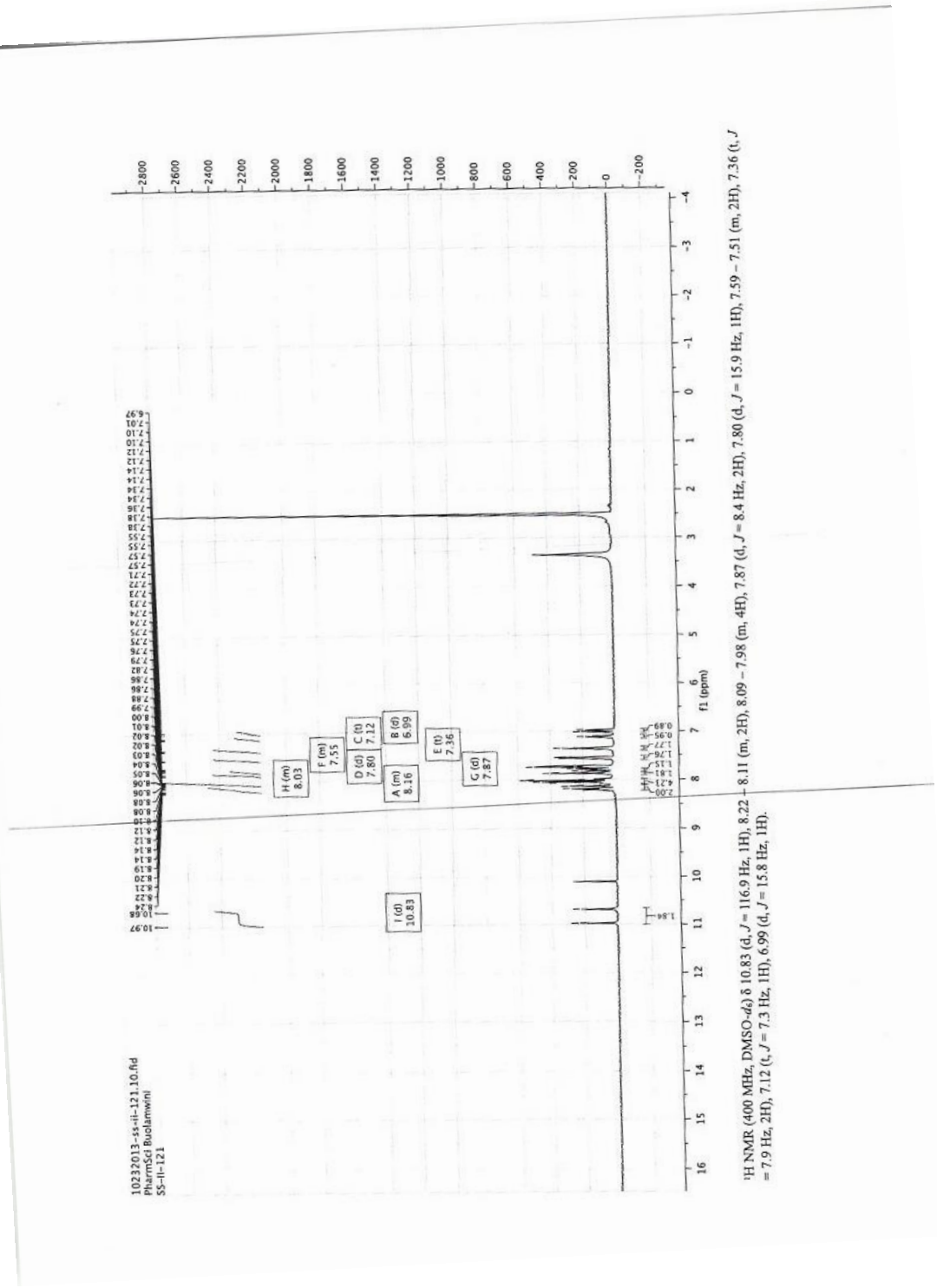



PharmSci Buolamwini
SS-II-119
11.791
11.675
8.936
8.931
8.862
8.857
8.497
8.492
8.475
8.470
8.412
8.407
8.391
8.385
8.332
8.269
7.701
7.696
7.684
7.679
7.673
7.652
7.646
7.636
7.630
7.625
7.614
7.609
7.599
7.593
7.588
7.577
7.572
7.492
7.488
7.473
7.467
7.463
7.448
7.434
7.430
7.426
7.412
7.329
7.323
7.316
7.310
7.306
7.156
7.134
7.106
7.084
3.348
2.514
ppm
1.00
0.99
1.02
1.01
4.05
3.07
1.96
1.02

Suppl. Mass spectrum and ^{1}H NMR Spectrum of **47**

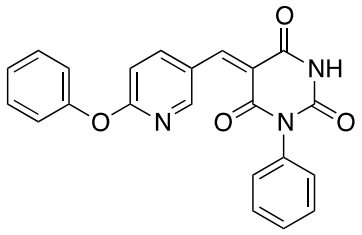






^{1}H NMR (400 MHz, DMSO-d_6) δ 10.83 (d, J = 116.9 Hz, 1H), 8.22 – 8.11 (m, 2H), 8.09 – 7.98 (m, 4H), 7.87 (d, J = 8.4 Hz, 2H), 7.80 (d, J = 15.9 Hz, 1H), 7.59 – 7.51 (m, 2H), 7.36 (t, J = 7.9 Hz, 2H), 7.12 (t, J = 7.3 Hz, 1H), 6.99 (d, J = 15.8 Hz, 1H).

Suppl. Mass spectrum and ^{1}H NMR Spectrum of **48**



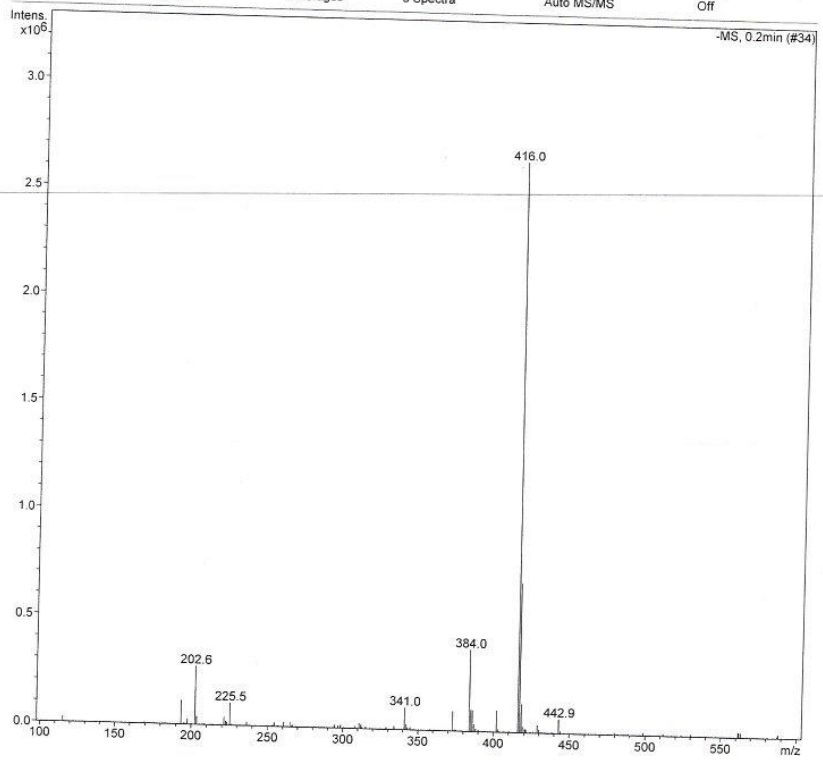
Display Report

Analysis Info

Analysis Name	102213-3.d	Acquisition Date	10/22/13 23:45:27
Method	Copy of XQ Default.ms	Operator	Administrator
Sample Name	ss-ii-123	Instrument	Esquire-LC_00018
Comment	ss-ii-123		

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Negative	Alternating Ion Polarity	n/a
Mass Range Mode	Std/Normal	Scan Begin	100.00 m/z	Scan End	600.00 m/z
Capillary Exit	-111.9 Volt	Skim 1	-37.5 Volt	Trap Drive	42.6
Accumulation Time	2638 µs	Averages	5 Spectra	Auto MS/MS	Off



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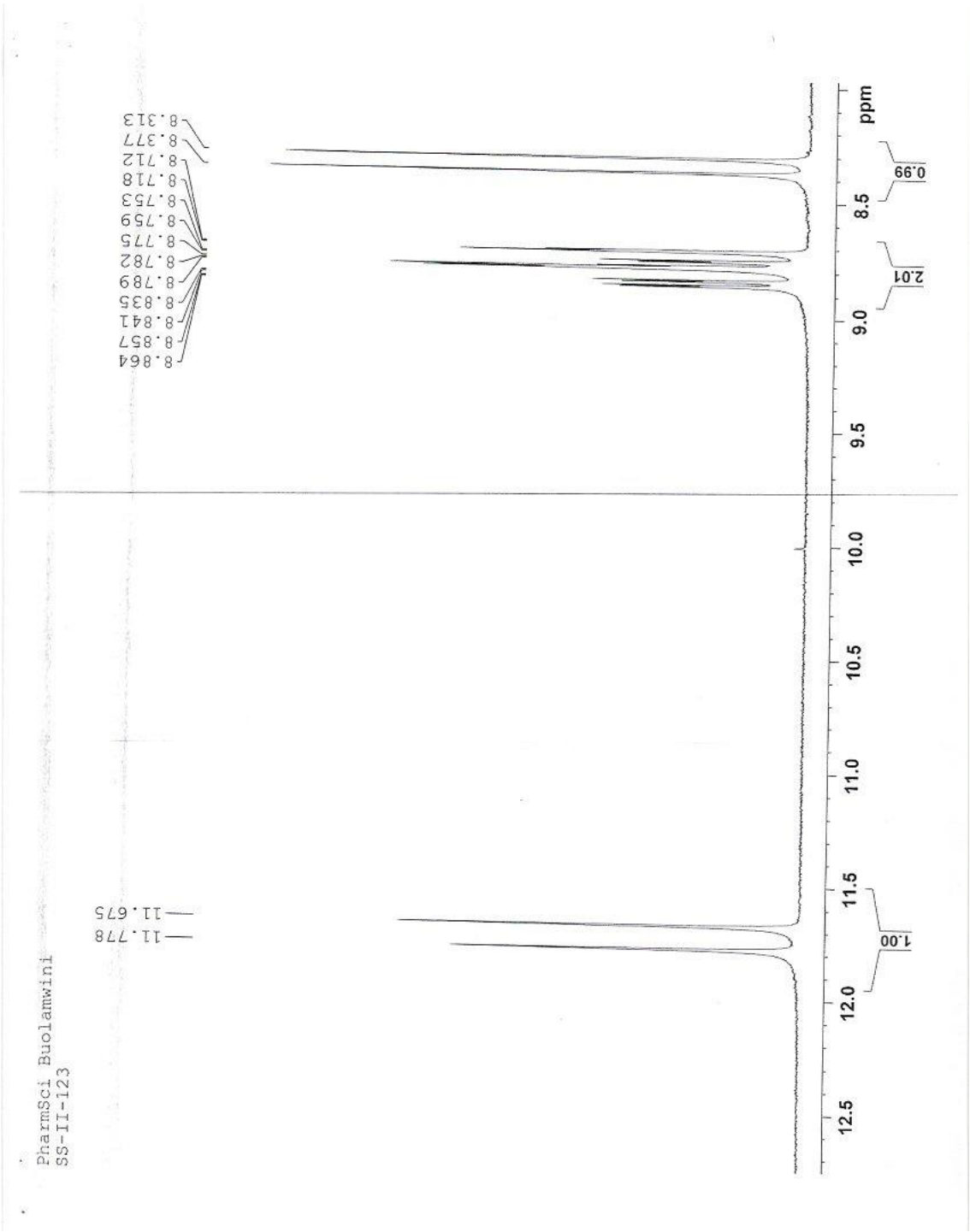
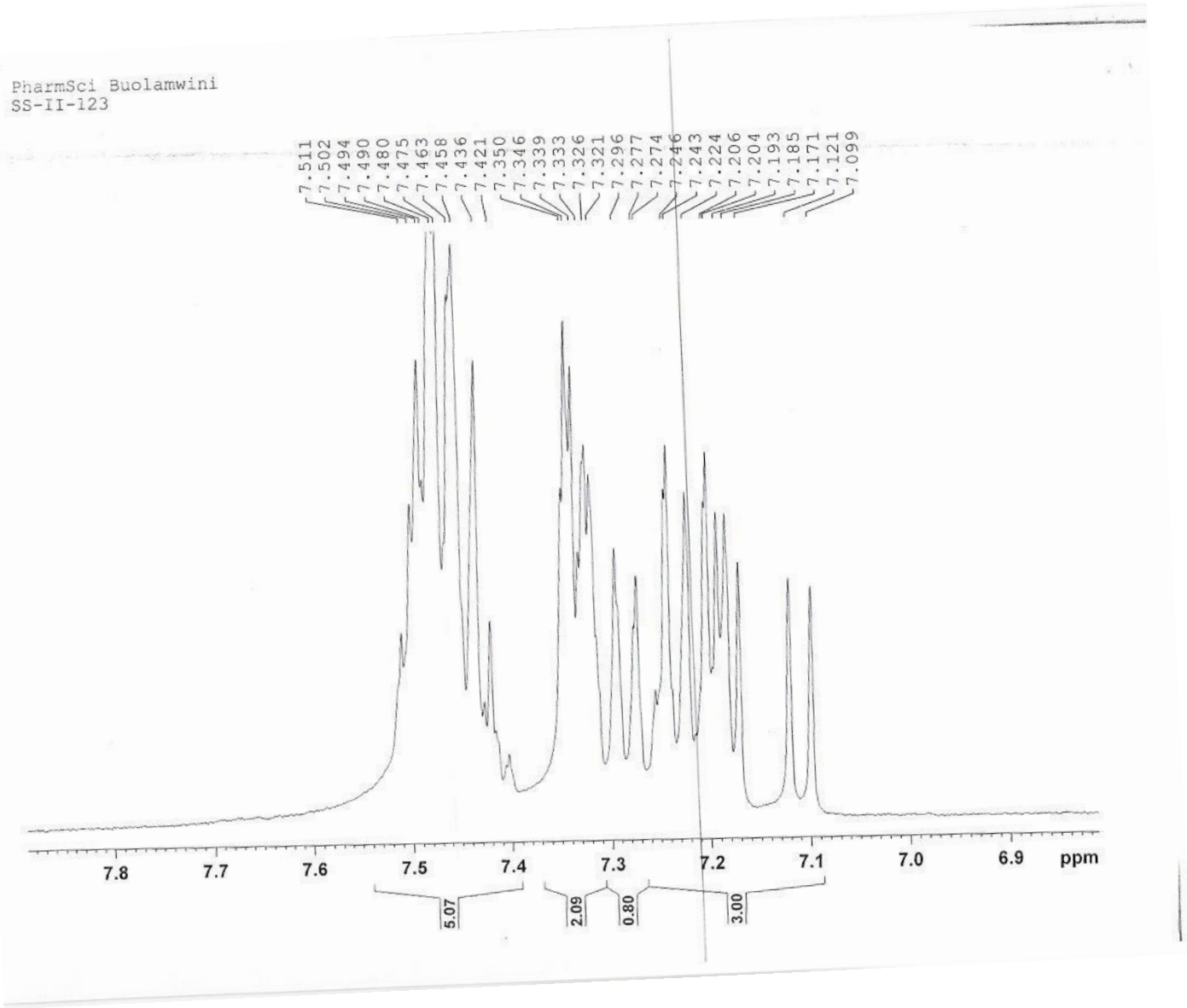
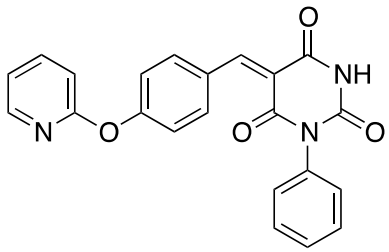
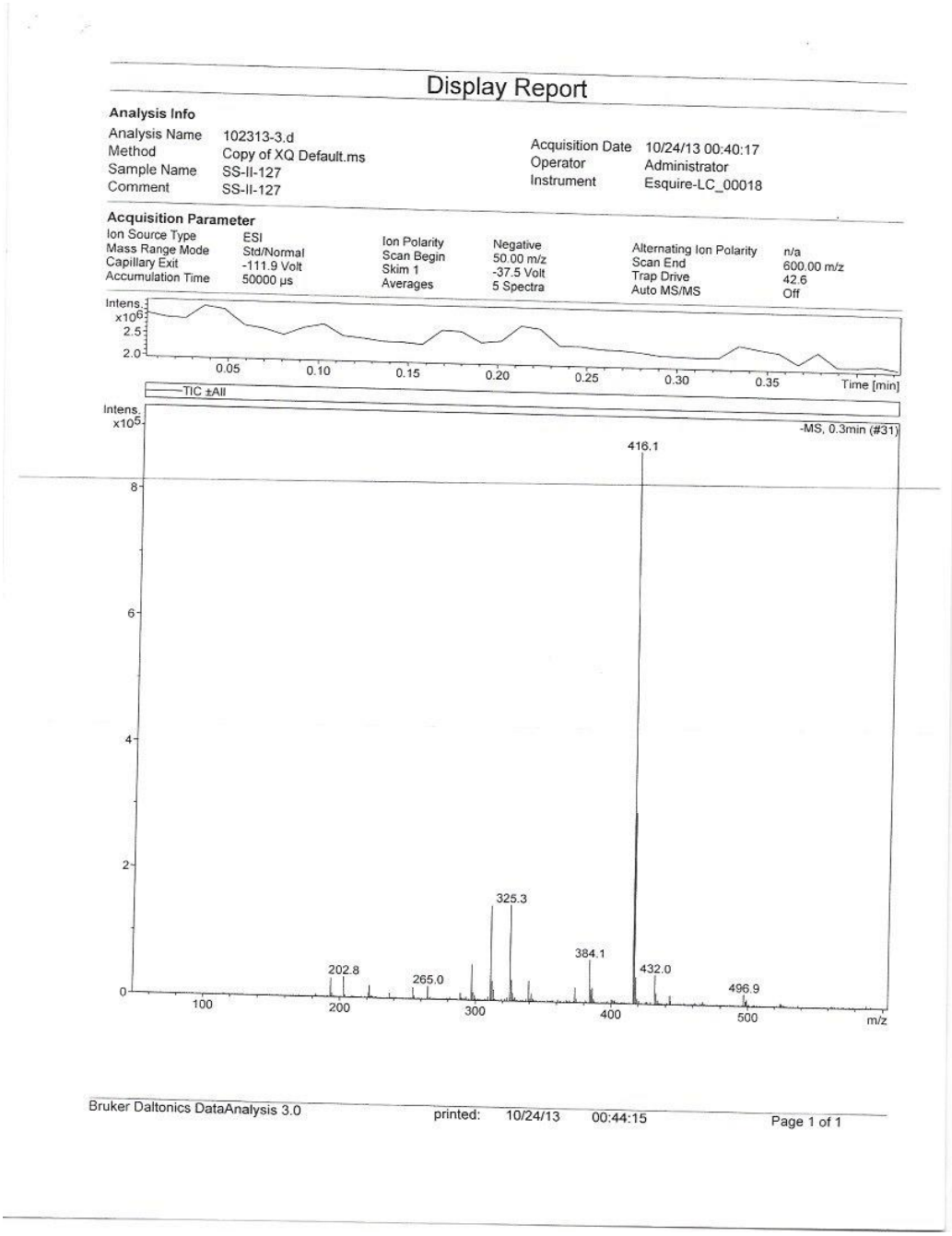

