Electronic Supporting Information (ESI)

3-(Benzo[d][1,3]dioxol-5-ylamino)-N-(4-fluorophenyl)thiophene-2-carboxamide overcomes cancer chemoresistance via inhibition of angiogenesis and P-glycoprotein efflux pump activity†‡

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† *IIIM Publication number. IIIM/1756/2015*

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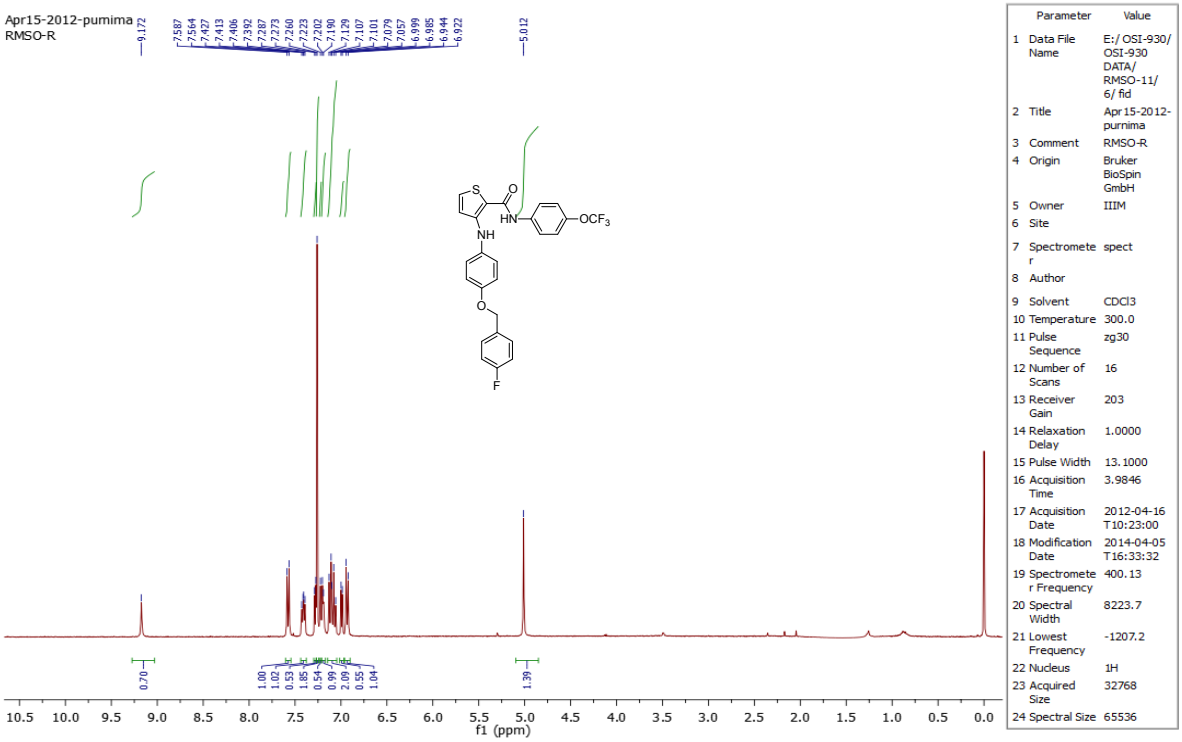
S1. Scanned copies of ^{1}H, ^{13}C, DEPT, ^{19}F-NMR copies of 1a-w.

*3-((4-((4-Fluorobenzyl)oxy)phenyl)amino)-N-(4-(trifluoromethoxy)phenyl)thiophene-2-carboxamide (**1a**).*



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5	Owner	IIIM
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7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
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16	Acquisition Time	3.9846
17	Acquisition Date	2012-04-16 T10:23:00
18	Modification Date	2014-04-05 T16:33:32
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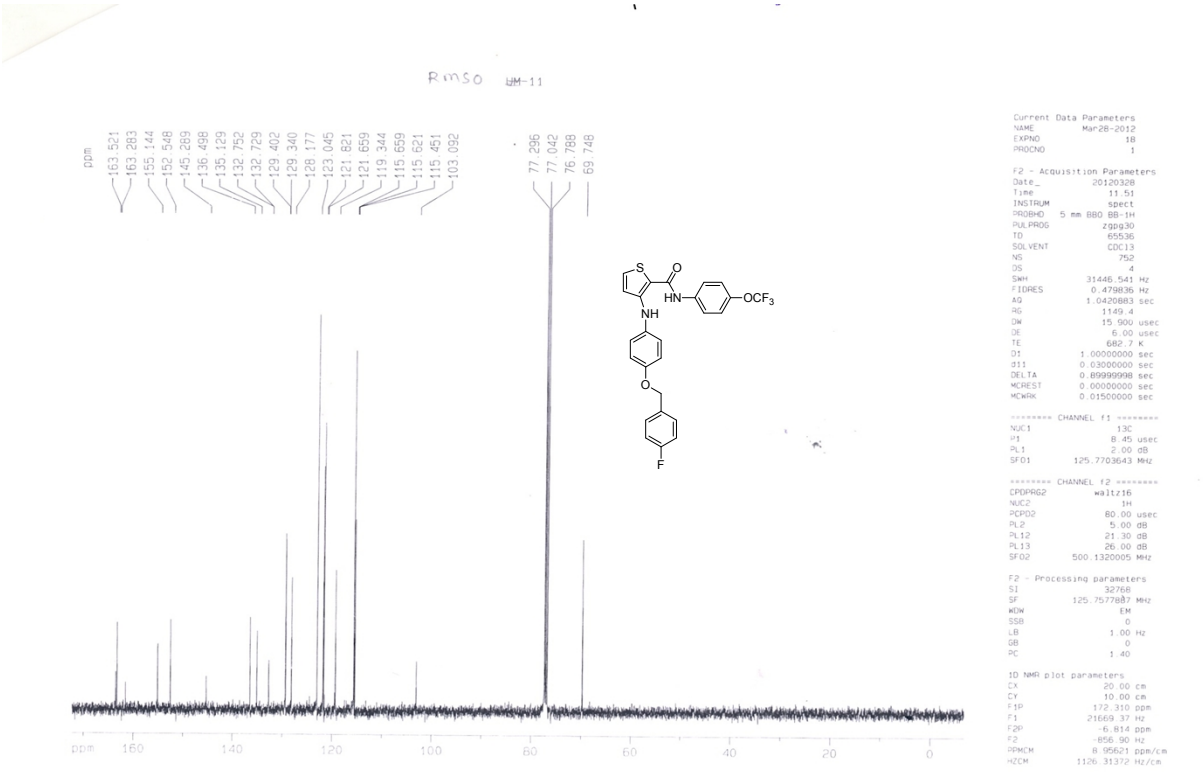
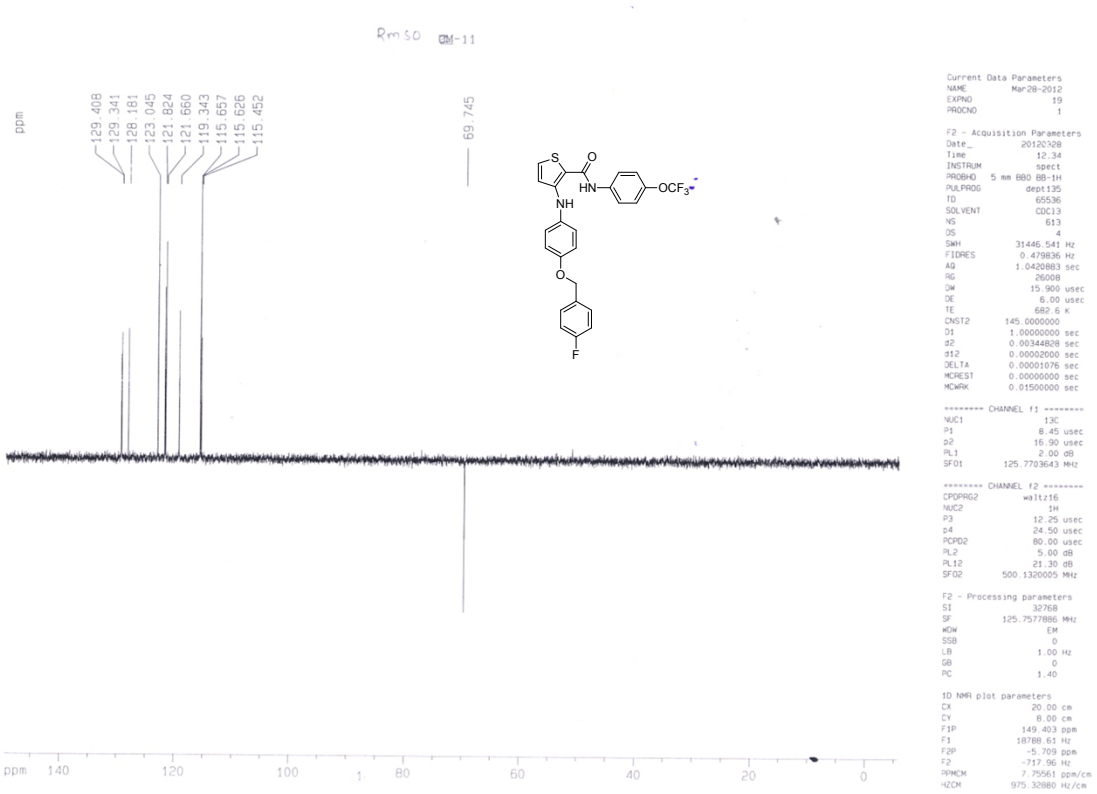
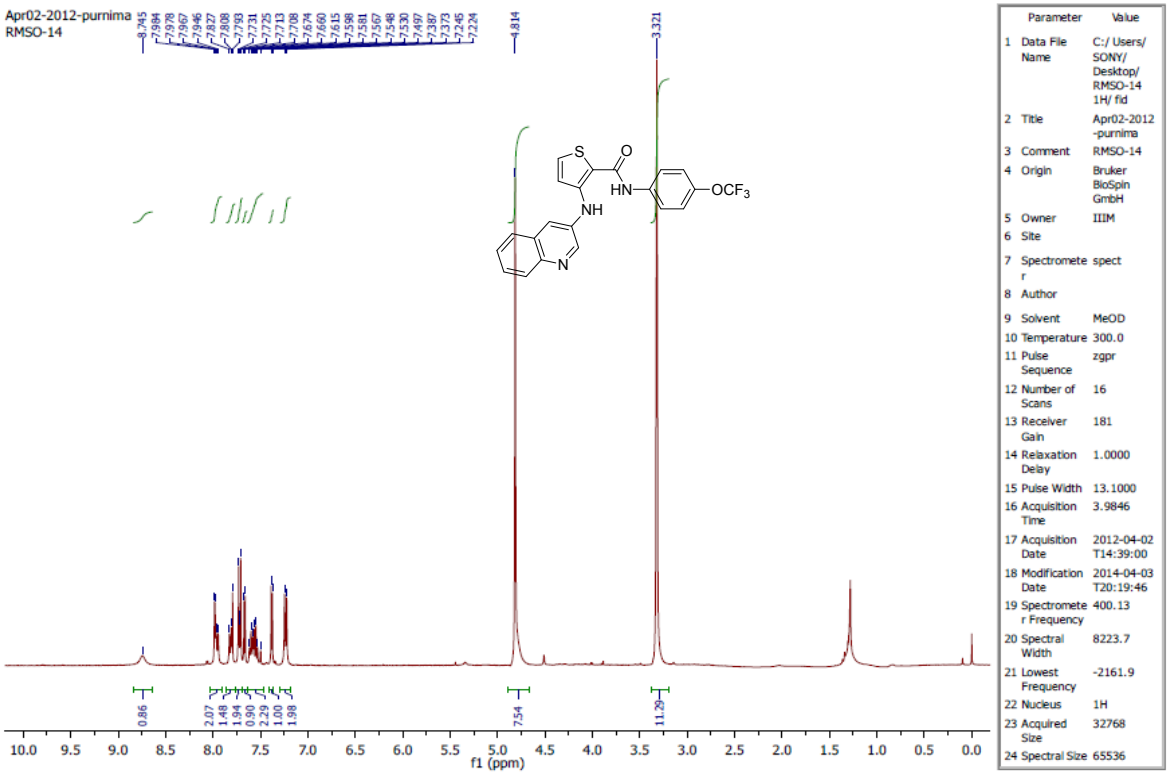
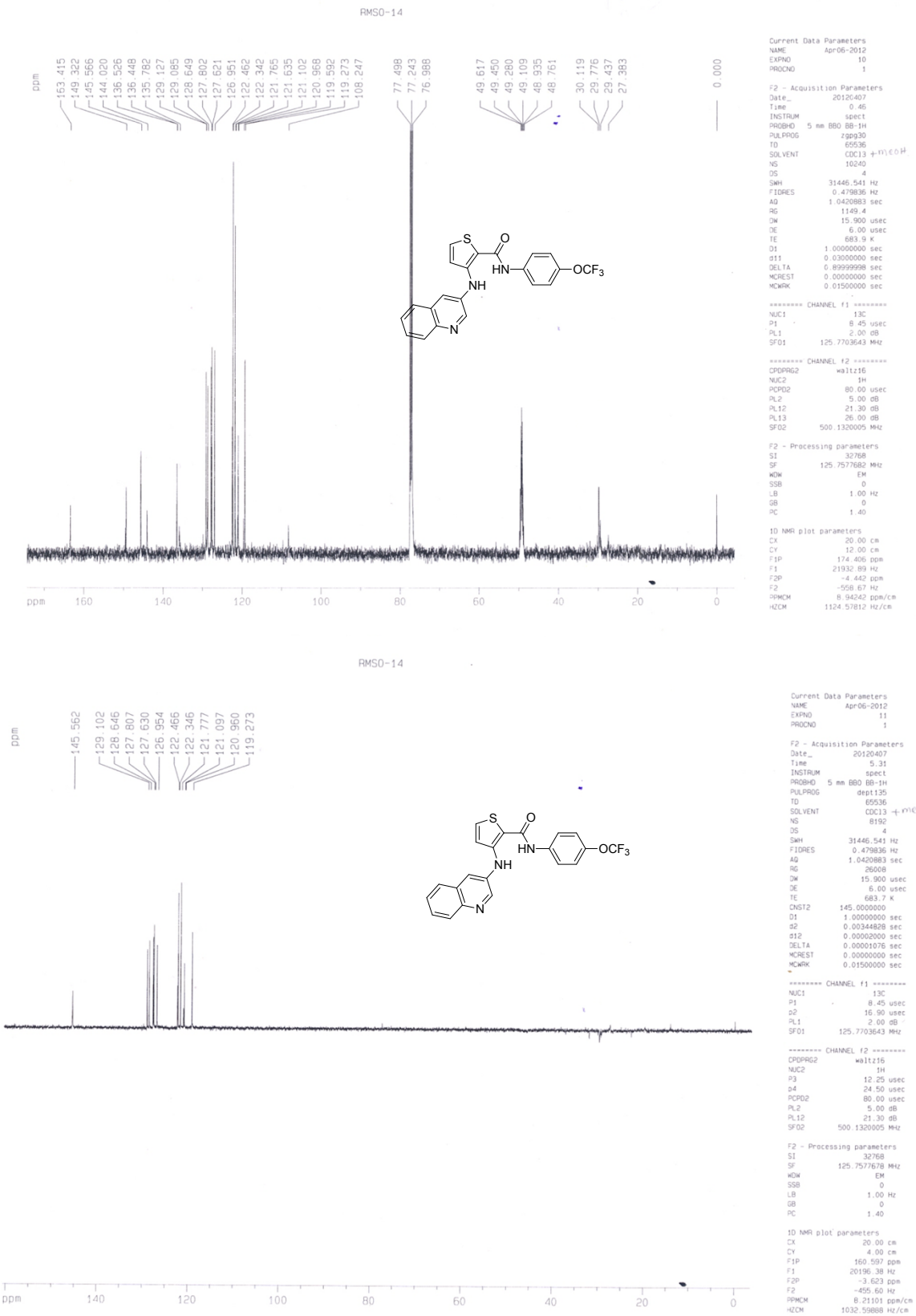




*3-(Quinolin-3-ylamino)-N-(4-(trifluoromethoxy)phenyl)thiophene-2-carboxamide (**1b**).*

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122.462
122.342
121.765
121.635
121.102
120.968
119.592
119.273
108.247
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76.988
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49.280
49.109
48.935
48.761
30.119
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29.437
27.383
0.000
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O
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OCF3
NH
N
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DELTA 0.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
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PL1 2.00 dB
SF01 125.7703643 MHz
======== CHANNEL f2 ========
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NUC2 1H
PCPD2 80.00 usec
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PL12 21.30 dB
PL13 26.00 dB
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SSB 0
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127.630
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PROCNO 1
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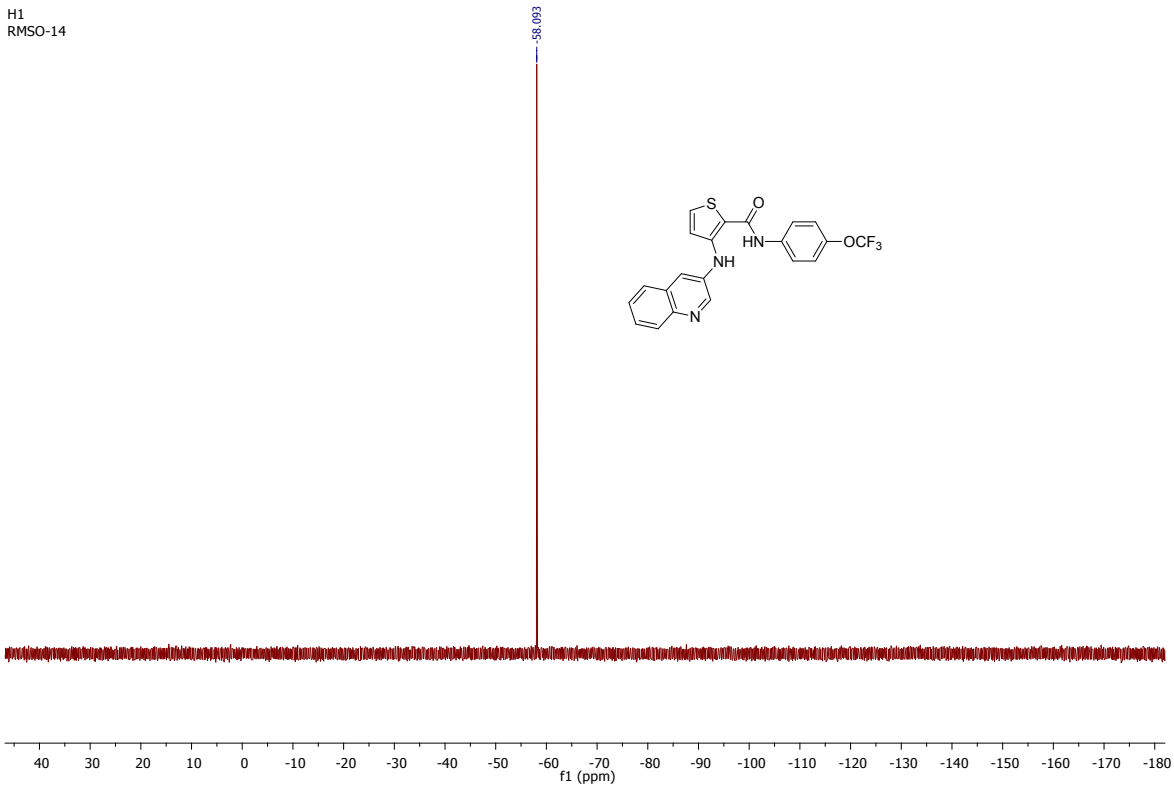
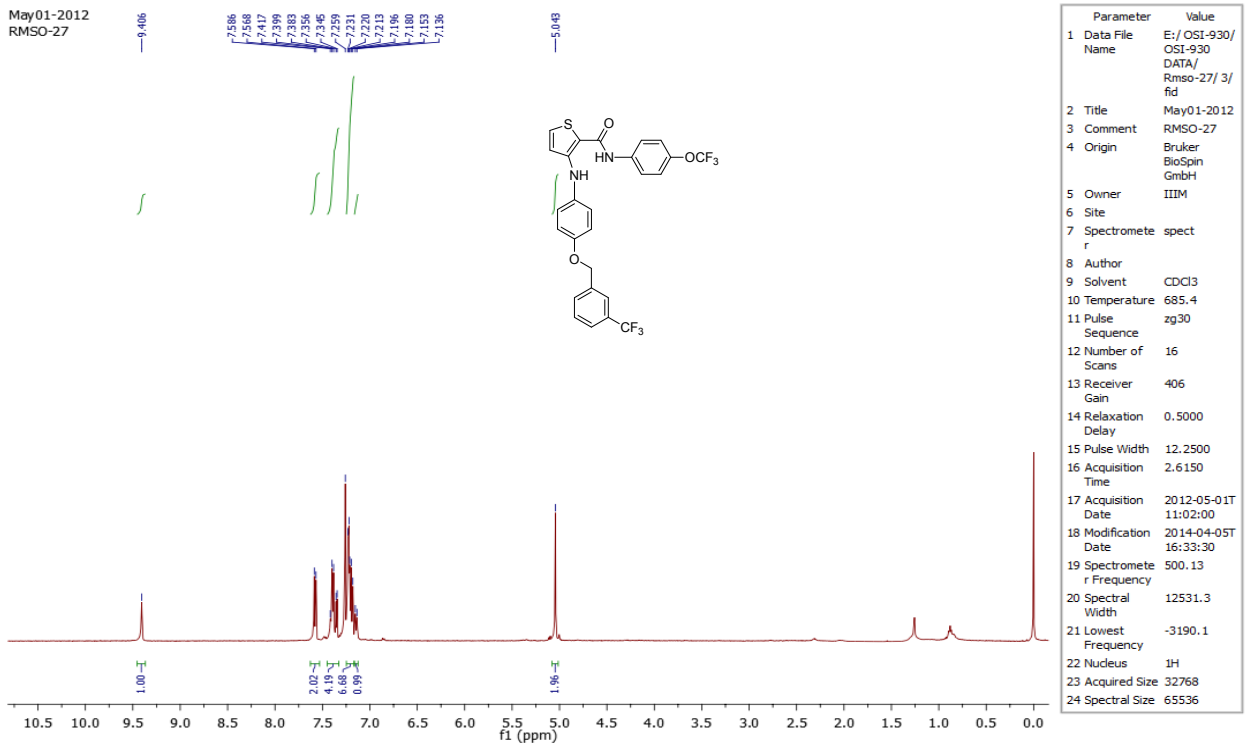


*N-(4-(Trifluoromethoxy)phenyl)-3-((4-((3-(trifluoromethyl)benzyl)oxy)phenyl)amino)thiophene-2-carboxamide (**1c**).*



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7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
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11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	406
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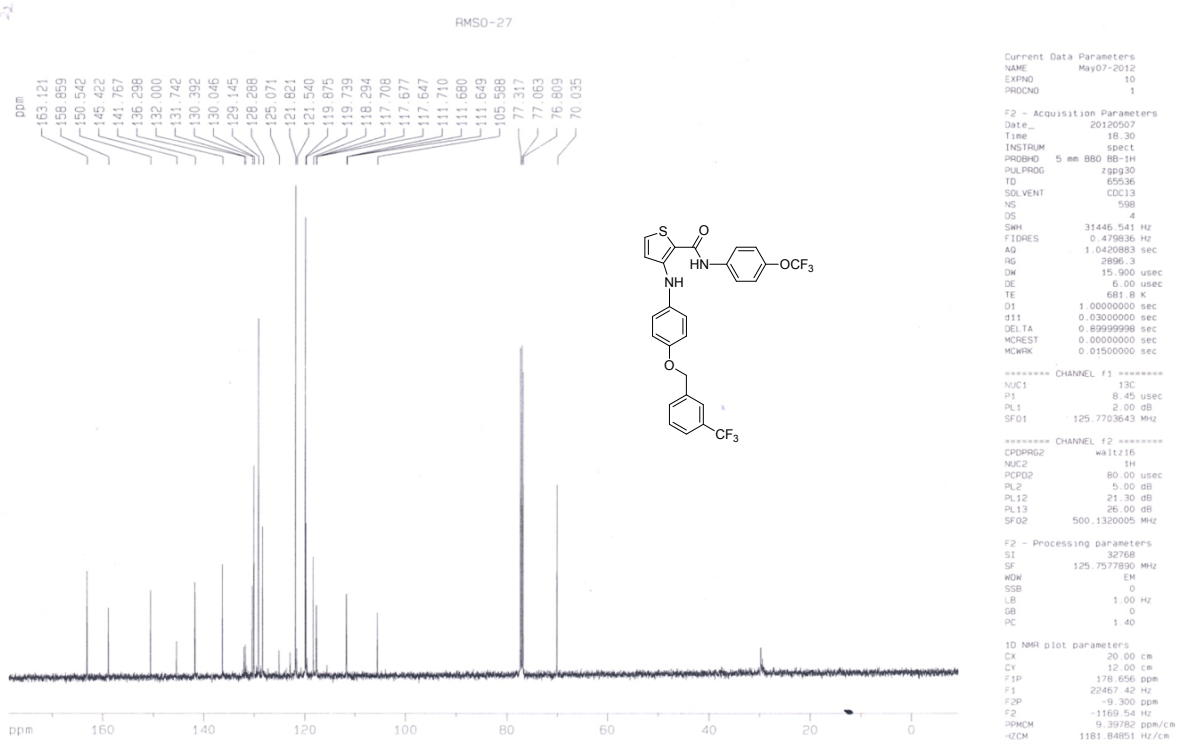


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TD                          65536
SOLVENT                   CDCl3
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FIDRES                  0.479836 Hz
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DE                         6.00 usec
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d11                    0.03000000 sec
DELTA                  0.89999998 sec
MCREST                 0.00000000 sec
MCWRK                  0.01500000 sec

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NUC1                         13C
P1                          8.45 usec
PL1                         2.00 dB
SF01                125.7703643 MHz

======== CHANNEL f2 ========
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NUC2                         1H
PCPD2                      80.00 usec
PL2                         5.00 dB
PL12                       21.30 dB
PL13                       26.00 dB
SF02                500.1320005 MHz

