Supporting Information

Cyclin-Dependent Kinase (CDK) Inhibitors: Structure-Activity Relationships and Insights into the CDK-2 Selectivity of 6-Substituted 2-Arylaminopurines

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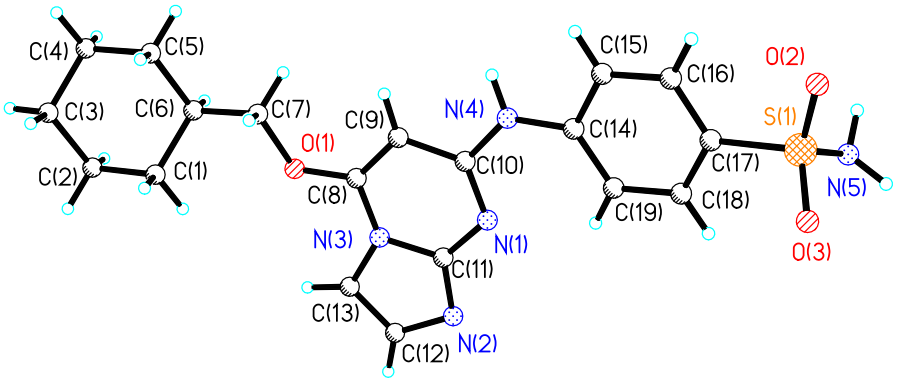
Structure, Crystal Data and Structure Refinement for Compound 102

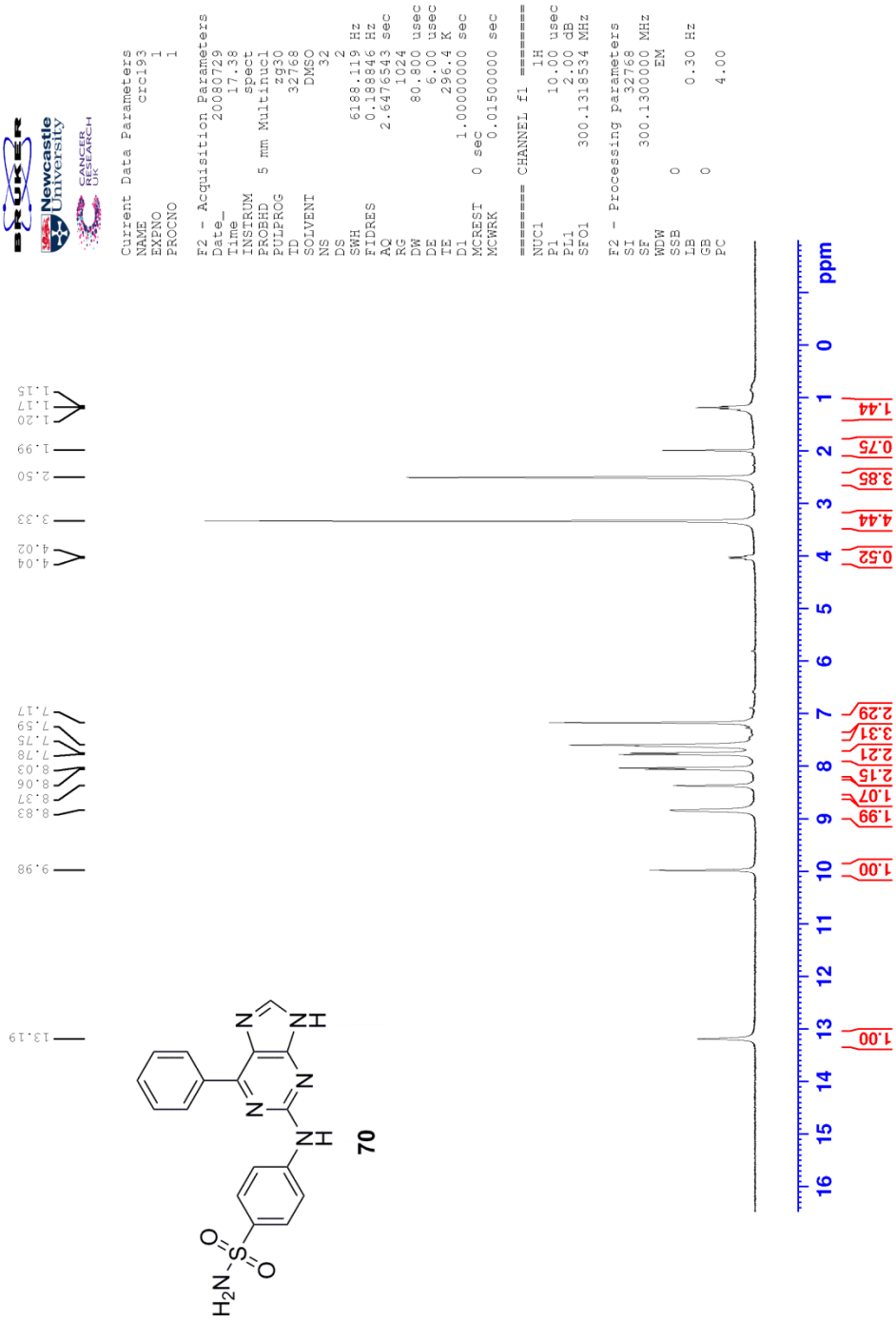


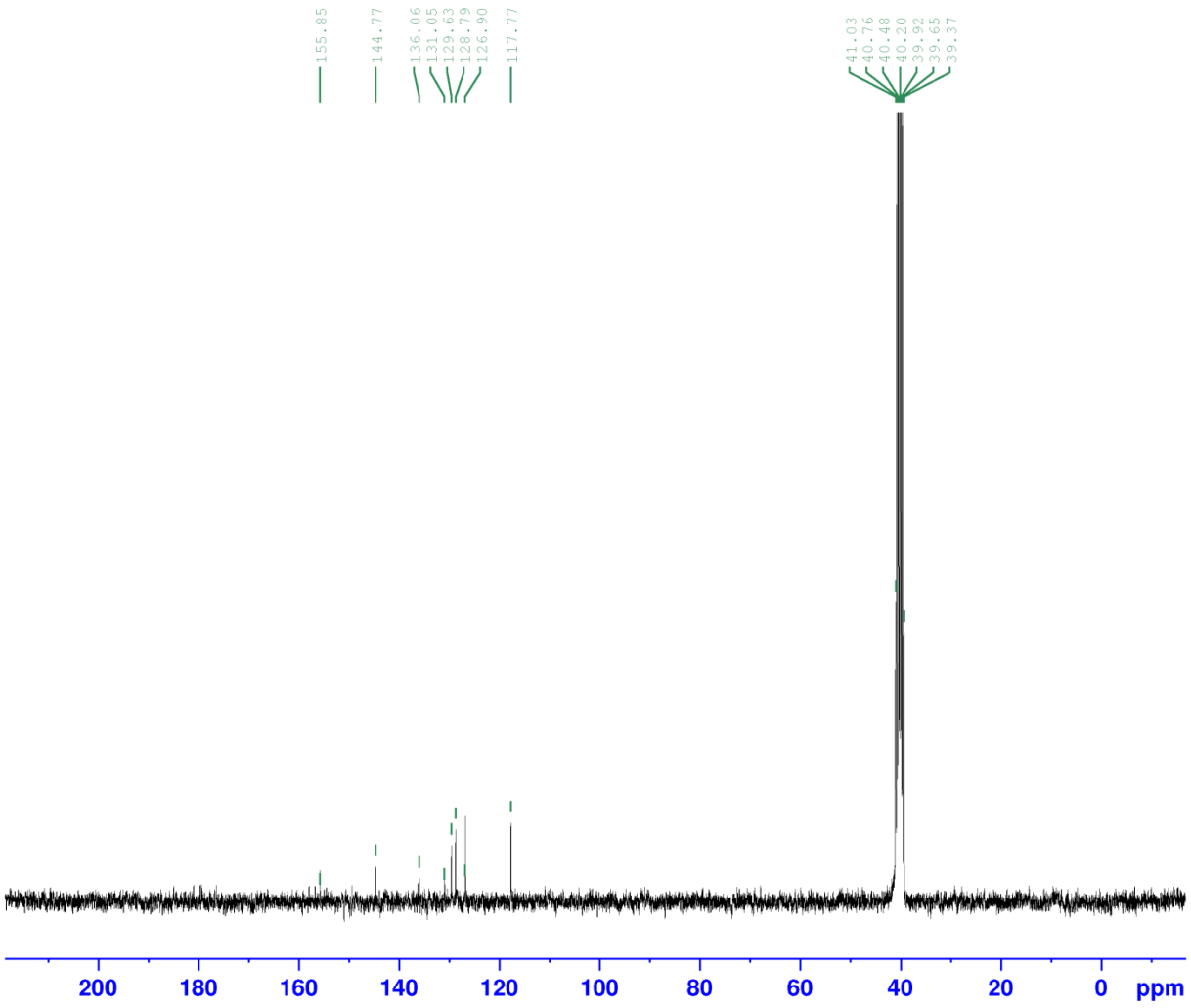
Identification code	**102**	
Chemical formula (moiety)	$C_{19}H_{23}N_5O_3S$	
Chemical formula (total)	$C_{19}H_{23}N_5O_3S$	
Formula weight	401.48	
Temperature	120(2) K	
Radiation, wavelength	synchrotron, 0.69110 Å	
Crystal system, space group	triclinic, $P\bar{1}$	
Unit cell parameters	a = 8.596(4) Å	α = 98.186(4)°
	b = 10.212(4) Å	β = 93.564(4)°
	c = 11.060(5) Å	γ = 90.221(5)°
Cell volume	959.0(7) Å^3	
Z	2	
Calculated density	1.390 g/cm^3	
Absorption coefficient μ	0.200 mm^{-1}	

F(000)	424
Crystal colour and size	colourless, 0.08 × 0.02 × 0.02 mm^3
Reflections for cell refinement	5638 (θ range 2.8 to 30.1°)
Data collection method	Bruker APEX2 CCD diffractometer
	thin-slice ω scans
θ range for data collection	2.8 to 29.6°
Index ranges	h –12 to 12, k –14 to 14, l –15 to 15
Completeness to θ = 25.0°	96.9 %
Intensity decay	15%
Reflections collected	9602
Independent reflections	5232 (R_{int} = 0.0265)
Reflections with $F^2>2\sigma$	4548
Absorption correction	semi-empirical from equivalents
Min. and max. transmission	0.9842 and 0.9960
Structure solution	direct methods
Refinement method	Full-matrix least-squares on F^2
Weighting parameters a, b	0.0645, 0.2799
Data / restraints / parameters	5232 / 0 / 265
Final R indices [$F^2>2\sigma$]	R1 = 0.0408, wR2 = 0.1106
R indices (all data)	R1 = 0.0471, wR2 = 0.1158
Goodness-of-fit on F^2	1.033
Largest and mean shift/su	0.001 and 0.000
Largest diff. peak and hole	0.46 and –0.41 e $Å^{-3}$

^{1}H and ^{13}C NMR Spectra and HPLC Traces for Compounds 70, 73, 83, 90, 91 and 98.