PharmSci Buolamwini
SS-II-123
11.675
11.778
8.313
8.377
8.712
8.718
8.753
8.759
8.775
8.782
8.789
8.835
8.841
8.857
8.864
ppm
0.99
2.01
1.00

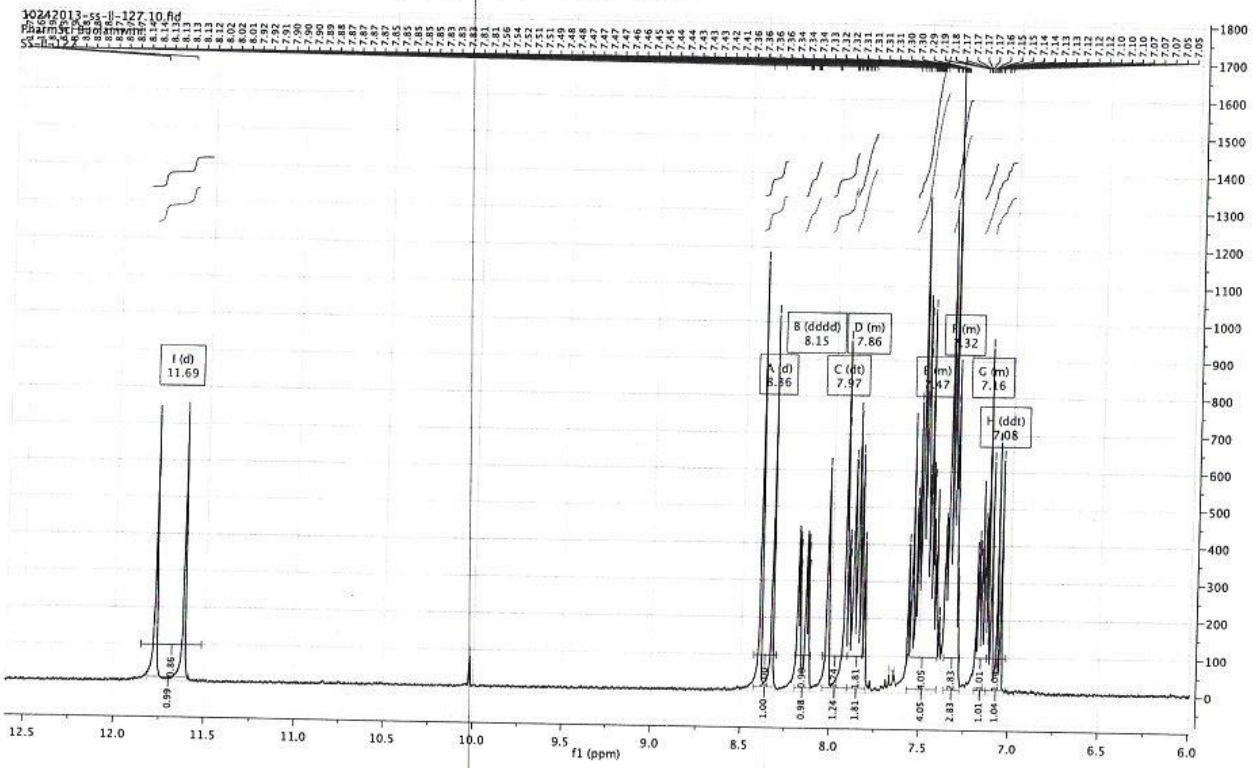

PharmSci Buolamwini
SS-II-123
7.511
7.502
7.494
7.490
7.480
7.475
7.463
7.458
7.436
7.421
7.350
7.346
7.339
7.333
7.326
7.321
7.296
7.277
7.274
7.246
7.243
7.224
7.206
7.204
7.193
7.185
7.171
7.121
7.099
7.8
7.7
7.6
7.5
7.4
7.3
7.2
7.1
7.0
6.9
ppm
5.07
2.09
0.80
3.00

Suppl. Mass spectrum and ^{1}H NMR Spectrum of **49**

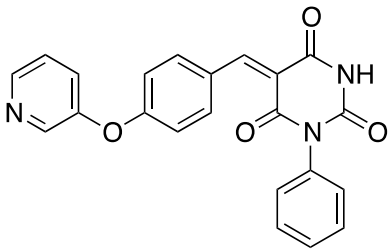




^{1}H NMR (400 MHz, DMSO-d_6) δ 11.69 (d, J = 63.4 Hz, 1H), 8.36 (d, J = 27.1 Hz, 1H), 8.15 (dddd, J = 18.6, 4.9, 2.1, 0.8 Hz, 1H), 7.97 (dt, J = 39.2, 2.0 Hz, 2H), 7.90 – 7.80 (m, 2H), 7.57 – 7.40 (m, 4H), 7.37 – 7.28 (m, 3H), 7.19 – 7.13 (m, 1H), 7.08 (ddt, J = 21.5, 8.3, 0.8 Hz, 1H).



Suppl. Mass spectrum and ^{1}H NMR Spectrum of **50**



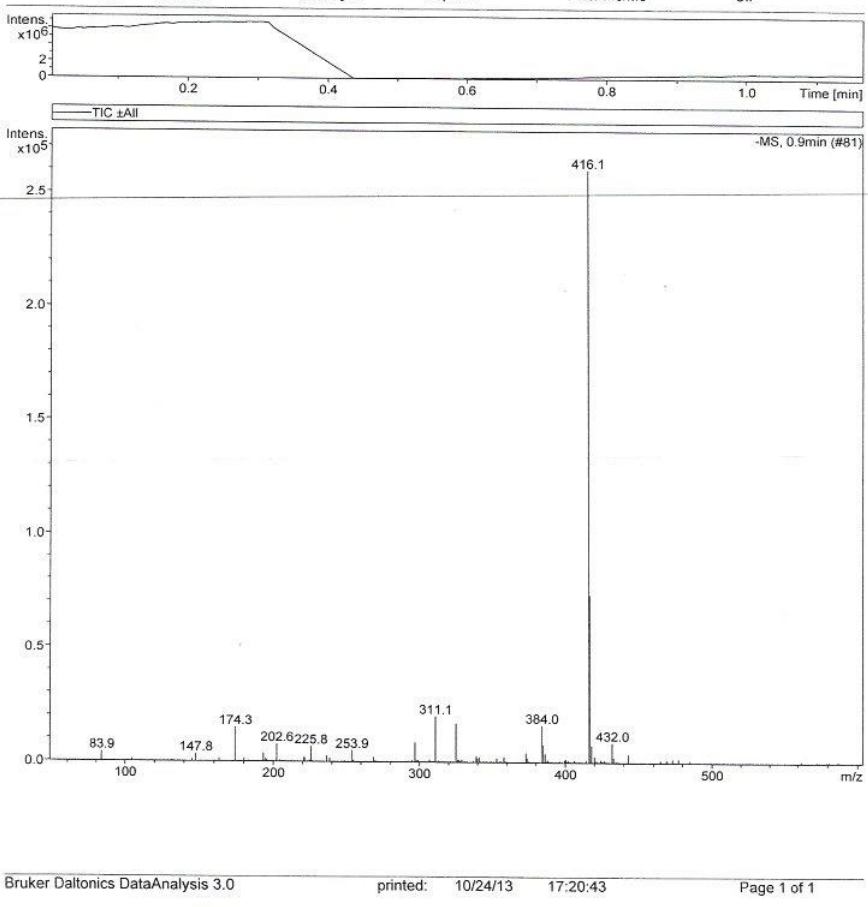
Display Report

Analysis Info

Analysis Name	102413-3.d	Acquisition Date	10/24/13 17:15:35
Method	Copy of Copy of CJJ.M	Operator	Default
Sample Name	sws-ii-129RE	Instrument	Esquire-LC_00018
Comment	ss-ii-129RE		

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	n/a
Mass Range Mode	Std/Normal	Scan Begin	50.00 m/z	Scan End	600.00 m/z
Capillary Exit	112.0 Volt	Skim 1	37.6 Volt	Trap Drive	37.2
Accumulation Time	29862 µs	Averages	5 Spectra	Auto MS/MS	Off



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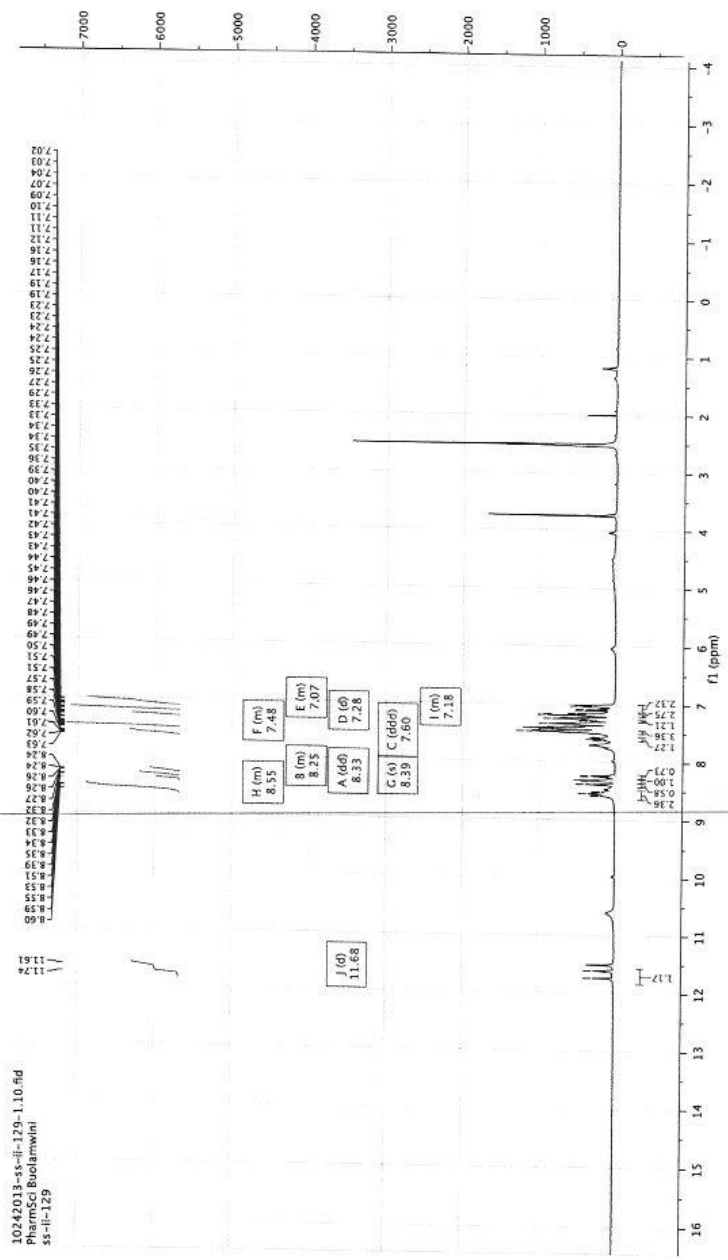
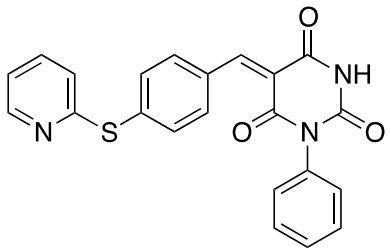


^{1}H NMR (400 MHz, DMSO-d_6) δ 11.68 (d, J = 50.7 Hz, 1H), 8.65 – 8.49 (m, 2H), 8.39 (s, 1H), 8.33 (dd, J = 6.6, 2.3 Hz, 1H), 8.28 – 8.21 (m, 1H), 7.60 (ddd, J = 12.9, 8.4, 4.8 Hz, 1H), 7.51 – 7.44 (m, 3H), 7.28 (d, J = 8.2 Hz, 1H), 7.21 – 7.15 (m, 2H), 7.13 – 7.00 (m, 2H).

Suppl. Mass spectrum and ^{1}H NMR Spectrum of **51**



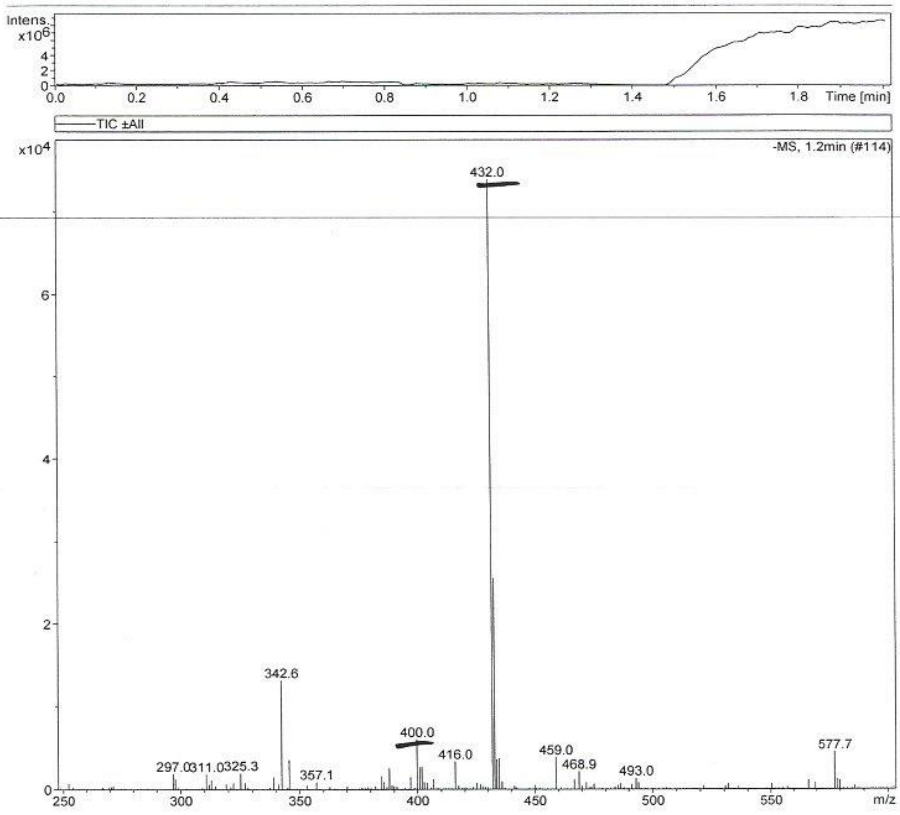
Display Report

Analysis Info

Analysis Name	102413-2.d	Acquisition Date	10/24/13 17:12:14
Method	Copy of Copy of CJJ.M	Operator	Default
Sample Name	sws-ii-125RE	Instrument	Esquire-LC_00018
Comment	ss-ii-125RE		

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Negative	Alternating Ion Polarity	n/a
Mass Range Mode	Std/Normal	Scan Begin	100.00 m/z	Scan End	600.00 m/z
Capillary Exit	-113.1 Volt	Skim 1	-38.4 Volt	Trap Drive	43.1
Accumulation Time	50000 µs	Averages	5 Spectra	Auto MS/MS	Off