F2 - Processing parameters
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GB                               0
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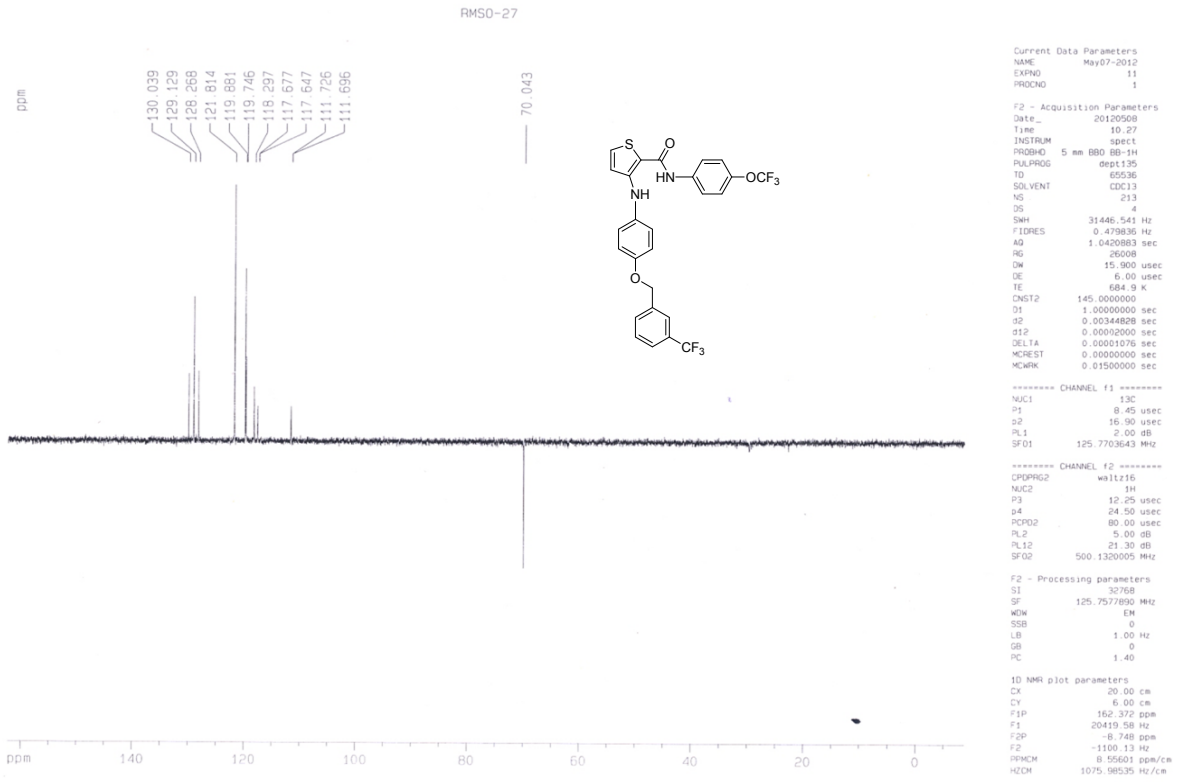


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SOLVENT                   CDCl3
NS                             213
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NUC1                         13C
P1                          8.45 usec
p2                         16.90 usec
PL1                         2.00 dB
SF01                125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                  waltz16
NUC2                         1H
P3                         12.25 usec
p4                         24.50 usec
PCPD2                      80.00 usec
PL2                         5.00 dB
PL12                       21.30 dB
SF02                500.1320005 MHz

F2 - Processing parameters
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1D NMR plot parameters
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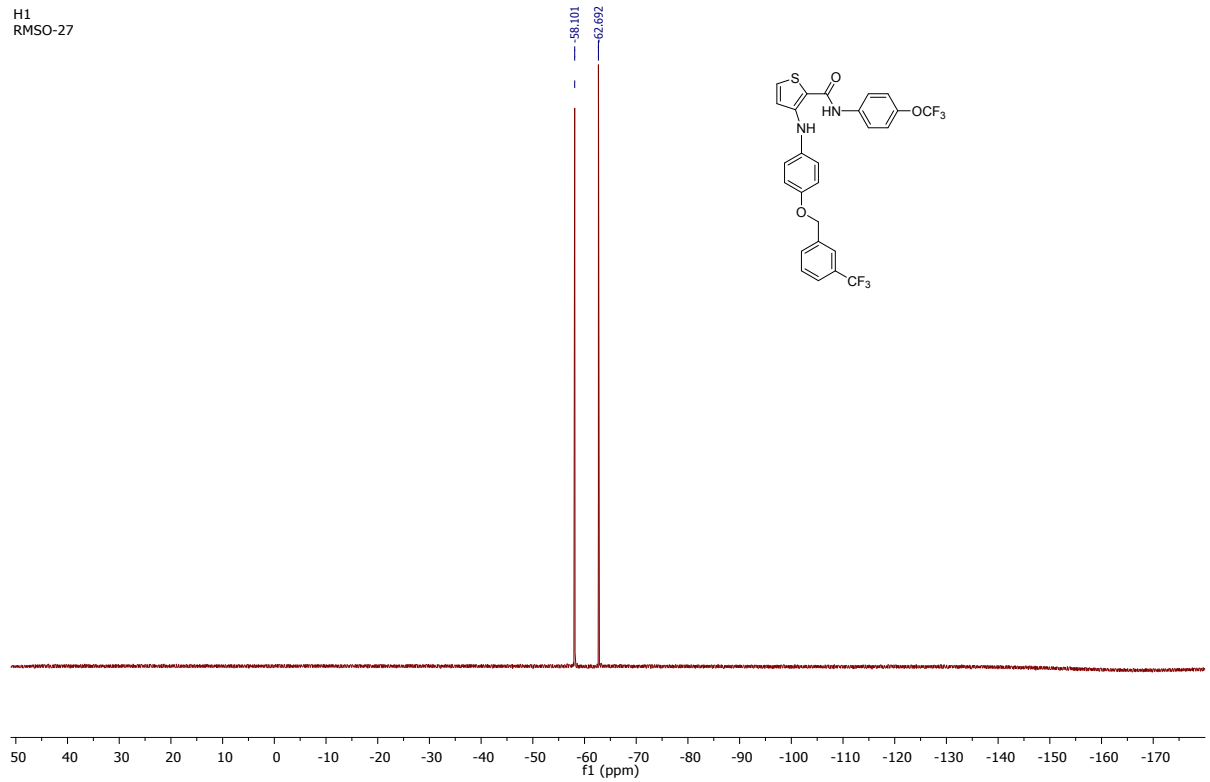
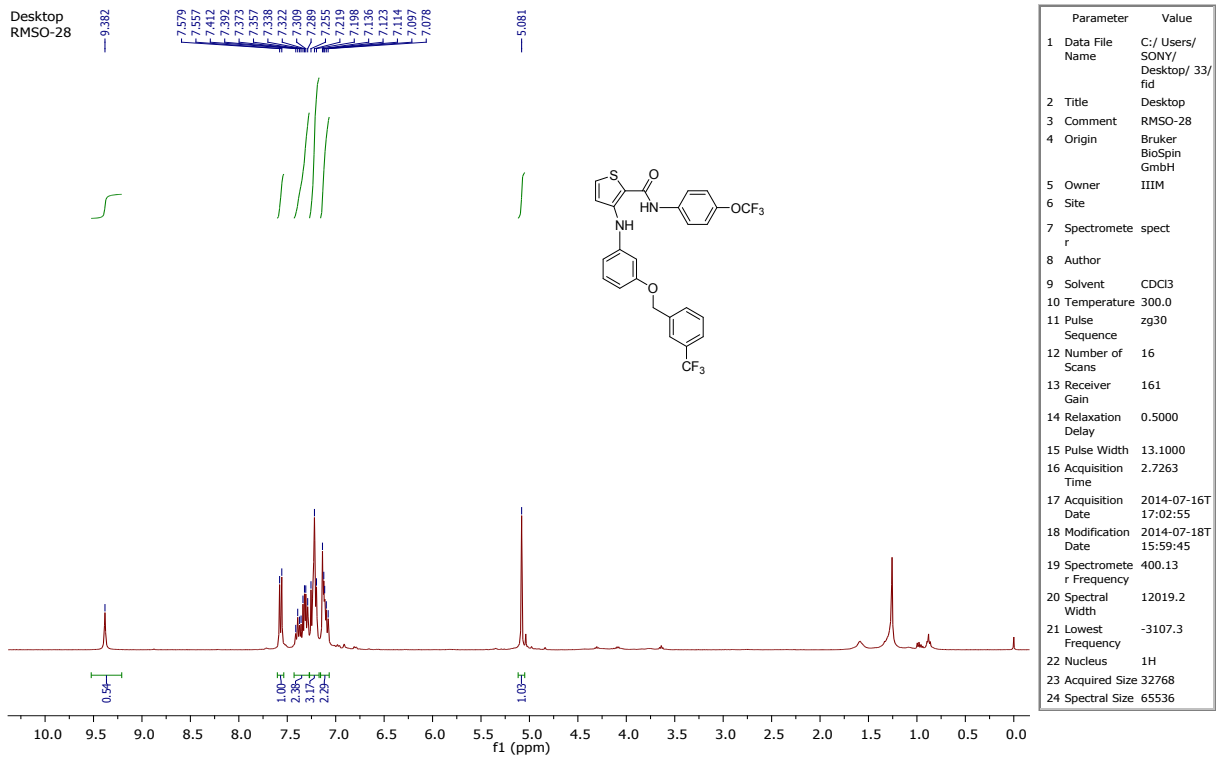


*N-(4-(Trifluoromethoxy)phenyl)-3-((3-((3-(trifluoromethyl)benzyl)oxy)phenyl)amino)thiophene-2-carboxamide (**1d**).*



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7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
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12	Number of Scans	16
13	Receiver Gain	161
14	Relaxation Delay	0.5000
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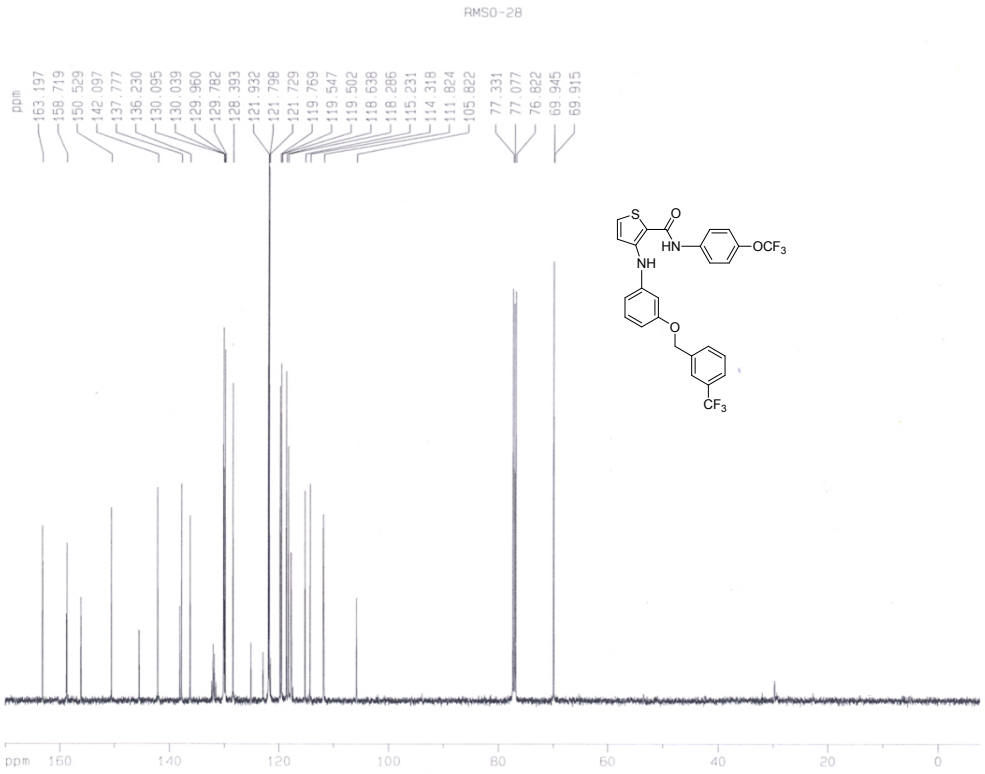


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TD                       65536
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FIDRES              0.479836 Hz
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RG                     1149.4
DW                     15.900 usec
DE                      6.00 usec
TE                     685.6 K
D1                  1.00000000 sec
d11                 0.03000000 sec
DELTA               0.89999998 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                       8.45 usec
PL1                      2.00 dB
SFO1                125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
PCPD2                   80.00 usec
PL2                      5.00 dB
PL12                    21.30 dB
PL13                    26.00 dB
SFO2                500.1320005 MHz

F2 - Processing parameters
SI                         32768
SF                  125.7577890 MHz
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SSB                            0
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GB                             0
PC                      1.40

1D NMR plot parameters
CX                      20.00 cm
CY                      16.00 cm
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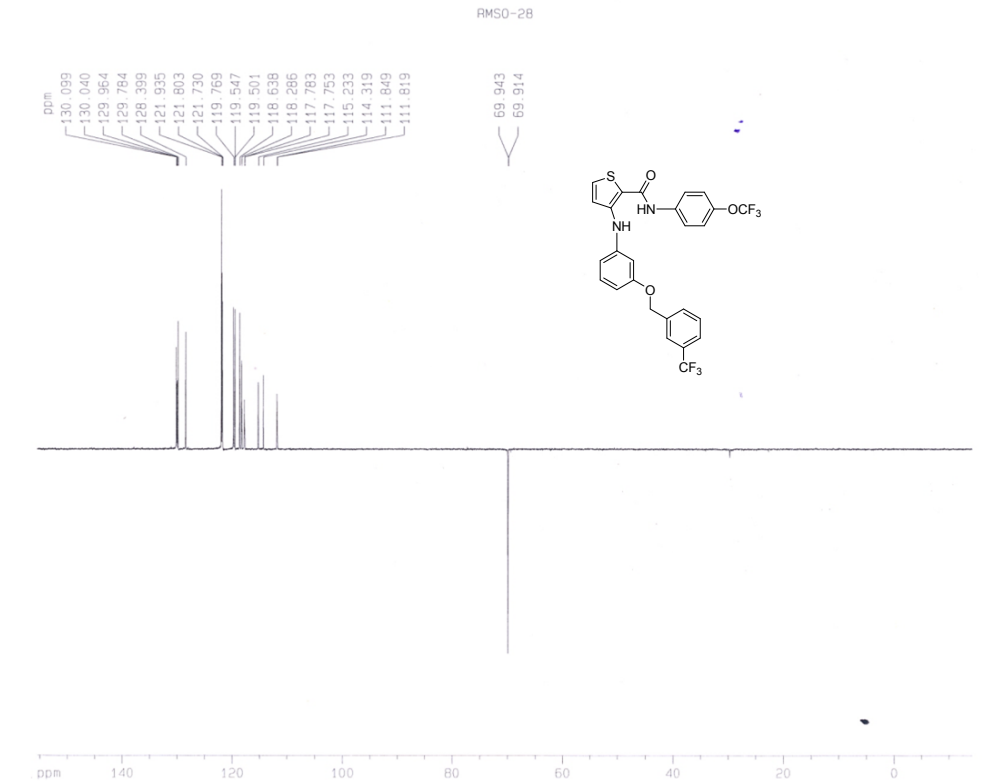


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FIDRES              0.479836 Hz
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RG                       26008
DW                     15.900 usec
DE                      6.00 usec
TE                     685.7 K
CNST2               145.0000000
D1                  1.00000000 sec
d2                  0.00344828 sec
d12                 0.00002000 sec
DELTA               0.00001076 sec
MCREST              0.00000000 sec
MCWRK               0.01500000 sec

======== CHANNEL f1 ========
NUC1                      13C
P1                       8.45 usec
p2                      16.90 usec
PL1                      2.00 dB
SFO1                125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                waltz16
NUC2                       1H
P3                      12.25 usec
p4                      24.50 usec
PCPD2                   80.00 usec
PL2                      5.00 dB
PL12                    21.30 dB
SFO2                500.1320005 MHz

F2 - Processing parameters
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SF                  125.7577890 MHz
WDW                           EM
SSB                            0
LB                      1.00 Hz
GB                             0
PC                      1.40

1D NMR plot parameters
CX                      20.00 cm
CY                       6.00 cm
F1P                   155.472 ppm
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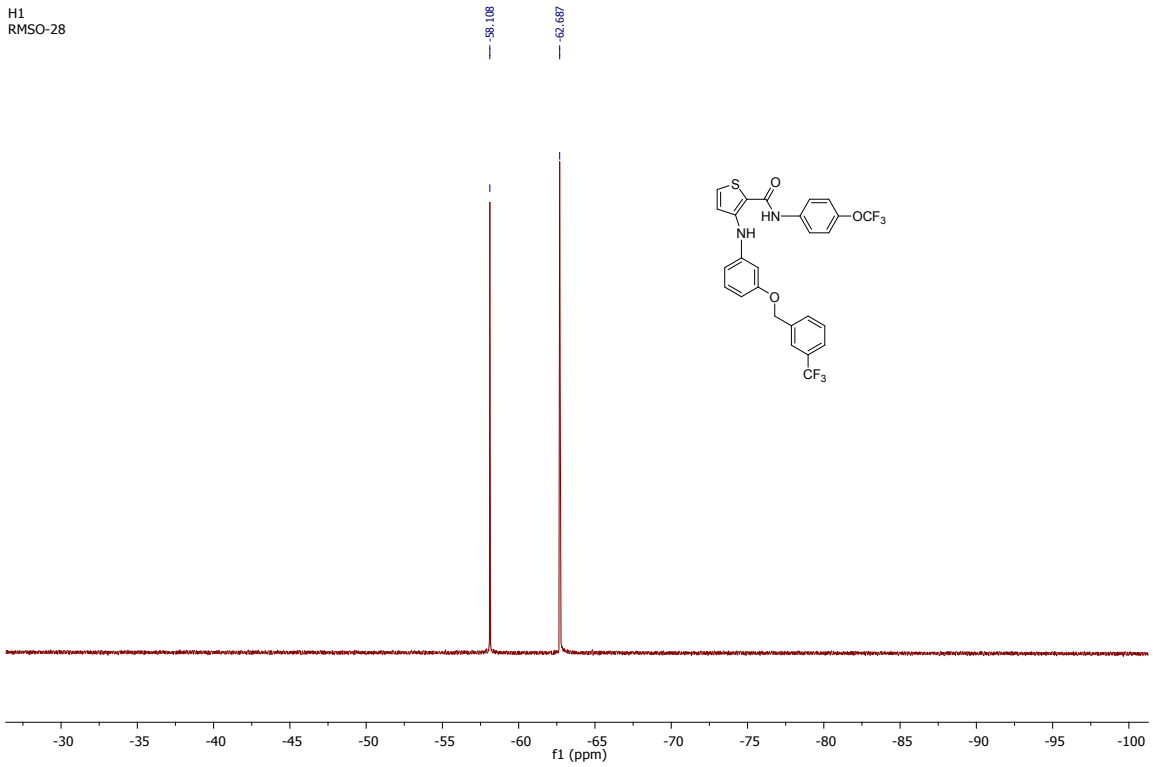
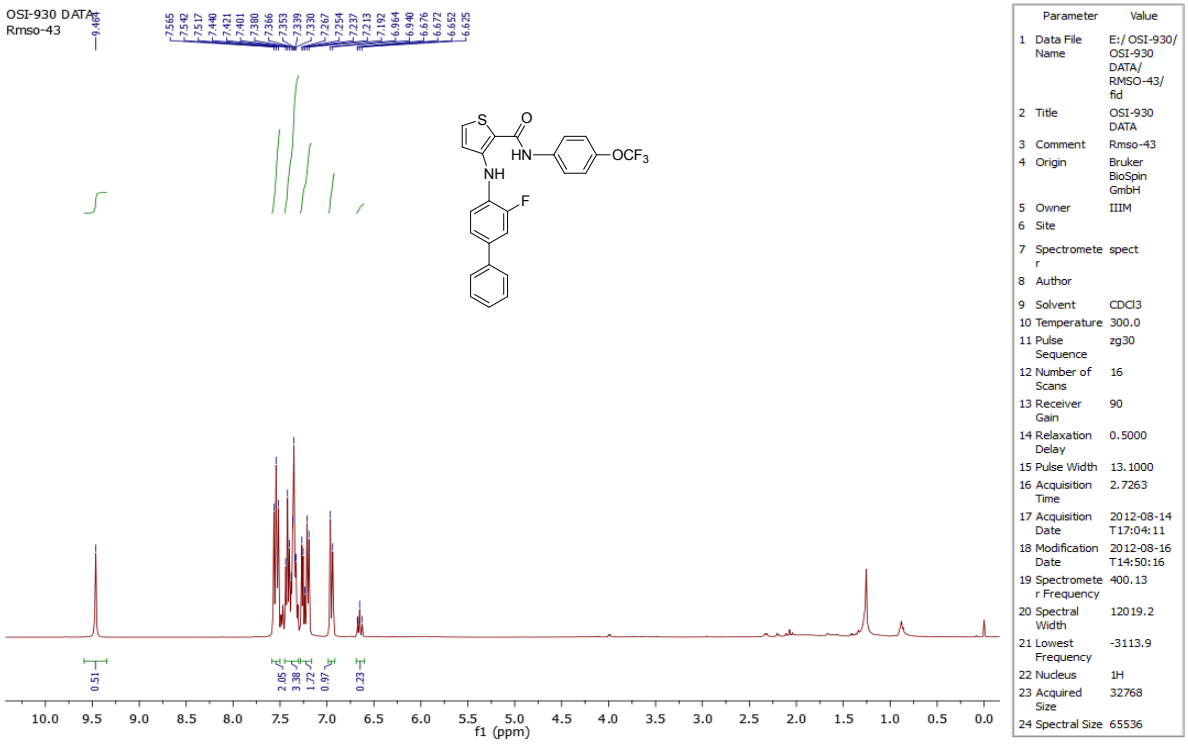
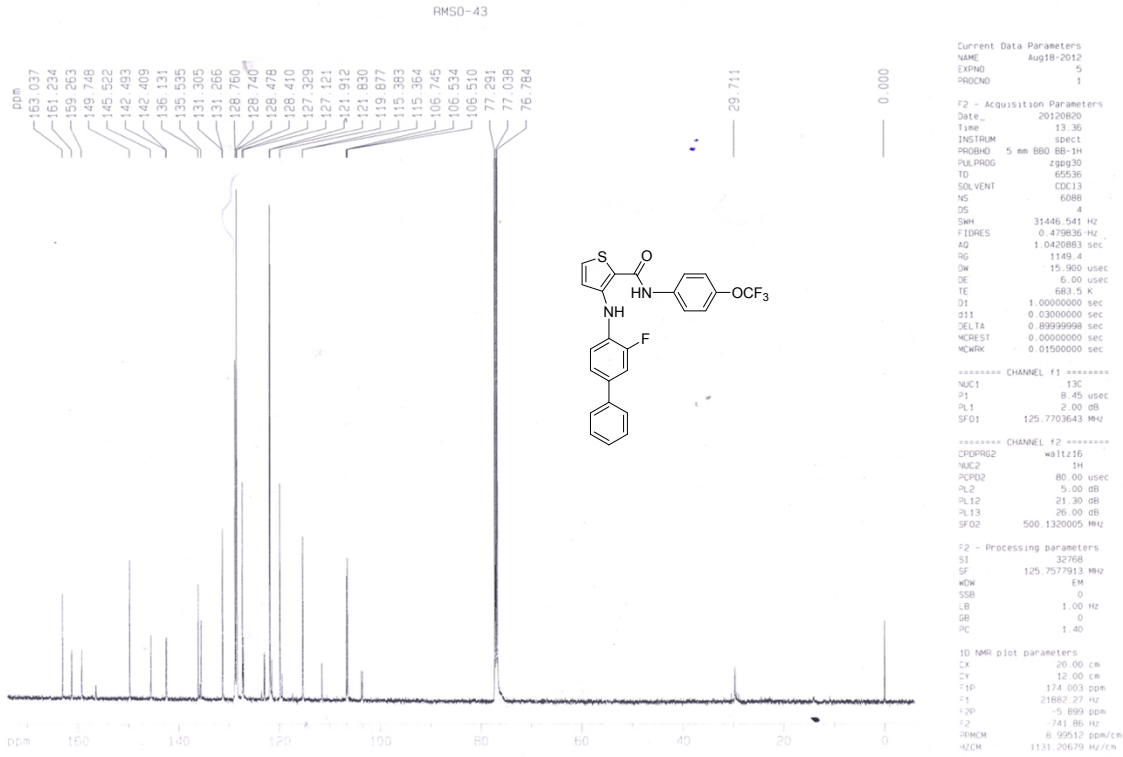


*3-((3-Fluoro-[1,1'-biphenyl]-4-yl)amino)-N-(4-(trifluoromethoxy)phenyl)thiophene-2-carboxamide (**1e**).*



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SOLVENT            CDCl3
NS                  6088
DS                     4
SWH           31446.541 Hz
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RG                1149.4
DW                15.900 usec
DE                 6.00 usec
TE                683.5 K
D1             1.00000000 sec
d11            0.03000000 sec
DELTA          0.89999998 sec
MCREST         0.00000000 sec
MCWRK          0.01500000 sec

======== CHANNEL f1 ========
NUC1                  13C
P1                 8.45 usec
PL1                2.00 dB
SFO1         125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
PCPD2             80.00 usec
PL2                5.00 dB
PL12              21.30 dB
PL13              26.00 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
SI                 32768
SF          125.7577913 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40

1D NMR plot parameters
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CY                12.00 cm
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F1             21882.27 Hz
F2P               -5.899 ppm
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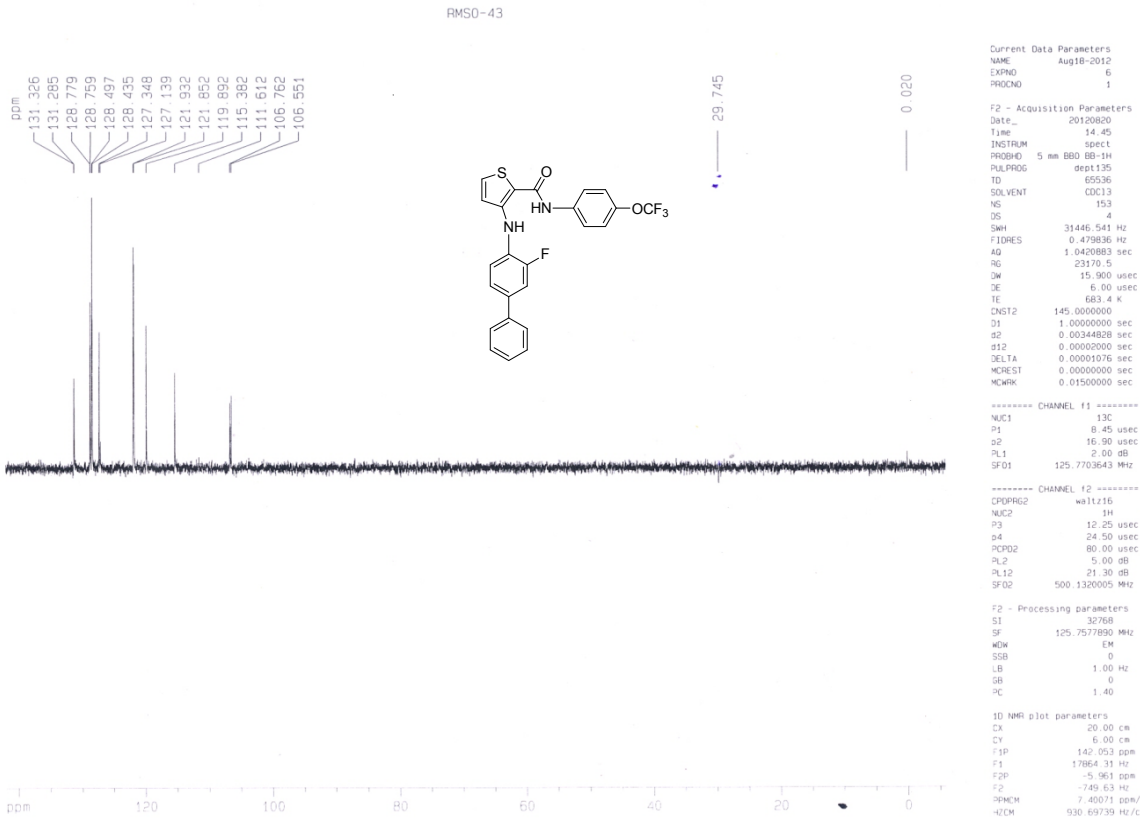