4-(6-Phenyl-9*H*-purin-2-ylamino)benzenesulfonamide (70)



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EXPNO                  2
PROCNO                 1

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PROBHD   5 mm Multinucl
PULPROG          zgpg30
TD                35968
SOLVENT            DMSO
NS                 3600
DS                    4
SWH           17985.611 Hz
FIDRES         0.500045 Hz
AQ            0.9999104 sec
RG                  181
DW                27.800 usec
DE                 6.00 usec
TE                313.9 K
D1           1.00000000 sec
d11          0.03000000 sec
DELTA        0.89999998 sec
MCREST   0 sec
MCWRK        0.01500000 sec

======== CHANNEL f1 ========
NUC1                13C
P1                 7.20 usec
PL1                1.00 dB
SFO1         75.4752653 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2             10.00 usec
PL2                2.00 dB
PL12               2.00 dB
PL13             120.00 dB
SFO2        300.1312005 MHz

F2 - Processing parameters
SI                 32768
SF           75.4677567 MHz
WDW                   EM
SSB      0
LB                 1.50 Hz
GB       0
PC                 1.40
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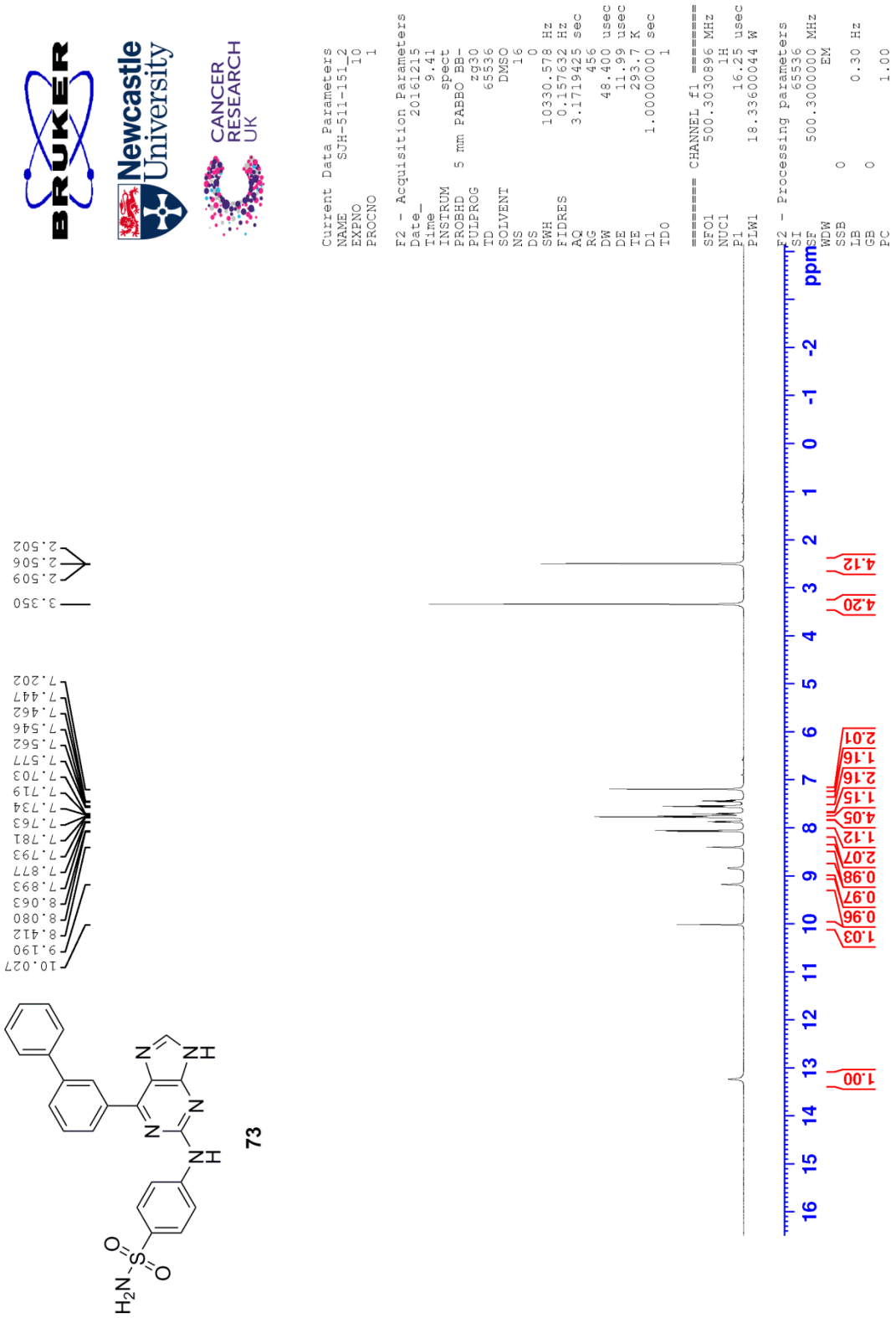
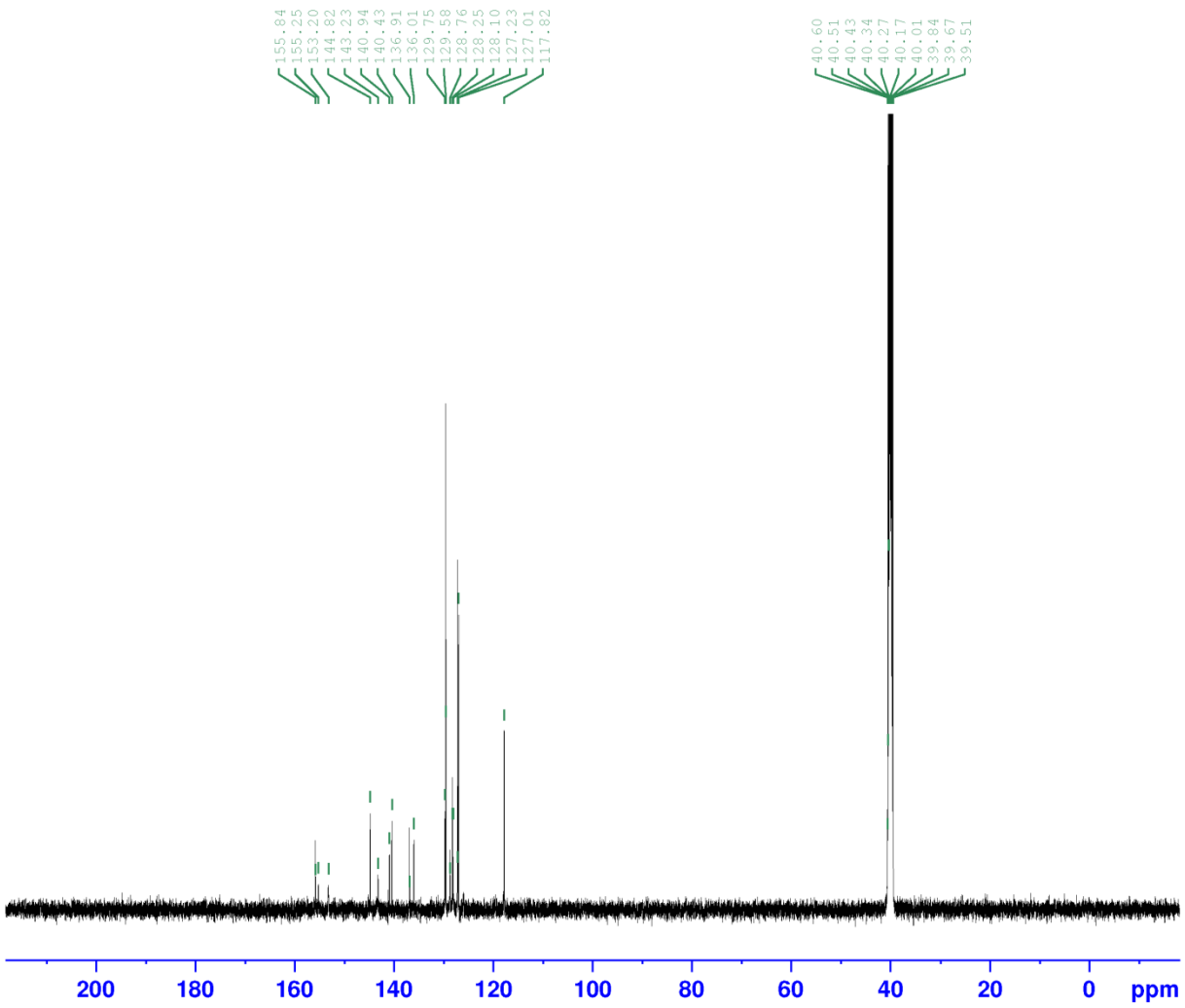
4-((6-([1,1'-biphenyl]-3-yl)-9*H*-purin-2-yl)amino)benzenesulfonamide (73)



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PROCNO                1

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Time                4.13
INSTRUM            spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                65536
SOLVENT            DMSO
NS                 5120
DS                    2
SWH            29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                  456
DW               16.800 usec
DE                 7.68 usec
TE                297.2 K
D1           2.00000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        125.8131151 MHz
NUC1                 13C
P1                  9.75 usec
PLW1        82.38999939 W