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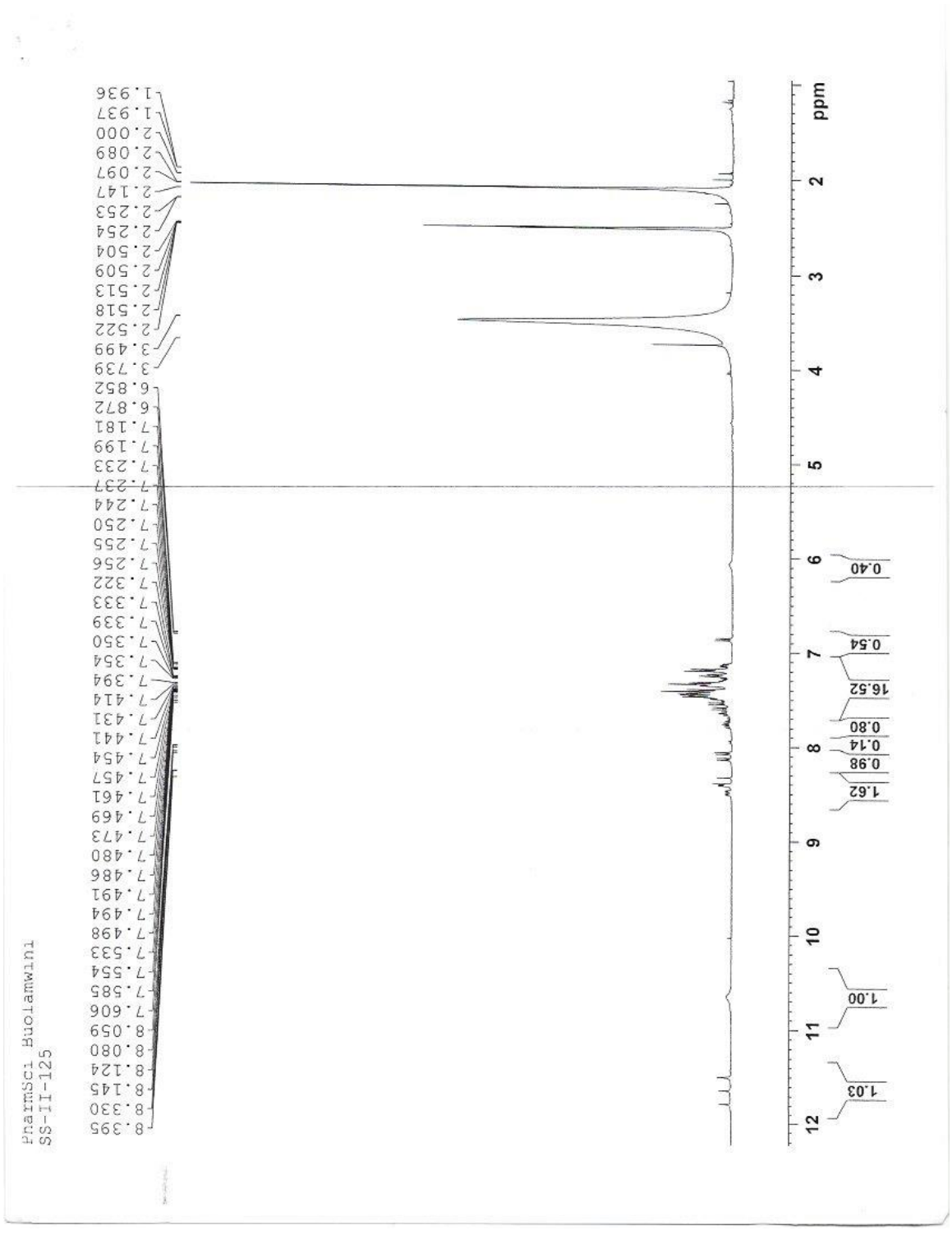
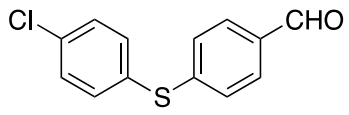
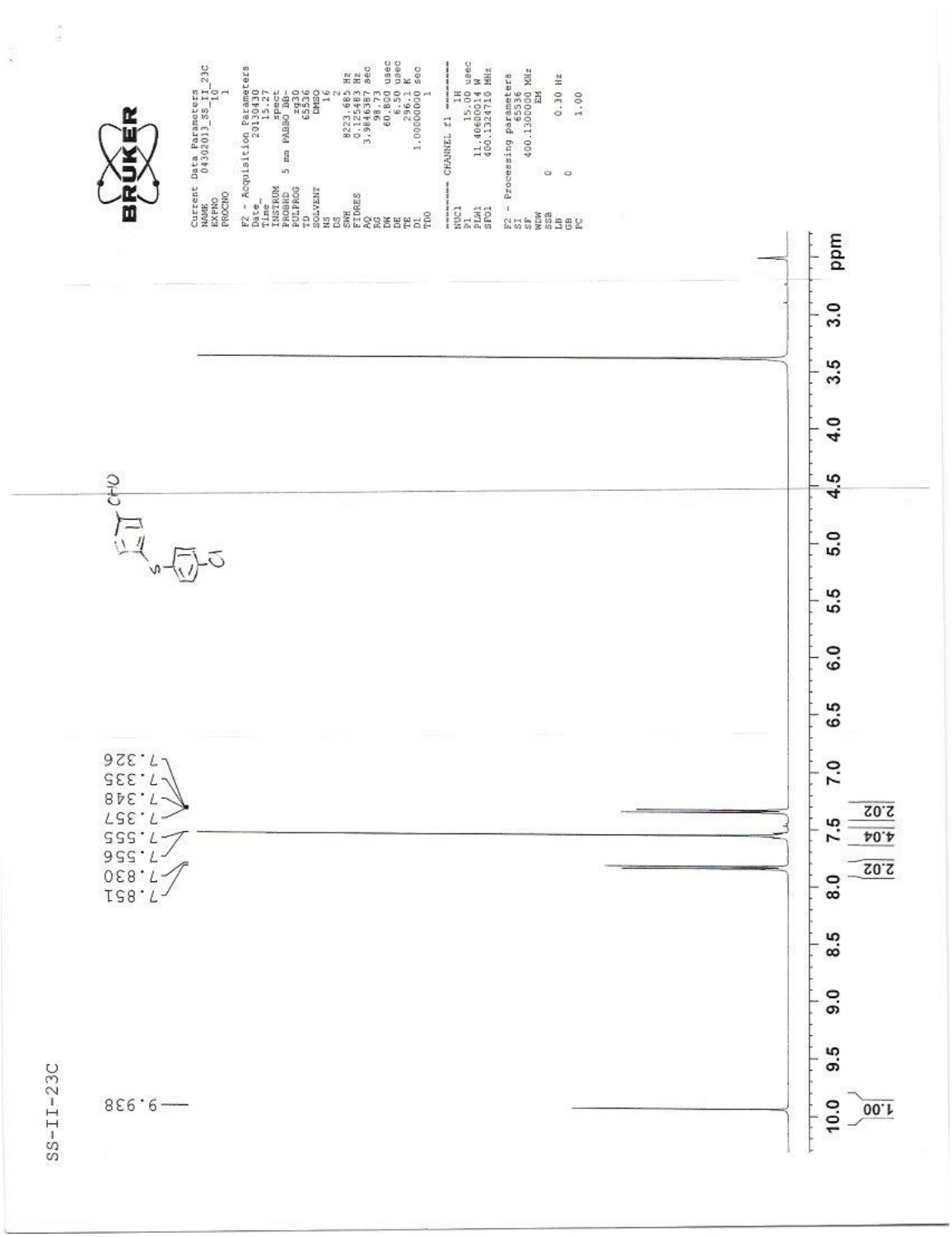
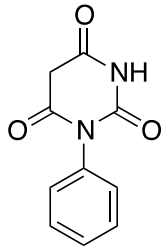

PharmSci Ruolamwini
SS-II-125
8.395
8.330
8.145
8.124
8.080
8.059
7.606
7.585
7.554
7.533
7.498
7.494
7.491
7.486
7.480
7.473
7.469
7.461
7.457
7.454
7.441
7.431
7.414
7.394
7.354
7.350
7.339
7.333
7.322
7.256
7.255
7.250
7.244
7.237
7.233
7.199
7.181
6.872
6.852
3.739
3.499
2.522
2.518
2.513
2.509
2.504
2.254
2.253
2.147
2.097
2.089
2.000
1.937
1.936
ppm
1.03
1.00
0.40
0.54
16.52
0.80
0.14
0.98
1.62

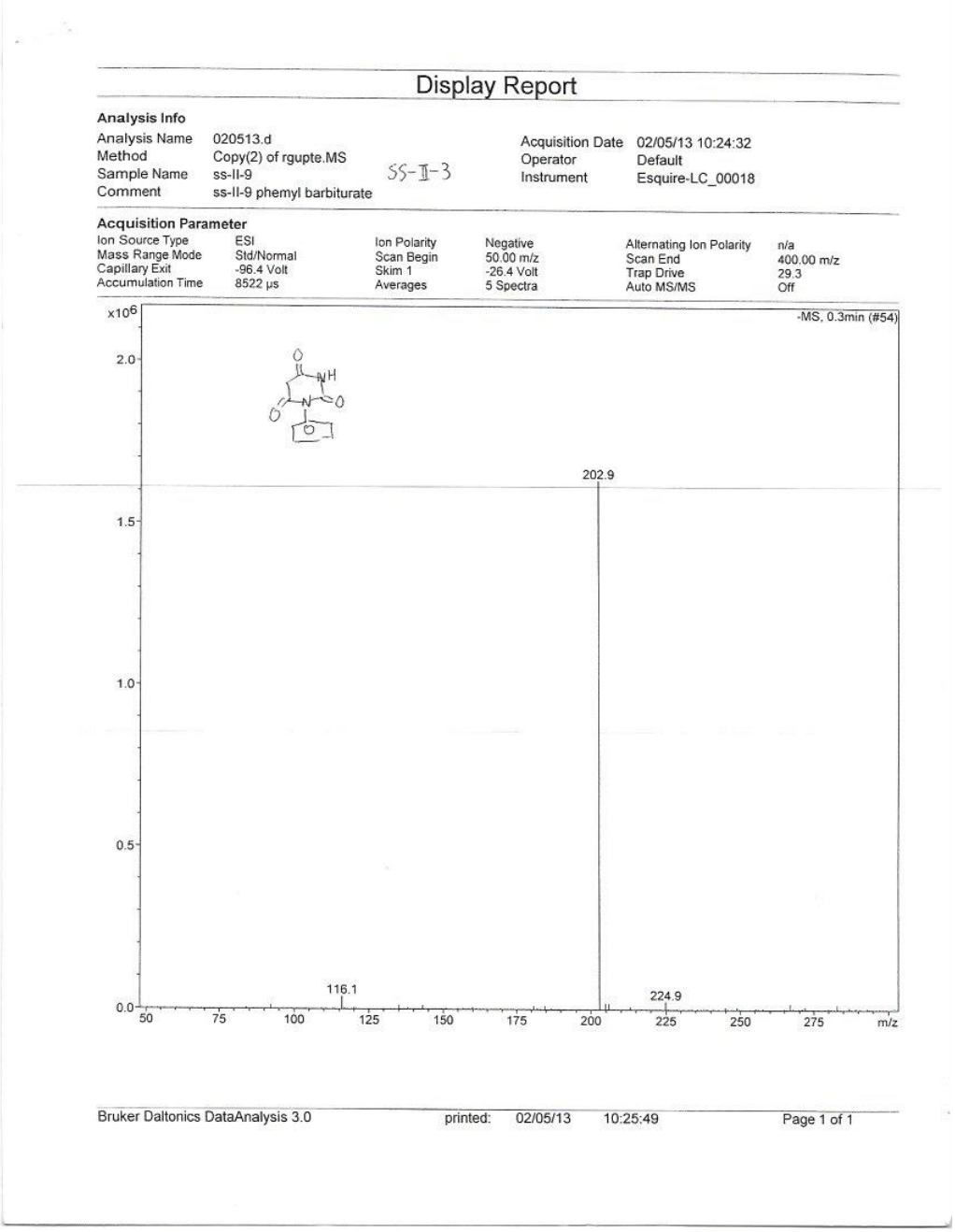
Suppl. ^{1}H NMR Spectrum of **52**

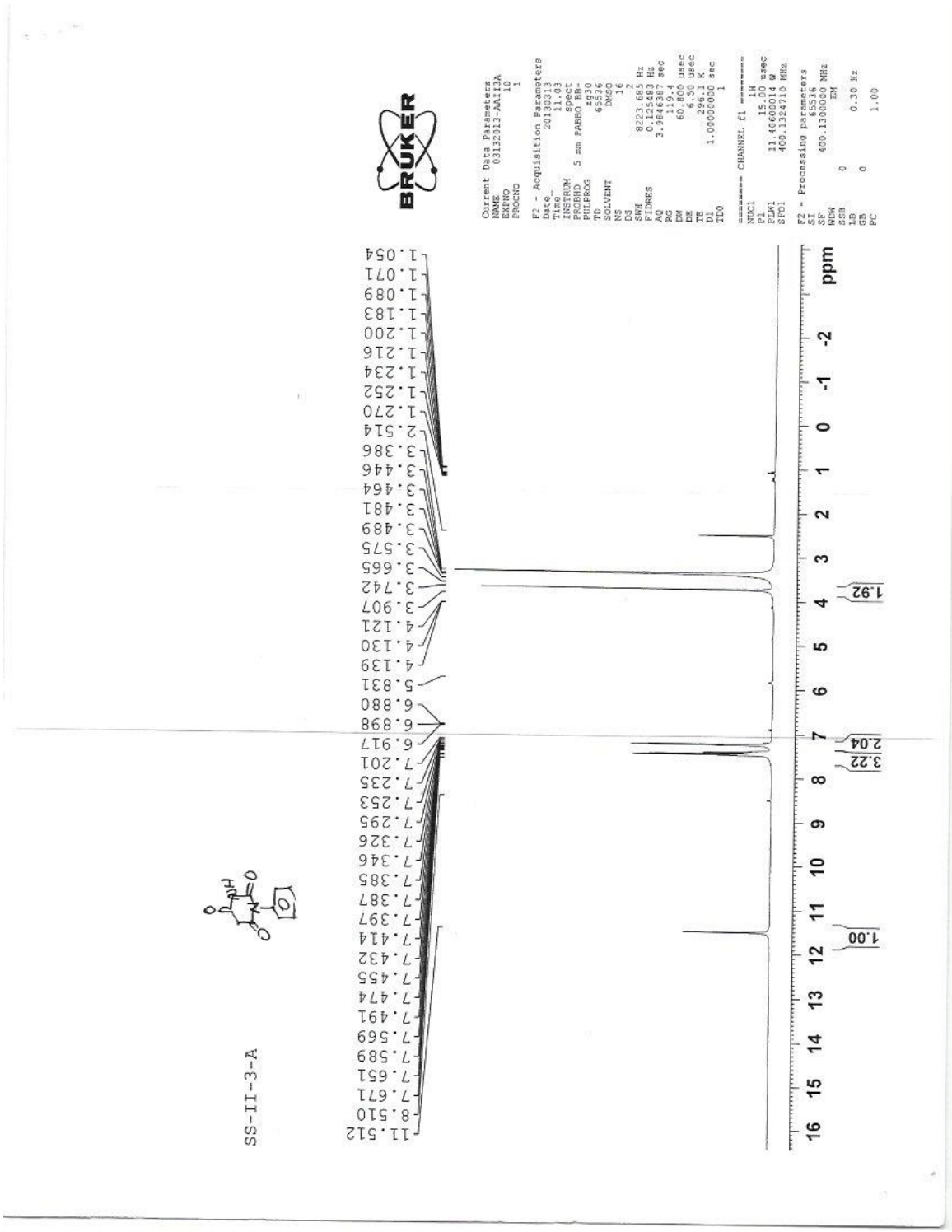




Suppl. Mass spectrum and ^{1}H NMR Spectrum of **53**






SS-II-3-A
BRUKER
Current Data Parameters
NAME 03132013-AA110
EXPNO 10
PROCNO 1
F2 - Acquisition Parameters
Date_ 20130313
Time 11.03
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zg30
TD 65536
SOLVENT DMSO
NS 16
DS 2
SWH 8223.685 Hz
FIDRES 0.125483 Hz
AQ 3.9846587 sec
RG 114.4
DW 60.800 usec
DE 6.50 usec
TE 296.1 K
D1 1.00000000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 1H
P1 15.00 usec
PLW1 11.40600014 W
SFO1 400.1324710 MHz
F2 - Processing parameters
SI 65536
SF 400.1300000 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 1.00
11.512
8.510
7.671
7.651
7.589
7.569
7.491
7.474
7.455
7.432
7.414
7.397
7.387
7.385
7.346
7.326
7.295
7.253
7.235
7.201
6.917
6.898
6.880
5.831
4.139
4.130
4.121
3.907
3.742
3.665
3.575
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1.270
1.252
1.234
1.216
1.200
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1.071
1.054
1.92
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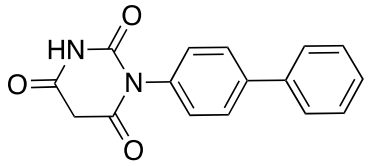
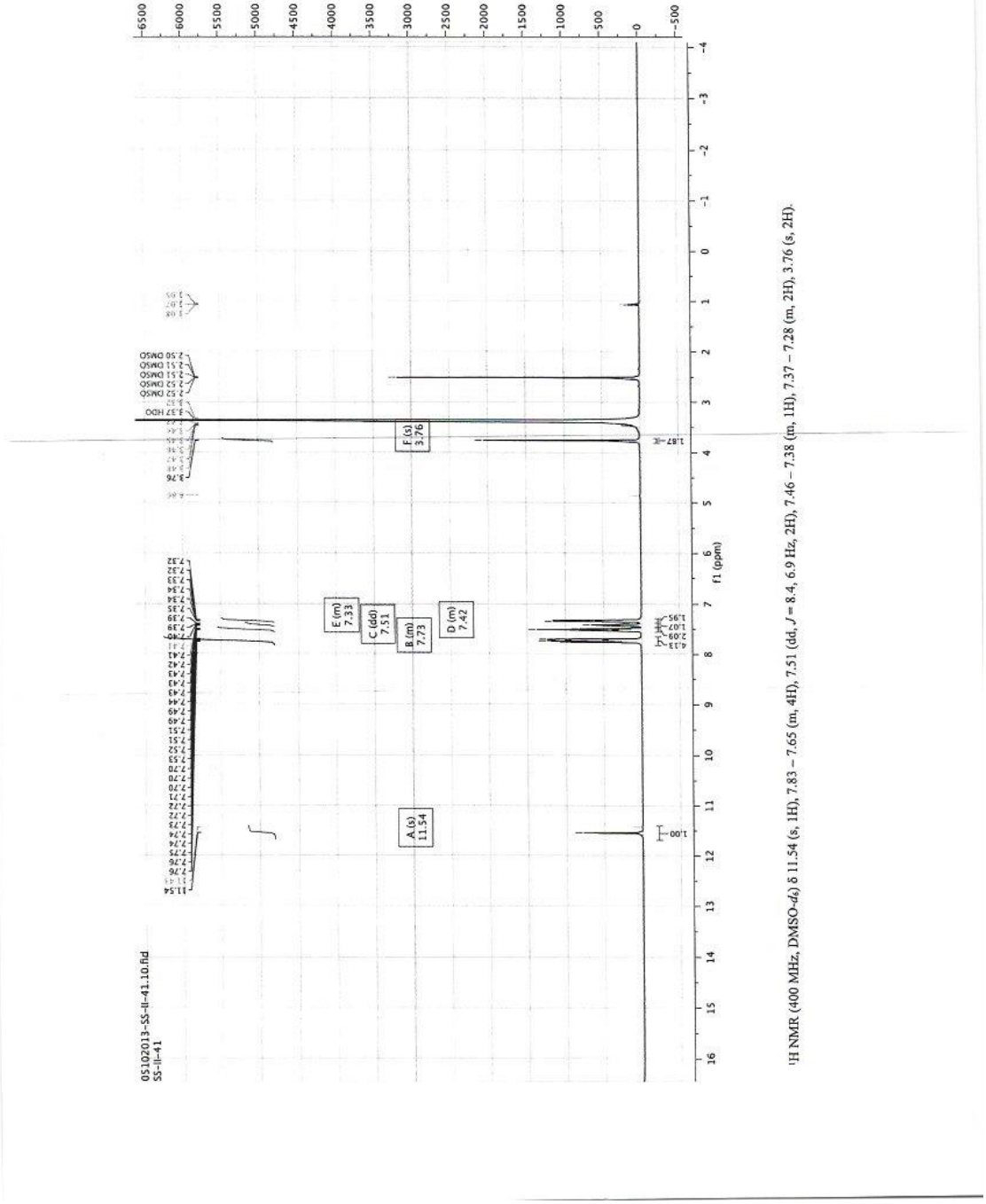
3.22
1.00
ppm

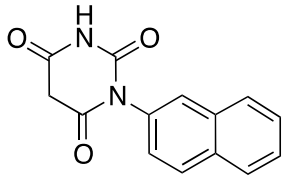
Suppl. ^{1}H NMR Spectrum of **54**





^{1}H NMR (400 MHz, DMSO-d_6) δ 11.54 (s, 1H), 7.83 – 7.65 (m, 4H), 7.51 (dd, J = 8.4, 6.9 Hz, 2H), 7.46 – 7.38 (m, 1H), 7.37 – 7.28 (m, 2H), 3.76 (s, 2H).