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MCREST         0.00000000 sec
MCWRK          0.01500000 sec

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NUC1                  13C
P1                 8.45 usec
P2                16.90 usec
PL1                2.00 dB
SFO1         125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2           waltz16
NUC2                  1H
P3                12.25 usec
P4                24.50 usec
PCPD2             80.00 usec
PL2                5.00 dB
PL12              21.30 dB
SFO2         500.1320005 MHz

F2 - Processing parameters
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SF          125.7577890 MHz
WDW                   EM
SSB                    0
LB                 1.00 Hz
GB                     0
PC                 1.40

1D NMR plot parameters
CX                20.00 cm
CY                 6.00 cm
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F1             17864.31 Hz
F2P               -5.961 ppm
F2              -749.63 Hz
PPMCM          7.40071 ppm/cm
HZCM        930.69739 Hz/cm
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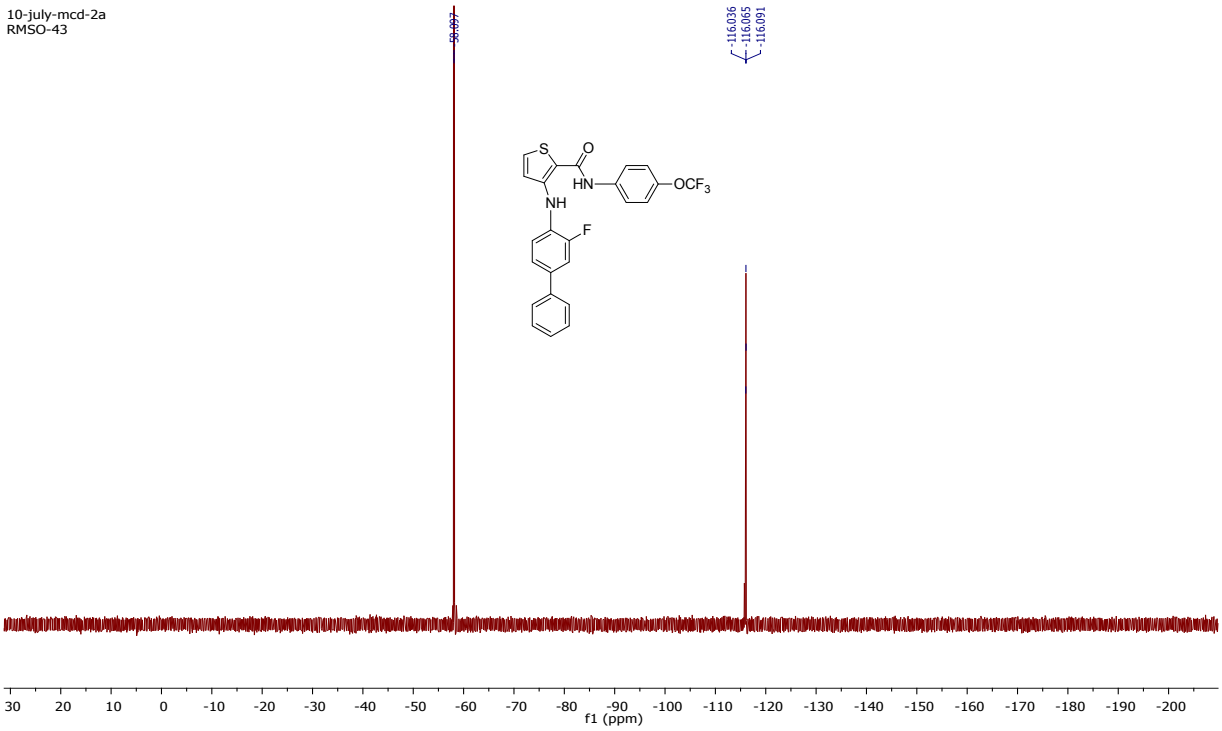
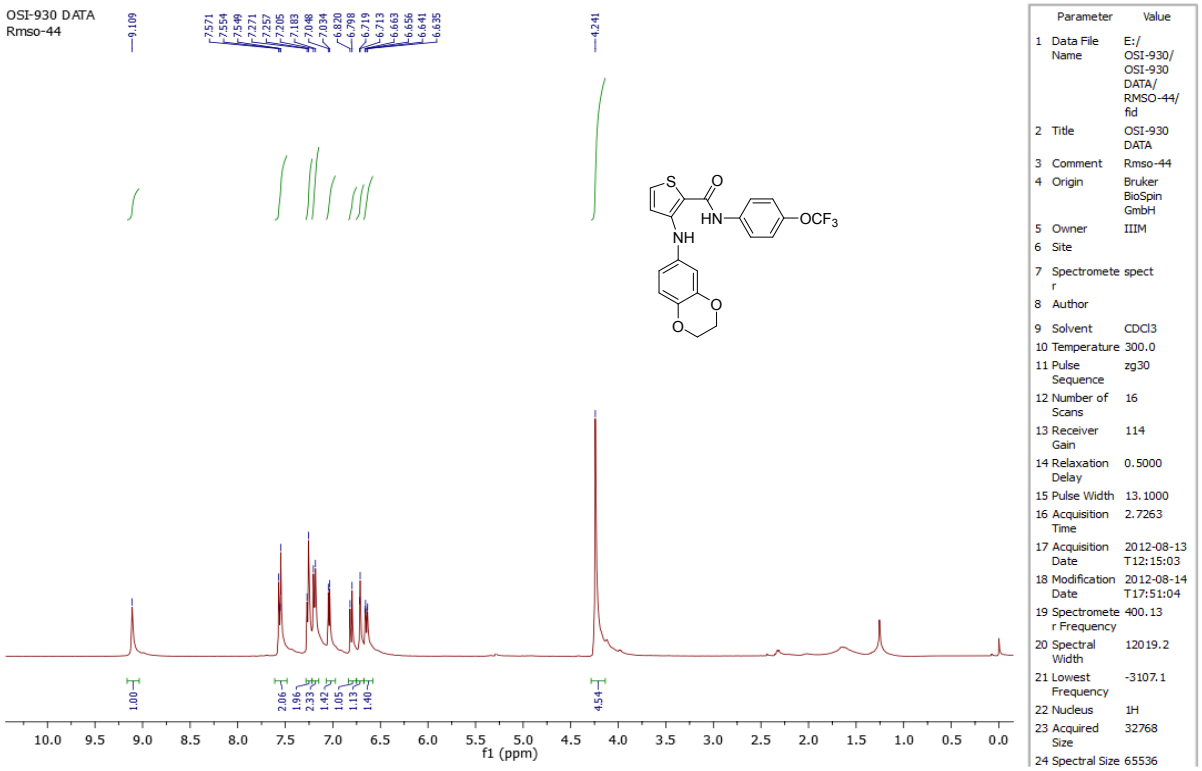
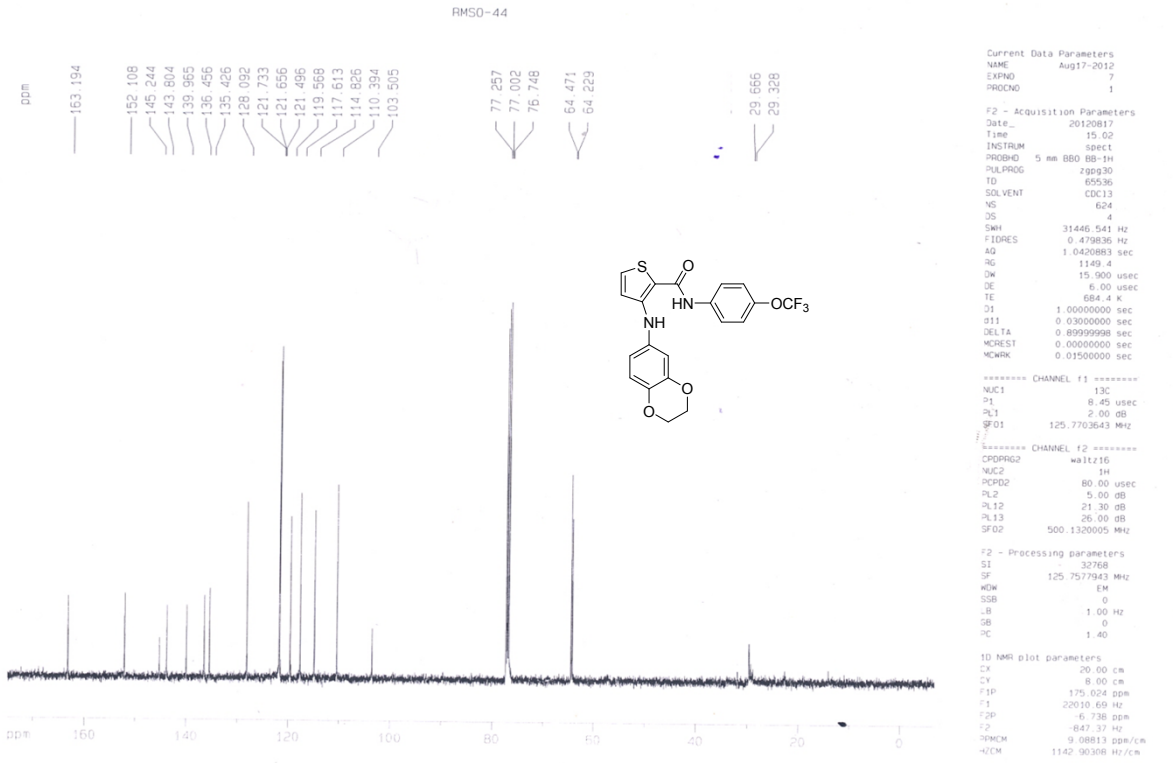


*3-((2,3-Dihydrobenzo[b][1,4]dioxin-6-yl)amino)-N-(4-(trifluoromethoxy)phenyl)thiophene-2-carboxamide (**1f**).*



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Current Data Parameters
NAME                  Aug17-2012
EXPNO                          7
PROCNO                         1

F2 - Acquisition Parameters
Date_                   20120817
Time                       15.02
INSTRUM                    spect
PROBHD    5 mm BBO BB-1H
PULPROG                  zgpg30
TD                        65536
SOLVENT                   CDCl3
NS                          624
DS                            4
SWH                   31446.541 Hz
FIDRES                0.479836 Hz
AQ                    1.0420883 sec
RG                       1149.4
DW                      15.900 usec
DE                       6.00 usec
TE                       684.4 K
D1                    1.00000000 sec
d11                   0.03000000 sec
DELTA                 0.89999998 sec
MCREST                0.00000000 sec
MCWRK                 0.01500000 sec

======== CHANNEL f1 ========
NUC1                        13C
P1                         8.45 usec
PL1                        2.00 dB
SFO1                125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
PCPD2                     80.00 usec
PL2                        5.00 dB
PL12                      21.30 dB
PL13                      26.00 dB
SFO2                500.1320005 MHz

F2 - Processing parameters
SI                         32768
SF                  125.7577943 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40

1D NMR plot parameters
CX                         20.00 cm
CY                          8.00 cm
F1P                       175.024 ppm
F1                      22010.69 Hz
F2P                      -6.738 ppm
F2                       -847.37 Hz
PPMCM                   9.08813 ppm/cm
HZCM                 1142.90308 Hz/cm
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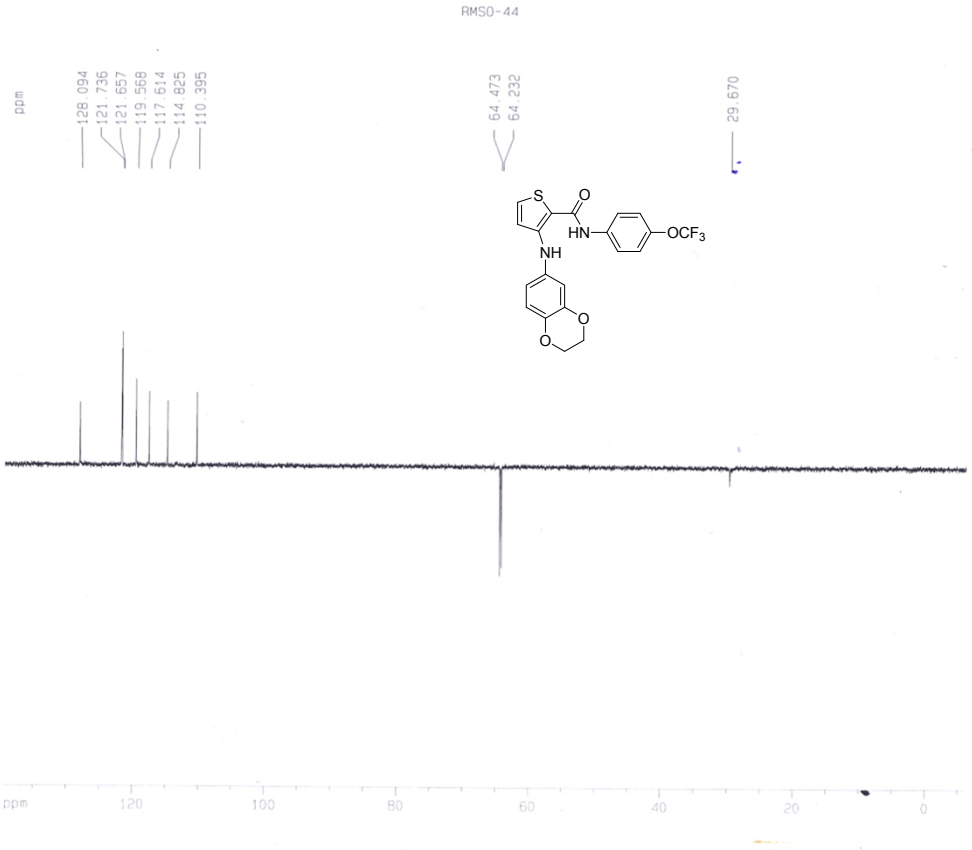


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Current Data Parameters
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EXPNO                          8
PROCNO                         1

F2 - Acquisition Parameters
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Time                       15.22
INSTRUM                    spect
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PULPROG                 dept135
TD                        65536
SOLVENT                   CDCl3
NS                          226
DS                            4
SWH                   31446.541 Hz
FIDRES                0.479836 Hz
AQ                    1.0420883 sec
RG                       23170.5
DW                      15.900 usec
DE                       6.00 usec
TE                       684.0 K
CNST2                145.0000000
D1                    1.00000000 sec
d2                    0.00344828 sec
d12                   0.00002000 sec
DELTA                 0.00001076 sec
MCREST                0.00000000 sec
MCWRK                 0.01500000 sec

======== CHANNEL f1 ========
NUC1                        13C
P1                         8.45 usec
p2                        16.90 usec
PL1                        2.00 dB
SFO1                125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2                 waltz16
NUC2                        1H
P3                        12.25 usec
p4                        24.50 usec
PCPD2                     80.00 usec
PL2                        5.00 dB
PL12                      21.30 dB
SFO2                500.1320005 MHz

F2 - Processing parameters
SI                         32768
SF                  125.7577940 MHz
WDW                           EM
SSB                            0
LB                          1.00 Hz
GB                             0
PC                          1.40

1D NMR plot parameters
CX                         20.00 cm
CY                          3.00 cm
F1P                       139.418 ppm
F1                      17532.86 Hz
F2P                      -6.205 ppm
F2                       -780.33 Hz
PPMCM                   7.28113 ppm/cm
HZCM                 915.65924 Hz/cm
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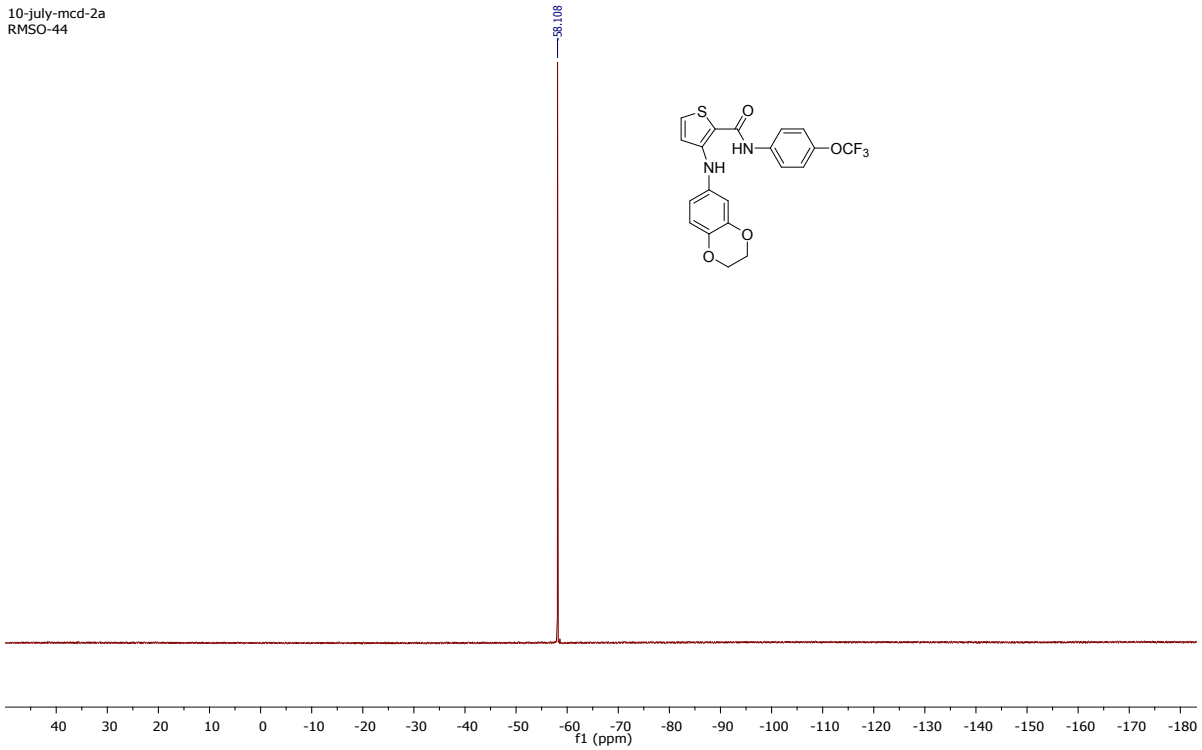
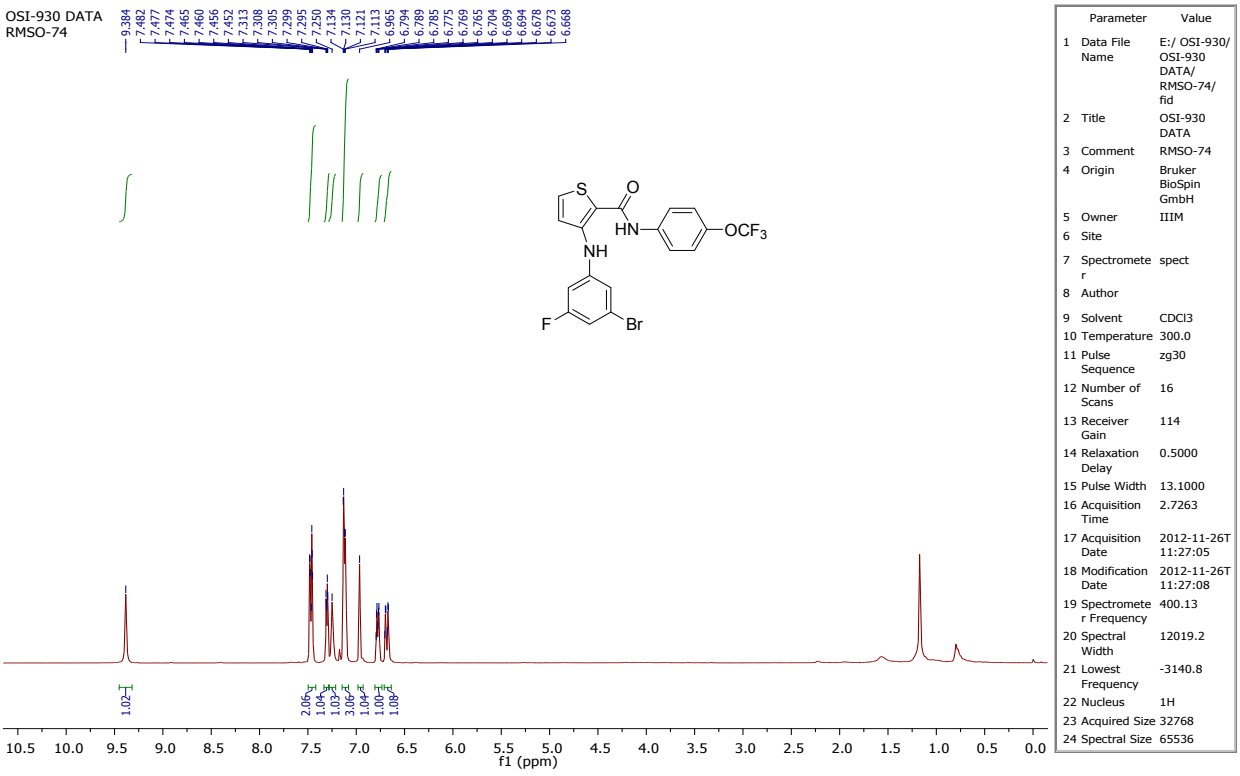


*3-((3-Bromo-5-fluorophenyl)amino)-N-(4-(trifluoromethoxy)phenyl)thiophene-2-carboxamide (**1g**).*



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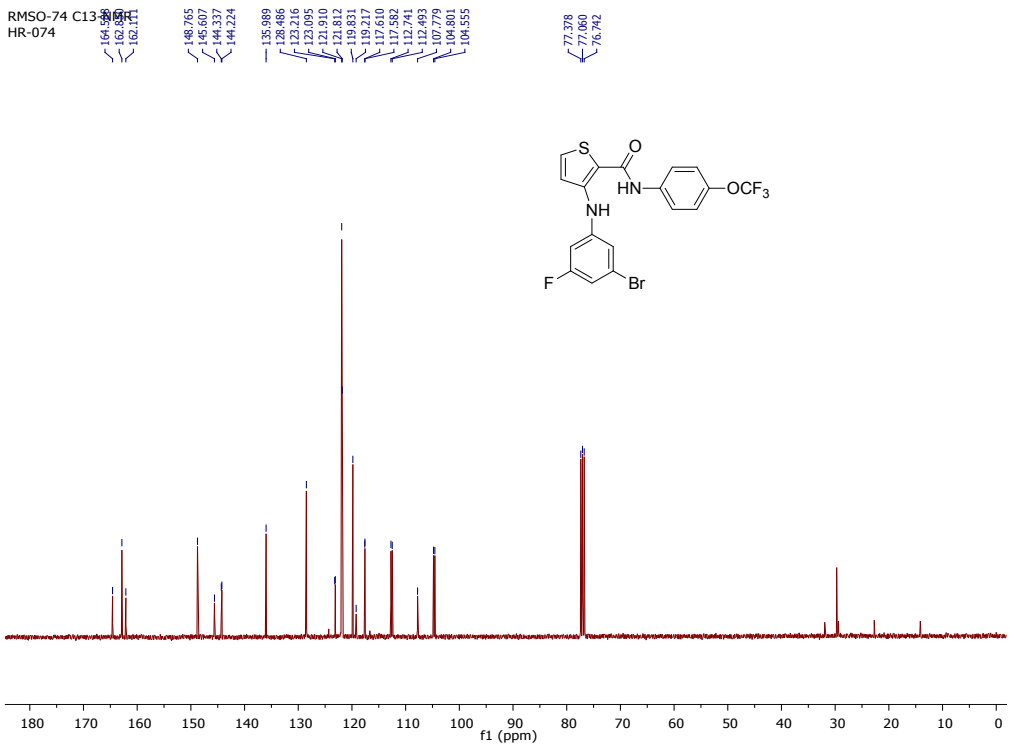
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	114
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2012-11-26T 11:27:05
18	Modification Date	2012-11-26T 11:27:08
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3140.8
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



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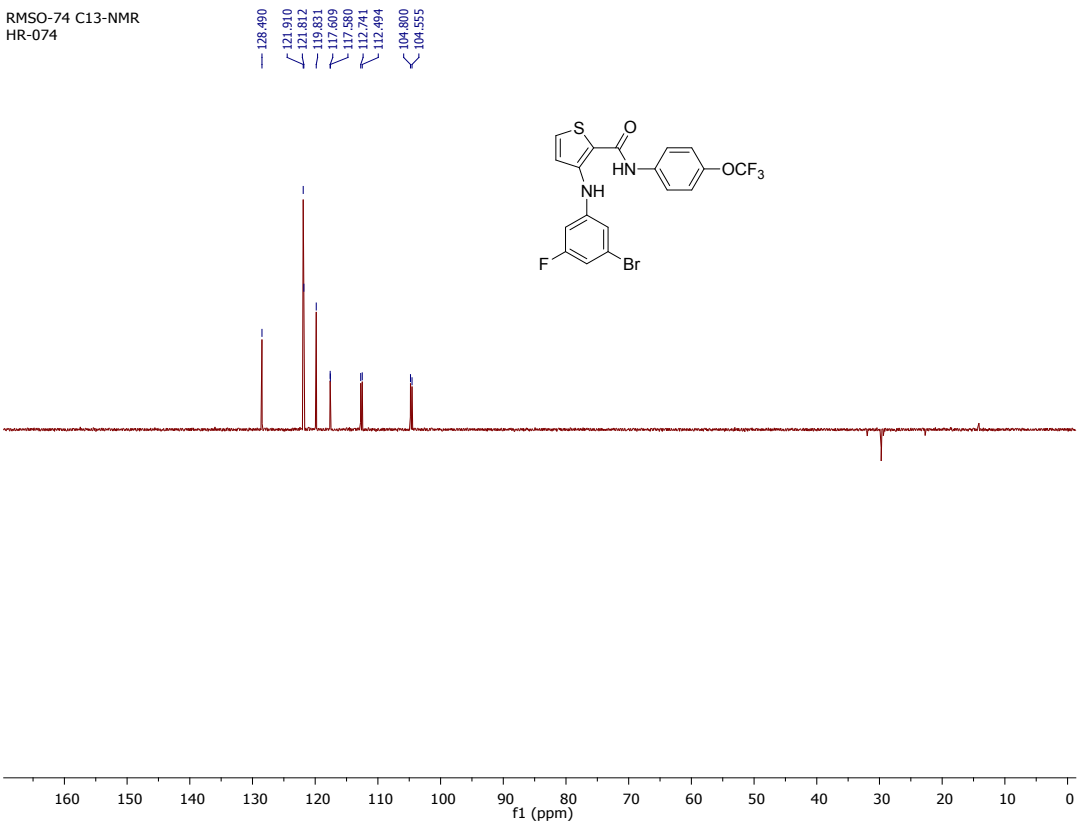
2	Title	RMSO-74 C13-NMR
3	Comment	HR-074
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Number of Scans	404
13	Receiver Gain	128
14	Relaxation Delay	1.0000
15	Pulse Width	9.2000
16	Acquisition Time	1.2976
17	Acquisition Date	2013-02-19T 15:16:19
18	Modification Date	2013-02-20T 12:52:40
19	Spectrometer Frequency	100.61
20	Spectral Width	25252.5
21	Lowest Frequency	-2565.5
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