======== CHANNEL f2 ========
SFO2        500.3020012 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2             80.00 usec
PLW2        18.33600044 W
PLW12        0.75654000 W
PLW13        0.38053000 W

F2 - Processing parameters
SI                65536
SF          125.8005350 MHz
WDW                  EM
SSB      0
LB                1.00 Hz
GB       0
PC                1.40
```

Data File D:\DATASHARE\28SEPT15\28SEP15_06.D
Sample Name: SJH-511-151

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Acq. Instrument : Analytical HPLC 1               Location : Vial 74
Injection Date  : 9/28/2015 5:44:00 PM                 Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SEP2015\28SEP15_DCM_LM_SJH 2015-09-28 16-08-17\XSELECT_
                  ACIDIC.M
Last changed    : 6/5/2014 7:30:31 AM
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                  M)
Last changed    : 9/29/2015 9:46:10 AM by Lauren Molyneux
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Method Info     :

                  using C18-AR col 2 from anal. HPLC
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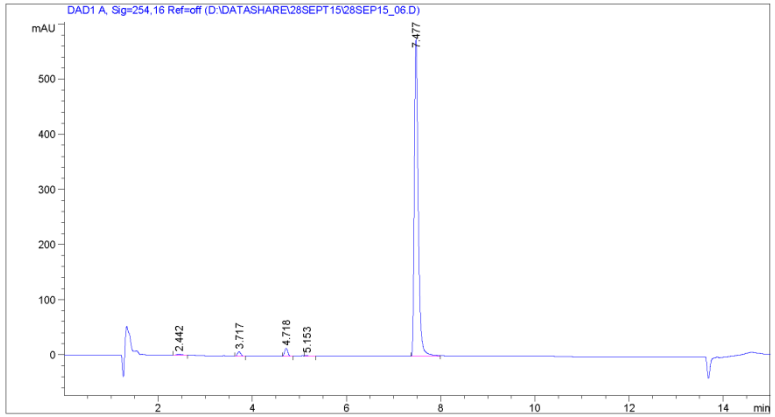


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==================================================================
                          Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 A, Sig=254,16 Ref=off
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	2.442	BB	0.1432	13.67263	1.36124	0.4048
2	3.717	BB	0.0711	37.88163	8.32149	1.1216

Data File D:\DATASHARE\28SEPT15\28SEP15_06.D
Sample Name: SJH-511-151

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
3	4.718	BB	0.0708	64.37805	14.22685	1.9061
4	5.153	VB	0.0826	8.94327	1.61479	0.2648
5	7.477	BB	0.0858	3252.59448	576.41913	96.3027

Totals : 3377.47006 601.94349

==========

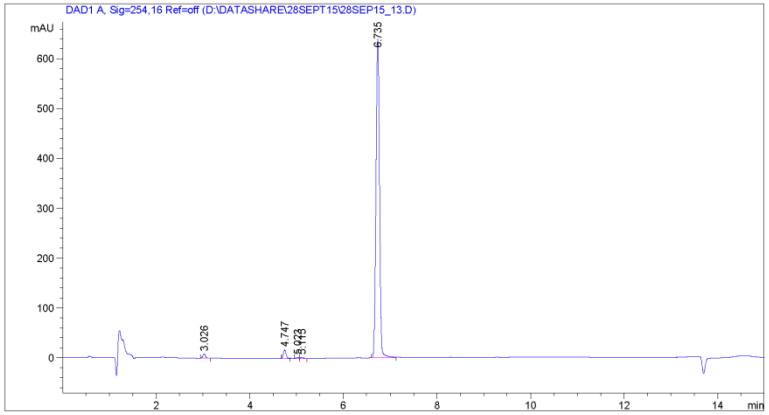
*** End of Report ***

Data File D:\DATASHARE\28SEPT15\28SEP15_13.D
Sample Name: SJH-511-151

==========

Acq. Operator : Lauren Molyneux Seq. Line : 13
Acq. Instrument : Analytical HPLC 1 Location : Vial 74
Injection Date : 9/28/2015 7:52:30 PM Inj : 1
Inj Volume : 5.000 µl
Acq. Method : C:\CHEM32\1\DATA\SEP2015\28SEP15_DCM_LM_SJH 2015-09-28 16-08-17\XSELECT_BASIC.M
Last changed : 6/5/2014 7:31:00 AM
Analysis Method : C:\CHEM32\1\DATA\201509\JEP-514-098-006.D\DA.M (20150612 JEP-489-208-+ACID.M)
Last changed : 9/29/2015 9:46:10 AM by Lauren Molyneux
(modified after loading)
Method Info :

using C18-AR col 2 from anal. HPLC



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Area Percent Report

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Sorted By : Signal
Multiplier: : 1.0000
Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

Signal 1: DAD1 A, Sig=254,16 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	3.026	BB	0.0643	34.73341	8.38657	1.0264
2	4.747	BB	0.0629	68.75916	17.11348	2.0320

Data File D:\DATASHARE\28SEPT15\28SEP15_13.D
Sample Name: SJH-511-151

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
3	5.023	BV	0.0600	6.52823	1.65744	0.1929
4	5.115	VB	0.0656	7.20858	1.69594	0.2130
5	6.735	BB	0.0815	3266.64380	640.38068	96.5356

Totals : 3383.87318 669.23411

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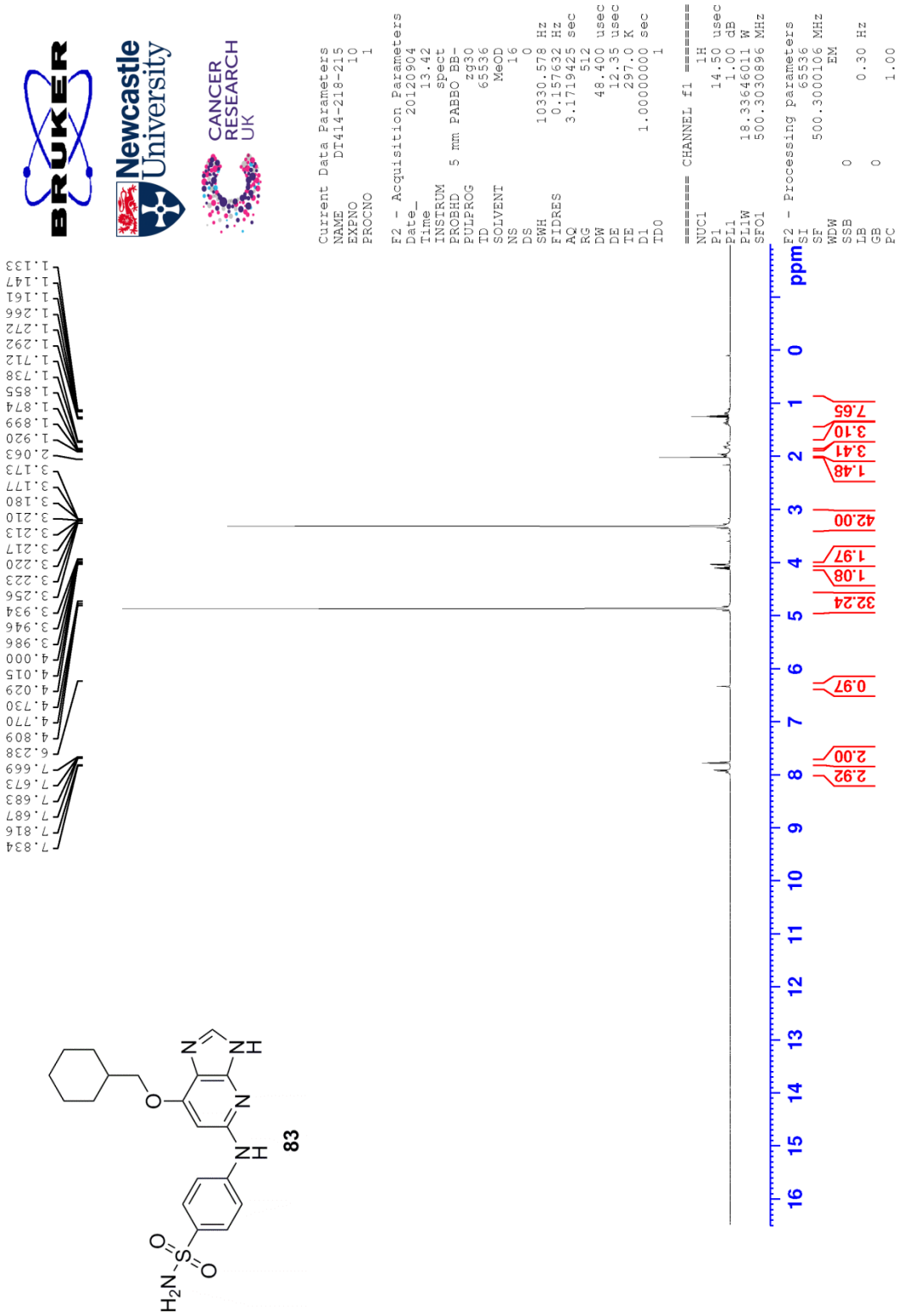
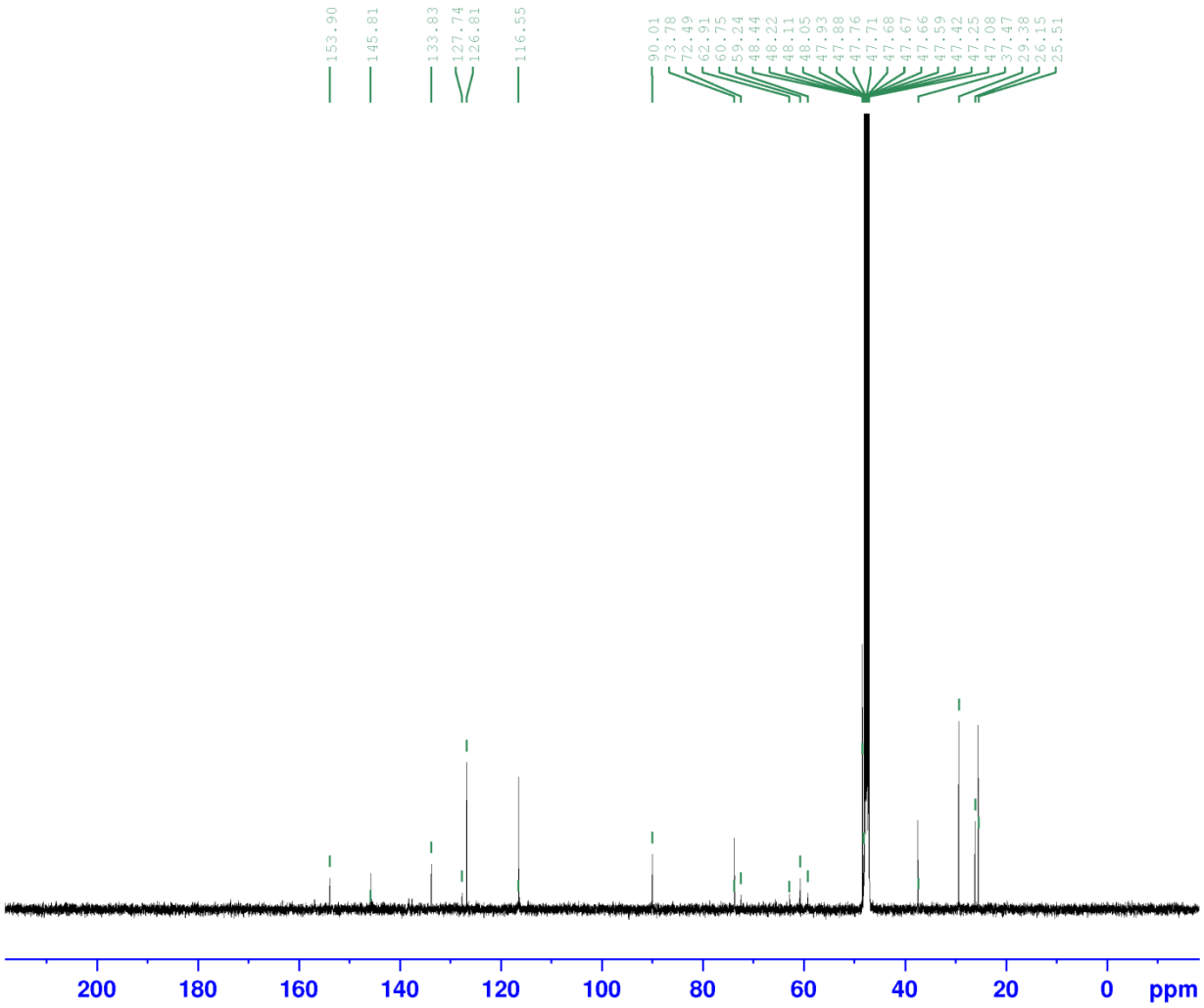
*** End of Report ***

4-((7-(Cyclohexylmethoxy)-3*H*-imidazo[4,5-*b*]pyridin-5-yl)amino) benzenesulfonamide (83)



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PROCNO                1

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Time               15.08
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PULPROG          zgpg30
TD                65536
SOLVENT            MeOD
NS                 7680
DS                    2
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                  456
DW                16.800 usec
DE                 7.68 usec
TE                297.3 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        125.8131151 MHz
NUC1                 13C
P1                  9.75 usec
PLW1        82.38999939 W

======== CHANNEL f2 ========
SFO2        500.3020012 MHz
NUC2                  1H
CPDPRG[2         waltz16
PCPD2              80.00 usec
PLW2        18.33600044 W
PLW12        0.75654000 W
PLW13        0.38053000 W

F2 - Processing parameters
SI                 65536
SF          125.8005350 MHz
WDW                   EM
SSB      0
LB                 1.00 Hz
GB       0
PC                 1.40
```