Suppl. Mass spectrum of **55**



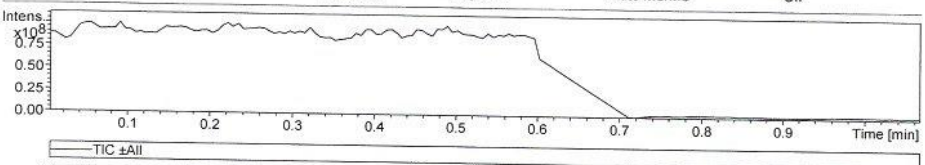
Display Report

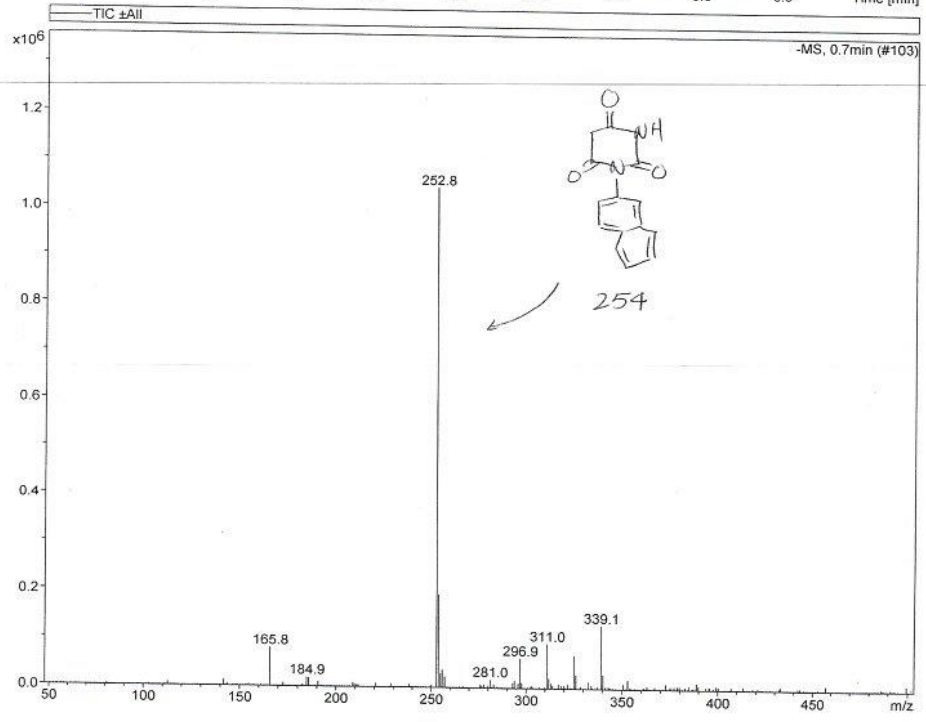
Analysis Info

Analysis Name	042313-1.d	Acquisition Date	04/23/13 11:46:49
Method	Copy of XQ Default.ms	Operator	Administrator
Sample Name	SS-II-31	Instrument	Esquire-LC_00018
Comment	ss-ii-31		

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Positive	Alternating Ion Polarity	n/a
Mass Range Mode	Std/Normal	Scan Begin	50.00 m/z	Scan End	500.00 m/z
Capillary Exit	101.0 Volt	Skim 1	29.8 Volt	Trap Drive	31.8
Accumulation Time	213 µs	Averages	5 Spectra	Auto MS/MS	Off





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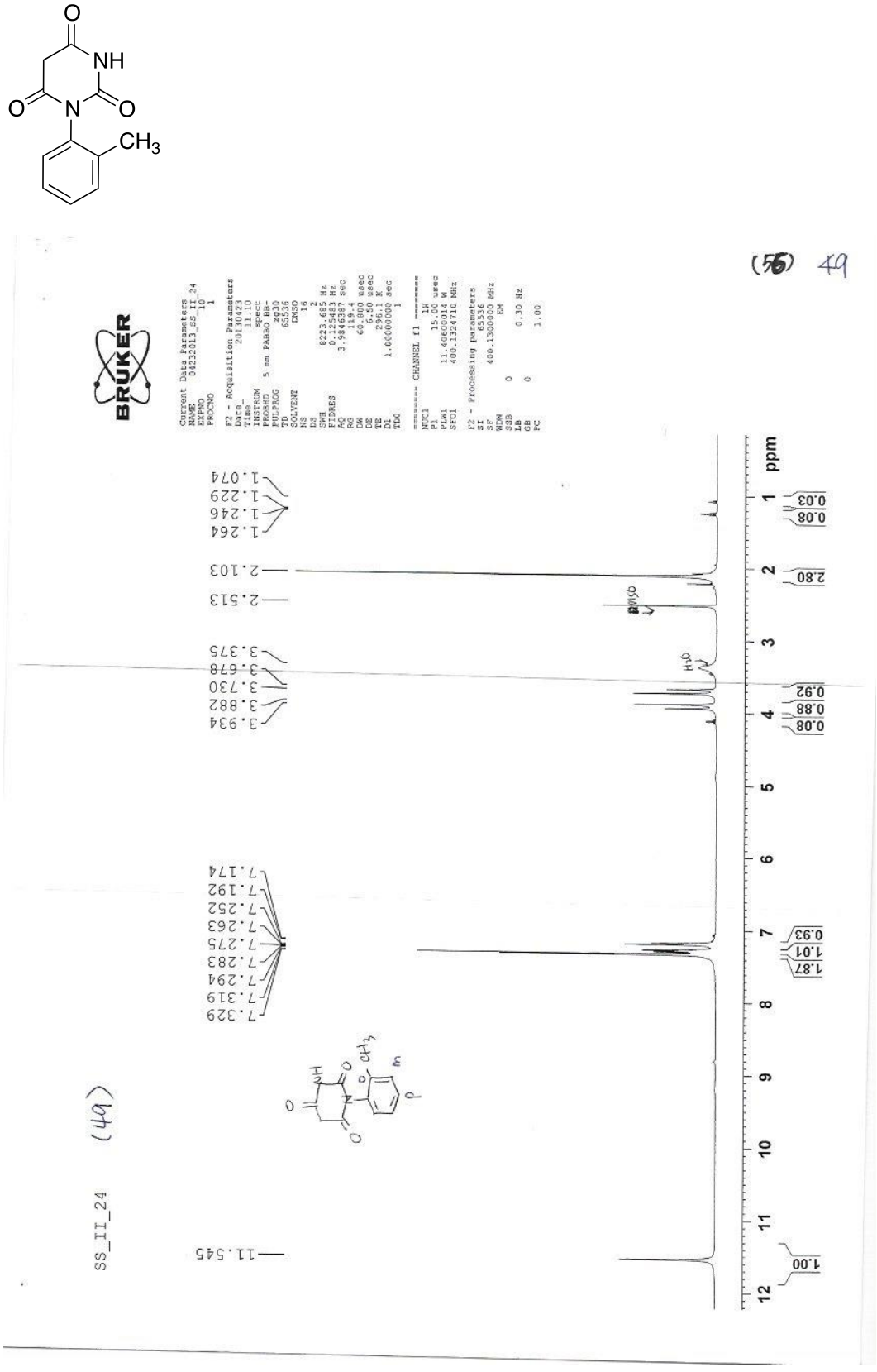
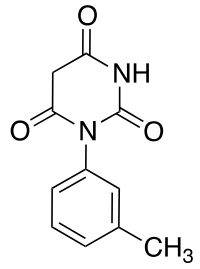
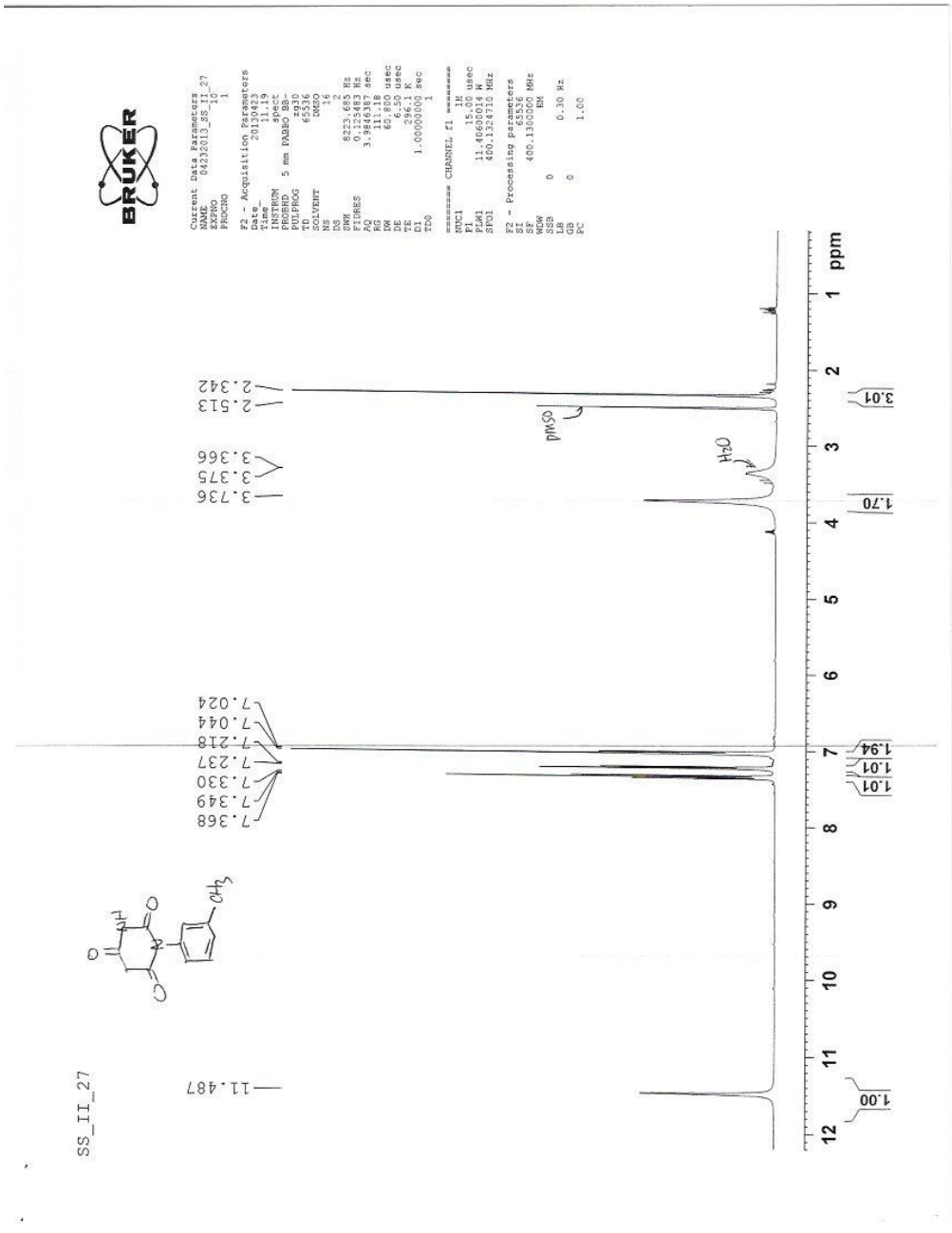
Suppl. ^{1}H NMR Spectrum of **56**