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1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-74 C13-NMR/ 35/ fid
2	Title	RMSO-74 C13-NMR
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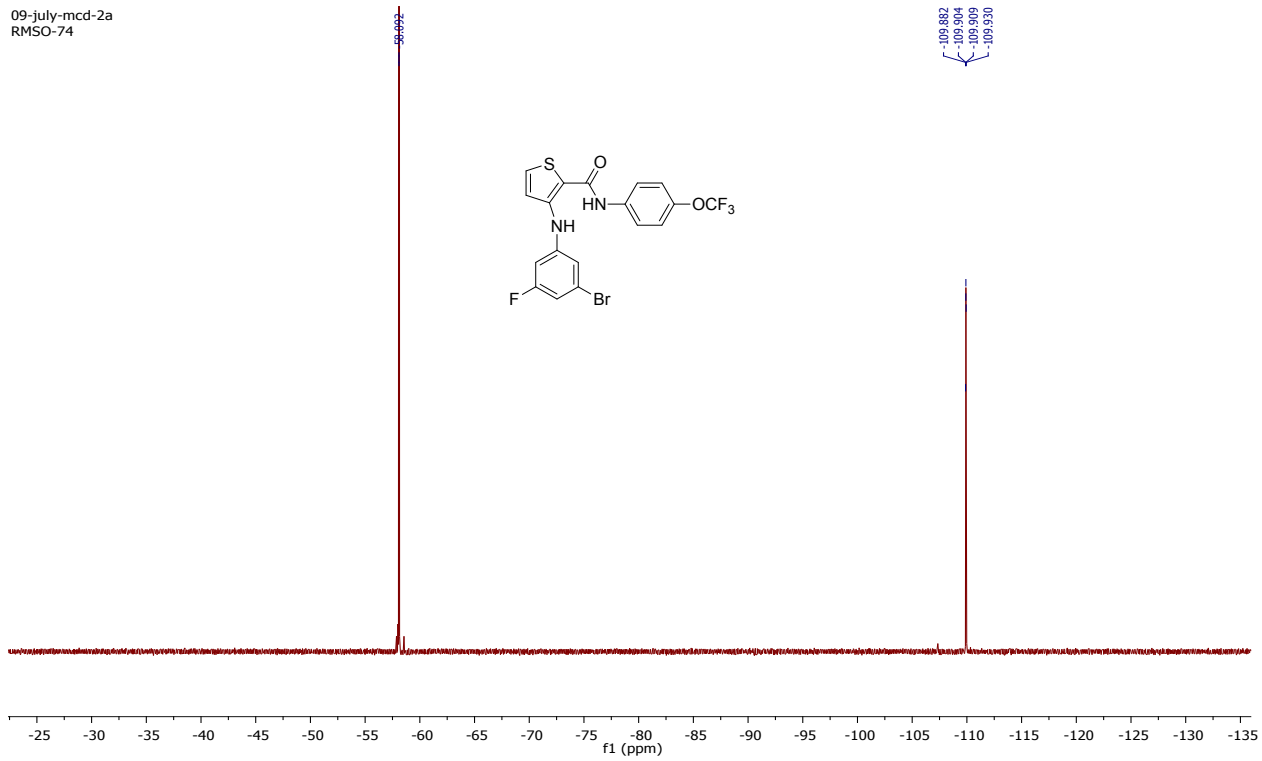
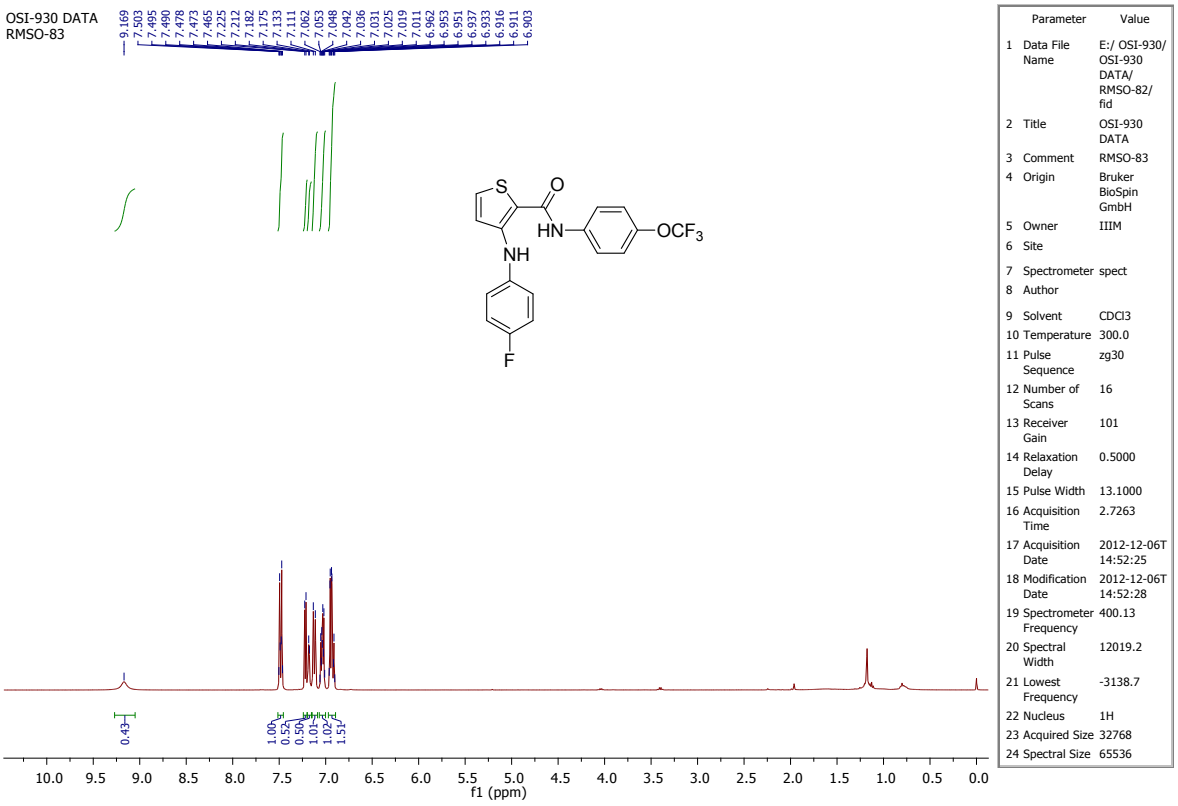
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	dept135
12	Number of Scans	250
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	9.2000
16	Acquisition Time	1.2976
17	Acquisition Date	2013-02-19 T15:30:56
18	Modification Date	2013-02-20 T12:52:40
19	Spectrometer Frequency	100.61
20	Spectral Width	25252.5
21	Lowest Frequency	-2565.5
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



*3-((4-Fluorophenyl)amino)-N-(4-(trifluoromethoxy)phenyl)thiophene-2-carboxamide (**1h**).*



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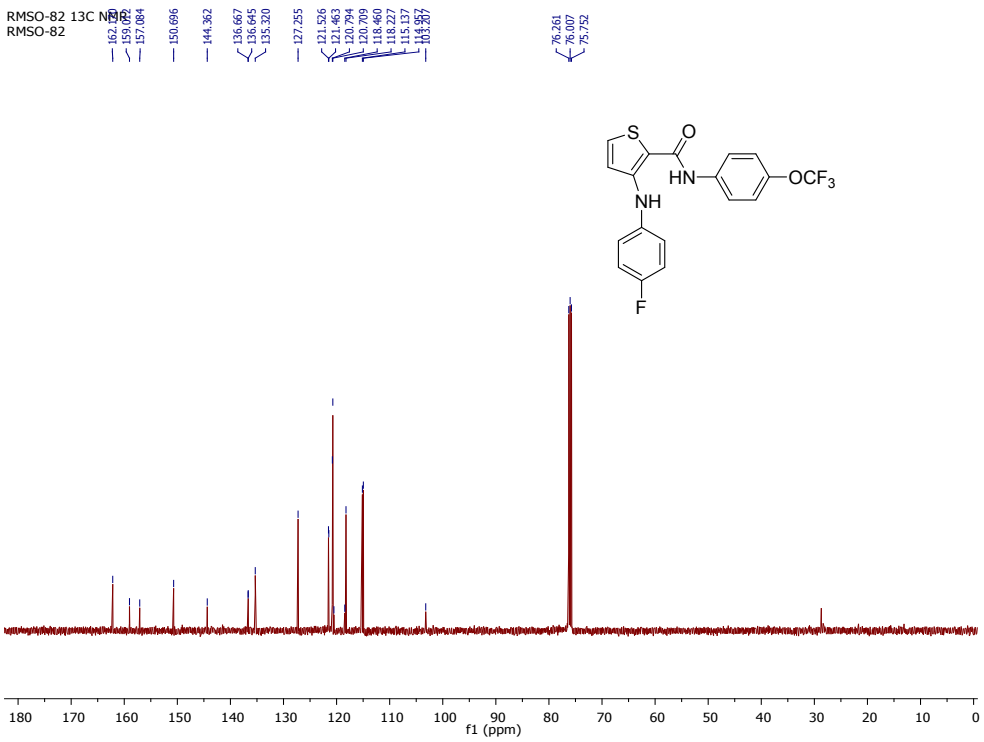
3	Comment	RMSO-83
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	101
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2012-12-06T 14:52:25
18	Modification Date	2012-12-06T 14:52:28
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3138.7
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



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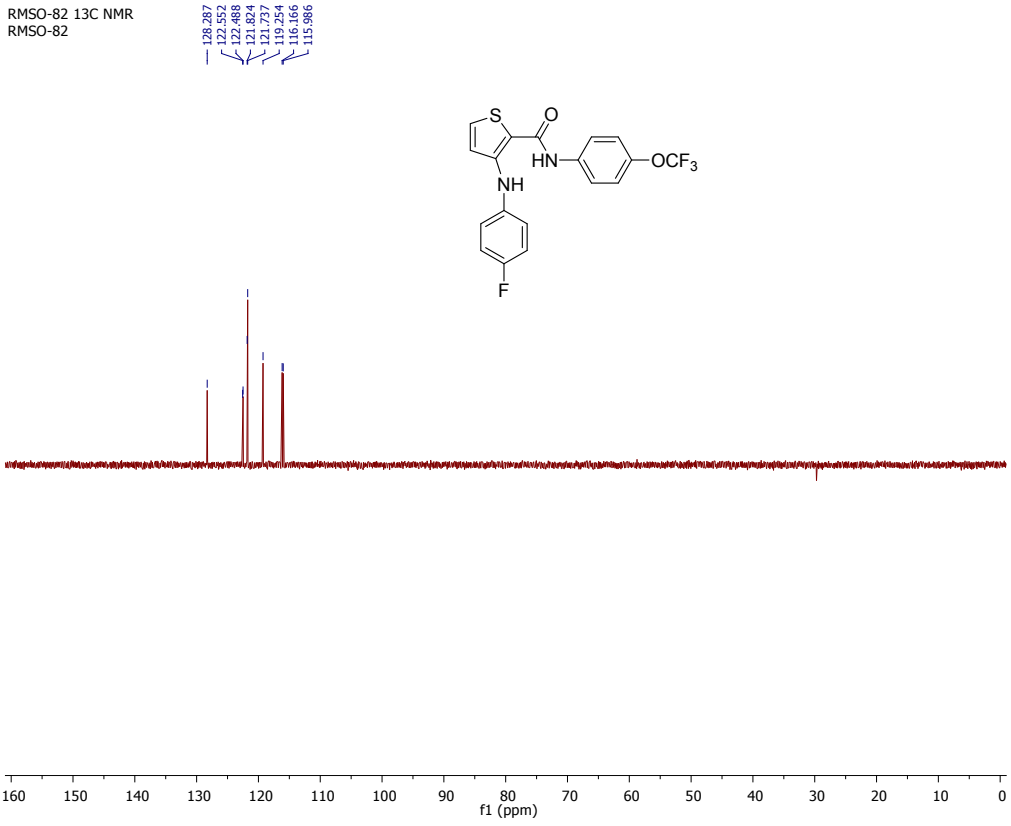
2	Title	RMSO-82 13C NMR
3	Comment	RMSO-82
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	685.3
11	Pulse Sequence	zgpg30
12	Number of Scans	800
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2012-12-28T 16:02:04
18	Modification Date	2012-12-28T 16:37:54
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3277.3
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



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3	Comment	RMSO-82
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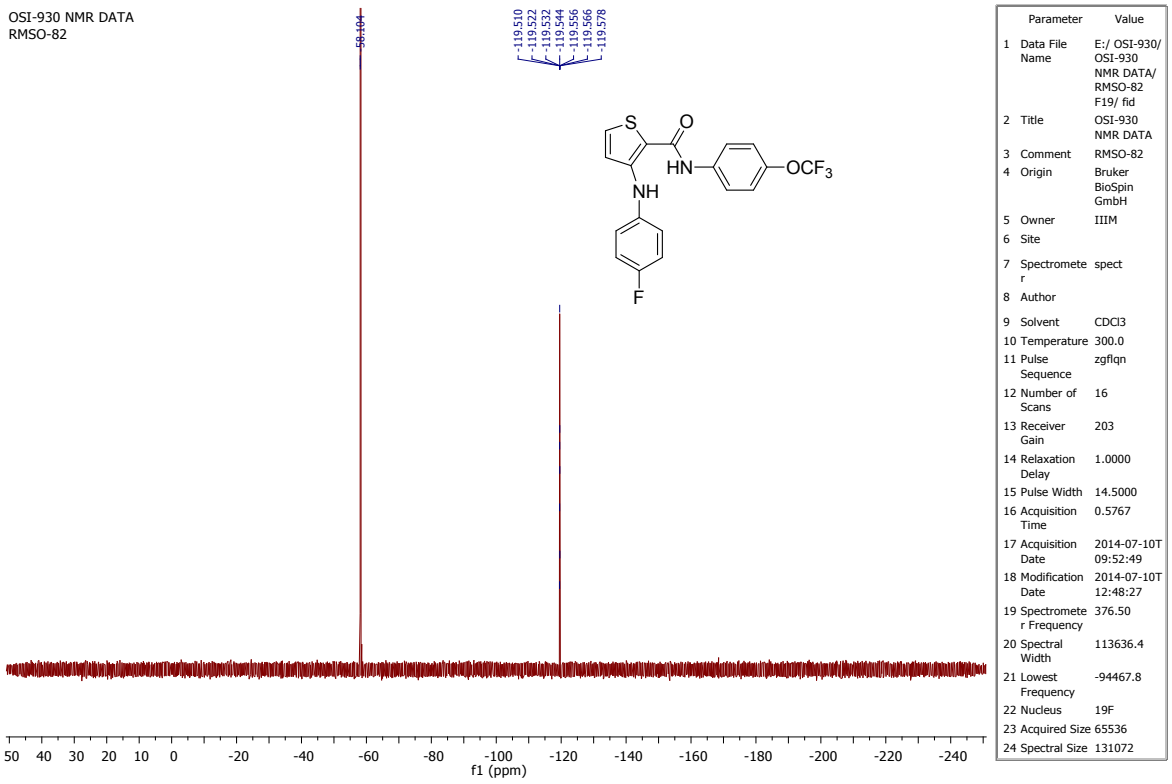
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	685.4
11	Pulse Sequence	dept135
12	Number of Scans	400
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2012-12-28T1 6:23:13
18	Modification Date	2012-12-28T1 6:45:36
19	Spectrometer Frequency	125.76
20	Spectral Width	30030.0
21	Lowest Frequency	-2439.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



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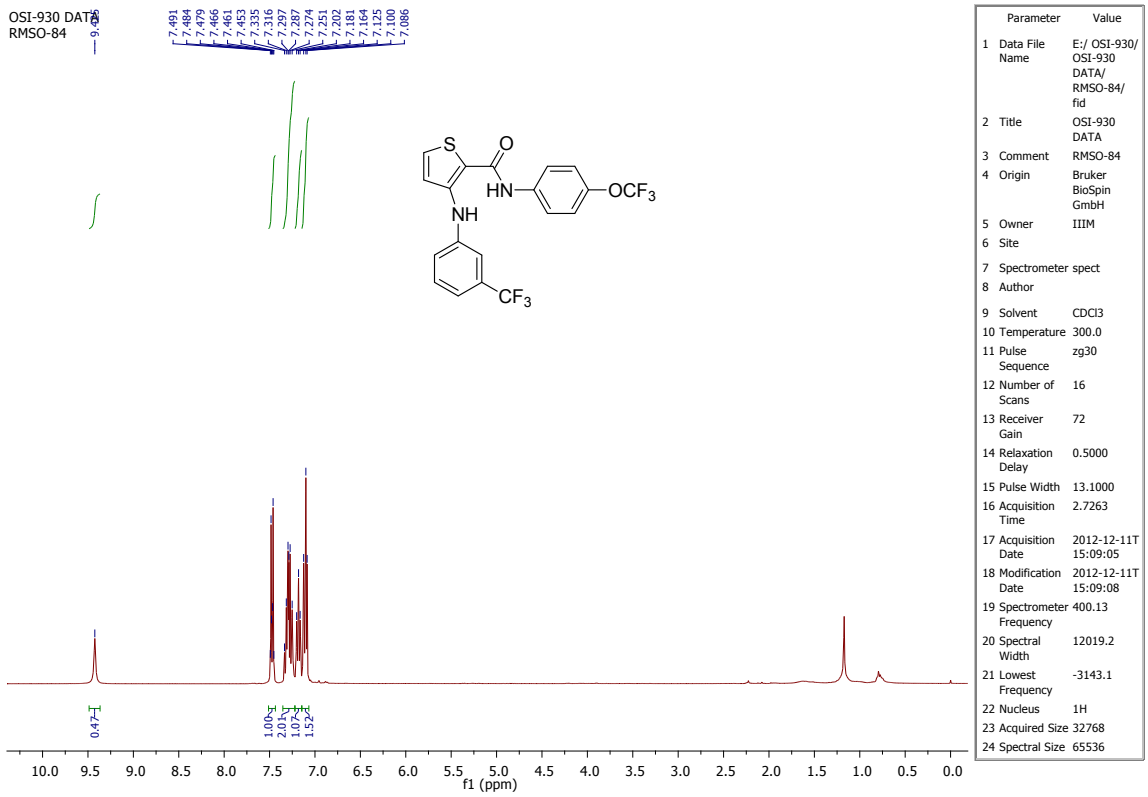
2	Title	OSI-930 NMR DATA
3	Comment	RMSO-82
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgflqn
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	14.5000
16	Acquisition Time	0.5767
17	Acquisition Date	2014-07-10T 09:52:49
18	Modification Date	2014-07-10T 12:48:27
19	Spectrometer Frequency	376.50
20	Spectral Width	113636.4
21	Lowest Frequency	-94467.8
22	Nucleus	19F
23	Acquired Size	65536
24	Spectral Size	131072

*N-(4-(Trifluoromethoxy)phenyl)-3-((3-(trifluoromethyl)phenyl)amino)thiophene-2-carboxamide (**1i**).*



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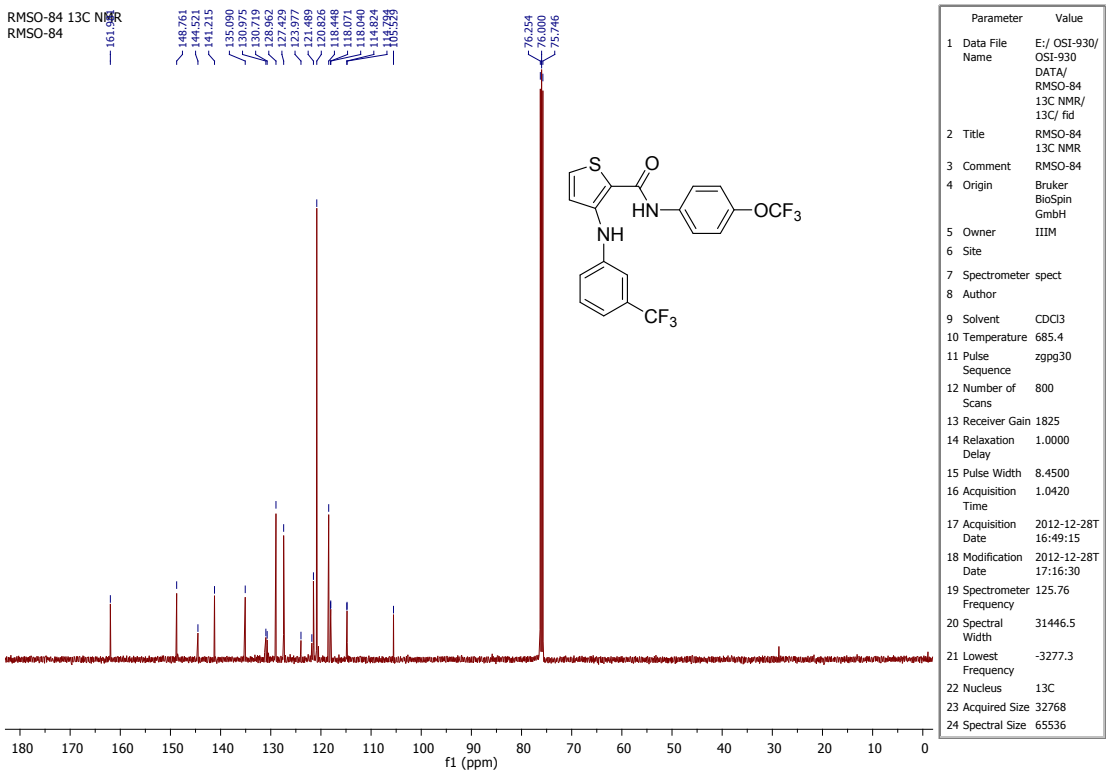
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	72
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2012-12-11T 15:09:05
18	Modification Date	2012-12-11T 15:09:08
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3143.1
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



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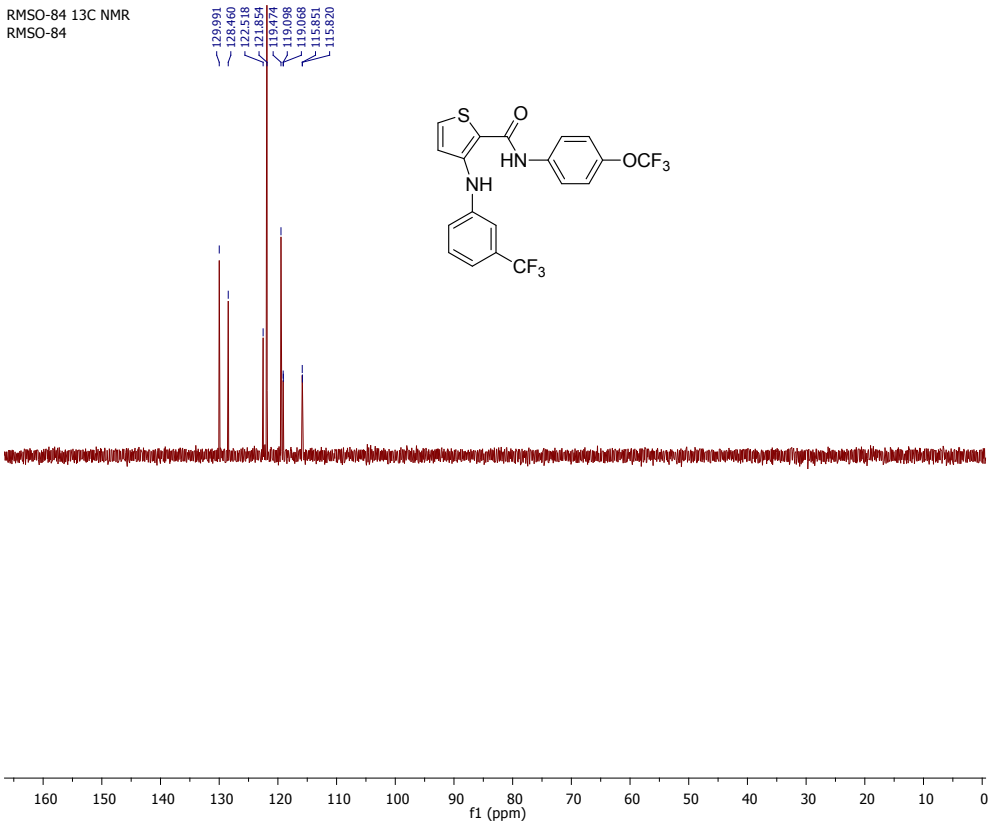
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	685.4
11	Pulse Sequence	zgpg30
12	Number of Scans	800
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2012-12-28T 16:49:15
18	Modification Date	2012-12-28T 17:16:30
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3277.3
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