Data File F:\04SEP12_08.D
Sample Name: DT-414-218-215

```
==========================================================================
Acq. Operator   : Karen Haggerty                 Seq. Line :   6
Acq. Instrument : Instrument 1                    Location : Vial 64
Injection Date  : 9/4/2012 5:46:15 PM                 Inj :   1
                                               Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SEP2012\04SEP12_HL_DT_SJC_SCOUT 2012-09-04 15-40-25\
                  XSELECT_ACIDIC.M
Last changed    : 9/4/2012 3:40:34 PM by Karen Haggerty
Analysis Method : F:\04SEP12_08.D\DA.M (XSELECT_ACIDIC.M)
Last changed    : 9/5/2012 7:13:27 AM by Karen Haggerty
                  (modified after loading)
Method Info     : Waters XSELECT CSH C18 3.5um 100 x 4.6mm
                  0.1% Formic Acid (aq)/MeCN, 1.0mL/min
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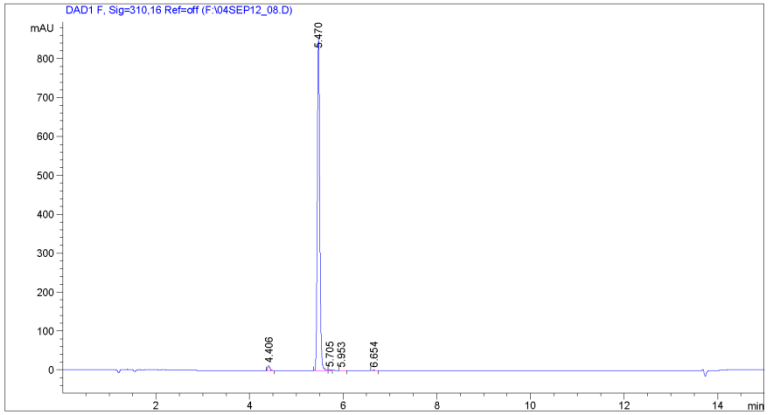


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Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 F, Sig=310,16 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   4.406 BB    0.0506   41.81723   12.62384   1.3518
   2   5.470 MF    0.0587 3036.96362  862.87885  98.1707
   3   5.705 MF    0.0683    6.52212    1.59071   0.2108
   4   5.953 FM    0.1187    4.02994 5.65722e-1   0.1303
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Data File F:\04SEP12_08.D
Sample Name: DT-414-218-215

```
Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   5   6.654 BB    0.0587    4.22257    1.10213   0.1365

Totals :                   3093.55548  878.76124


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Data File F:\04SEP12_18.D
Sample Name: DT-414-218-215

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Acq. Instrument : Instrument 1                    Location : Vial 64
Injection Date  : 9/4/2012 8:41:44 PM                 Inj :   1
                                                Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\SEP2012\04SEP12_HL_DT_SJC_SCOUT 2012-09-04 15-40-25\
                  XSELECT_BASIC.M
Last changed    : 7/11/2012 11:31:43 AM by Karen Haggerty
Analysis Method : F:\04SEP12_18.D\DA.M (XSELECT_BASIC.M)
Last changed    : 9/5/2012 7:17:56 AM by Karen Haggerty
                  (modified after loading)
Method Info     : Waters XSELECT CSH C18 3.5um 100 x 4.6mm
                  0.1% Ammonia (aq)/MeCN, 1.0mL/min
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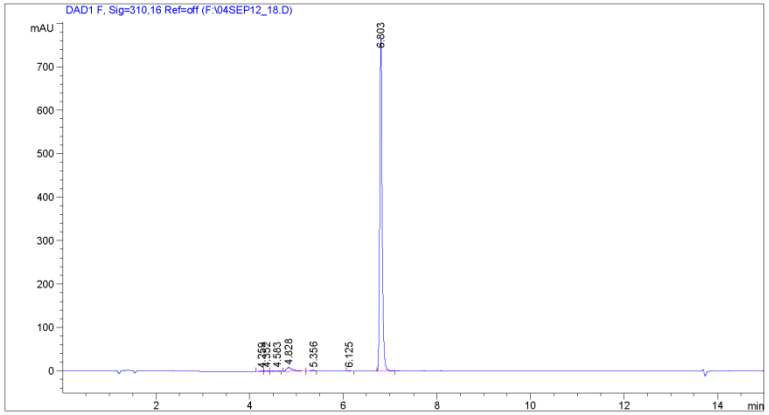


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==========================================================================
                              Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 F, Sig=310,16 Ref=off
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Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	4.259	MF	0.0786	5.62544	1.19343	0.1860
2	4.352	FM	0.0717	7.68639	1.78712	0.2541
3	4.583	FM	0.1167	15.16913	2.16556	0.5015
4	4.828	FM	0.1581	84.12363	8.86909	2.7814