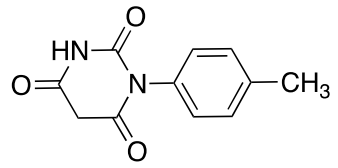


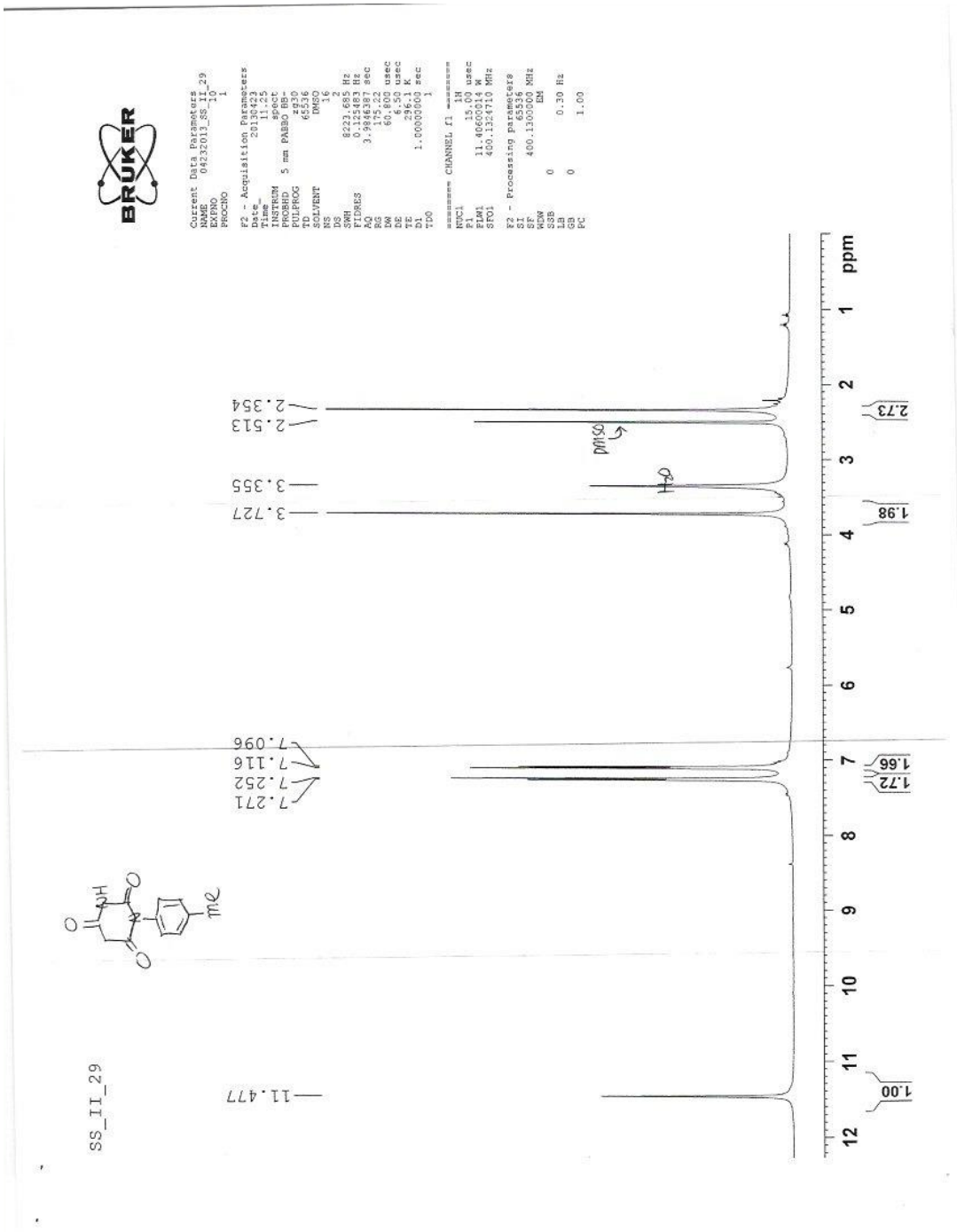
Suppl. ^{1}H NMR Spectrum of **57**



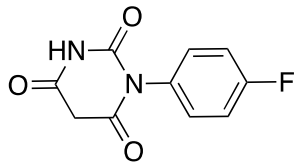


Suppl. NMR Spectrum of **58**





Suppl. Mass spectrum and ^{1}H NMR Spectrum of **59**



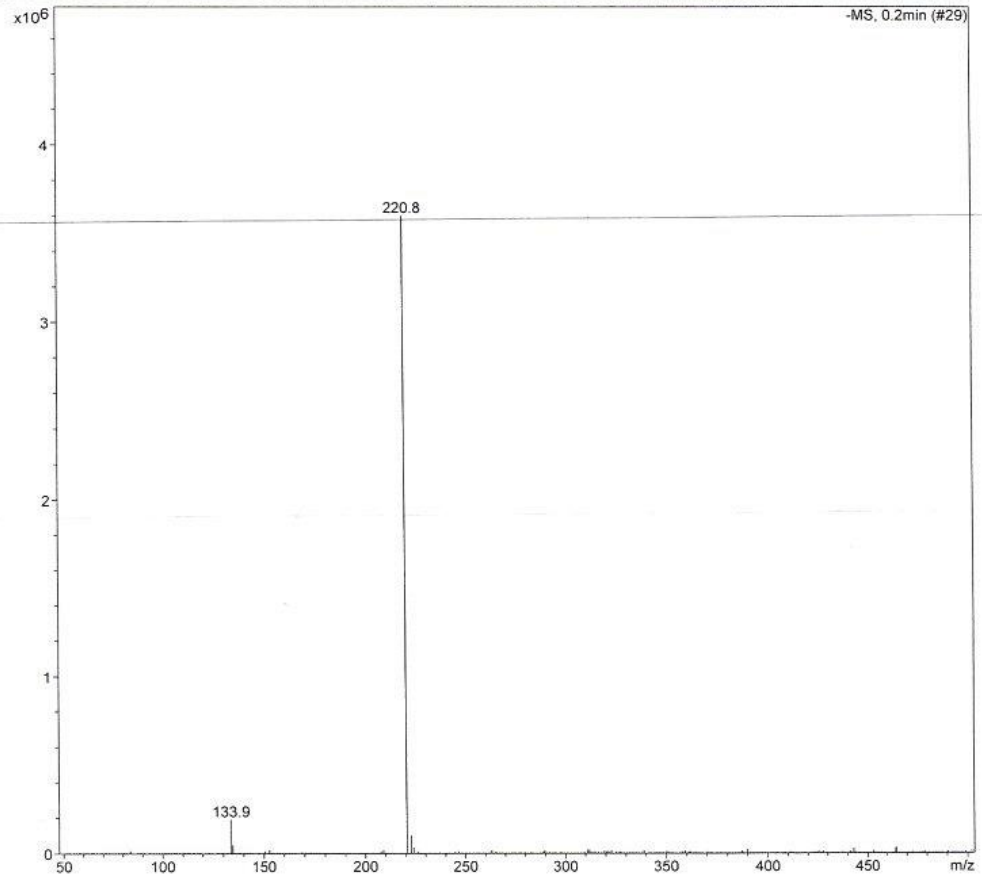
Display Report

Analysis Info

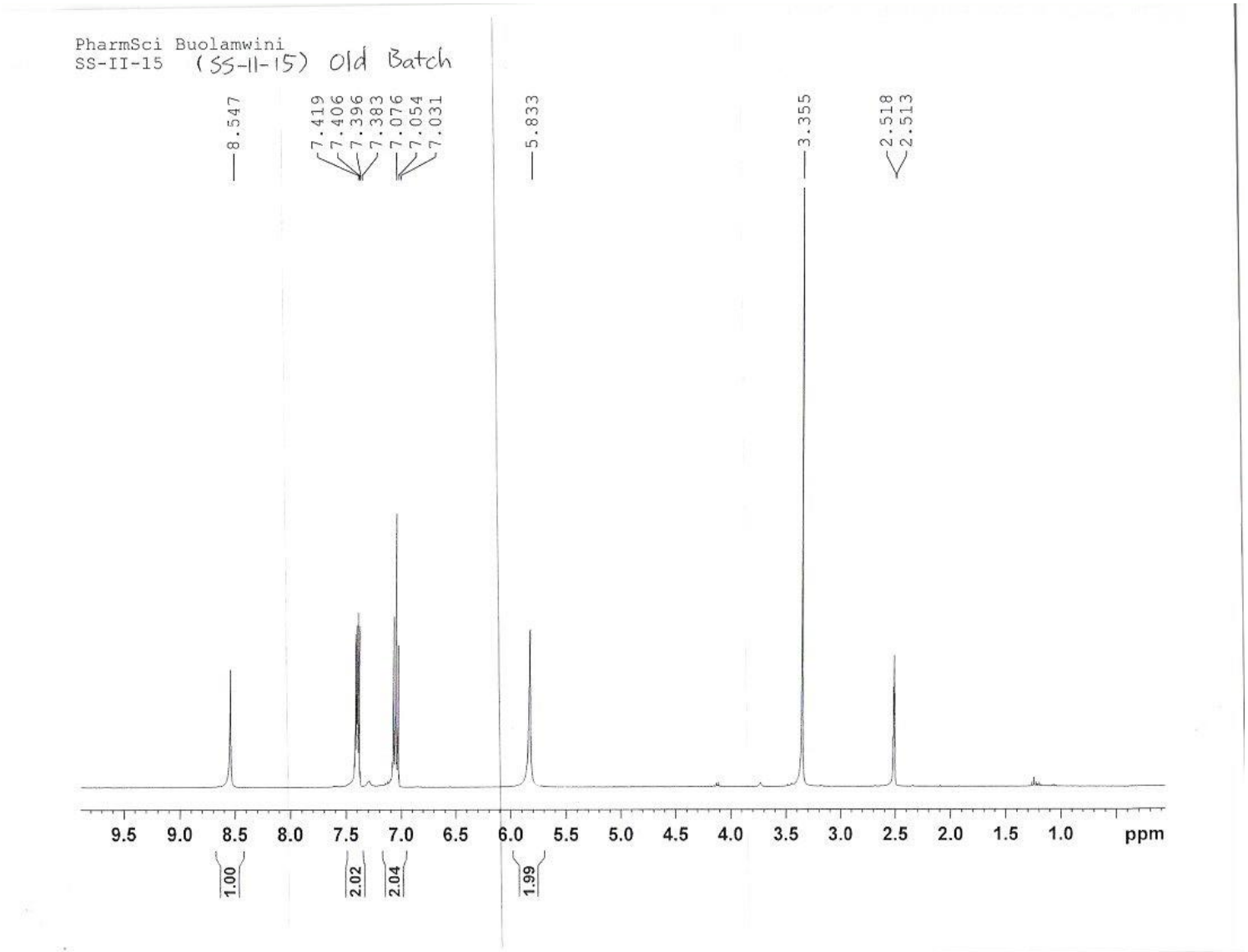
Analysis Name	032713.d	Acquisition Date	03/27/13 10:35:39
Method	Copy(2) of rgupte.MS	Operator	Default
Sample Name	ss-II-15	Instrument	Esquire-LC_00018
Comment	ss-II-15		

Acquisition Parameter

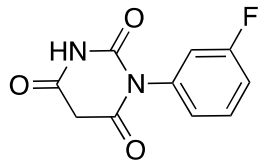
Ion Source Type	ESI	Ion Polarity	Negative	Alternating Ion Polarity	n/a
Mass Range Mode	Std/Normal	Scan Begin	50.00 m/z	Scan End	500.00 m/z
Capillary Exit	-98.1 Volt	Skim 1	-27.6 Volt	Trap Drive	30.2
Accumulation Time	3934 µs	Averages	5 Spectra	Auto MS/MS	Off

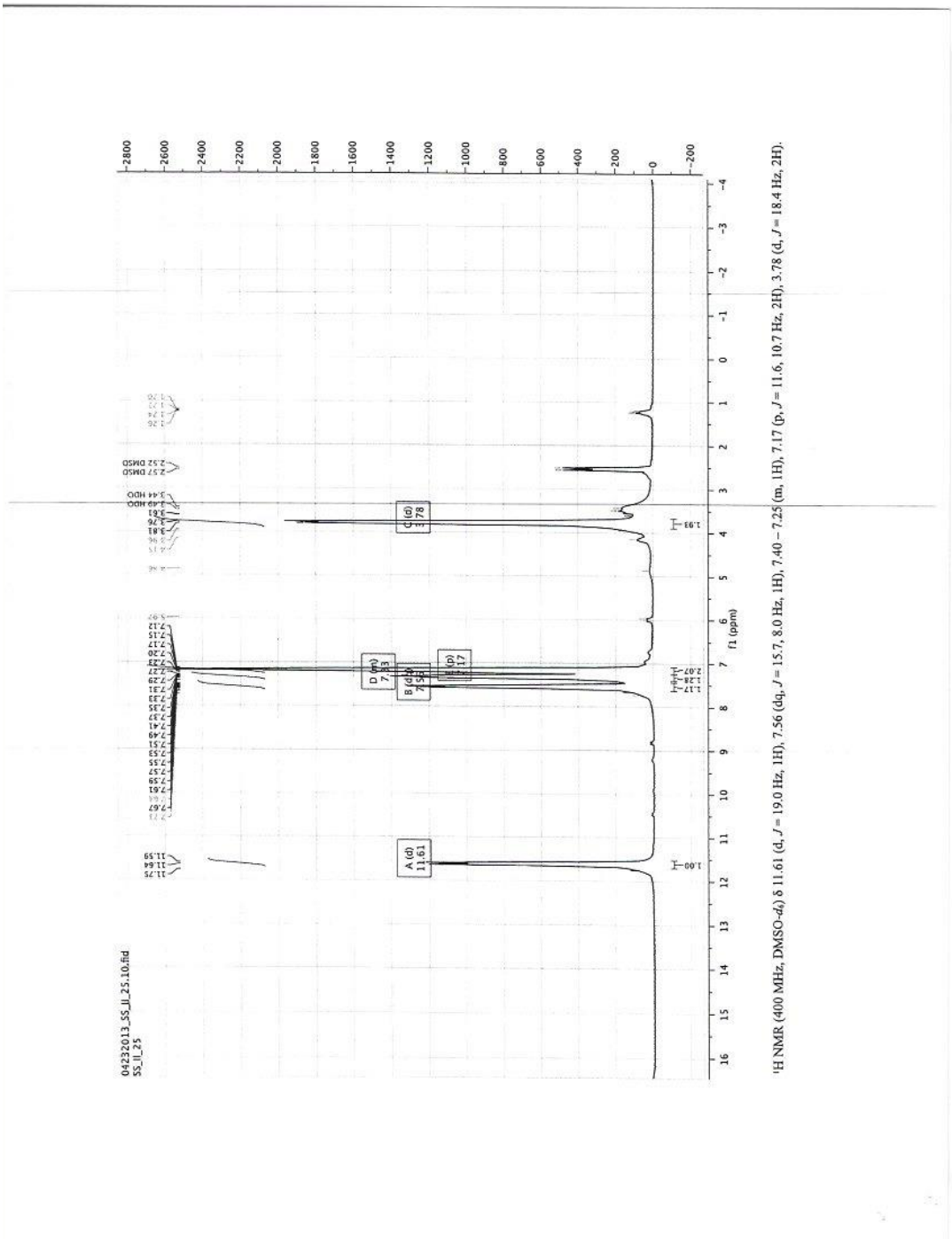


Bruker Daltonics DataAnalysis 3.0 printed: 03/27/13 10:37:22 Page 1 of 1


PharmSci Buolamwini
SS-II-15 (SS-II-15) Old Batch
8.547
7.419
7.406
7.396
7.383
7.076
7.054
7.031
5.833
3.355
2.518
2.513
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 ppm
1.00
2.02
2.04
1.99

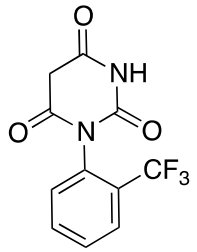
Suppl. ^{1}H NMR Spectrum of **60**

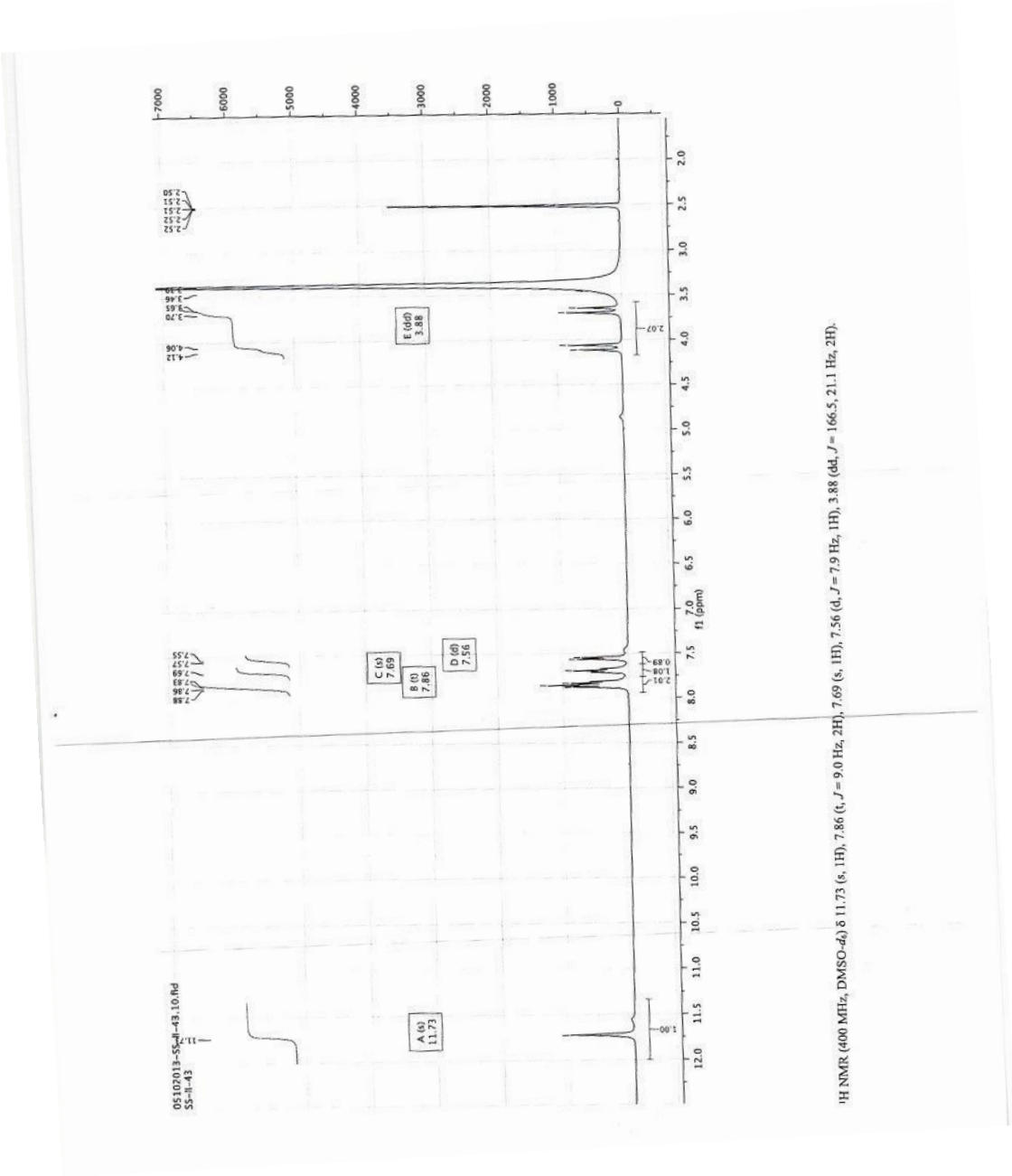




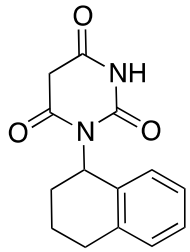
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.61 (d, J = 19.0 Hz, 1H), 7.56 (dq, J = 15.7, 8.0 Hz, 1H), 7.40 – 7.25 (m, 1H), 7.17 (p, J = 11.6, 10.7 Hz, 2H), 3.78 (d, J = 18.4 Hz, 2H).

Suppl. ^{1}H NMR Spectrum of **61**





Suppl. Mass spectrum of **62**



(62) 55

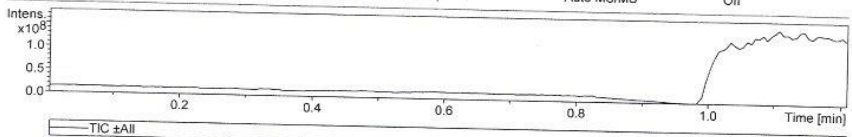
Display Report

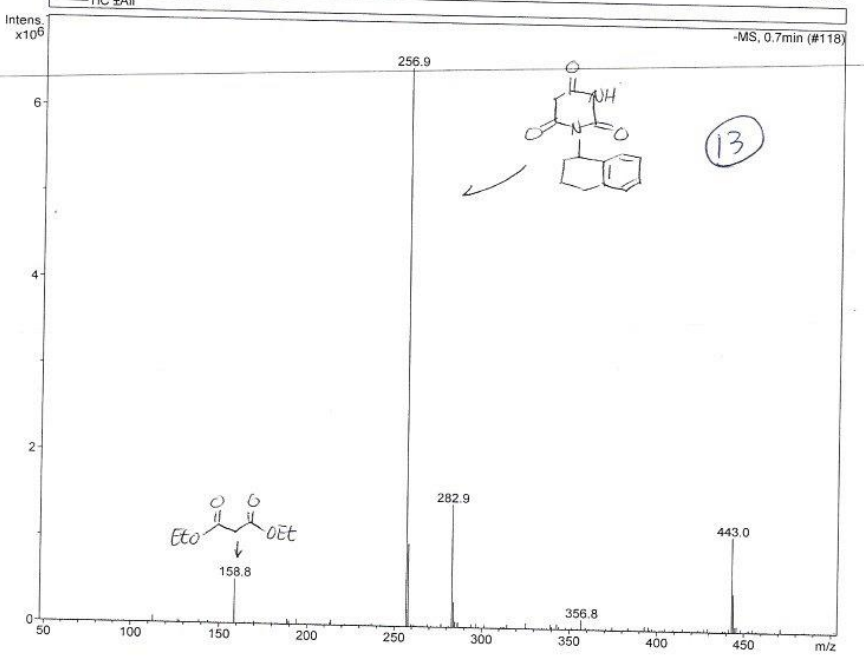
Analysis Info

Analysis Name	042313-2.d	Acquisition Date	04/23/13 11:50:56
Method	Copy of XQ Default.ms	Operator	Administrator
Sample Name	SS-II-35	Instrument	Esquire-LC_00018
Comment	ss-ii-35		

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Negative	Alternating Ion Polarity	n/a
Mass Range Mode	Std/Normal	Scan Begin	50.00 m/z	Scan End	500.00 m/z
Capillary Exit	-101.4 Volt	Skim 1	-30.1 Volt	Trap Drive	39.0
Accumulation Time	1321 µs	Averages	5 Spectra	Auto MS/MS	Off





(13)