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3	Comment	RMSO-84
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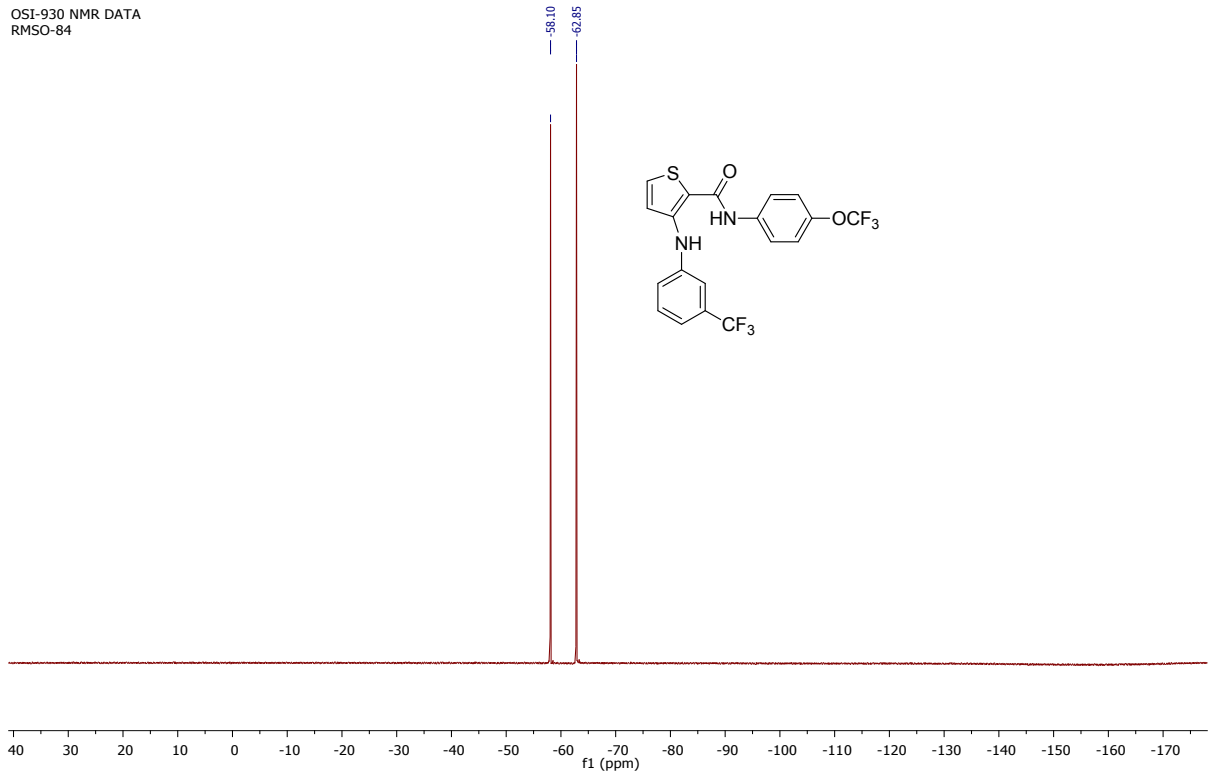
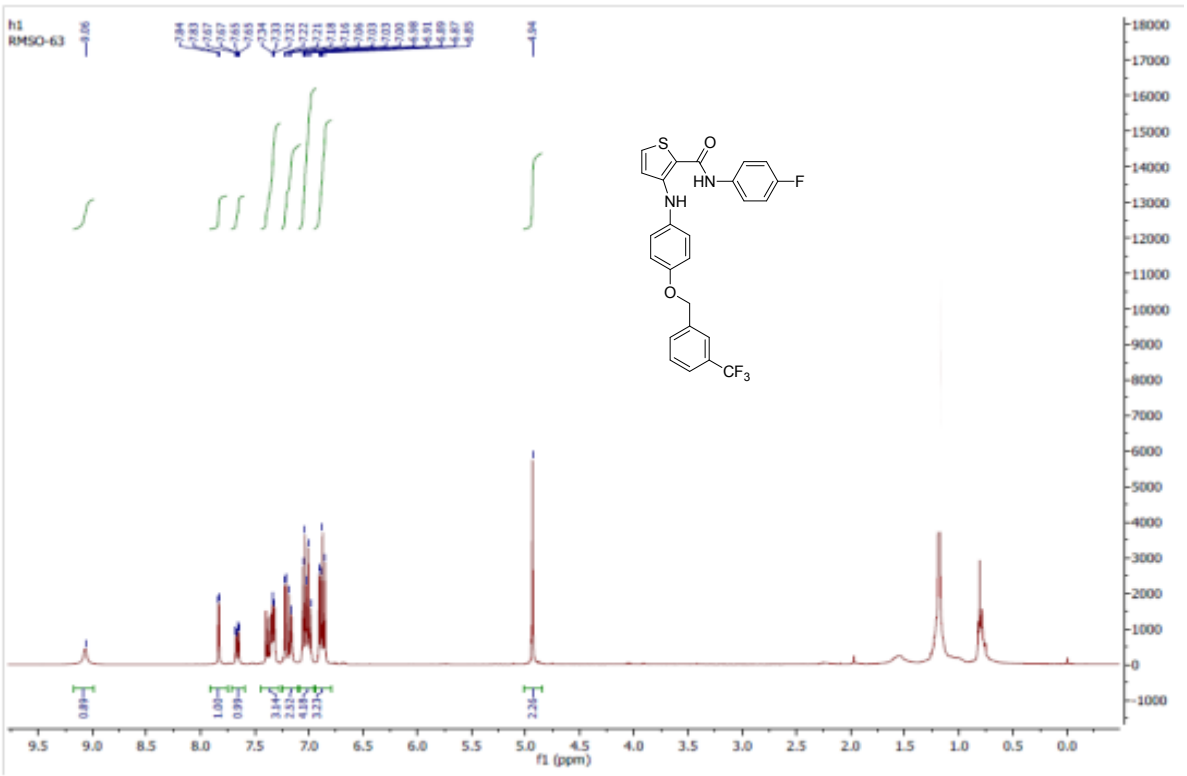
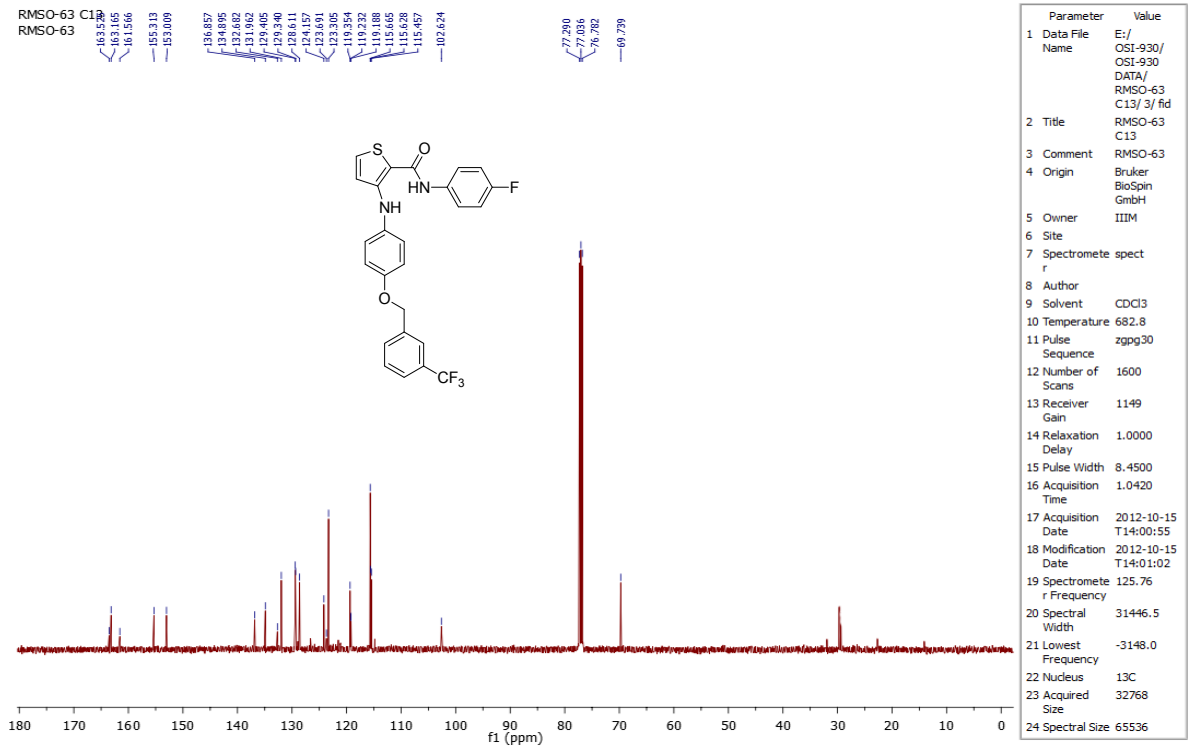
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	685.5
11	Pulse Sequence	dept135
12	Number of Scans	400
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2012-12-28T1 7:21:15
18	Modification Date	2012-12-28T1 7:26:14
19	Spectrometer Frequency	125.76
20	Spectral Width	30030.0
21	Lowest Frequency	-2439.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



N-(4-Fluorophenyl)-3-((4-((3-(trifluoromethyl)benzyl)oxy)phenyl)amino)thiophene-2-carboxamide ***(1j).***





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2	Title	RMSO-63 C13
3	Comment	RMSO-63
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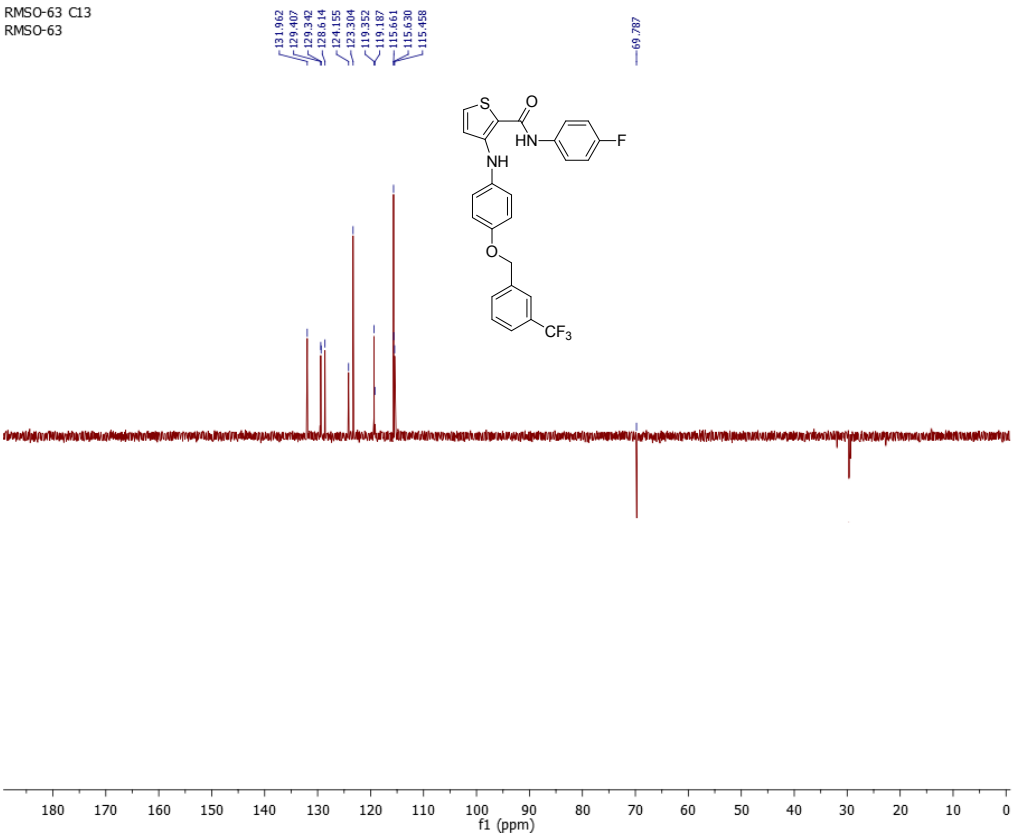
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	682.8
11	Pulse Sequence	zgpg30
12	Number of Scans	1600
13	Receiver Gain	1149
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2012-10-15 T14:00:55
18	Modification Date	2012-10-15 T14:01:02
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3148.0
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-63 C13/ 4/ fid
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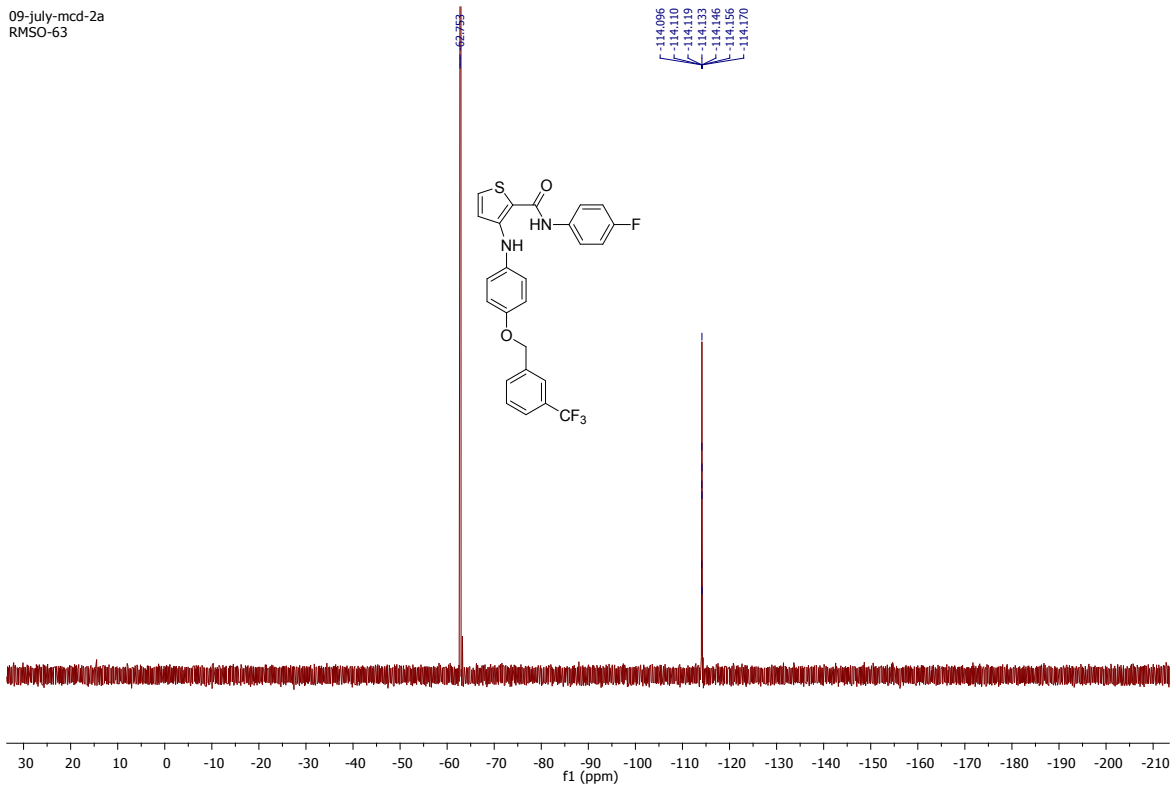
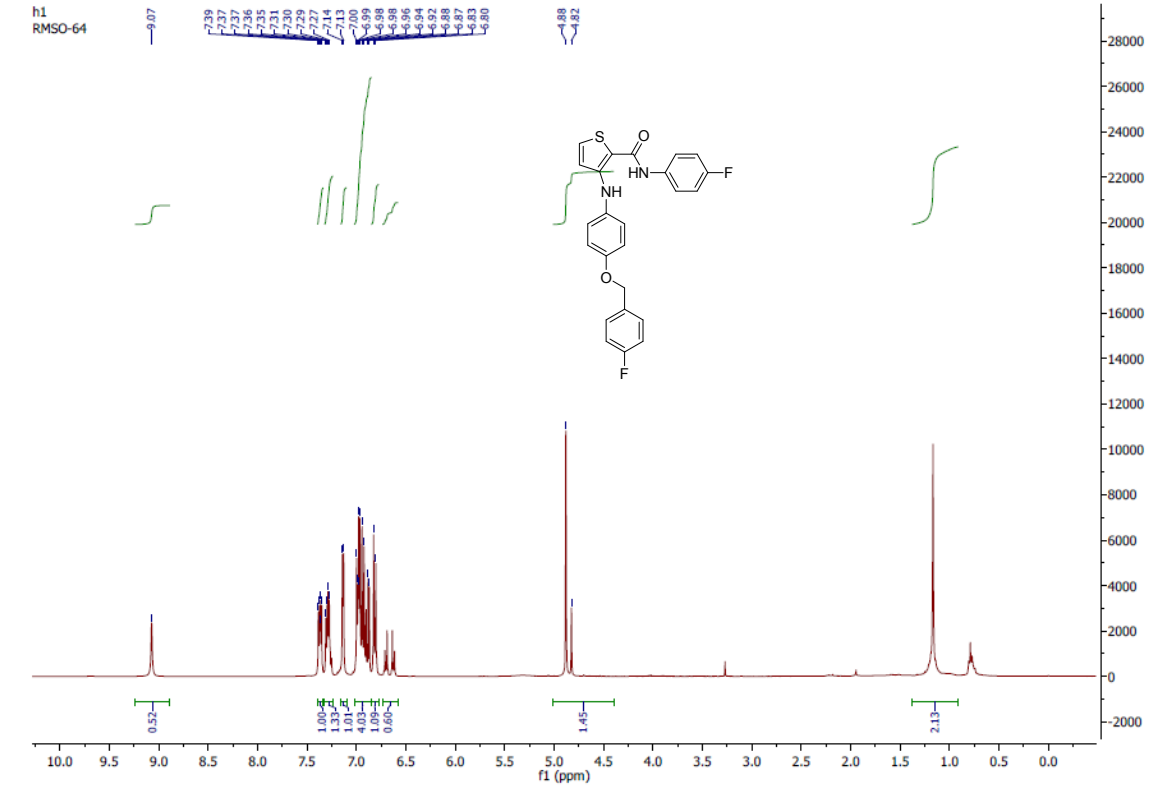
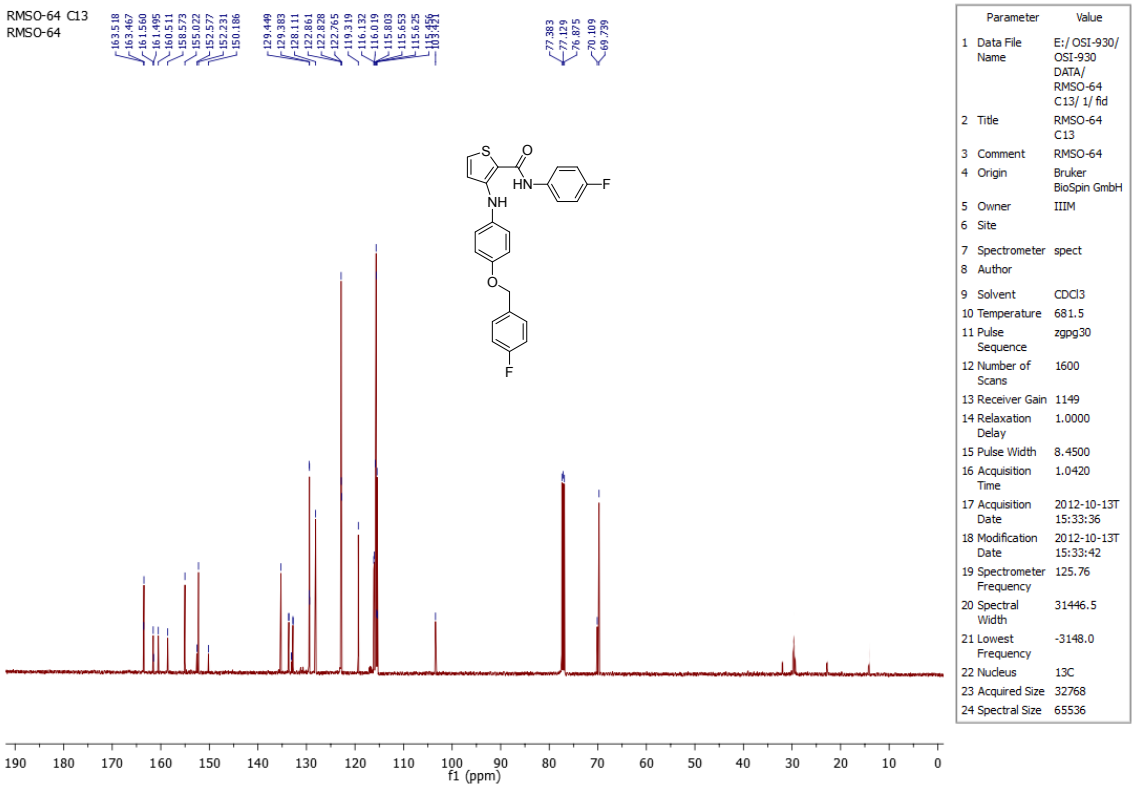
3	Comment	RMSO-63
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	682.6
11	Pulse Sequence	dept135
12	Number of Scans	800
13	Receiver Gain	23170
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2012-10-15T 14:29:06
18	Modification Date	2012-10-15T 14:29:12
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3148.0
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



*3-((4-((4-Fluorobenzyl)oxy)phenyl)amino)-N-(4-fluorophenyl)thiophene-2-carboxamide (**1k**).*





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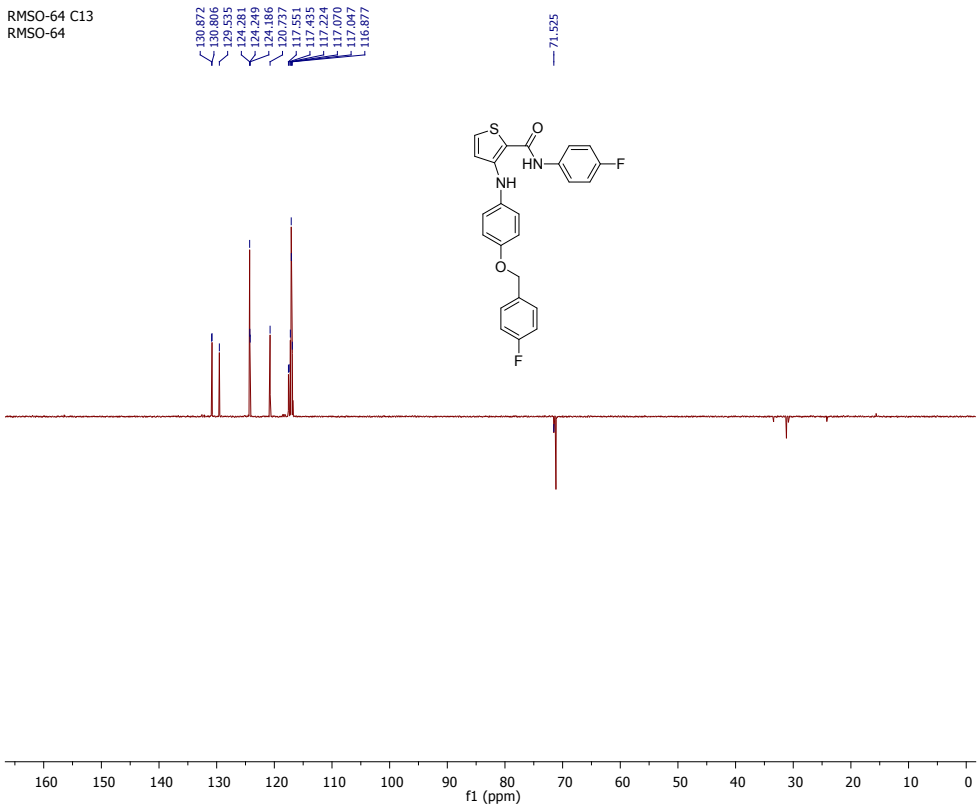
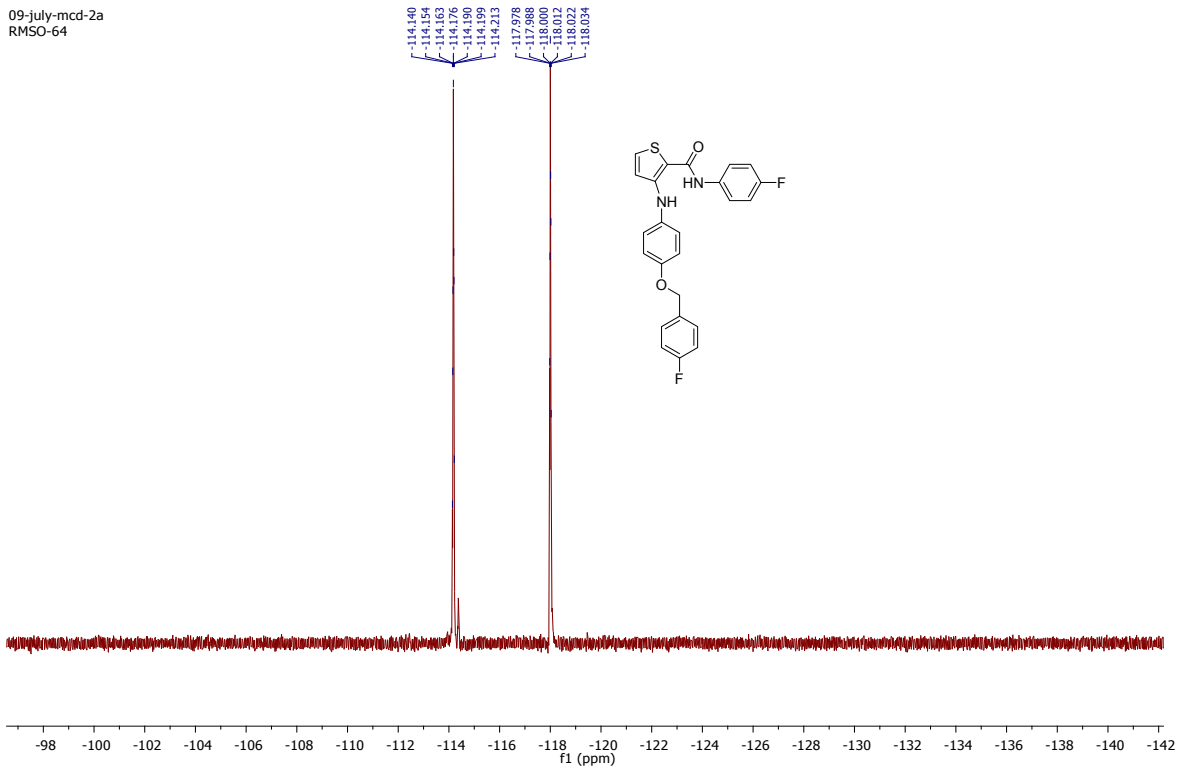
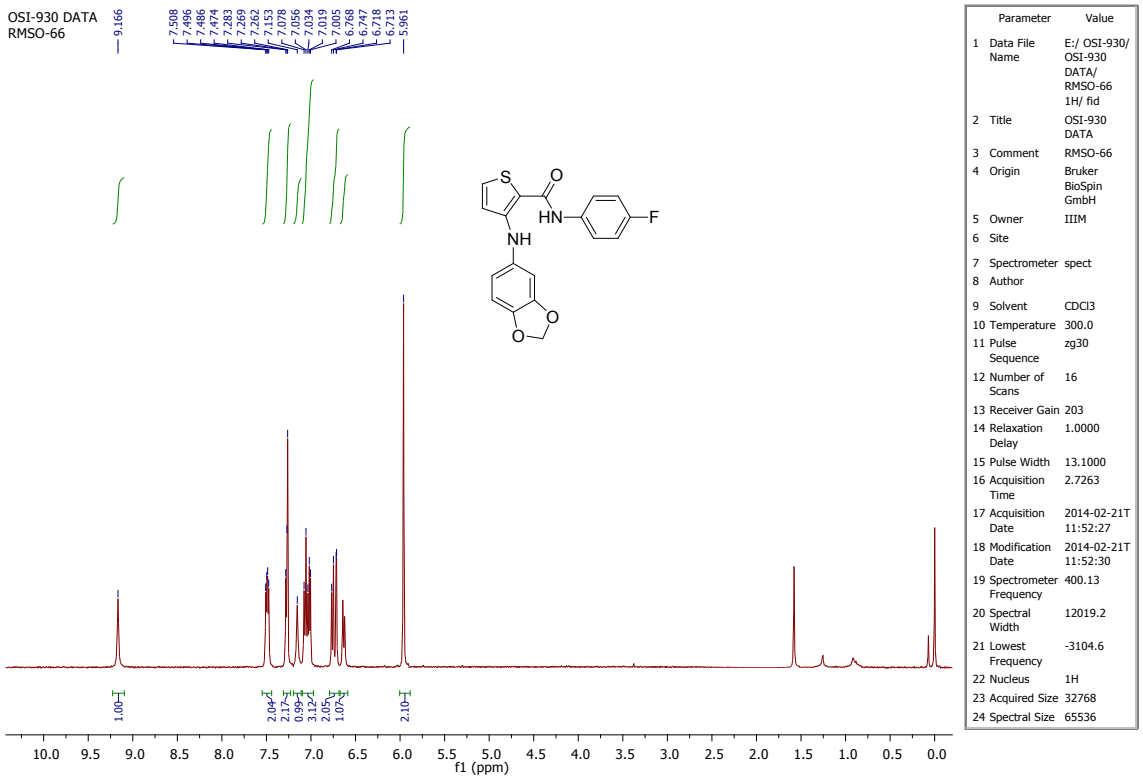
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-64 C13/ 1/ fid
2	Title	RMSO-64 C13
3	Comment	RMSO-64
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	681.5
11	Pulse Sequence	zgpg30
12	Number of Scans	1600
13	Receiver Gain	1149
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2012-10-13T 15:33:36
18	Modification Date	2012-10-13T 15:33:42
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3148.0
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