Data File F:\04SEP12_18.D
Sample Name: DT-414-218-215

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
5	5.356	FM	0.1040	14.91038	2.38899	0.4930
6	6.125	BB	0.0583	6.22366	1.63944	0.2058
7	6.803	BB	0.0581	2890.73706	765.21002	95.5781
Totals :				3024.47570	783.25366	

```
==========================================================================
                          *** End of Report ***
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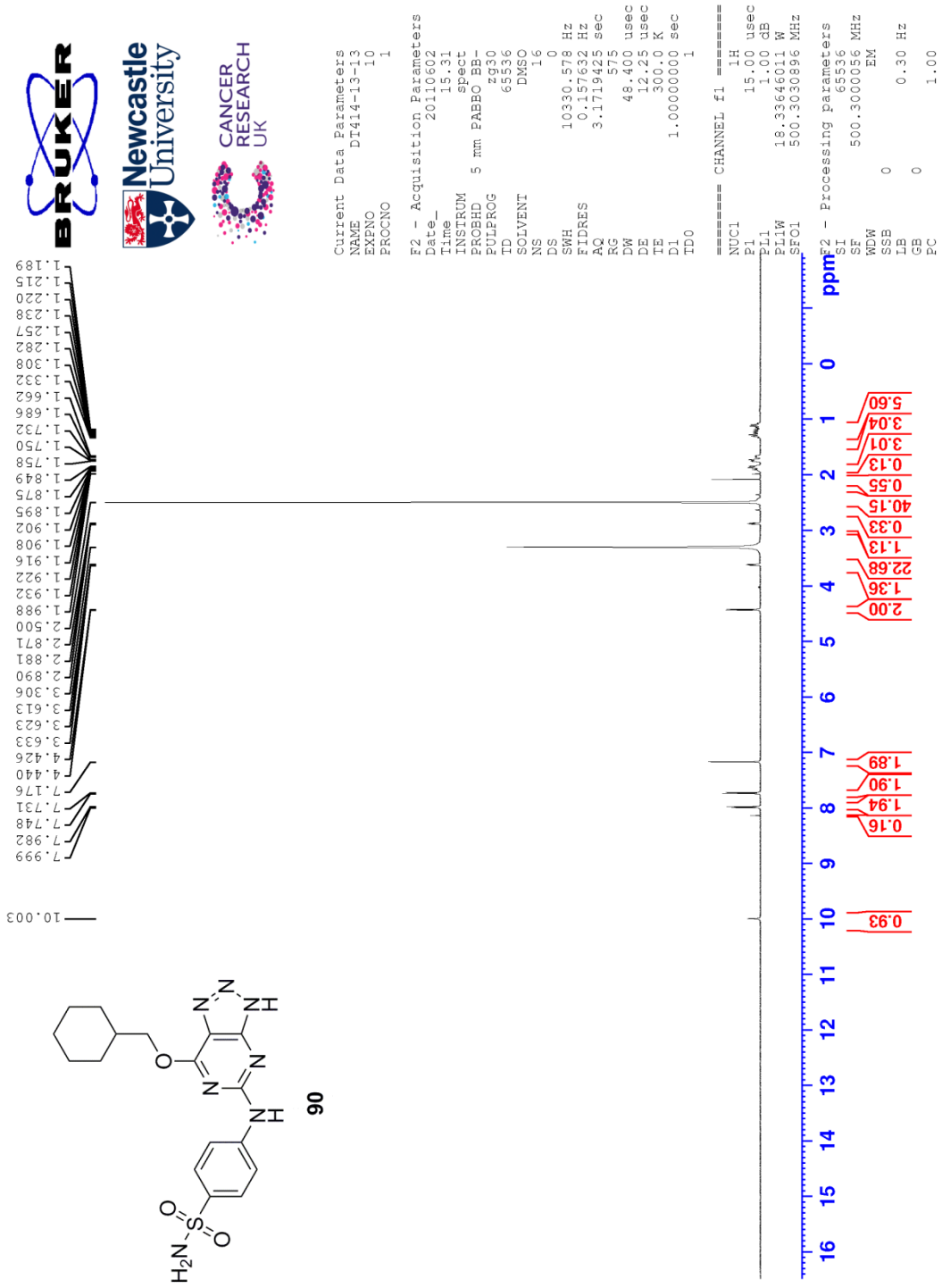
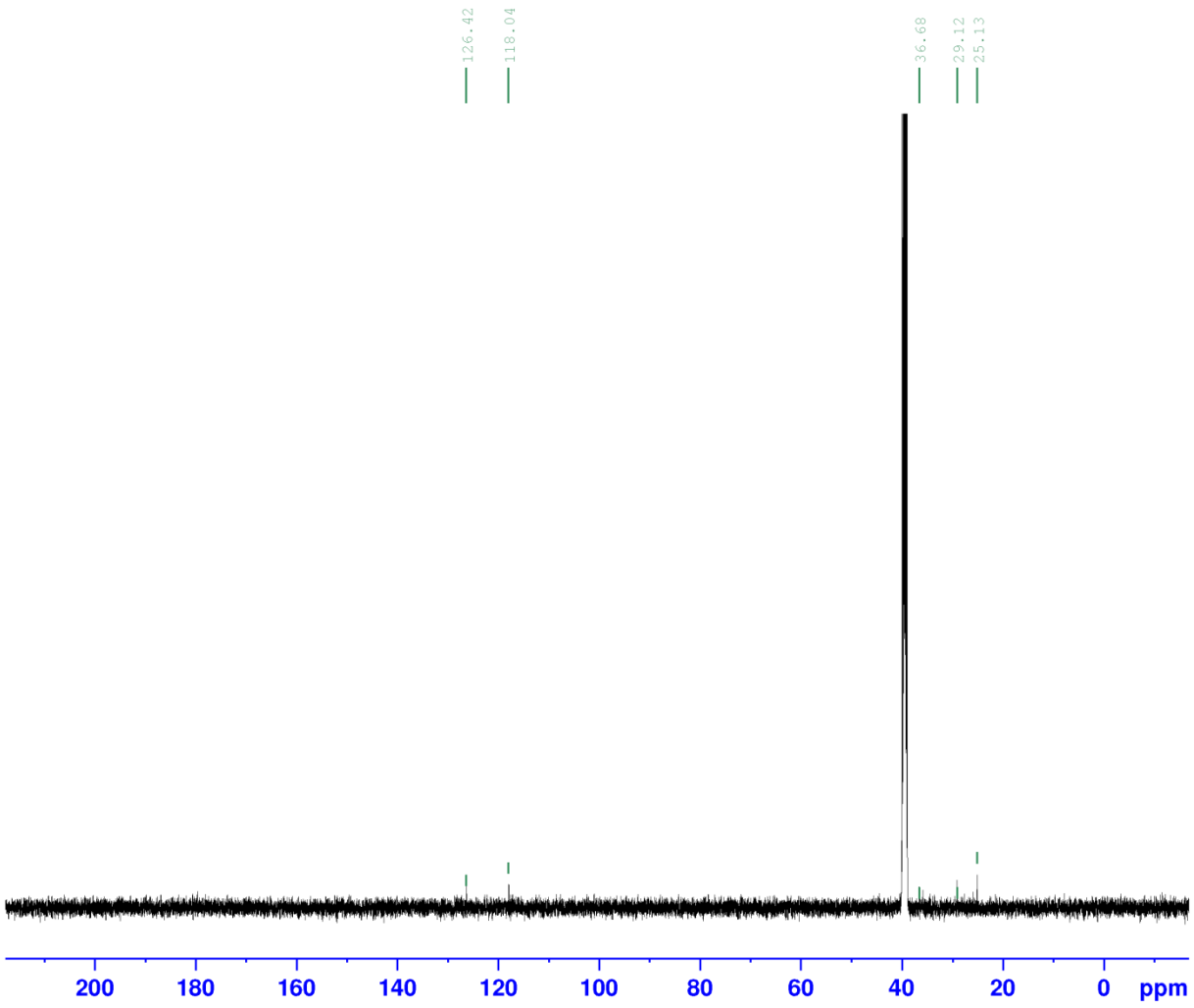
4-((7-(Cyclohexylmethoxy)-3*H*-[1,2,3]triazolo[4,5-*d*]pyrimidin-5-yl)amino)-benzenesulfonamide (90)



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PROCNO                1

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Time               22.46
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PULPROG          zgpg30
TD                65536
SOLVENT            DMSO
NS                 2560
DS                    2
SWH            29761.904 Hz
FIDRES         0.454131 Hz
AQ             1.1010048 sec
RG                  456
DW                16.800 usec
DE                 7.75 usec
TE                300.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
NUC1                 13C
P1                  9.38 usec
PL1      0 dB
PL1W        82.38987732 W
SFO1        125.8131151 MHz

======== CHANNEL f2 ========
CPDPRG[2         waltz16
NUC2                 1H
PCPD2              80.00 usec
PL2                 1.00 dB
PL12               17.00 dB
PL13               21.00 dB
PL2W        18.33646011 W
PL12W        0.46059108 W
PL13W        0.18336460 W
SFO2        500.3020012 MHz

F2 - Processing parameters
SI                 65536
SF          125.8005979 MHz
WDW                   EM
SSB      0
LB                  1.00 Hz
GB       0
PC                  1.40
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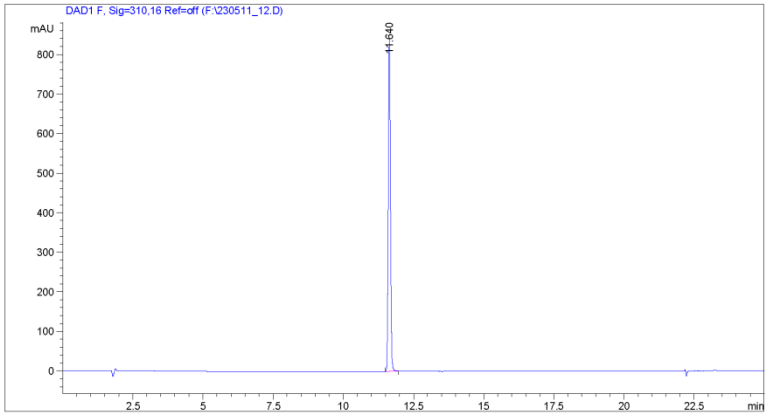
Data File F:\230511_12.D
Sample Name: DT-414-13-13

==========

Acq. Operator : Karen Haggerty Seq. Line : 8
Acq. Instrument : Instrument 1 Location : Vial 53
Injection Date : 5/23/2011 8:27:54 PM Inj : 1
Inj Volume : 5.000 µl
Different Inj Volume from Sequence ! Actual Inj Volume : 2.000 µl
Acq. Method : C:\CHEM32\1\DATA\KH0511\230511_AB_DT 2011-05-23 15-26-39\COL1-A2+B1-NO_REF_SHORT.M
Last changed : 5/23/2011 3:26:46 PM by Karen Haggerty
Analysis Method : F:\230511_12.D\DA.M (COL1-A2+B1-NO_REF_SHORT.M)
Last changed : 5/24/2011 7:55:13 AM by Karen Haggerty
(modified after loading)
Method Info : Waters XTerra RP18 5um, 150 x 4.6mm

Sample Info : Waters XTerra RP18 150 x 4.6mm, 0.1% Formic Acid (aq)/MeCN



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Area Percent Report

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Dilution: : 1.0000
Use Multiplier & Dilution Factor with ISTDs

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Sample Name: DT-414-13-13

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Totals : 4437.54443 842.14056

*** End of Report ***

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Acq. Operator   : Karen Haggerty                 Seq. Line :  16
Acq. Instrument : Instrument 1                    Location : Vial 53
Injection Date  : 5/24/2011 2:21:54 AM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 2.000 µl
Acq. Method     : C:\CHEM32\1\DATA\KH0511\230511_AB_DT 2011-05-23 15-26-39\COL1-A1+B1-NO_REF_
                  SHORT.M
Last changed    : 5/13/2011 3:07:11 PM by Karen Haggerty
Analysis Method : F:\230511_25.D\DA.M (COL1-A1+B1-NO_REF_SHORT.M)
Last changed    : 5/24/2011 7:58:32 AM by Karen Haggerty
                  (modified after loading)
Sample Info     : Waters XTerra RP18 150 x 4.6mm, 0.1% Ammonia (aq)/MeCN
```
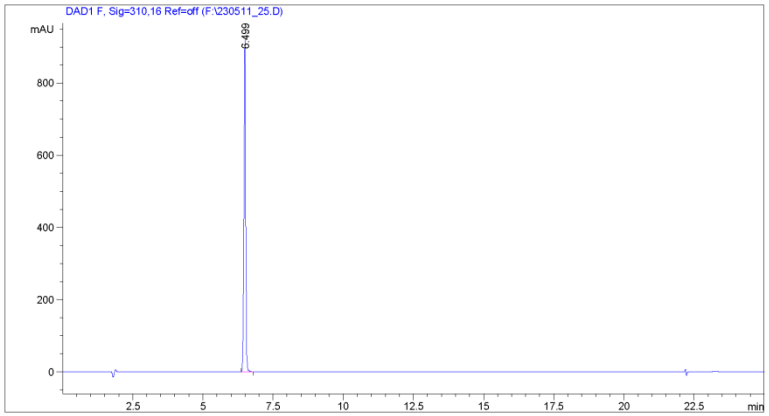
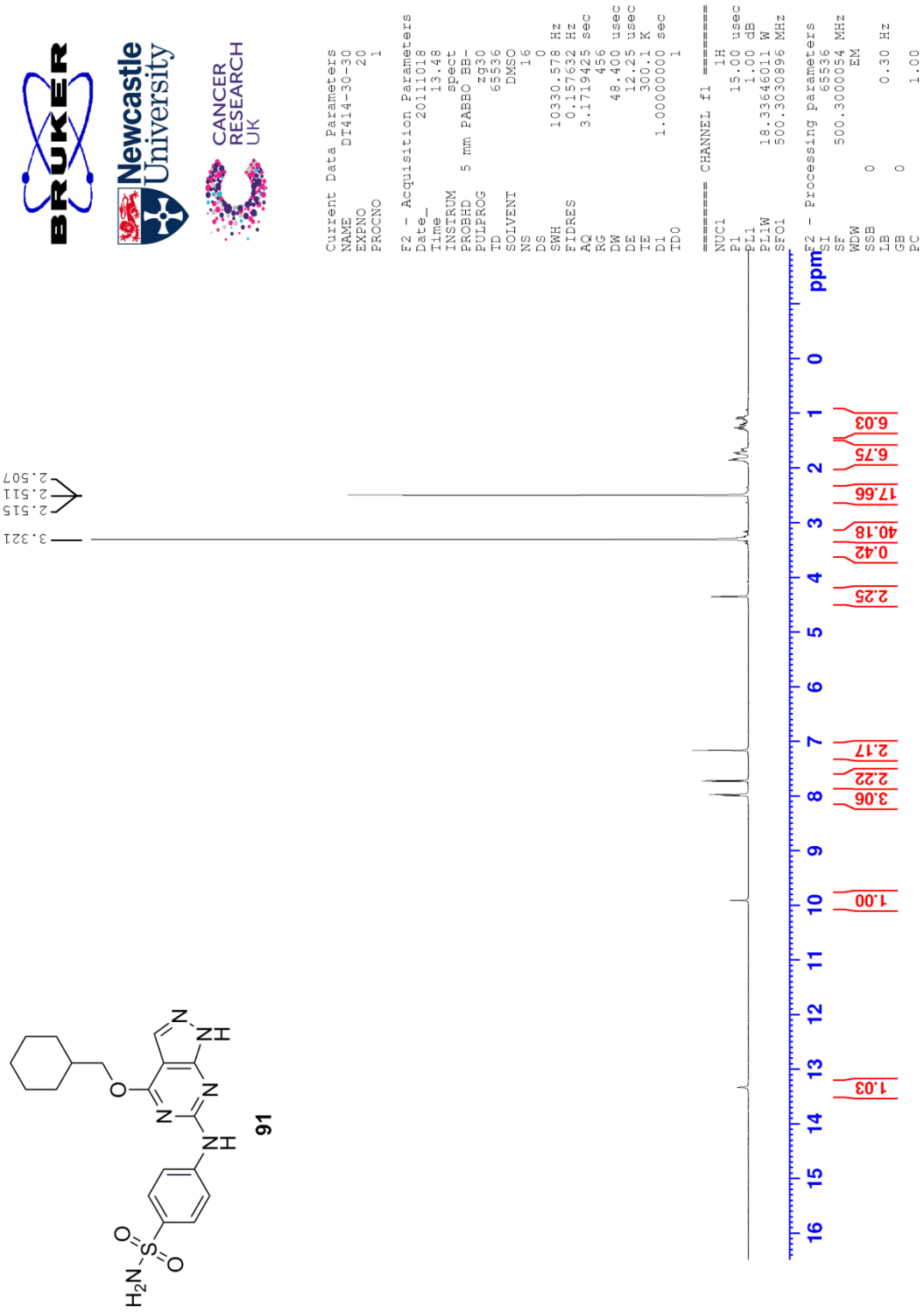