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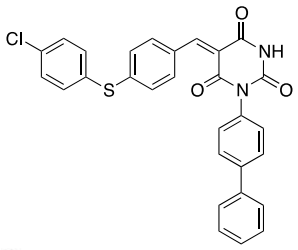
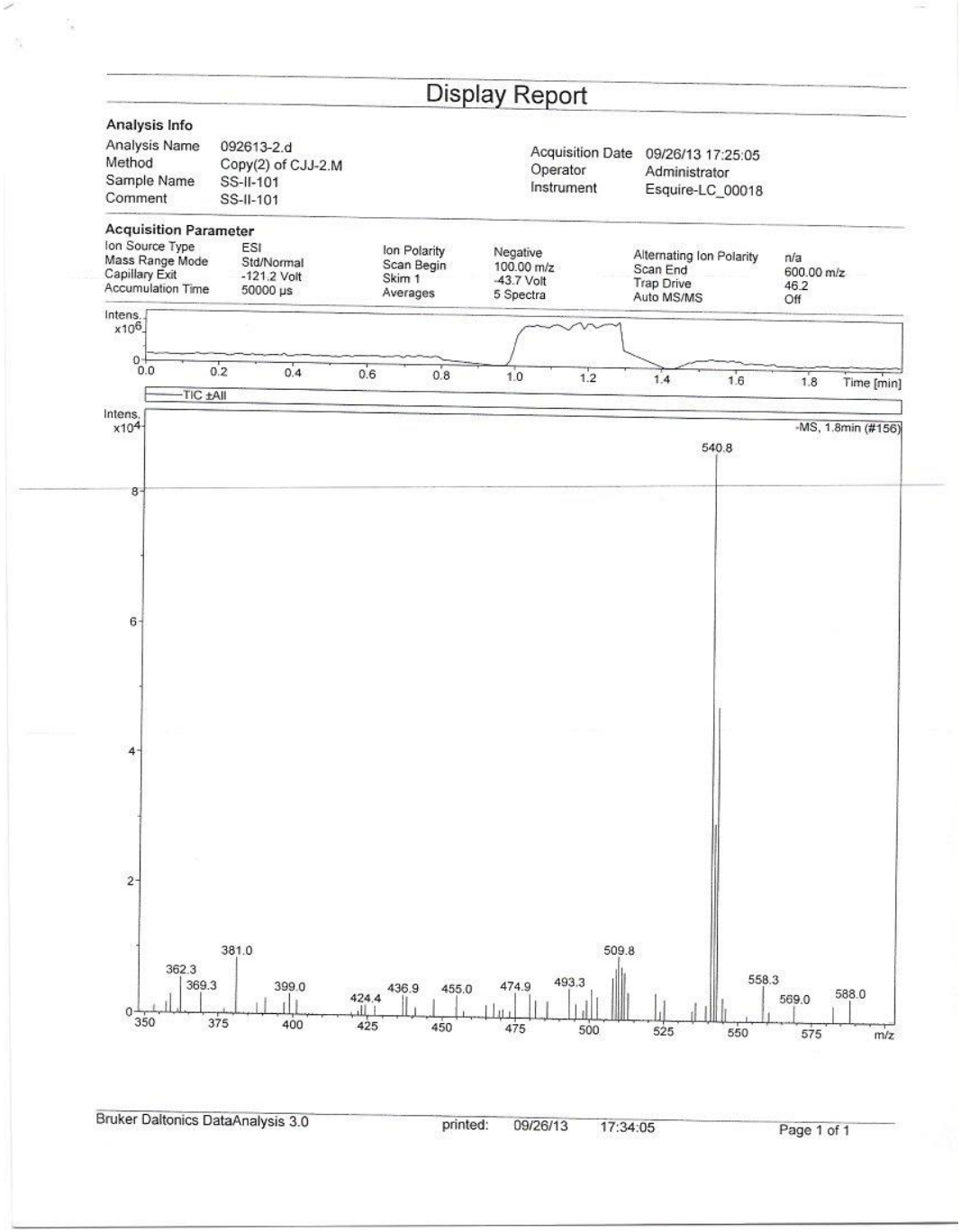
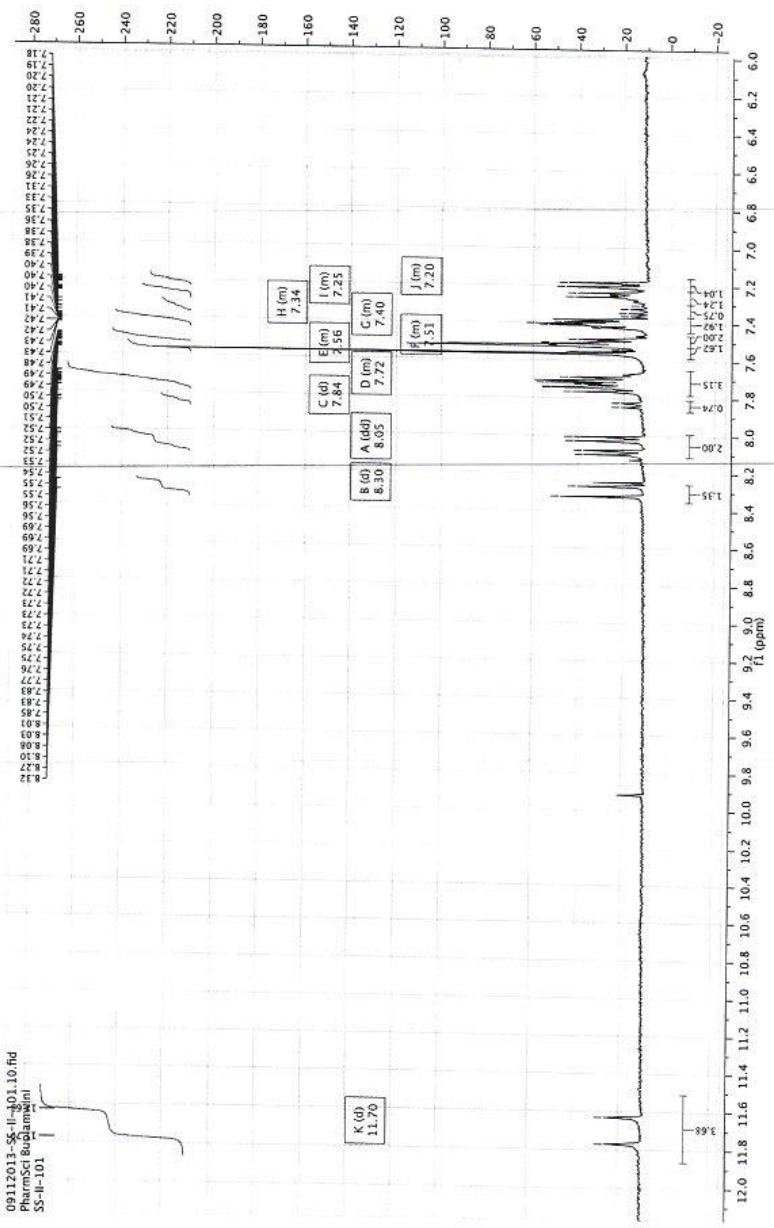
Suppl. Mass spectrum and ^{1}H NMR Spectrum of **63**

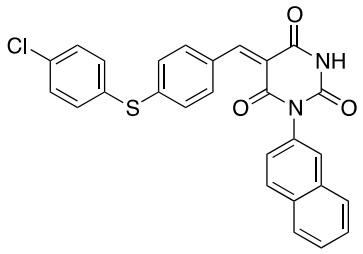


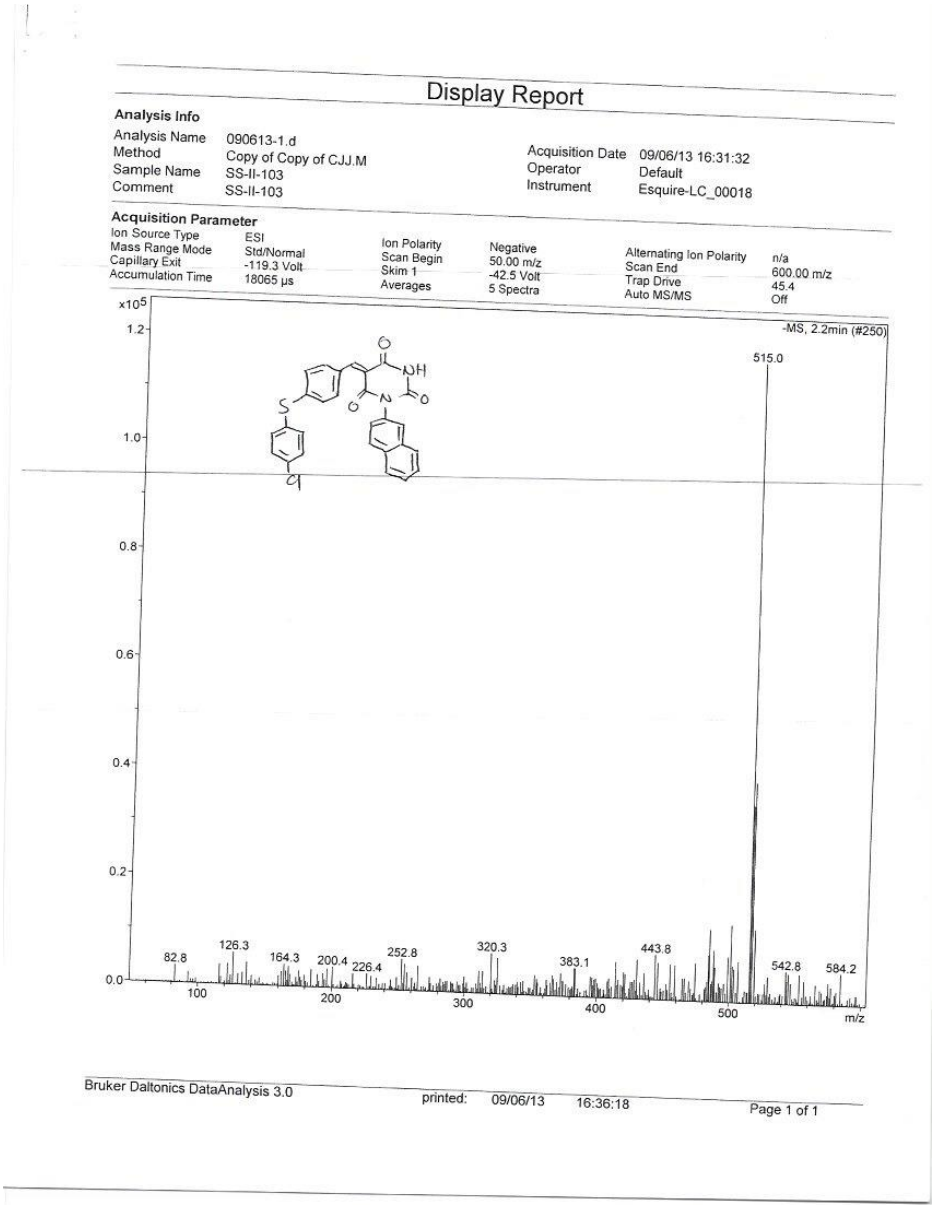


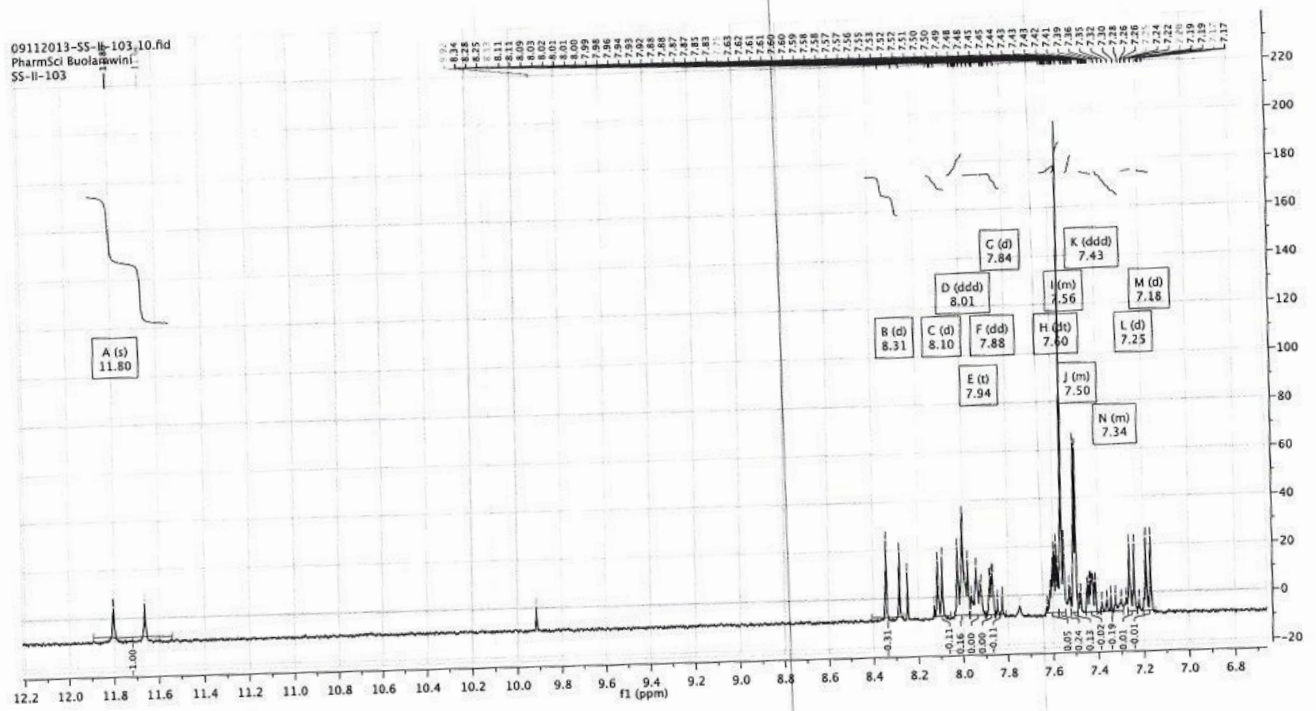


^{1}H NMR (400 MHz, DMSO-d_6) δ 11.70 (d, J = 56.1 Hz, 1H), 8.30 (d, J = 21.4 Hz, 1H), 8.05 (dd, J = 29.4, 8.6 Hz, 2H), 7.84 (d, J = 8.4 Hz, 1H), 7.78 – 7.65 (m, 5H), 7.59 – 7.53 (m, 2H), 7.53 – 7.47 (m, 2H), 7.45 – 7.37 (m, 2H), 7.37 – 7.30 (m, 1H), 7.30 – 7.23 (m, 2H), 7.23 – 7.16 (m, 1H).