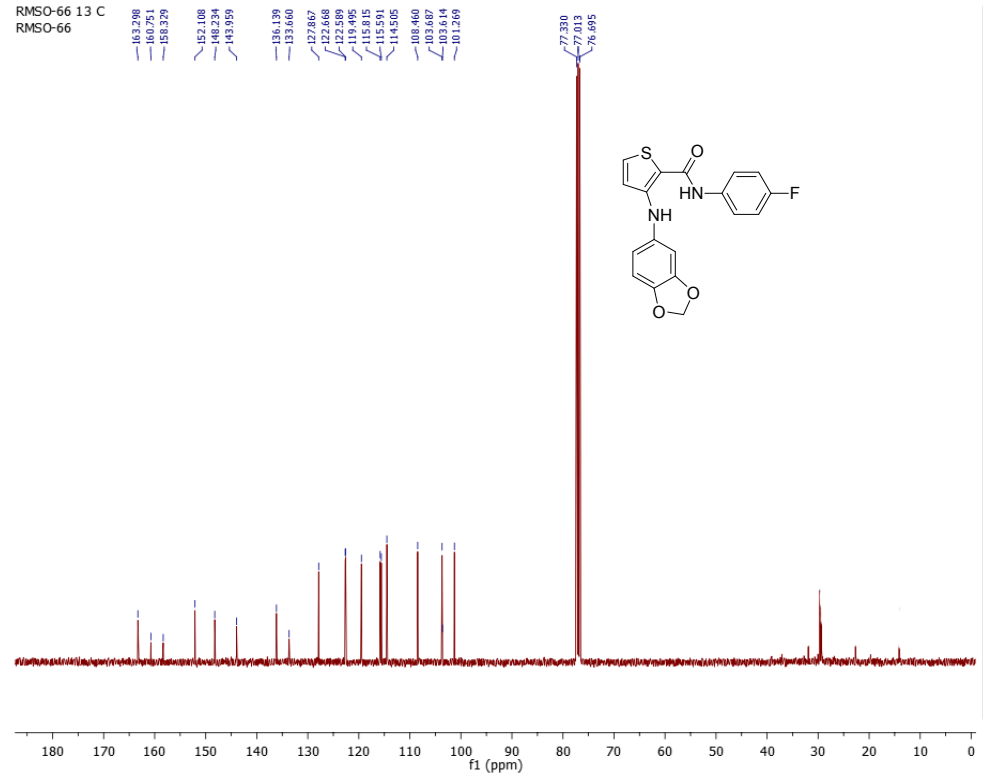
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-64 C13/ 2/ fid
2	Title	RMSO-64 C13
3	Comment	RMSO-64
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	681.5
11	Pulse Sequence	dept135
12	Number of Scans	800
13	Receiver Gain	23170
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2012-10-13T 16:01:47
18	Modification Date	2012-10-13T 16:01:54
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-2969.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



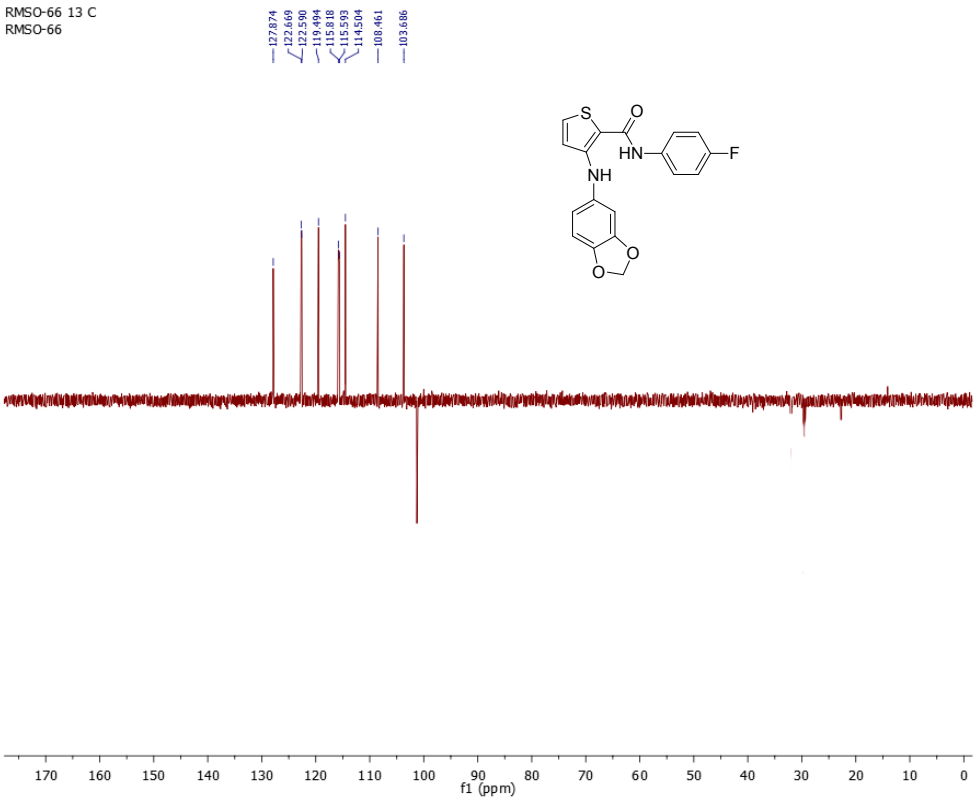
*3-(Benzo[d][1,3]dioxol-5-ylamino)-N-(4-fluorophenyl)thiophene-2-carboxamide (**11**).*



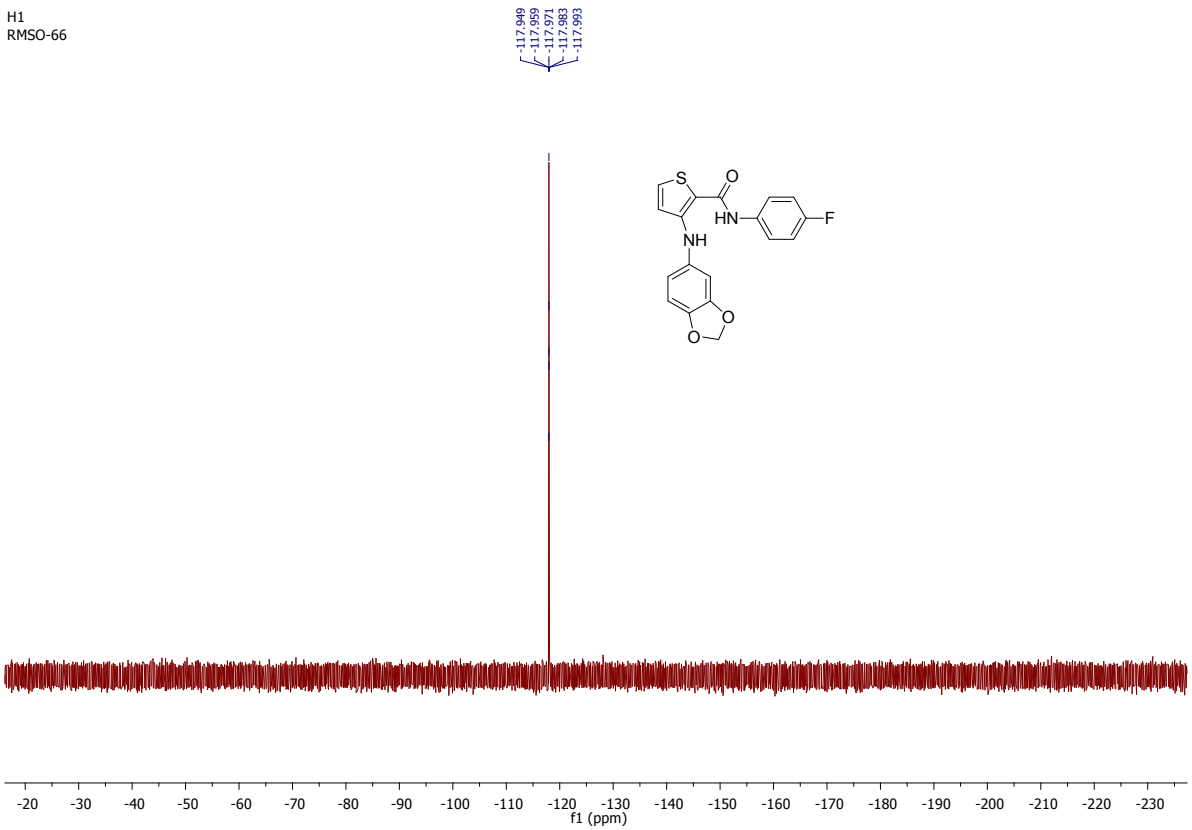
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-66 1H/ fid
2	Title	OSI-930 DATA
3	Comment	RMSO-66
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2014-02-21T 11:52:27
18	Modification Date	2014-02-21T 11:52:30
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3104.6
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



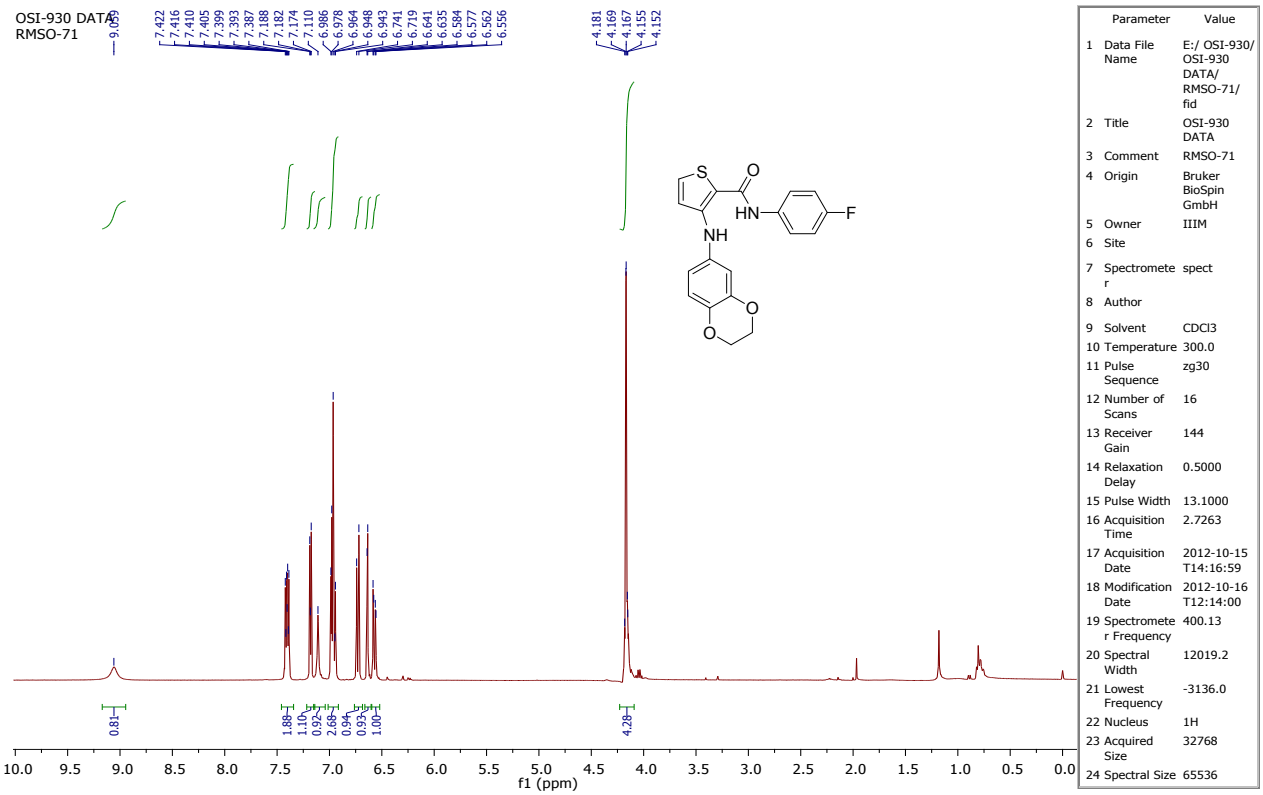
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-66 13 C/ 12/ fid
2	Title	RMSO-66 13 C
3	Comment	RMSO-66
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zgpg30
12	Number of Scans	1200
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	9.2000
16	Acquisition Time	1.2976
17	Acquisition Date	2012-10-15T 13:42:27
18	Modification Date	2012-10-16T 12:13:58
19	Spectrometer Frequency	100.61
20	Spectral Width	25252.5
21	Lowest Frequency	-2565.5
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



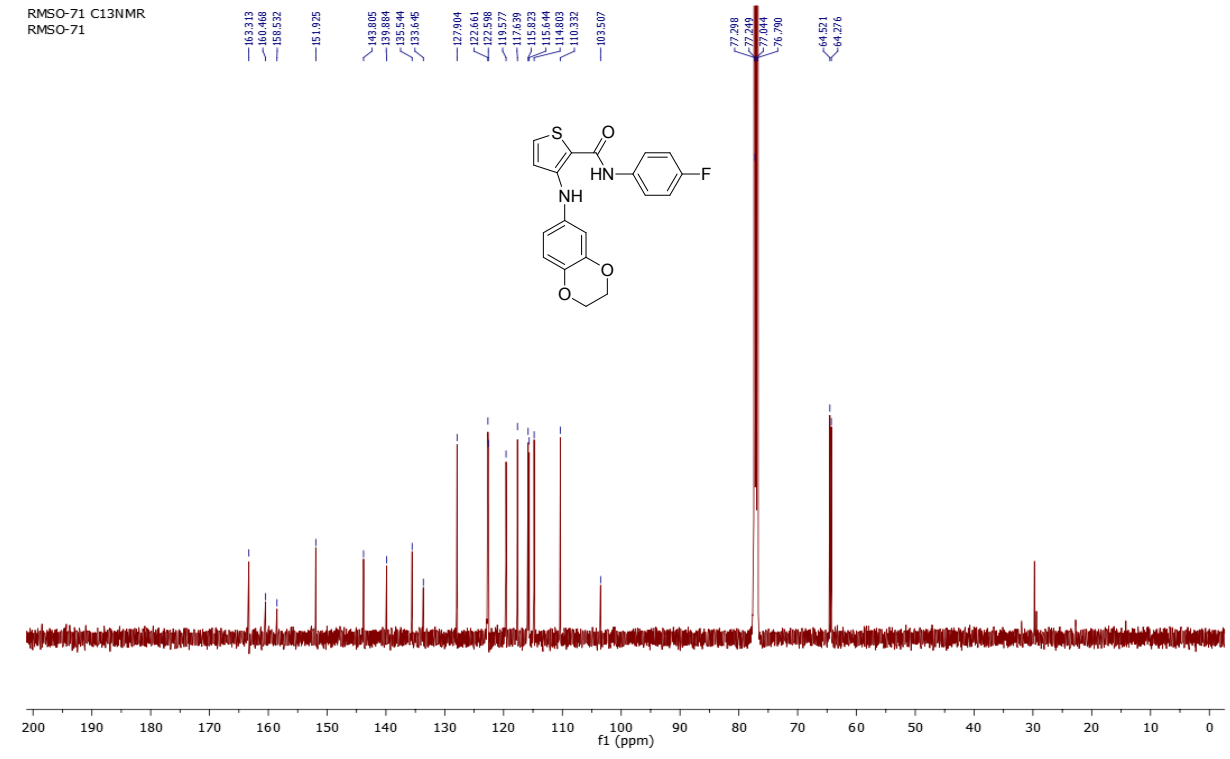
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-66 13 C/ 13/ fid
2	Title	RMSO-66 13 C
3	Comment	RMSO-66
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	dept135
12	Number of Scans	600
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	9.2000
16	Acquisition Time	1.2976
17	Acquisition Date	2012-10-15T 14:06:08
18	Modification Date	2012-10-16T 12:13:59
19	Spectrometer Frequency	100.61
20	Spectral Width	25252.5
21	Lowest Frequency	-2565.5
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

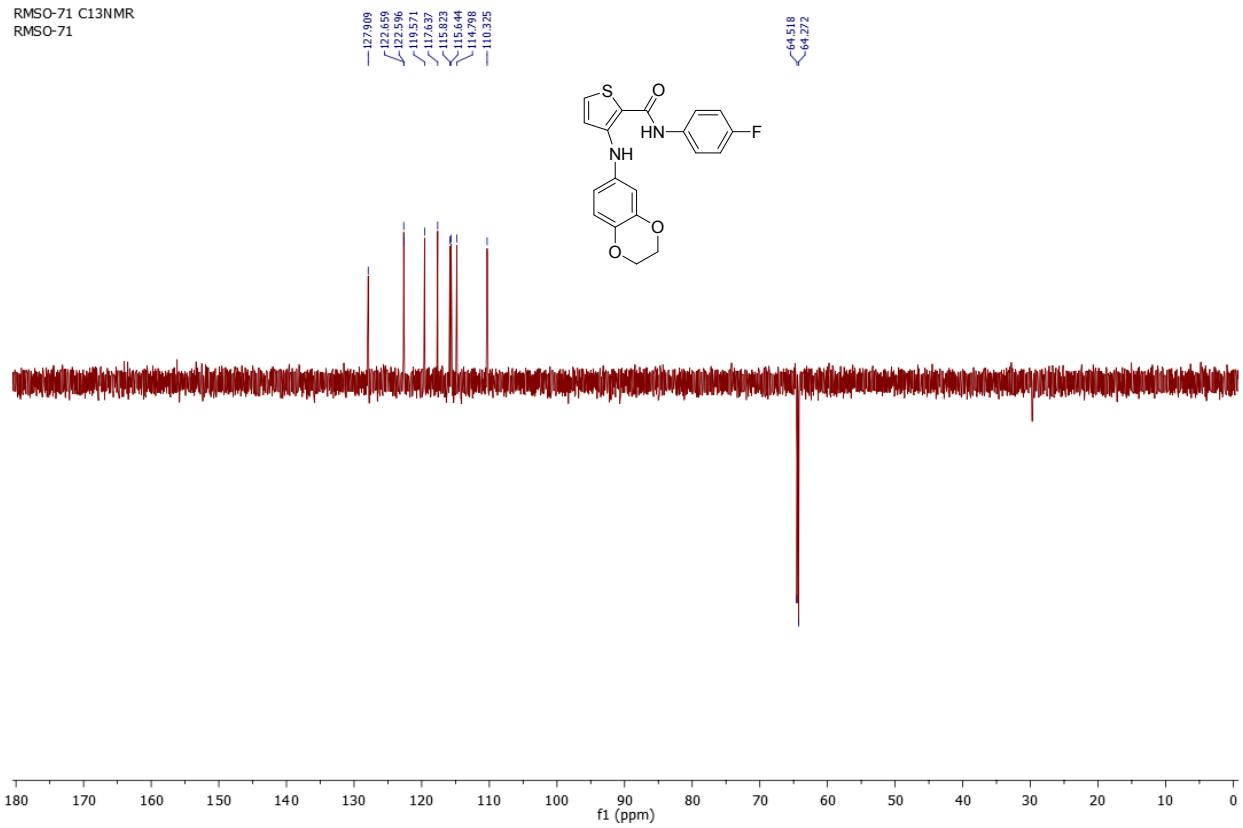


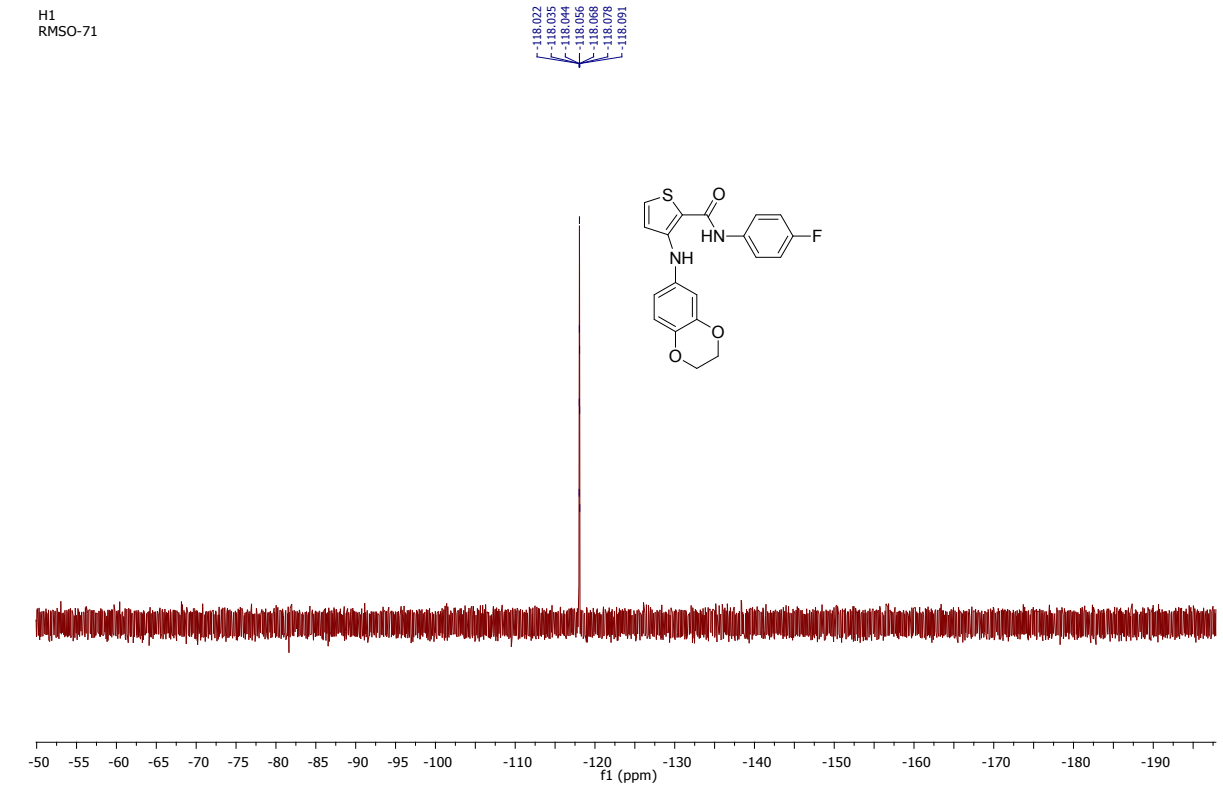
*3-((2,3-Dihydrobenzo[b][1,4]dioxin-6-yl)amino)-N-(4-fluorophenyl)thiophene-2-carboxamide (**1m**).*



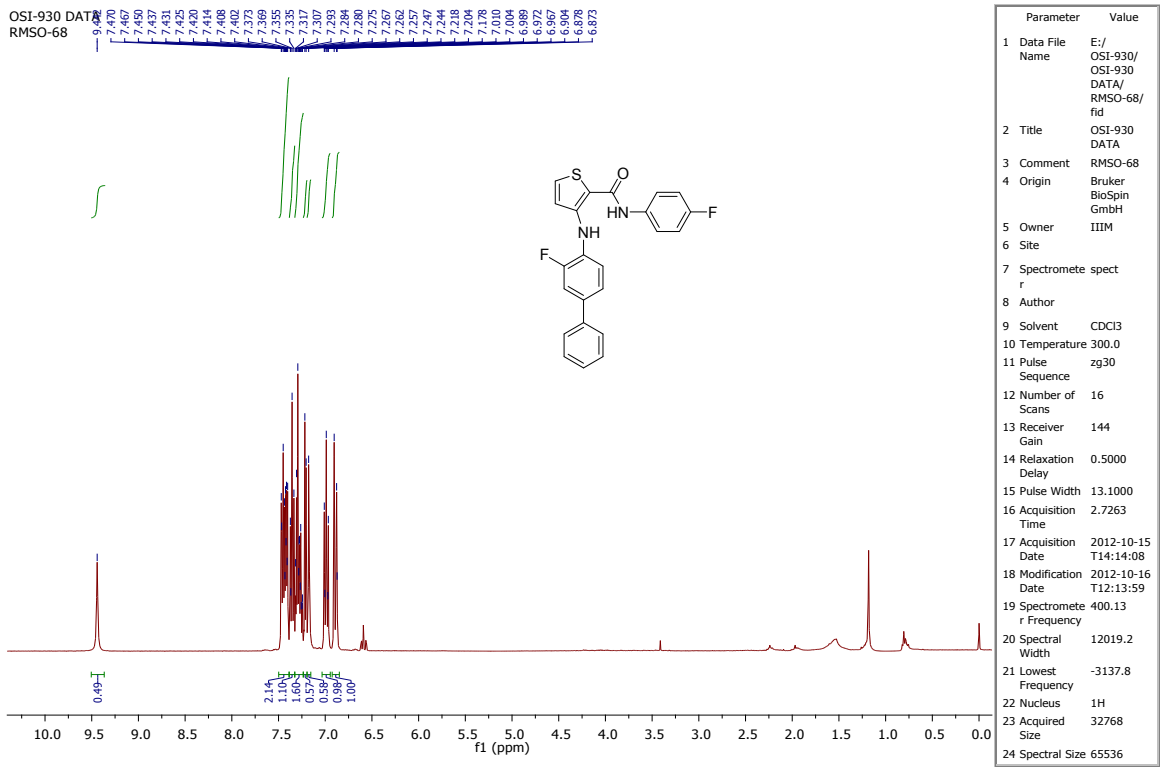
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-71/ fid
2	Title	OSI-930 DATA
3	Comment	RMSO-71
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	144
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2012-10-15 T14:16:59
18	Modification Date	2012-10-16 T12:14:00
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3136.0
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



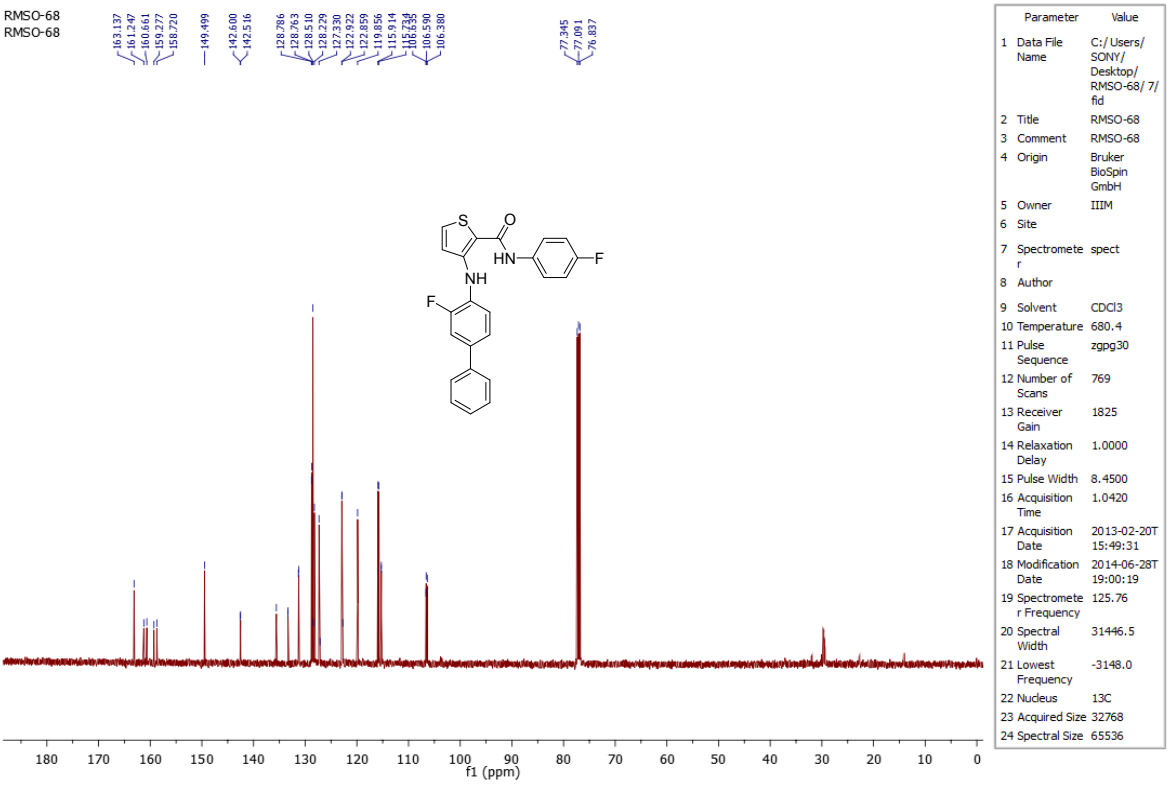

RMSO-71 C13NMR
RMSO-71
127.909
122.659
122.596
119.571
117.637
115.823
115.644
114.798
110.325
64.518
64.272
S
O
HN
F
NH
O
O
180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)