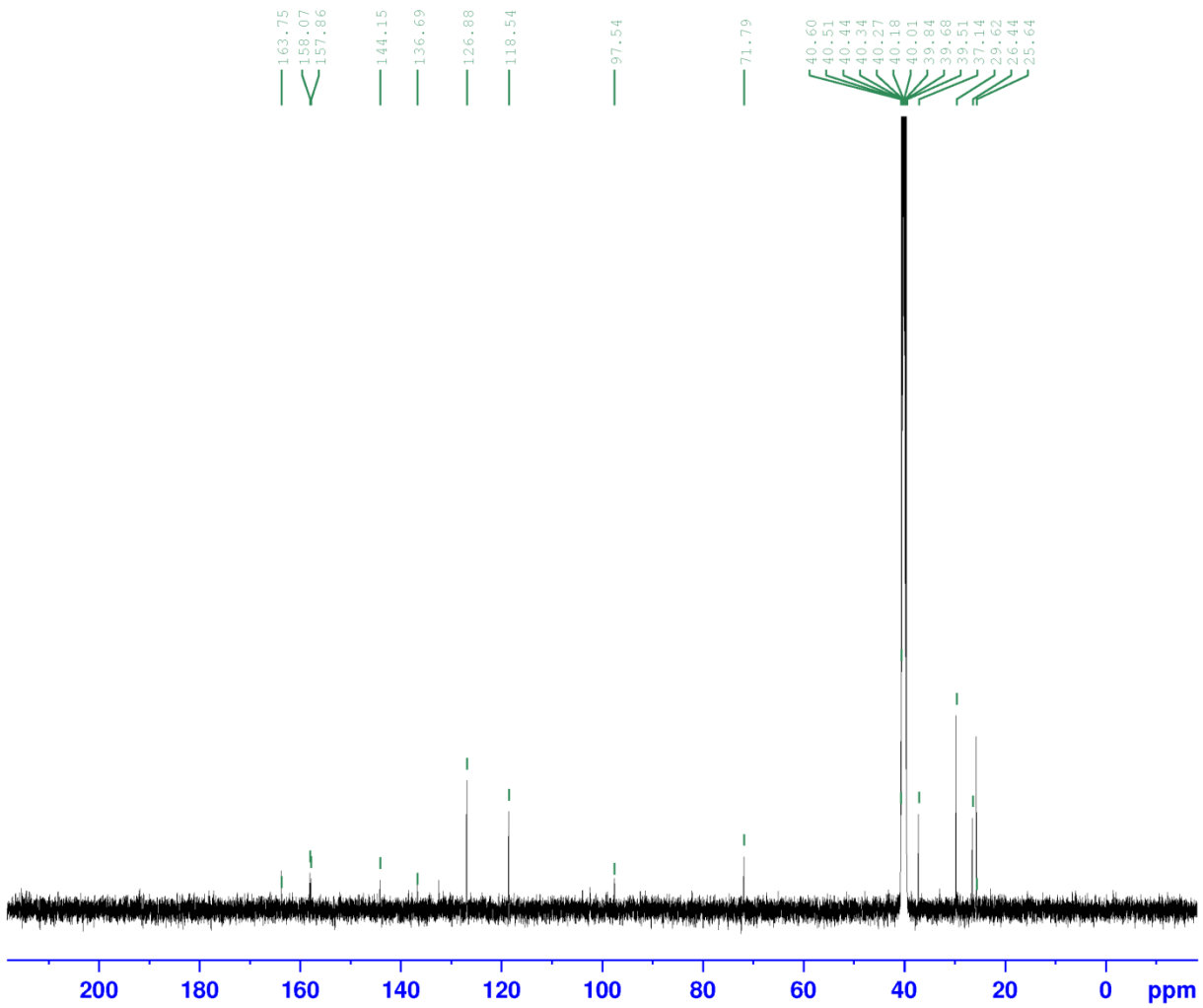

```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 F, Sig=310,16 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.499 BB    0.0678 4085.26587  920.34296 100.0000

Totals :                  4085.26587  920.34296
```


Data File F:\230511_25.D
Sample Name: DT-414-13-13

```
==================================================================
                        *** End of Report ***
```

4-((4-(Cyclohexylmethoxy)-1*H*-pyrazolo[3,4-*d*]pyrimidin-6-yl)amino)benzenesulfonamide (91)