Suppl. Mass spectrum and ^{1}H NMR Spectrum of **64**



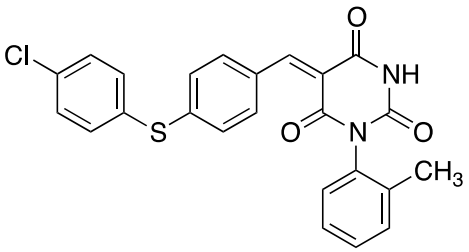


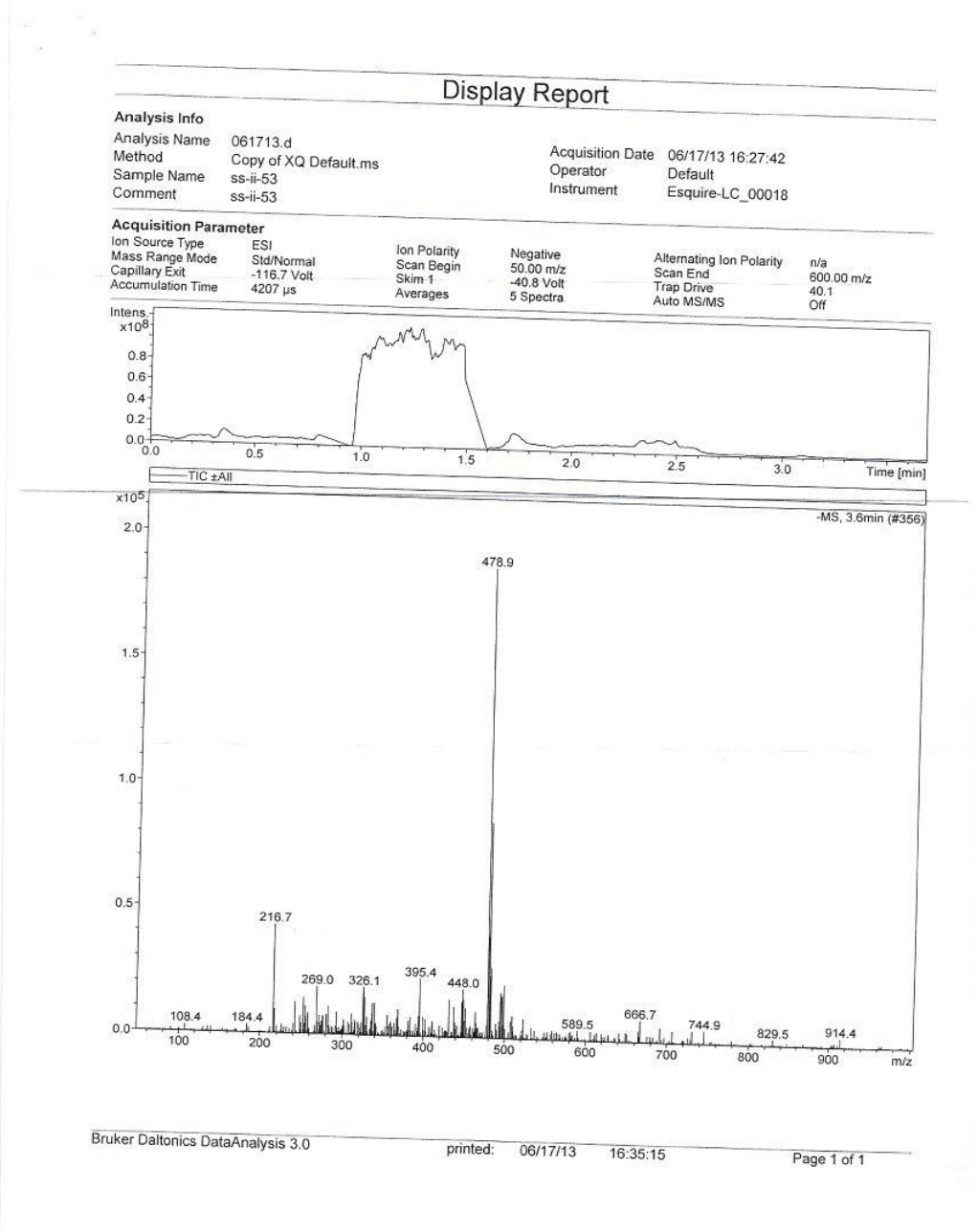


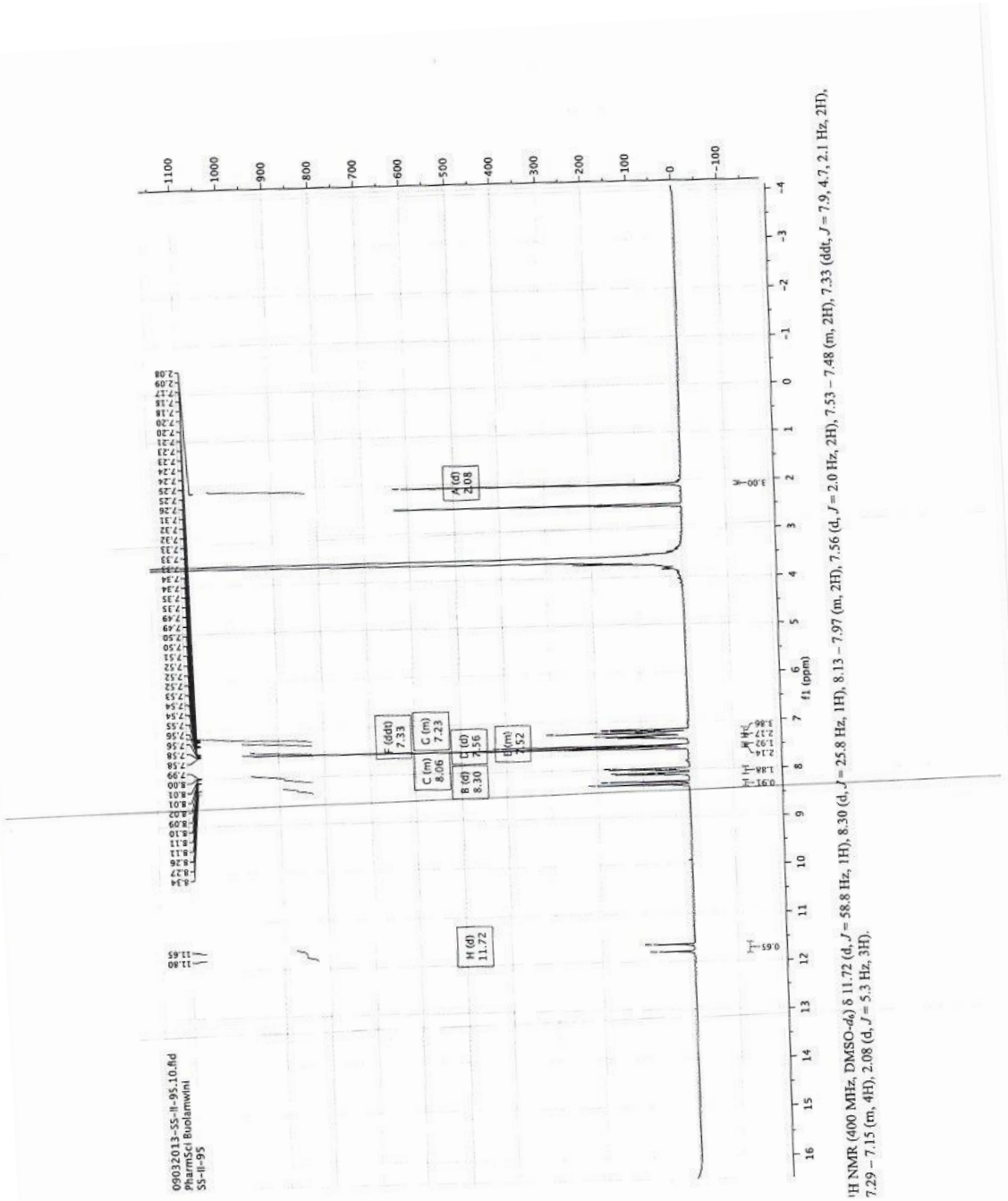
J=5.5Hz

^{1}H NMR (400 MHz, DMSO-d_6) δ 11.80 (d, -1H), 8.31 (d, J = 23.7 Hz, 1H), 8.10 (d, J = 8.7 Hz, 0H), 8.01 (ddd, J = 10.1, 7.3, 3.6 Hz, 2H), 7.94 (t, J = 8.6 Hz, 2H), 7.88 (dd, J = 5.1, 2.0 Hz, 1H), 7.60 (dt, J = 6.6, 3.2 Hz, 1H), 7.58 – 7.54 (m, 3H), 7.52 – 7.49 (m, 2H), 7.43 (ddd, J = 8.7, 4.9, 2.0 Hz, 1H), 7.25 (d, J = 8.6 Hz, 1H), 7.18 (d, J = 8.6 Hz, 1H).

Suppl. Mass spectrum and ^{1}H NMR Spectrum of **65**

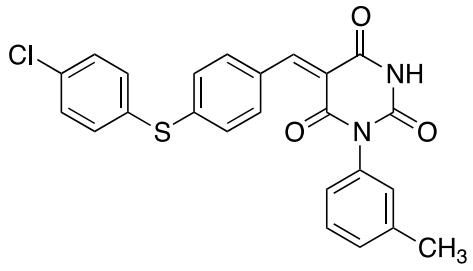


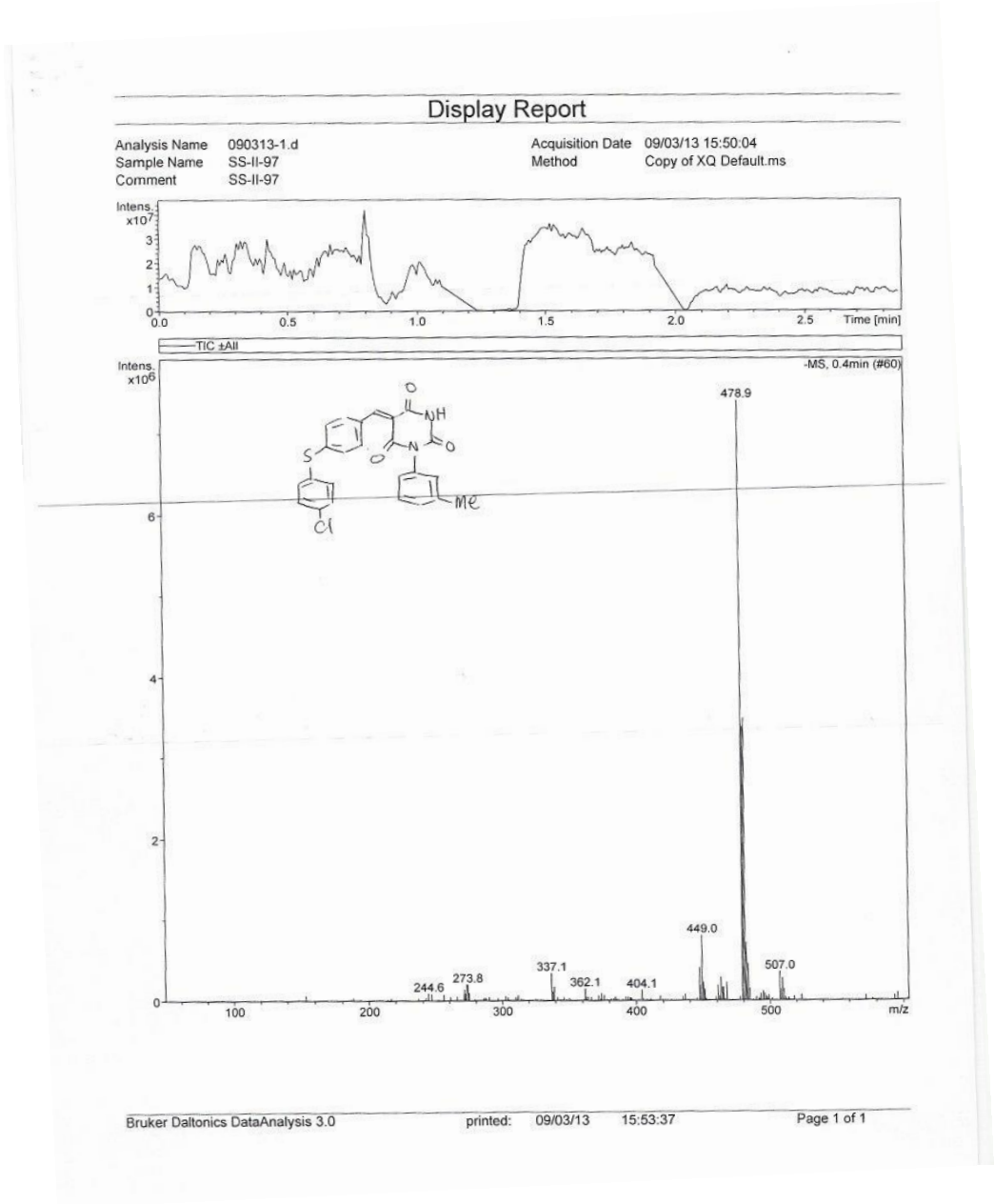


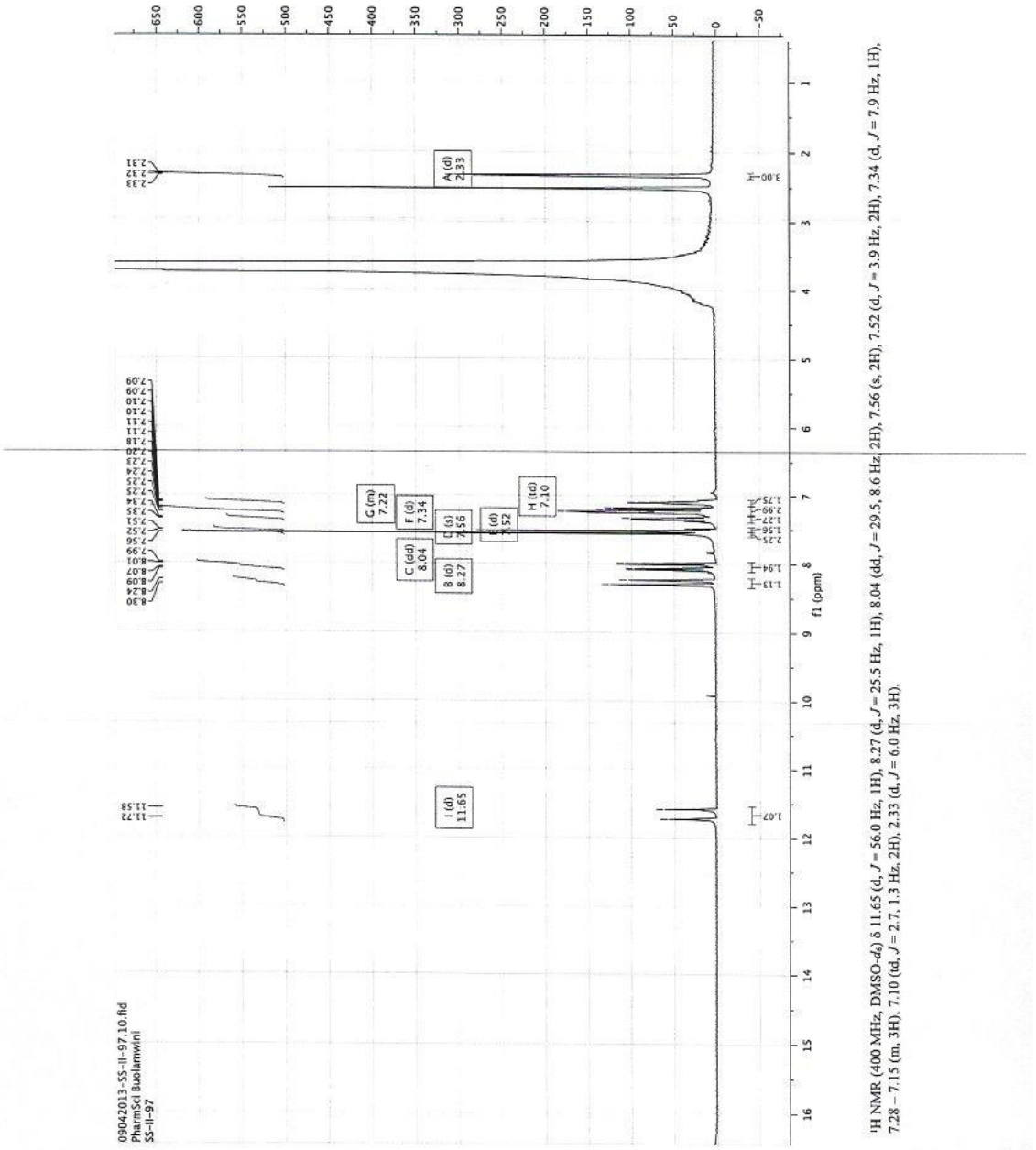


^{1}H NMR (400 MHz, DMSO-d_6) δ 11.72 (d, J = 58.8 Hz, 1H), 8.30 (d, J = 25.8 Hz, 1H), 8.13 – 7.97 (m, 2H), 7.56 (d, J = 2.0 Hz, 2H), 7.53 – 7.48 (m, 2H), 7.33 (ddt, J = 7.9, 4.7, 2.1 Hz, 2H), 7.29 – 7.15 (m, 4H), 2.08 (d, J = 5.3 Hz, 3H).

Suppl. Mass spectrum and ^{1}H NMR Spectrum of **66**

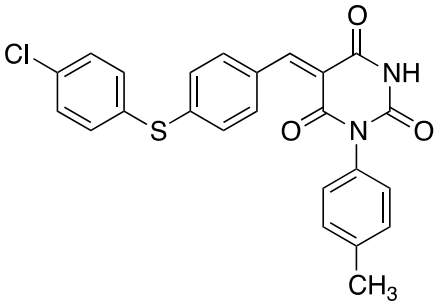


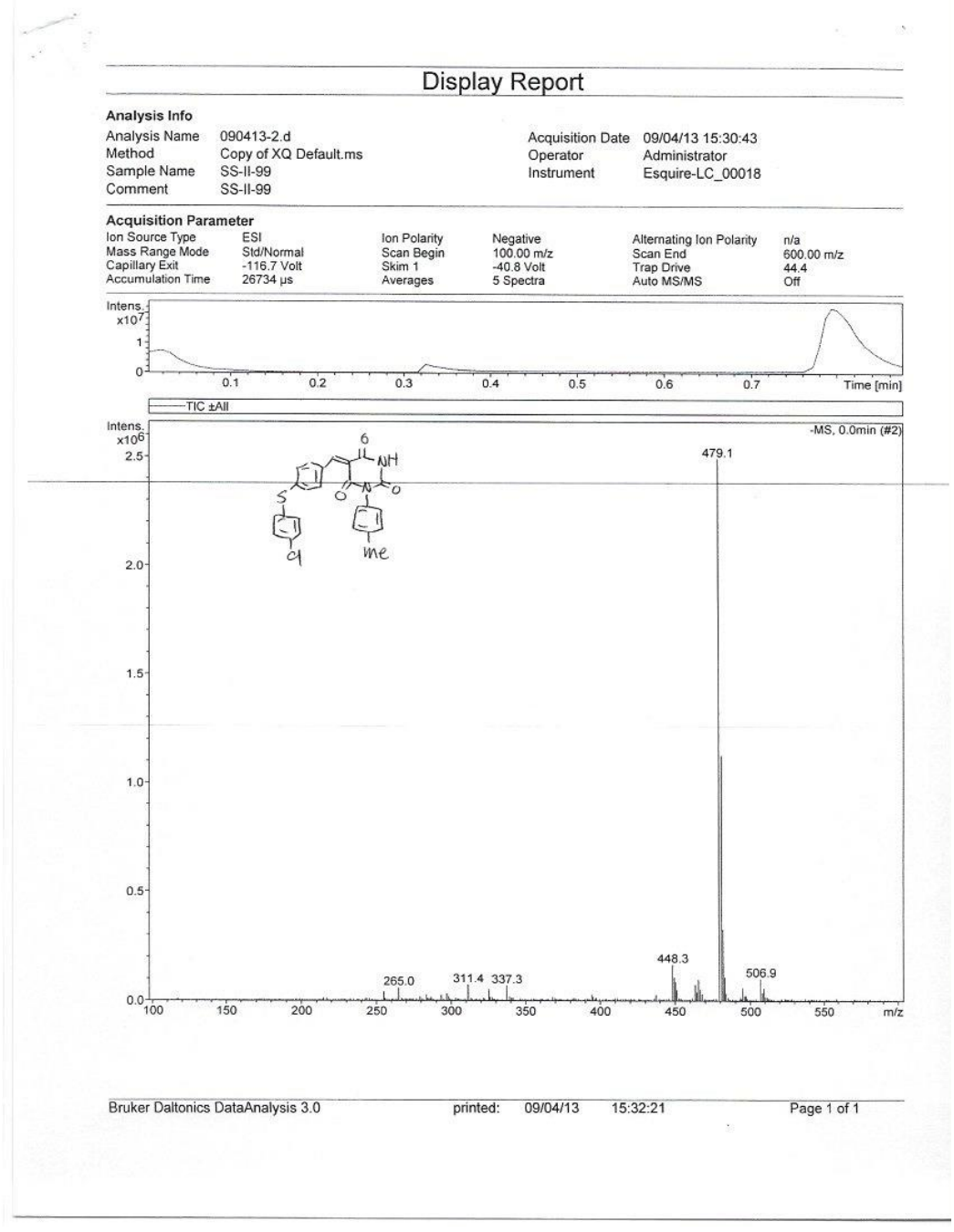




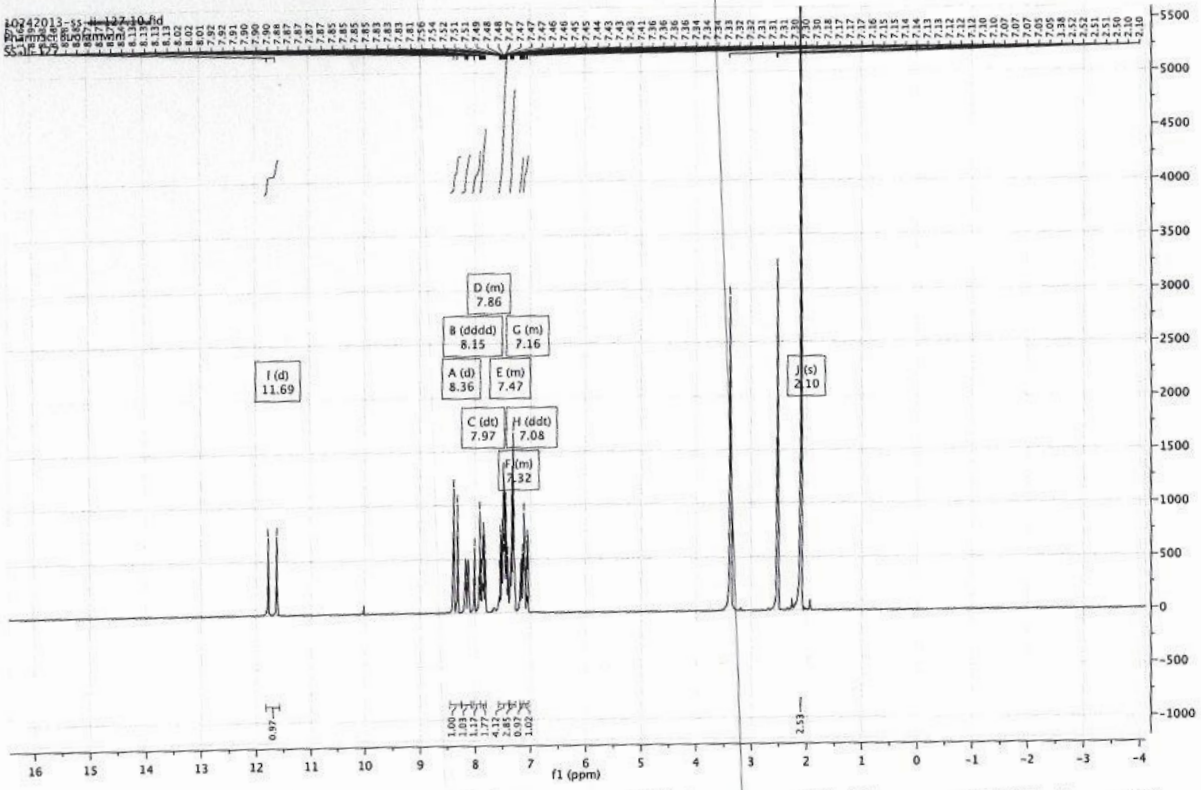
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.65 (d, J = 56.0 Hz, 1H), 8.27 (d, J = 25.5 Hz, 1H), 8.04 (dd, J = 29.5, 8.6 Hz, 2H), 7.56 (s, 2H), 7.52 (d, J = 3.9 Hz, 2H), 7.34 (d, J = 7.9 Hz, 1H), 7.28 – 7.15 (m, 3H), 7.10 (td, J = 2.7, 1.3 Hz, 2H), 2.33 (d, J = 6.0 Hz, 3H).