H1
RMSO-71
118.022
118.035
118.044
118.056
118.068
118.078
118.091
S
O
HN
F
NH
O
O
-50 -55 -60 -65 -70 -75 -80 -85 -90 -95 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190
f1 (ppm)

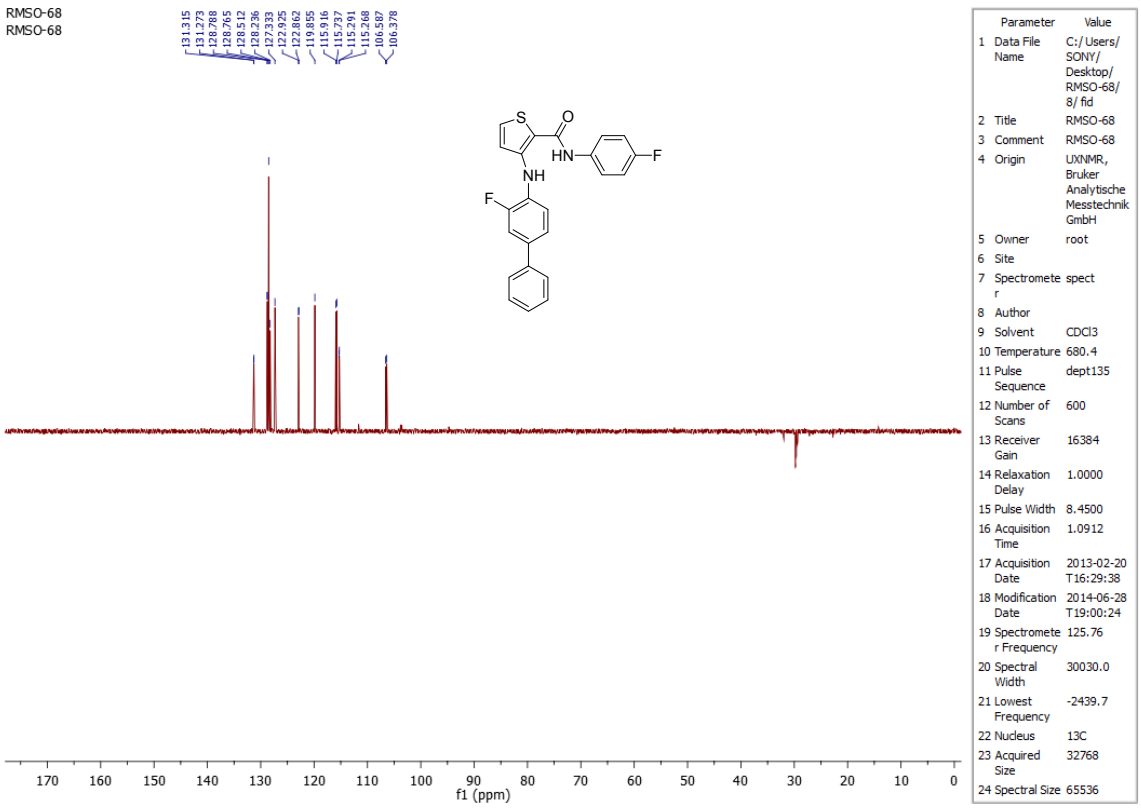
*3-((3-Fluoro-[1,1'-biphenyl]-4-yl)amino)-N-(4-fluorophenyl)thiophene-2-carboxamide (**1n**).*

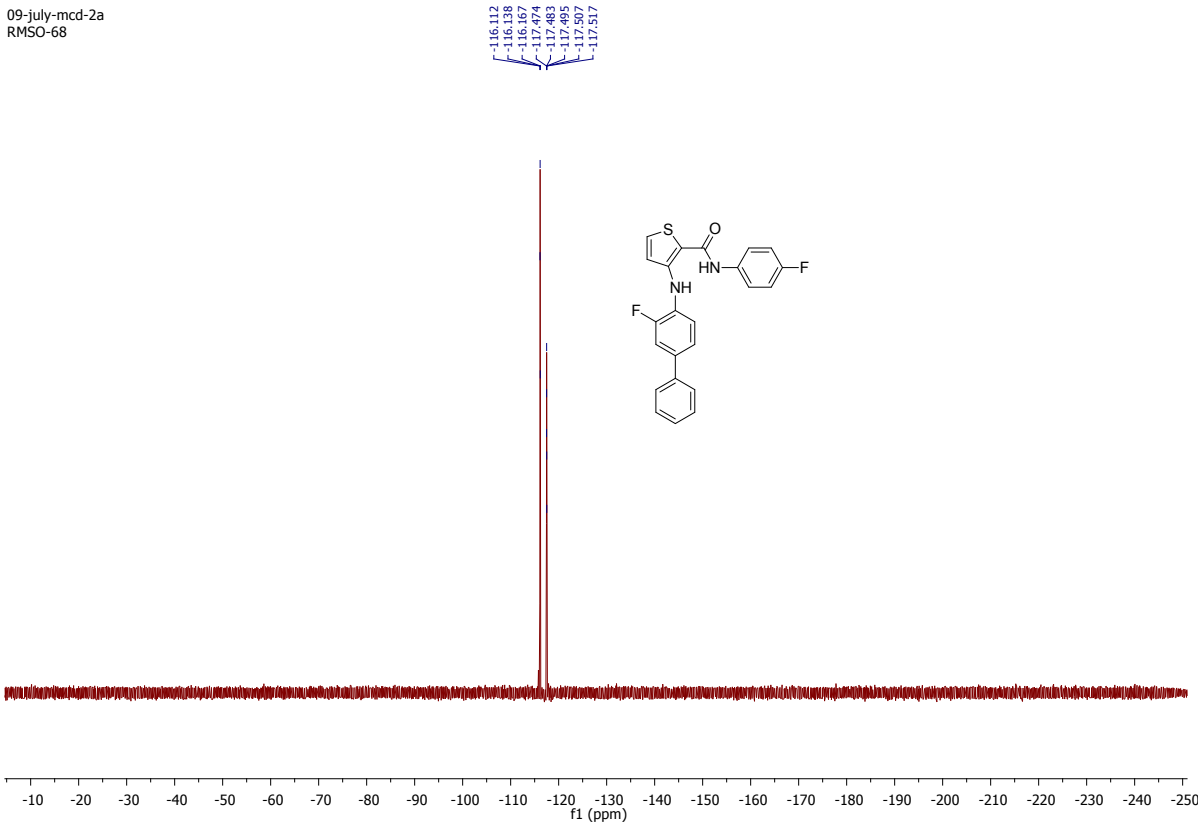


	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-68/ fid
2	Title	OSI-930 DATA
3	Comment	RMSO-68
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	144
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2012-10-15 T14:14:08
18	Modification Date	2012-10-16 T12:13:59
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3137.8
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

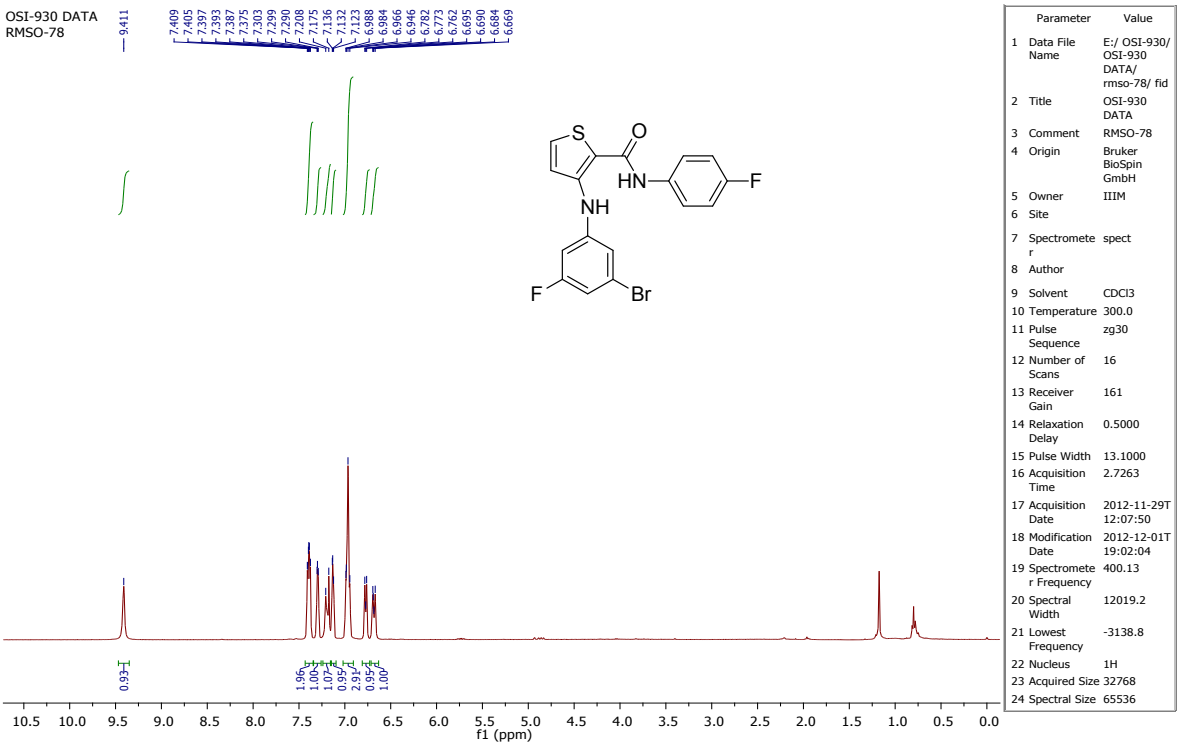


	Parameter	Value
1	Data File Name	C:/ Users/ SONY/ Desktop/ RMSO-68/ 7/ fid
2	Title	RMSO-68
3	Comment	RMSO-68
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	680.4
11	Pulse Sequence	zgpg30
12	Number of Scans	769
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2013-02-20T 15:49:31
18	Modification Date	2014-06-28T 19:00:19
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3148.0
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536

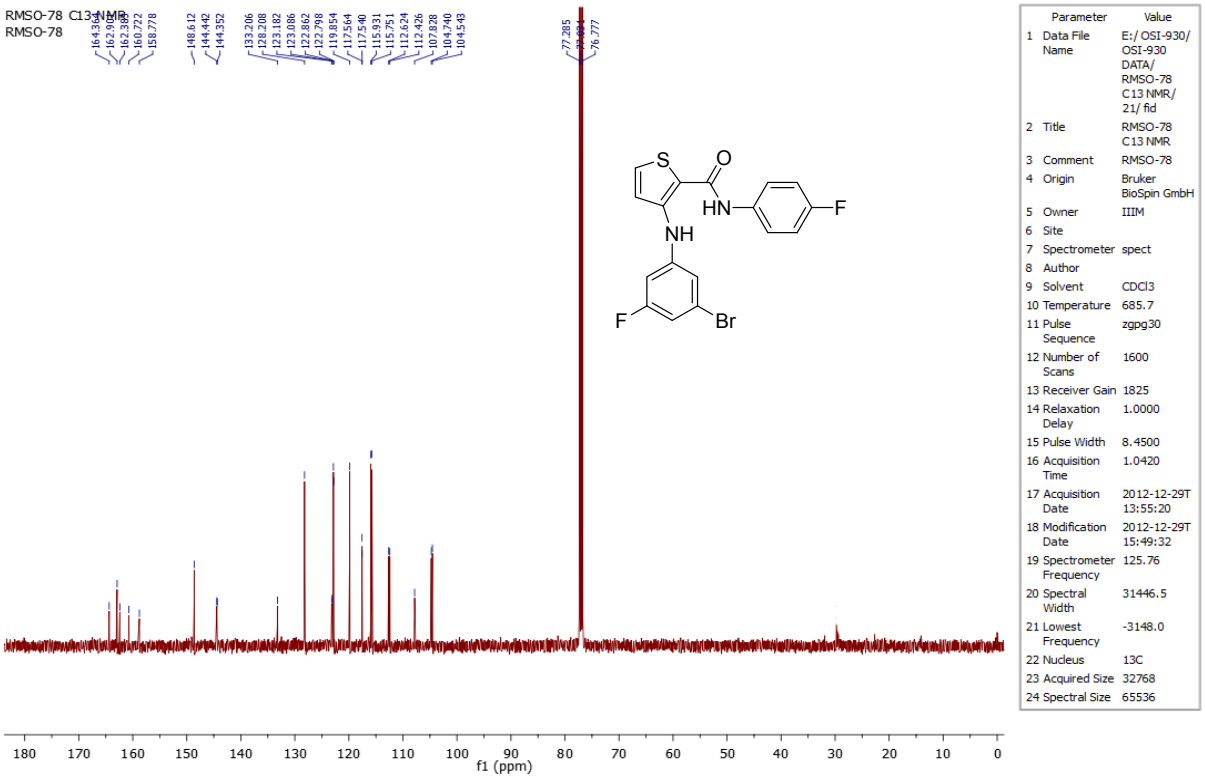

RMSO-68
RMSO-68
131.315
131.273
128.788
128.765
128.512
128.236
127.333
122.925
122.862
119.855
115.916
115.737
115.291
115.268
106.587
106.378
S
O
HN
F
NH
F
170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)
Parameter Value
1 Data File Name C:/Users/SONY/Desktop/RMSO-68/8/fid
2 Title RMSO-68
3 Comment RMSO-68
4 Origin UXNMR, Bruker Analytische Messtechnik GmbH
5 Owner root
6 Site
7 Spectrometer spect
8 Author
9 Solvent CDCl3
10 Temperature 680.4
11 Pulse Sequence dept135
12 Number of Scans 600
13 Receiver Gain 16384
14 Relaxation Delay 1.0000
15 Pulse Width 8.4500
16 Acquisition Time 1.0912
17 Acquisition Date 2013-02-20 T16:29:38
18 Modification Date 2014-06-28 T19:00:24
19 Spectrometer Frequency 125.76
20 Spectral Width 30030.0
21 Lowest Frequency -2439.7
22 Nucleus 13C
23 Acquired Size 32768
24 Spectral Size 65536


09-july-mcd-2a
RMSO-68
-116.112
-116.138
-116.167
-117.474
-117.483
-117.495
-117.507
-117.517
S
O
HN
F
NH
F
-10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250
f1 (ppm)

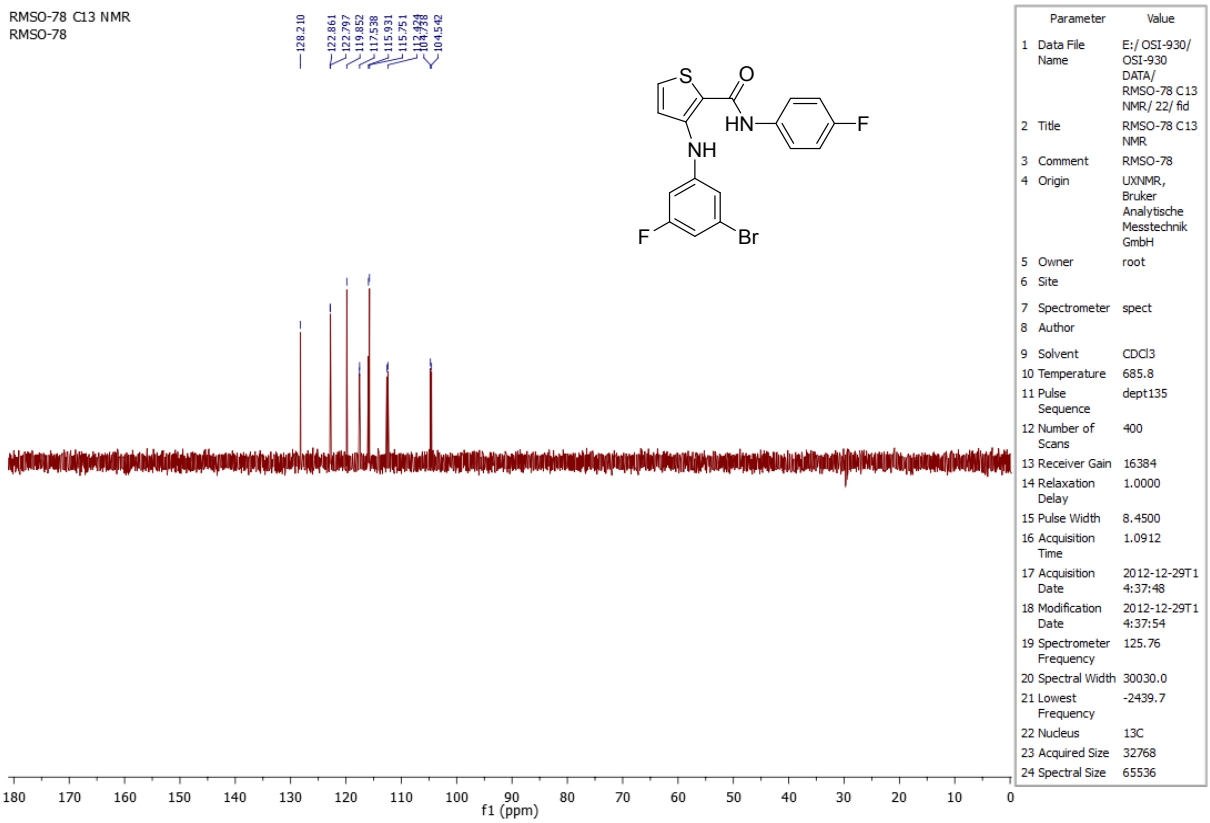
*3-((3-Bromo-5-fluorophenyl)amino)-N-(4-fluorophenyl)thiophene-2-carboxamide (**1o**).*



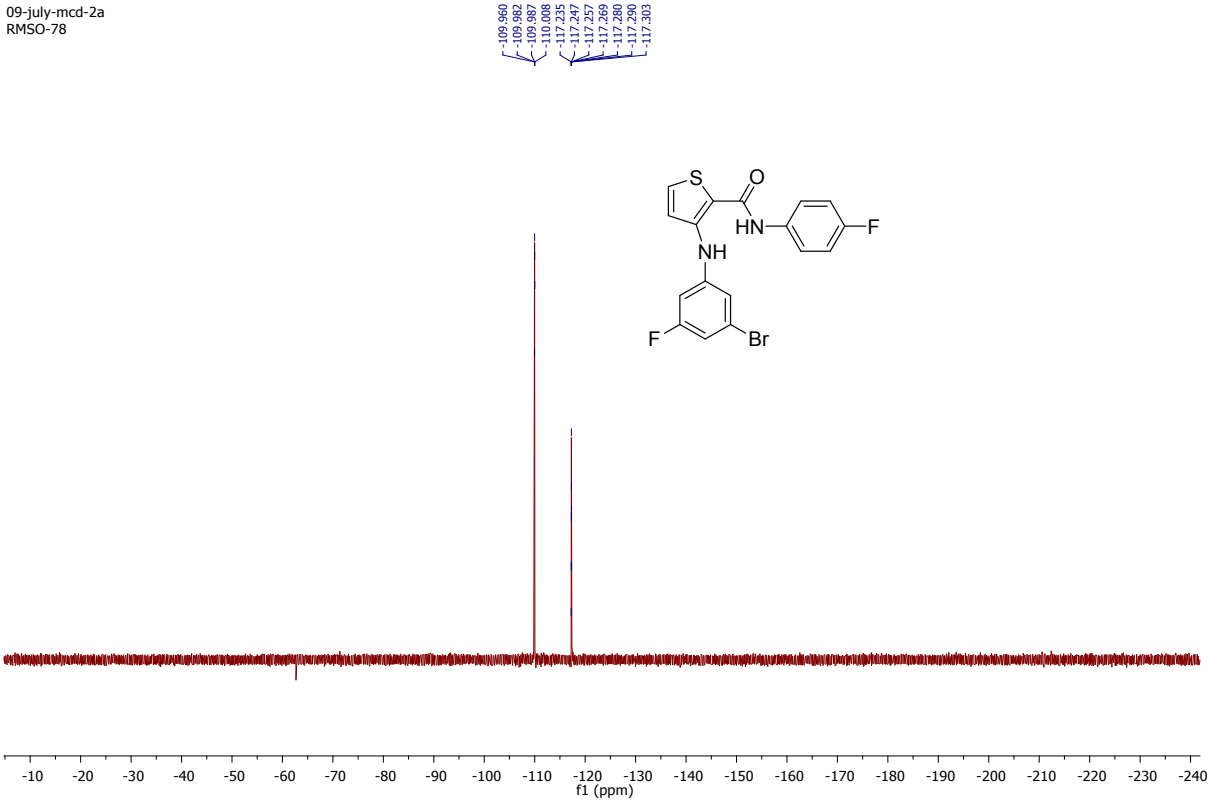
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ rmso-78/ fid
2	Title	OSI-930 DATA
3	Comment	RMSO-78
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	161
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2012-11-29T 12:07:50
18	Modification Date	2012-12-01T 19:02:04
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3138.8
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



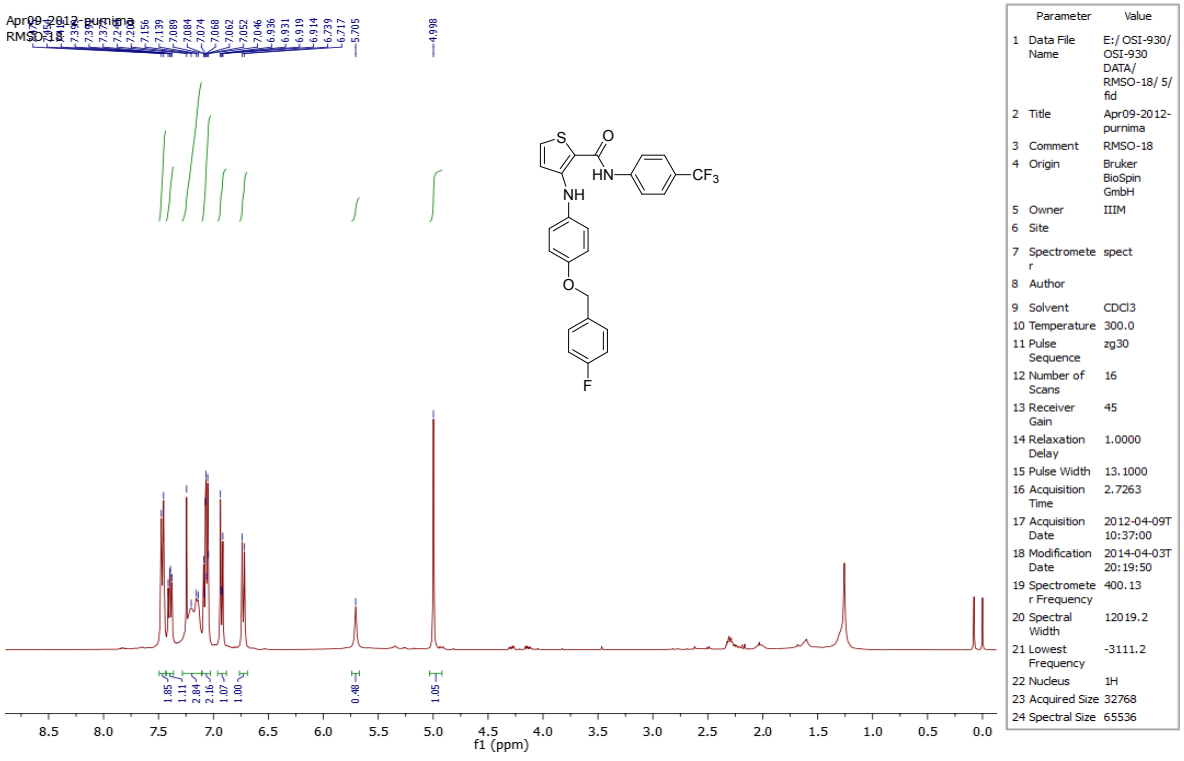
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-78 C13 NMR/ 21/ fid
2	Title	RMSO-78 C13 NMR
3	Comment	RMSO-78
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	685.7
11	Pulse Sequence	zgpg30
12	Number of Scans	1600
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2012-12-29T 13:55:20
18	Modification Date	2012-12-29T 15:49:32
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3148.0
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



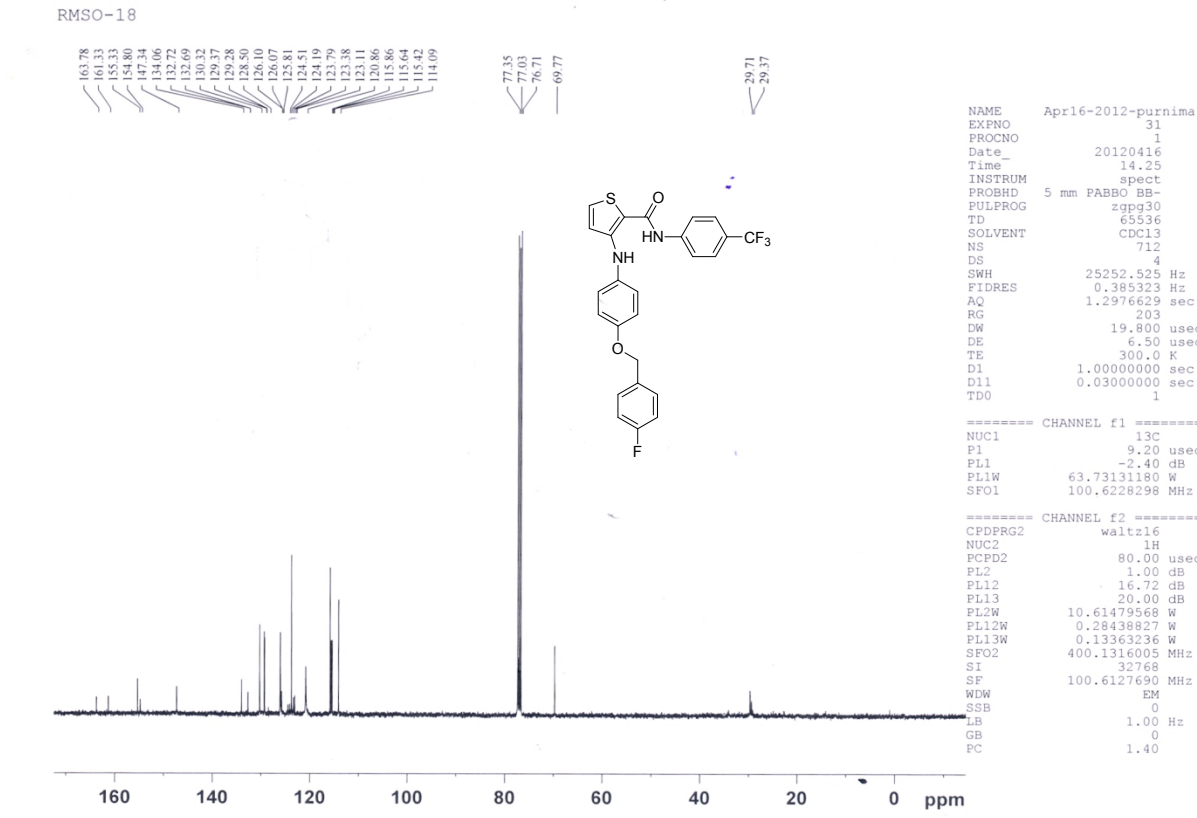
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-78 C13 NMR/ 22/ fid
2	Title	RMSO-78 C13 NMR
3	Comment	RMSO-78
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	685.8
11	Pulse Sequence	dept135
12	Number of Scans	400
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2012-12-29T14:37:48
18	Modification Date	2012-12-29T14:37:54
19	Spectrometer Frequency	125.76
20	Spectral Width	30030.0
21	Lowest Frequency	-2439.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