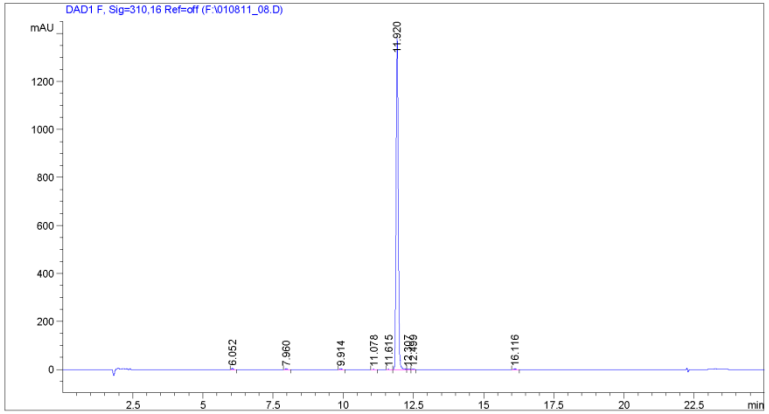





```
Current Data Parameters
NAME        DT414-30-30
EXPNO                10
PROCNO                1

F2 - Acquisition Parameters
Date_            20161218
Time                 1.29
INSTRUM             spect
PROBHD   5 mm PABBO BB-
PULPROG           zgpg30
TD                 65536
SOLVENT             DMSO
NS                   7680
DS                      2
SWH            29761.904 Hz
FIDRES          0.454131 Hz
AQ             1.1010048 sec
RG                    456
DW                 16.800 usec
DE                   7.68 usec
TE                  297.0 K
D1            2.00000000 sec
D11           0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
SFO1         125.8131151 MHz
NUC1                  13C
P1                   9.75 usec
PLW1         82.38999939 W

======== CHANNEL f2 ========
SFO2         500.3020012 MHz
NUC2                   1H
CPDPRG[2          waltz16
PCPD2               80.00 usec
PLW2         18.33600044 W
PLW12         0.75654000 W
PLW13         0.38053000 W

F2 - Processing parameters
SI                  65536
SF           125.8005350 MHz
WDW                    EM
SSB       0
LB                   1.00 Hz
GB        0
PC                   1.40
```

Data File F:\010811_08.D
Sample Name: DT-414-30

```
==================================================================
Acq. Operator   : Karen Haggerty                 Seq. Line :   6
Acq. Instrument : Instrument 1                    Location : Vial 5
Injection Date  : 8/1/2011 7:21:29 PM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 20.000 µl
Acq. Method     : C:\CHEM32\1\DATA\KH0811\010811_AB_DT_SJC_AES_SCOUT 2011-08-01 16-06-07\
                  COL1-A2+B1-NO_REF_SHORT.M
Last changed    : 8/1/2011 4:06:16 PM by Karen Haggerty
Analysis Method : F:\010811_08.D\DA.M (COL1-A2+B1-NO_REF_SHORT.M)
Last changed    : 8/2/2011 7:39:33 AM by Karen Haggerty
                  (modified after loading)
Method Info     : Waters XTerra RP18 5um, 150 x 4.6mm


Sample Info     : Waters XTerra RP18 150 x 4.6mm, 0.1% Formic Acid (aq)/M
                  eCN
```




```
==================================================================
                        Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs
```


Data File F:\010811_08.D
Sample Name: DT-414-30

Signal 1: DAD1 F, Sig=310,16 Ref=off

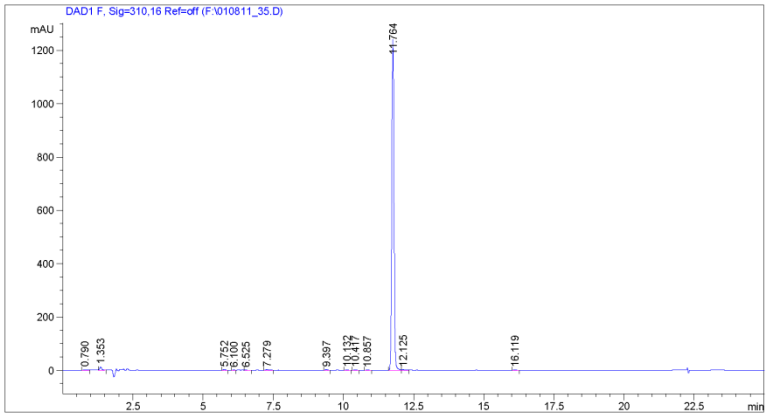
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.052	BB	0.0740	25.52725	5.31517	0.3474
2	7.960	BB	0.0912	20.18016	3.30745	0.2746
3	9.914	BB	0.0757	18.71260	3.78181	0.2546
4	11.078	BB	0.0770	6.96062	1.42470	0.0947
5	11.615	BB	0.0771	5.02495	1.02584	0.0684
6	11.920	MF	0.0871	7239.71875	1384.76477	98.5139
7	12.307	MF	0.1239	12.17315	1.63775	0.1656
8	12.499	MF	0.1261	8.56661	1.13197	0.1166
9	16.116	BB	0.0822	12.06865	2.26281	0.1642

Totals : 7348.93277 1404.65227

*** End of Report ***

Data File F:\010811_35.D
Sample Name: DT-414-30

```
==========================================================================
Acq. Operator   : Karen Haggerty                 Seq. Line :  27
Acq. Instrument : Instrument 1                    Location : Vial 5
Injection Date  : 8/2/2011 8:17:00 AM                 Inj :   1
                                                 Inj Volume : 5.000 µl
Different Inj Volume from Sequence !     Actual Inj Volume : 20.000 µl
Acq. Method     : C:\CHEM32\1\DATA\KH0811\010811_AB_DT_SJC_AES_SCOUT 2011-08-01 16-06-07\
                  COL1-A1+B1-NO_REF_SHORT.M
Last changed    : 7/29/2011 7:46:01 AM by Karen Haggerty
Analysis Method : F:\010811_35.D\DA.M (COL1-A1+B1-NO_REF_SHORT.M)
Last changed    : 8/2/2011 8:54:54 AM by Karen Haggerty
                  (modified after loading)
Sample Info     : Waters XTerra RP18 150 x 4.6mm, 0.1% Ammonia (aq)/MeCN
```




```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 F, Sig=310,16 Ref=off
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	0.790	BB	0.1065	14.46601	1.99842	0.2112
2	1.353	BB	0.0750	60.76270	12.00758	0.8871
3	5.752	BB	0.0716	18.74145	3.93454	0.2736

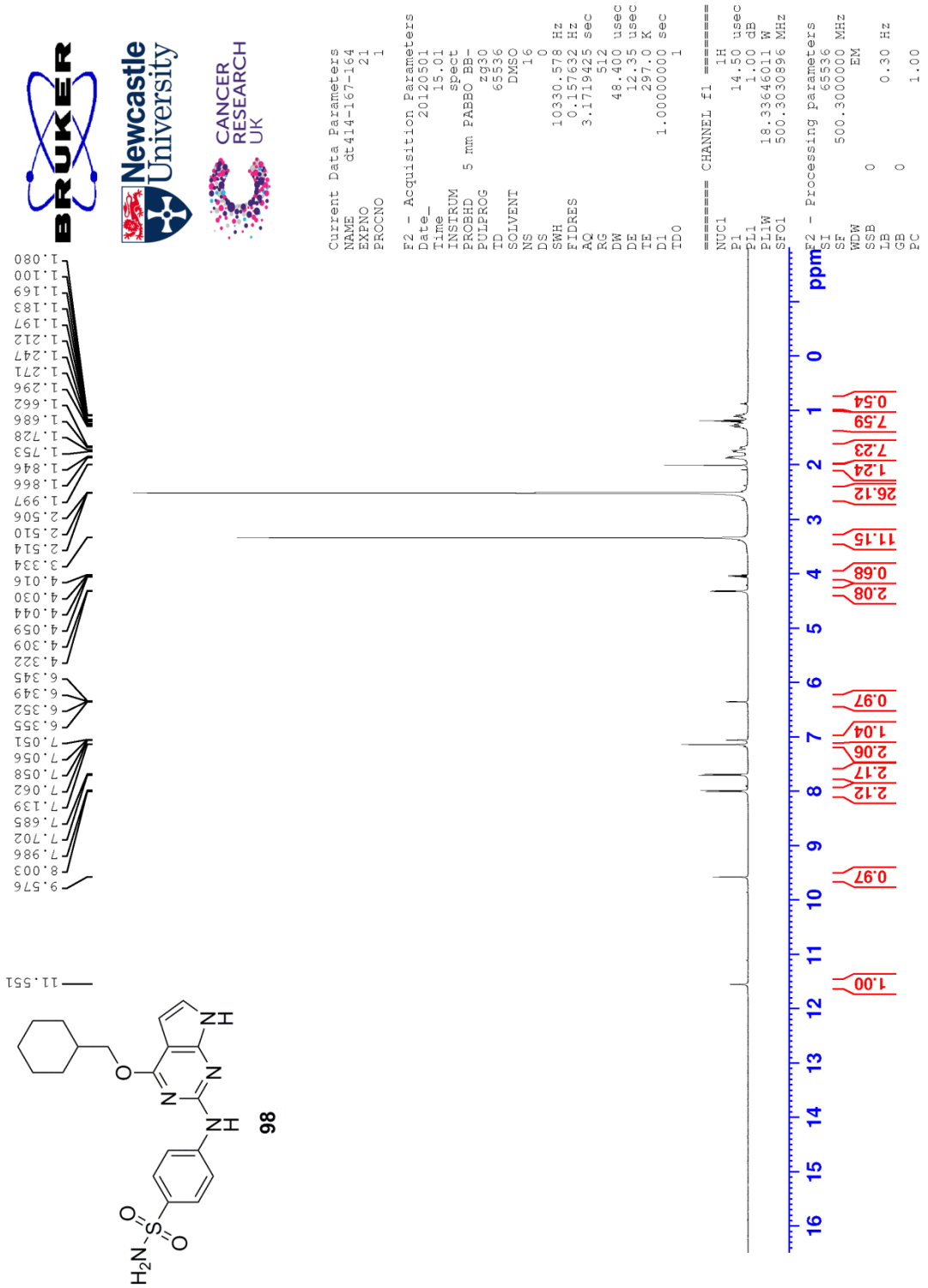
Data File F:\010811_35.D
Sample Name: DT-414-30

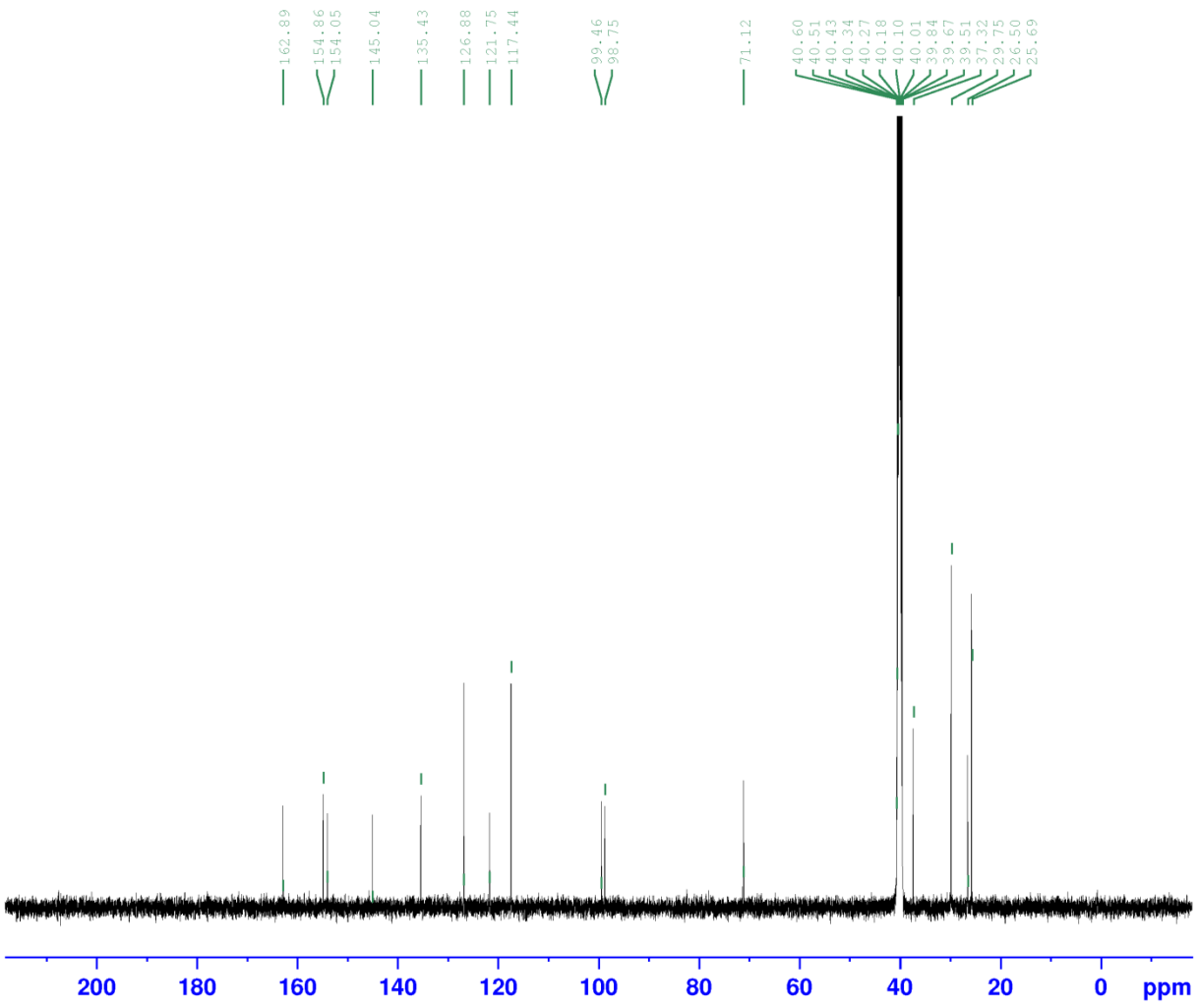
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
4	6.100	BV	0.0728	5.95042	1.22296	0.0869
5	6.525	VB	0.0796	5.99854	1.09959	0.0876
6	7.279	BB	0.0904	22.62056	3.75019	0.3302
7	9.397	BB	0.0759	16.29608	3.28337	0.2379
8	10.132	BB	0.0847	10.41924	1.87932	0.1521
9	10.417	BB	0.0823	12.94998	2.42372	0.1891
10	10.857	BB	0.0863	7.80855	1.37321	0.1140
11	11.764	BV	0.0823	6636.80615	1242.32788	96.8909
12	12.125	VB	0.1174	25.14643	2.95247	0.3671
13	16.119	BB	0.0828	11.80470	2.19319	0.1723

Totals : 6849.77082 1280.44645