Suppl. Mass spectrum and ^{1}H NMR Spectrum of **67**



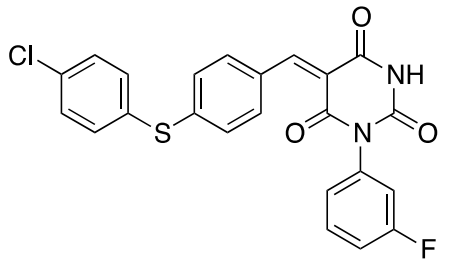


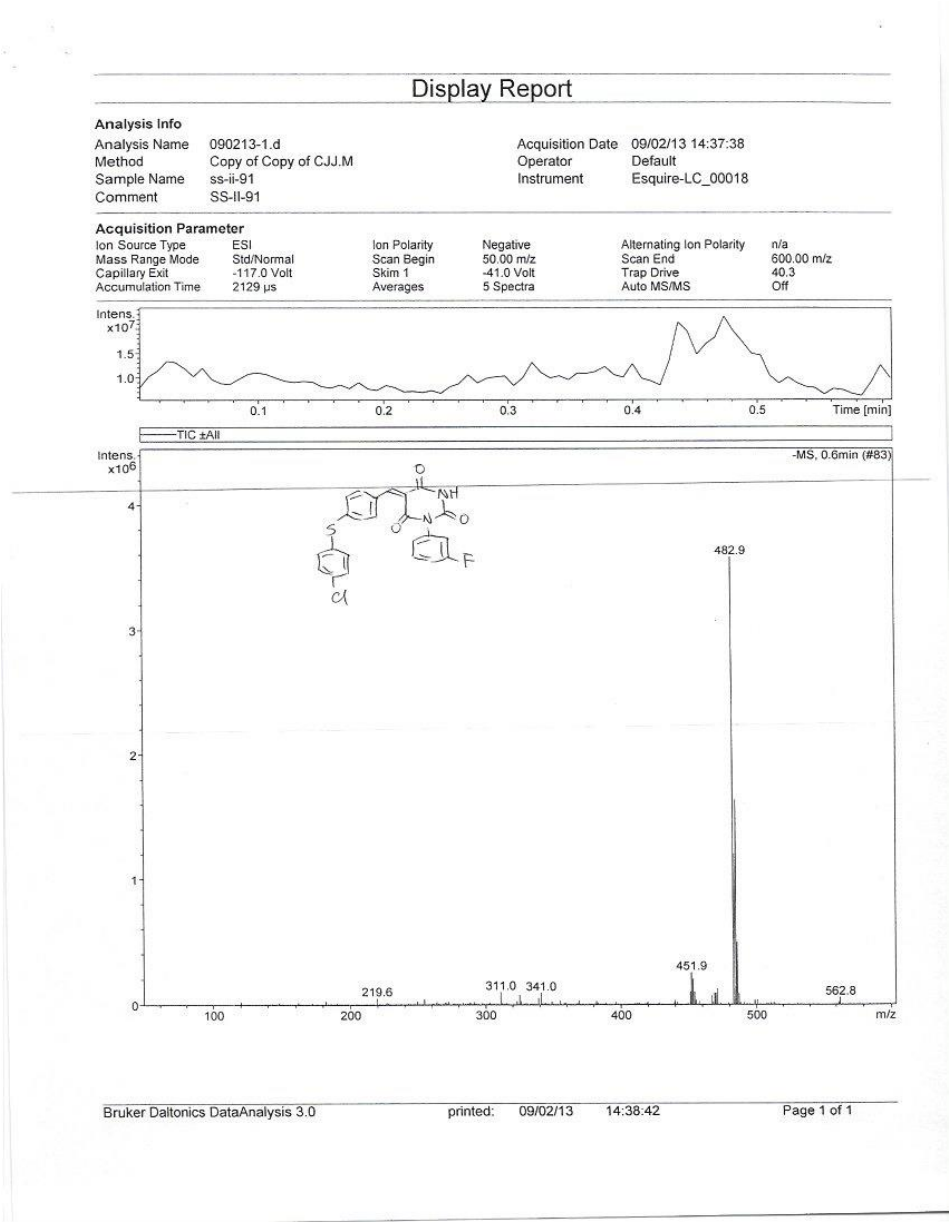
SS-11-99



^{1}H NMR (400 MHz, DMSO-d_6) δ 11.69 (d, J = 63.4 Hz, 1H), 8.36 (d, J = 27.1 Hz, 1H), 8.15 (dddd, J = 18.6, 4.9, 2.1, 0.8 Hz, 1H), 7.97 (dt, J = 39.1, 2.0 Hz, 1H), 7.91 – 7.80 (m, 2H), 7.57 – 7.39 (m, 4H), 7.37 – 7.27 (m, 2H), 7.20 – 7.13 (m, 1H), 7.08 (ddt, J = 21.5, 8.3, 0.8 Hz, 1H), 2.10 (s, 3H).

Suppl. Mass spectrum and ^{1}H NMR Spectrum of **68**





Display Report

Analysis Info

Analysis Name	090213-1.d	Acquisition Date	09/02/13 14:37:38
Method	Copy of Copy of CJJ.M	Operator	Default
Sample Name	ss-ii-91	Instrument	Esquire-LC_00018
Comment	SS-II-91		

Acquisition Parameter

Ion Source Type	ESI	Ion Polarity	Negative	Alternating Ion Polarity	n/a
Mass Range Mode	Std/Normal	Scan Begin	50.00 m/z	Scan End	600.00 m/z
Capillary Exit	-117.0 Volt	Skim 1	-41.0 Volt	Trap Drive	40.3
Accumulation Time	2129 µs	Averages	5 Spectra	Auto MS/MS	Off

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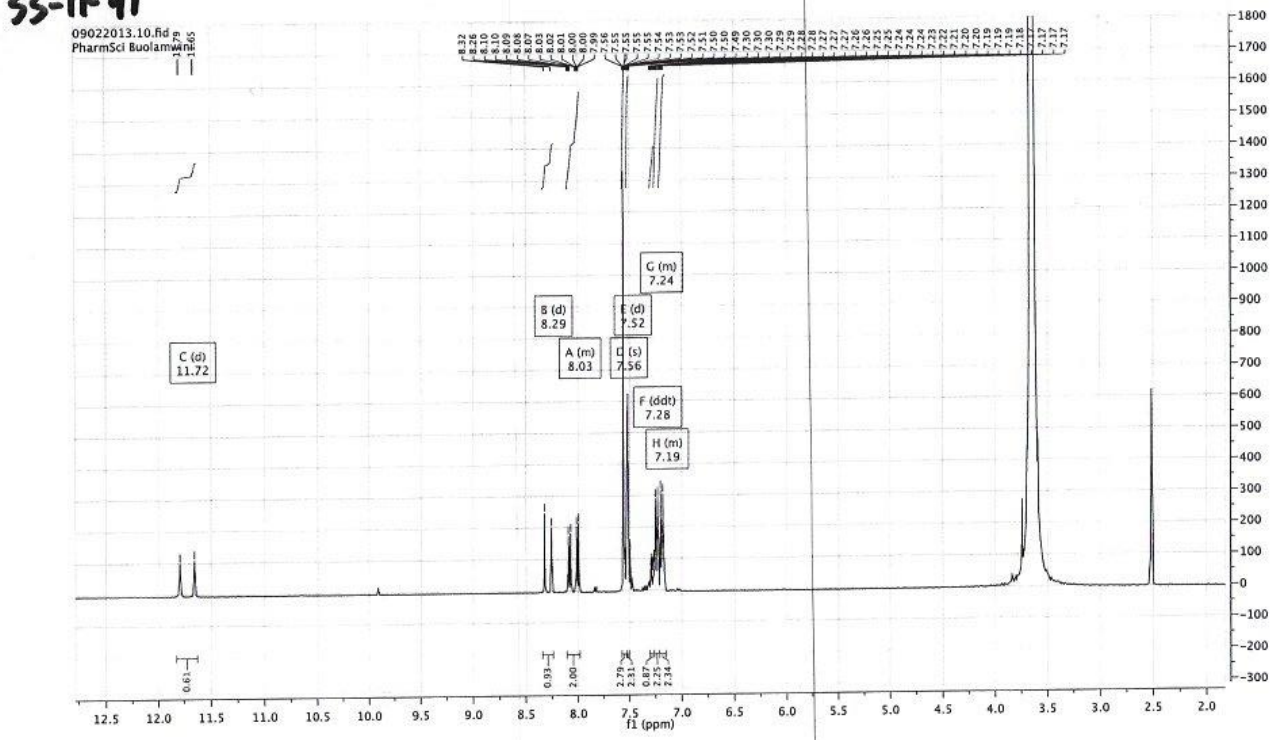
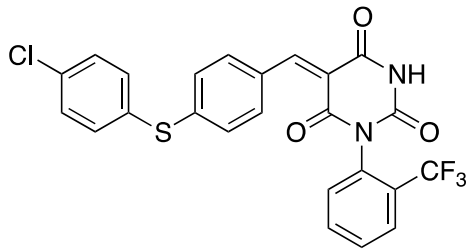
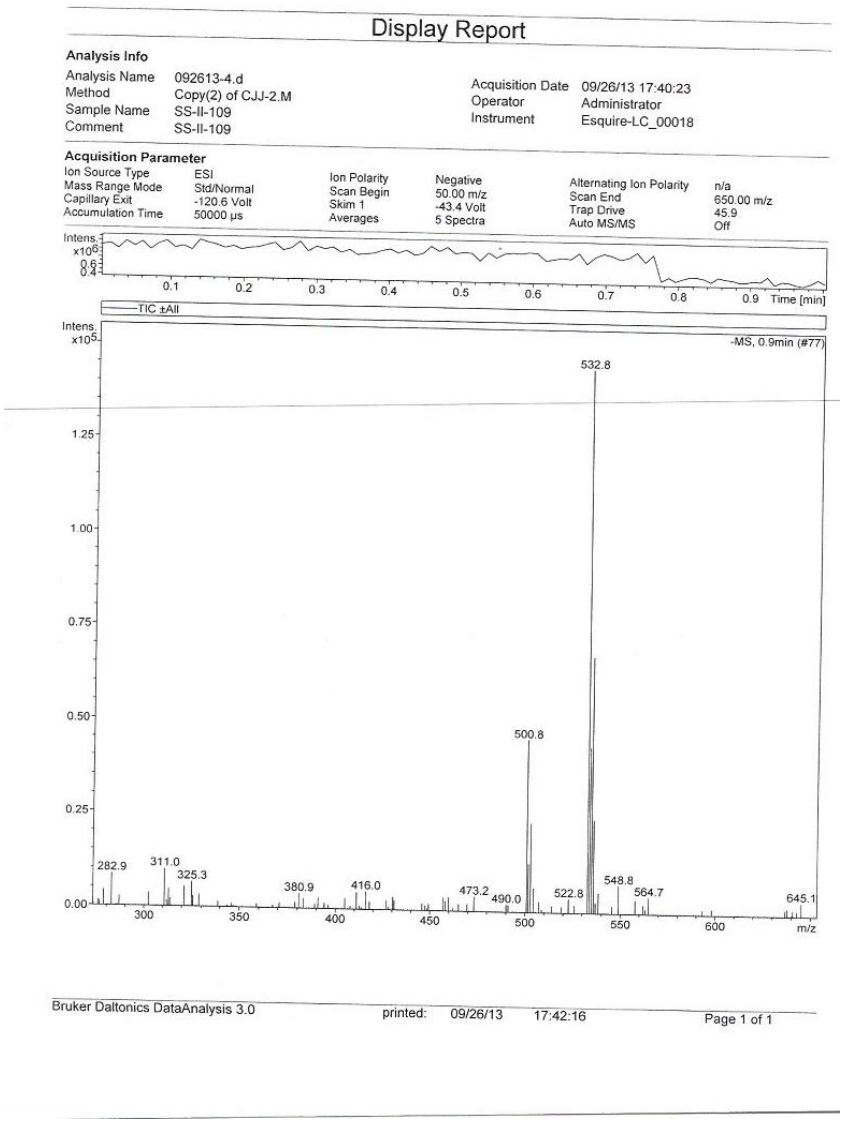


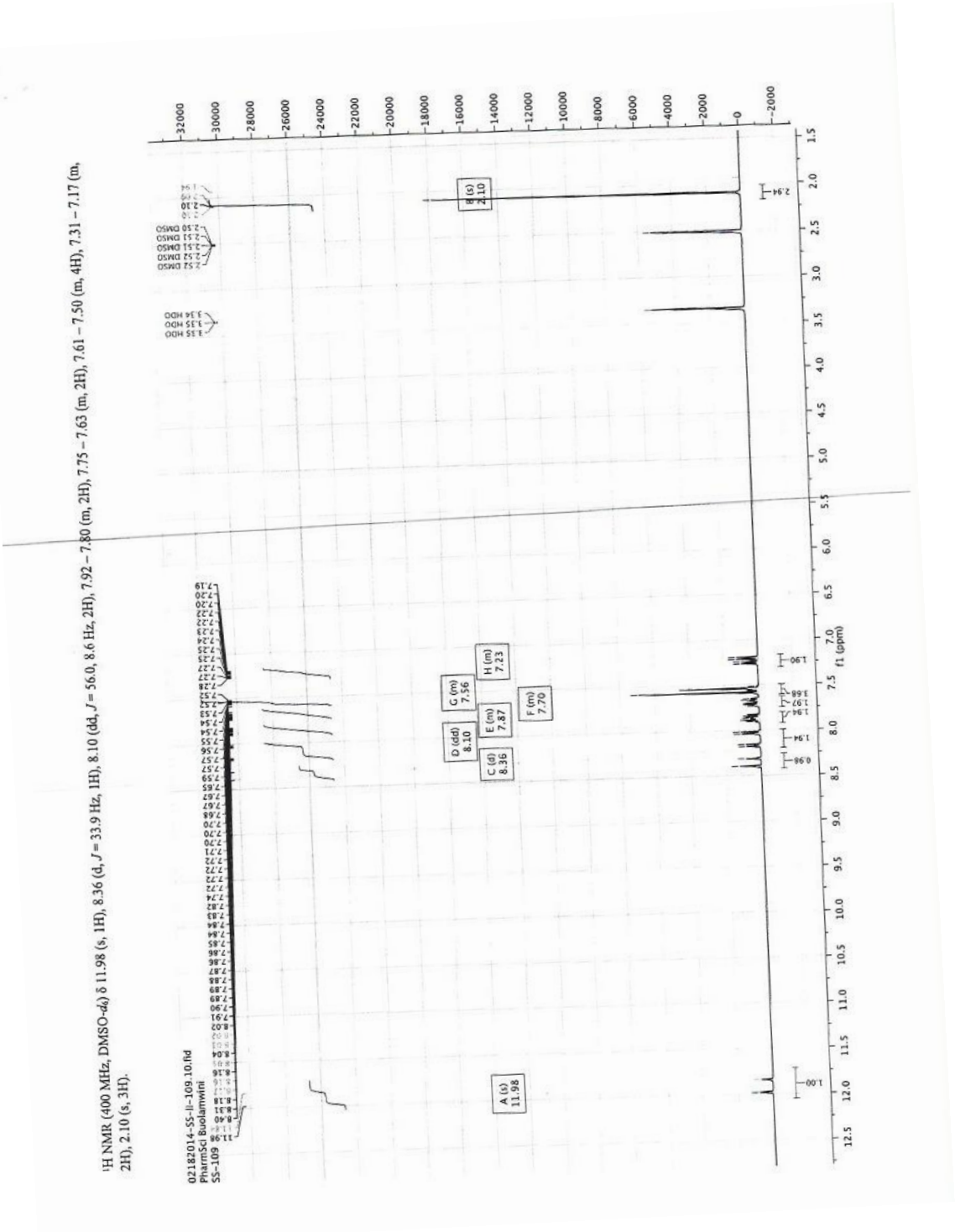
^{1}H NMR (400 MHz, DMSO-d_6) δ 11.72 (d, J = 55.8 Hz, 1H), 8.29 (d, J = 26.0 Hz, 1H), 8.11 – 7.98 (m, 2H), 7.56 (s, 3H), 7.52 (d, J = 3.3 Hz, 2H), 7.28 (ddt, J = 8.9, 2.5, 1.2 Hz, 1H), 7.26 – 7.21 (m, 2H), 7.21 – 7.15 (m, 2H).

Suppl. Mass spectrum and ^{1}H NMR Spectrum of **69**





^{1}H NMR (400 MHz, DMSO-d_6) δ 11.98 (s, 1H), 8.36 (d, J = 33.9 Hz, 1H), 8.10 (dd, J = 56.0, 8.6 Hz, 2H), 7.92 – 7.80 (m, 2H), 7.75 – 7.63 (m, 2H), 7.61 – 7.50 (m, 4H), 7.31 – 7.17 (m, 2H), 2.10 (s, 3H).



Suppl. Mass spectrum of **70**