```
==========================================================================
                          *** End of Report ***
```

4-((4-(Cyclohexylmethoxy)-7*H*-pyrrolo[2,3-*d*]pyrimidin-2-yl)amino)benzenesulfonamide (98)





Current Data Parameters
NAME DT-414-167-164
EXPNO 10
PROCNO 1

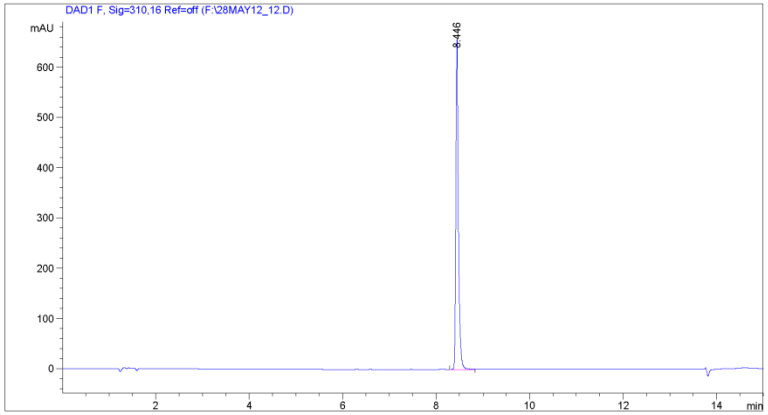
F2 - Acquisition Parameters
Date_ 20161218
Time 8.18
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT DMSO
NS 7680
DS 2
SWH 29761.904 Hz
FIDRES 0.454131 Hz
AQ 1.1010048 sec
RG 456
DW 16.800 usec
DE 7.68 usec
TE 296.8 K
D1 2.00000000 sec
D11 0.03000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 125.8131151 MHz
NUC1 13C
P1 9.75 usec
PLW1 82.38999939 W

======== CHANNEL f2 ========
SFO2 500.3020012 MHz
NUC2 1H
CPDPRG[2 waltz16
PCPD2 80.00 usec
PLW2 18.33600044 W
PLW12 0.75654000 W
PLW13 0.38053000 W

F2 - Processing parameters
SI 65536
SF 125.8005350 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

```
==================================================================
Acq. Operator   : Karen Haggerty                 Seq. Line :   8
Acq. Instrument : Instrument 1                    Location : Vial 65
Injection Date  : 5/28/2012 7:31:06 PM                 Inj :   1
                                               Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\MAY2012\28MAY12_SMM_BJC_DT 2012-05-28 16-18-11\XSELECT_
                  ACIDIC.M
Last changed    : 5/28/2012 4:18:19 PM by Karen Haggerty
Analysis Method : F:\28MAY12_12.D\DA.M (XSELECT_ACIDIC.M)
Last changed    : 5/29/2012 7:21:46 AM by Karen Haggerty
                  (modified after loading)
Method Info     : Waters XSELECT CSH C18 3.5um 100 x 4.6mm
                  0.1% Formic Acid (aq)/MeCN, 1.0mL/min
```

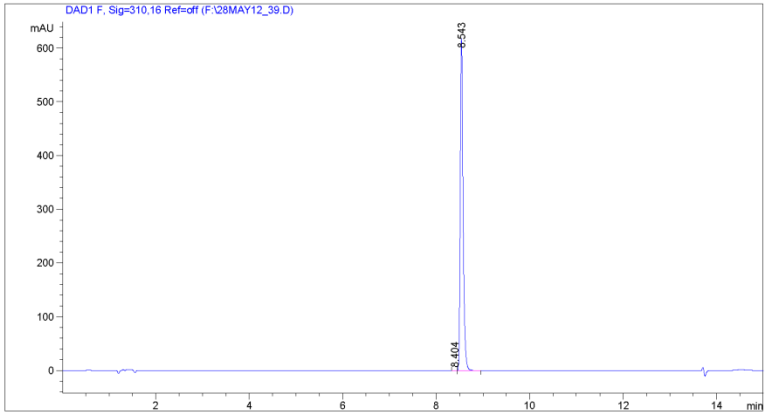



```
==================================================================
                         Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 F, Sig=310,16 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.446 MF    0.0665 2635.70703  660.25592 100.0000

Totals :                  2635.70703  660.25592
```


Data File F:\28MAY12_12.D
Sample Name: DT-414-164-167

```
==================================================================
                        *** End of Report ***
```

```
==================================================================
Acq. Operator   : Karen Haggerty                 Seq. Line :  22
Acq. Instrument : Instrument 1                    Location : Vial 65
Injection Date  : 5/29/2012 3:27:24 AM                Inj :   2
                                                Inj Volume : 5.000 µl
Acq. Method     : C:\CHEM32\1\DATA\MAY2012\28MAY12_SMM_BJC_DT 2012-05-28 16-18-11\XSELECT_
                  BASIC.M
Last changed    : 5/15/2012 3:52:00 PM by Karen Haggerty
Analysis Method : F:\28MAY12_39.D\DA.M (XSELECT_BASIC.M)
Last changed    : 5/29/2012 7:26:03 AM by Karen Haggerty
                  (modified after loading)
Method Info     : Waters XSELECT CSH C18 3.5um 100 x 4.6mm
                  0.1% Ammonia (aq)/MeCN, 1.0mL/min
```




```
==================================================================
                          Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier:                   :      1.0000
Dilution:                     :      1.0000
Use Multiplier & Dilution Factor with ISTDs


Signal 1: DAD1 F, Sig=310,16 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   8.404 MF    0.0617    3.12164 8.43640e-1   0.1223
   2   8.543 MF    0.0683 2548.83496  622.10461  99.8777

Totals :                  2551.95660  622.94825
```



```
==================================================================
                        *** End of Report ***
```