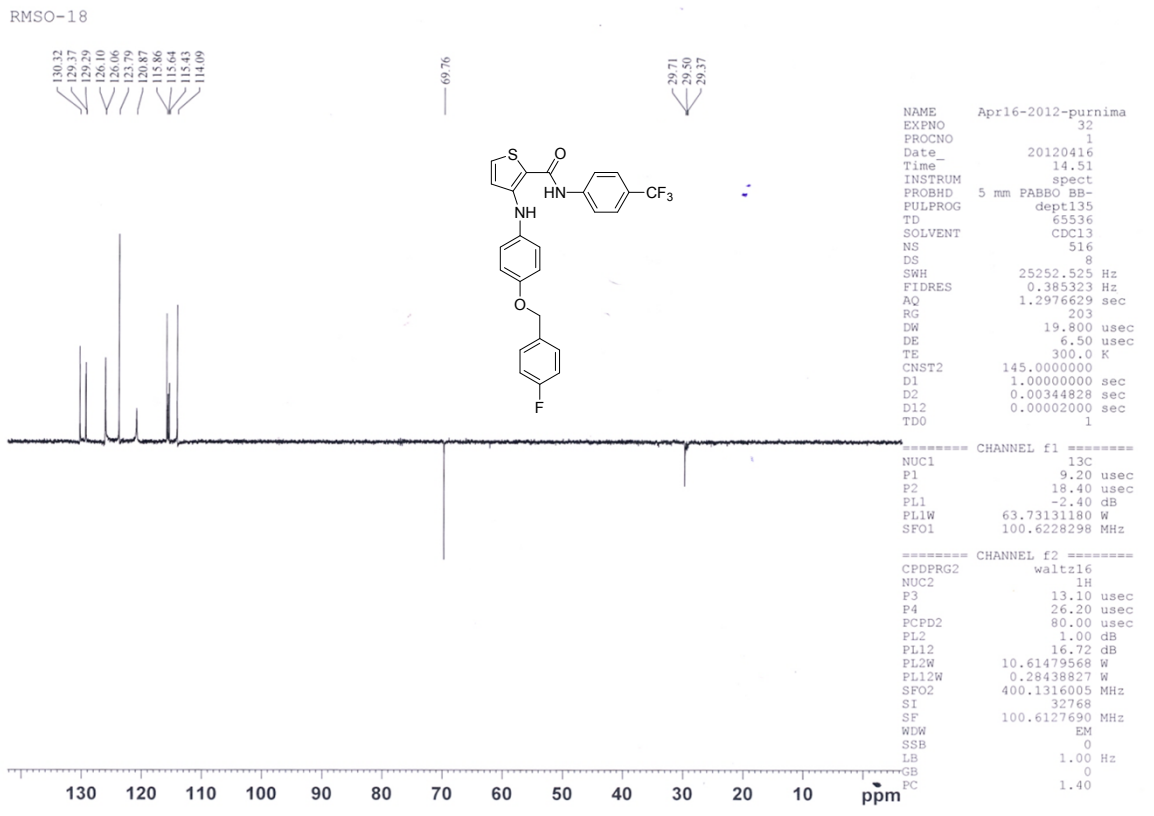
*3-((4-((4-Fluorobenzyl)oxy)phenyl)amino)-N-(4-(trifluoromethyl)phenyl)thiophene-2-carboxamide (**1p**).*

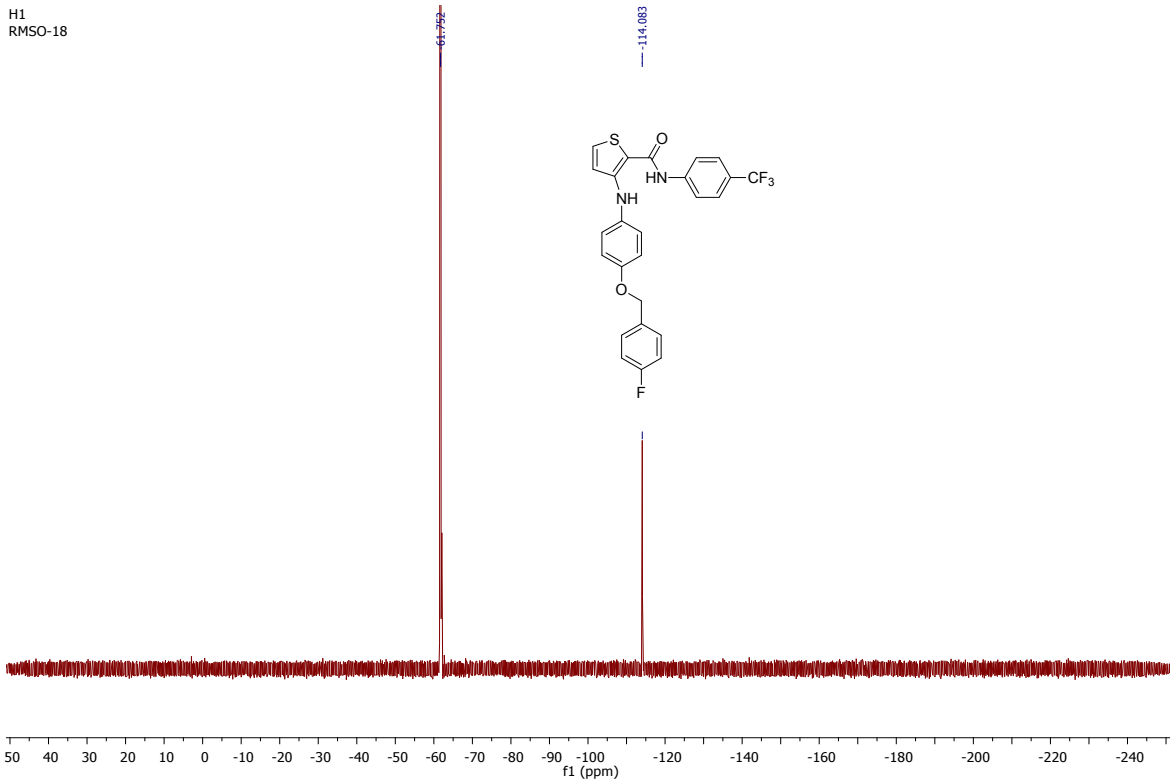


	Parameter	Value
1	Data File Name	E:/OSI-930/OSI-930 DATA/RMSO-18/5/fid
2	Title	Apr09-2012-purnima
3	Comment	RMSO-18
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	45
14	Relaxation Delay	1.0000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2012-04-09T 10:37:00
18	Modification Date	2014-04-03T 20:19:50
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3111.2
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

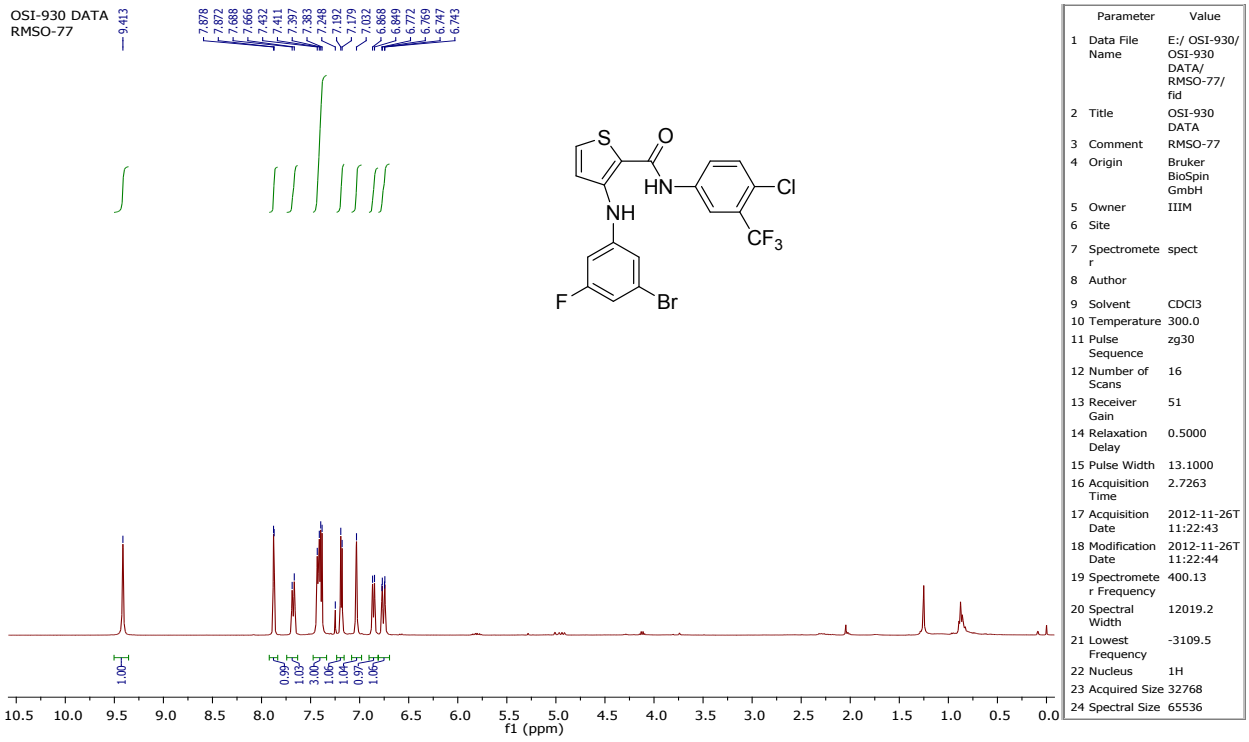


NAME	Apr16-2012-purnima
EXPNO	31
PROCNO	1
Date_	20120416
Time	14.25
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	712
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	203
DW	19.800 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.20 usec
PL1	-2.40 dB
PL1W	63.73131180 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.72 dB
PL13	20.00 dB
PL2W	10.61479568 W
PL12W	0.28438827 W
PL13W	0.13363236 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

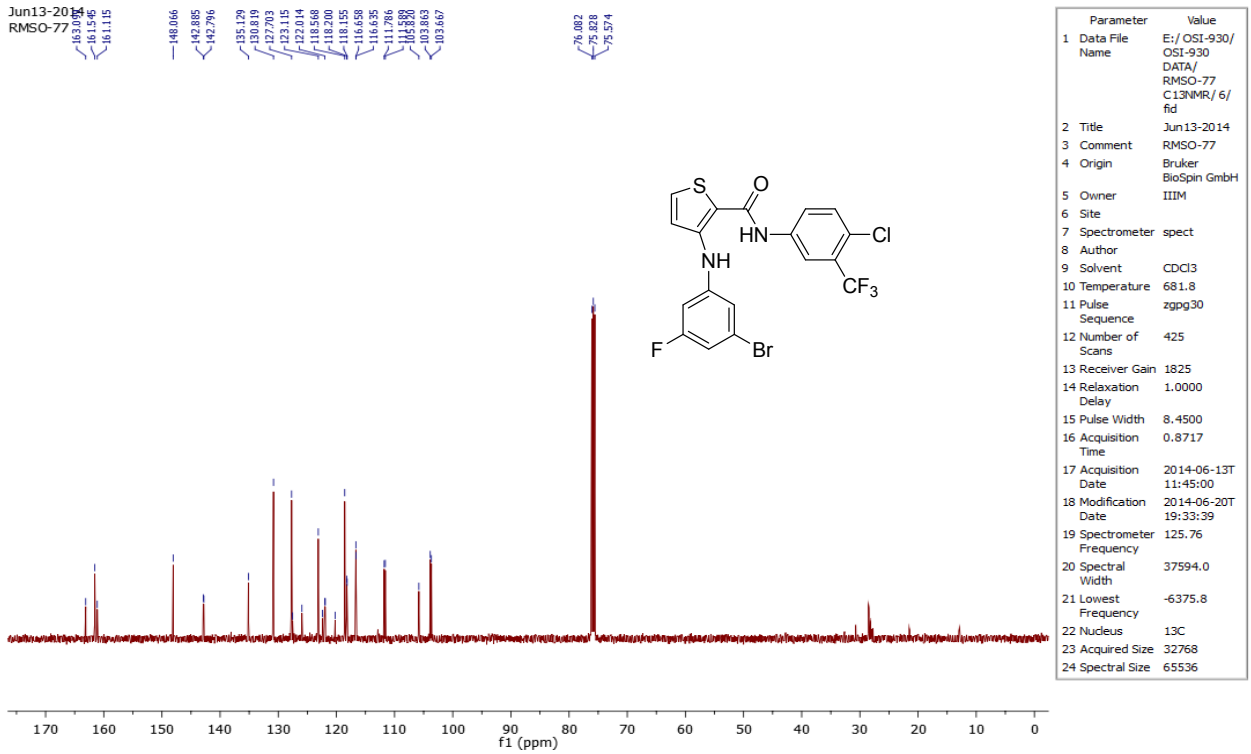

RMSO-18
130.32
129.37
129.29
126.10
126.06
123.79
120.87
115.86
115.64
115.43
114.09
69.76
29.71
29.50
29.37
NAME Apr16-2012-purnima
EXPNO 32
PROCNO 1
Date_ 20120416
Time 14.51
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 516
DS 8
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.20 usec
P2 18.40 usec
PL1 -2.40 dB
PL1W 63.73131180 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 13.10 usec
P4 26.20 usec
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.72 dB
PL2W 10.61479568 W
PL12W 0.28438827 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
S
O
HN
CF3
NH
O
F
130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


H1
RMSO-18
61.752
-114.083
S
O
HN
CF3
NH
O
F
50 40 30 20 10 0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -120 -140 -160 -180 -200 -220 -240
f1 (ppm)

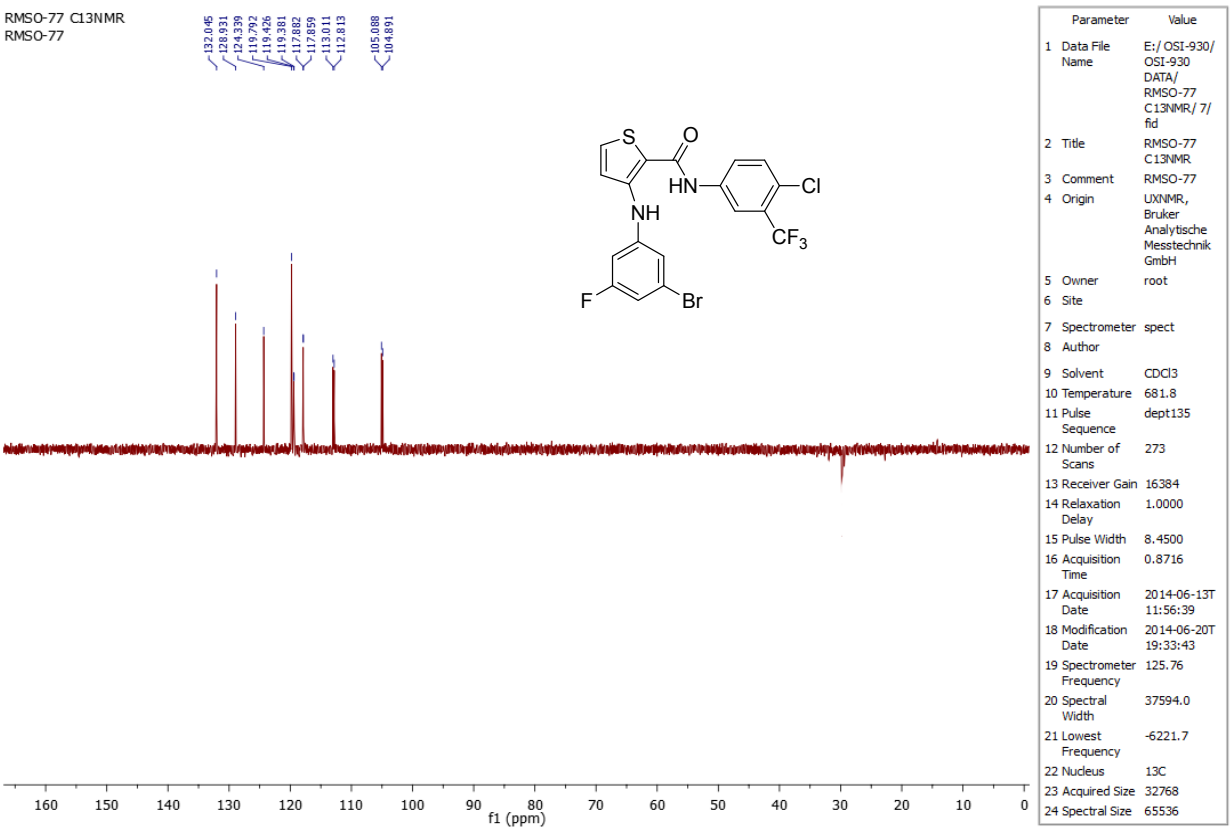
*3-((3-Bromo-5-fluorophenyl)amino)-N-(4-chloro-3-(trifluoromethyl)phenyl)thiophene-2-carboxamide (**1q**).*



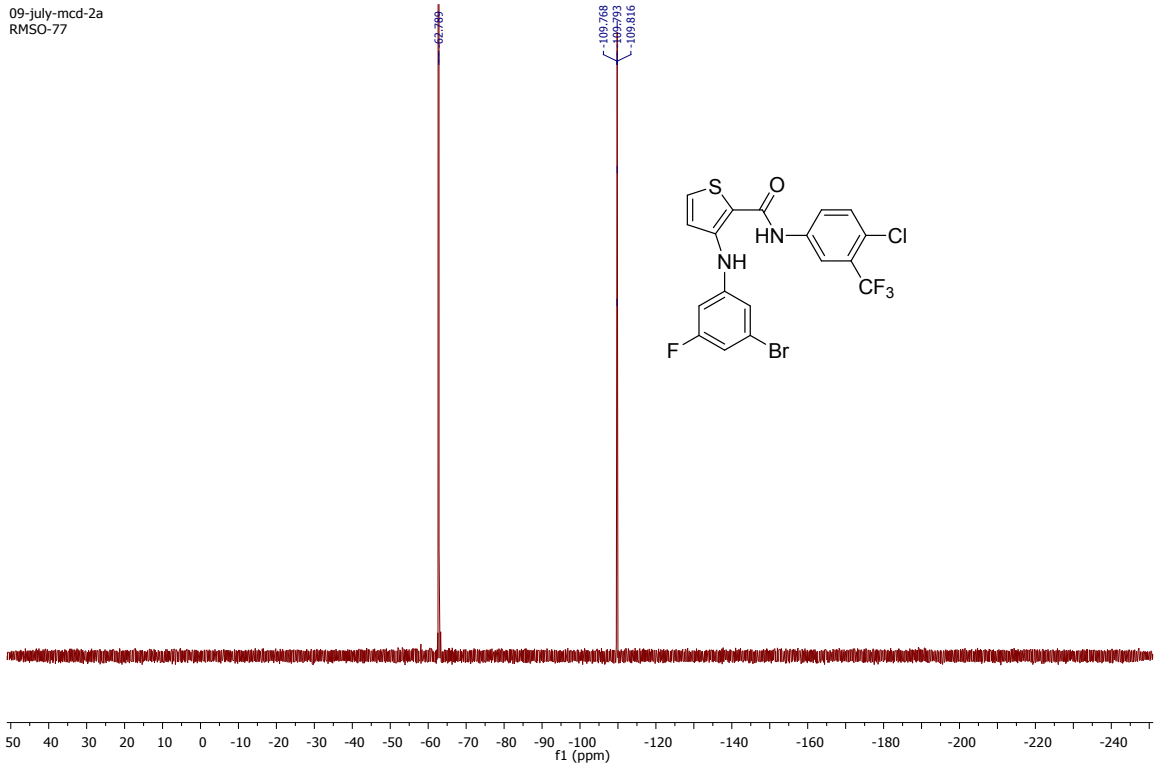
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-77/ fid
2	Title	OSI-930 DATA
3	Comment	RMSO-77
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	51
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2012-11-26T 11:22:43
18	Modification Date	2012-11-26T 11:22:44
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3109.5
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



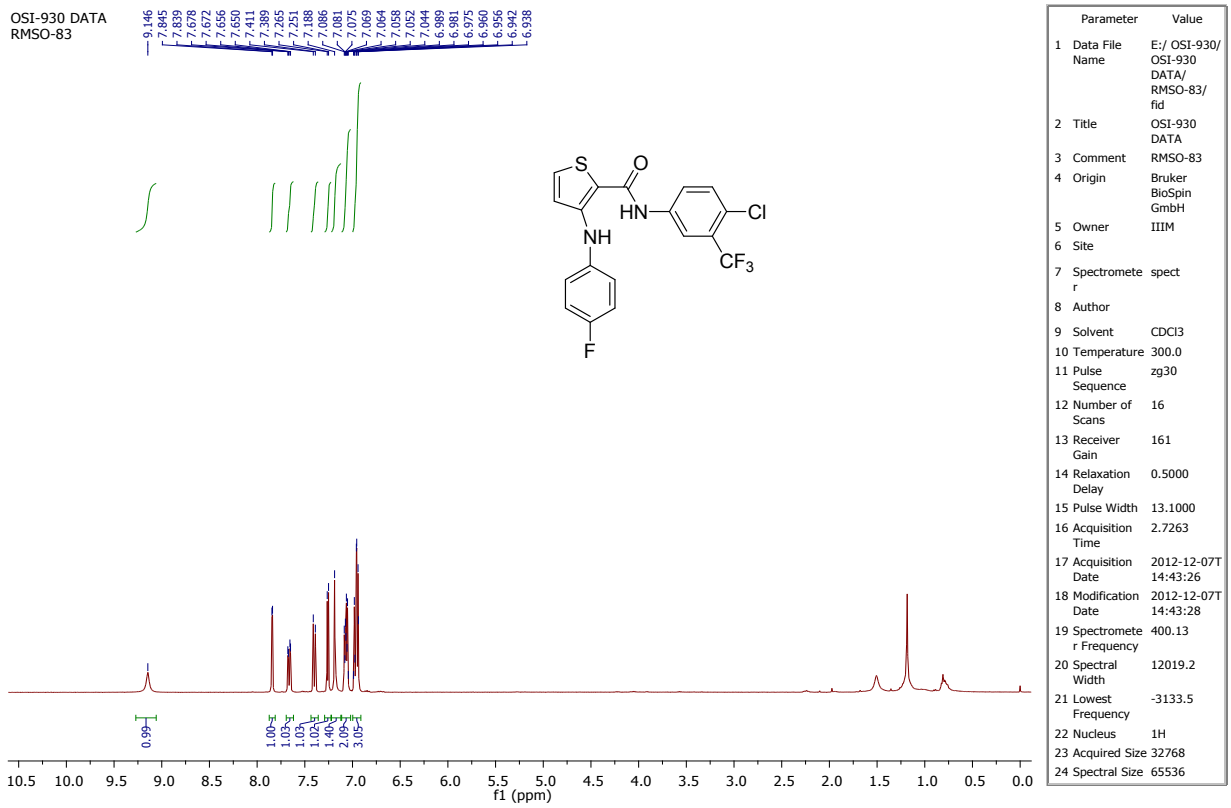
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-77 C13NMR/ 6/ fid
2	Title	Jun13-2014
3	Comment	RMSO-77
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	681.8
11	Pulse Sequence	zgpg30
12	Number of Scans	425
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	0.8717
17	Acquisition Date	2014-06-13T 11:45:00
18	Modification Date	2014-06-20T 19:33:39
19	Spectrometer Frequency	125.76
20	Spectral Width	37594.0
21	Lowest Frequency	-6375.8
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



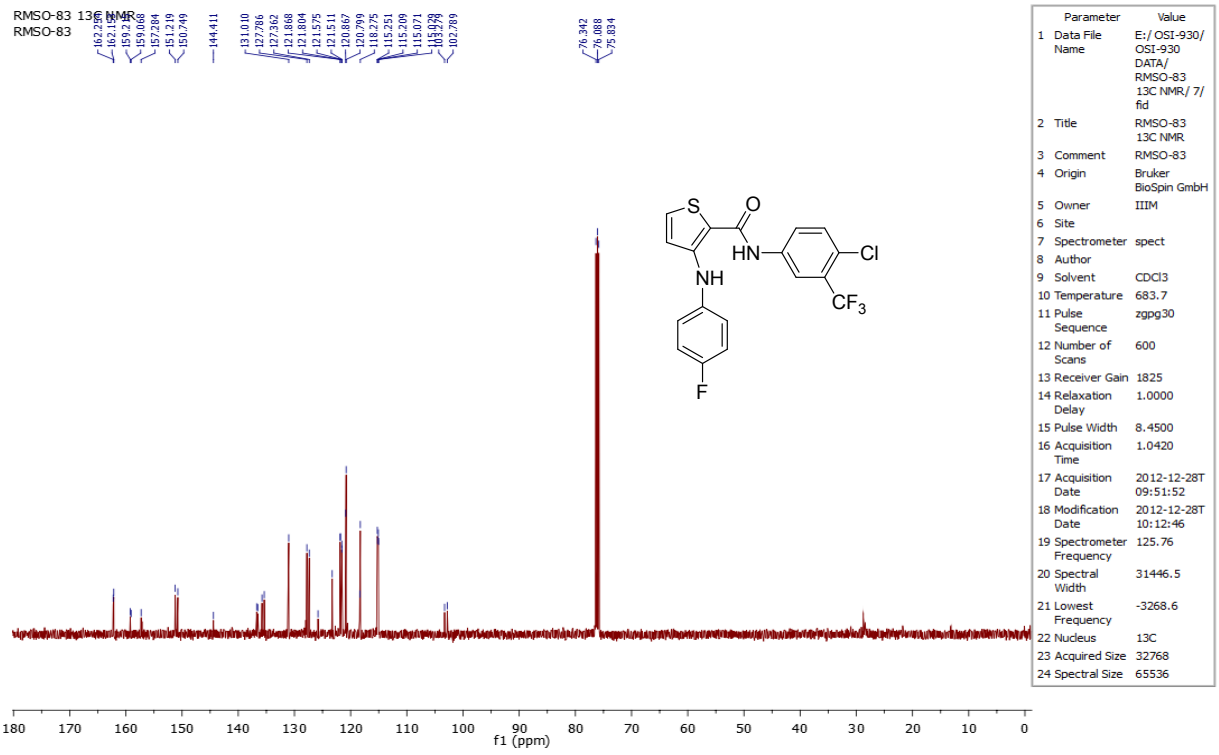
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-77 C13NMR/ 7/ fid
2	Title	RMSO-77 C13NMR
3	Comment	RMSO-77
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	681.8
11	Pulse Sequence	dept135
12	Number of Scans	273
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	0.8716
17	Acquisition Date	2014-06-13T 11:56:39
18	Modification Date	2014-06-20T 19:33:43
19	Spectrometer Frequency	125.76
20	Spectral Width	37594.0
21	Lowest Frequency	-6221.7
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



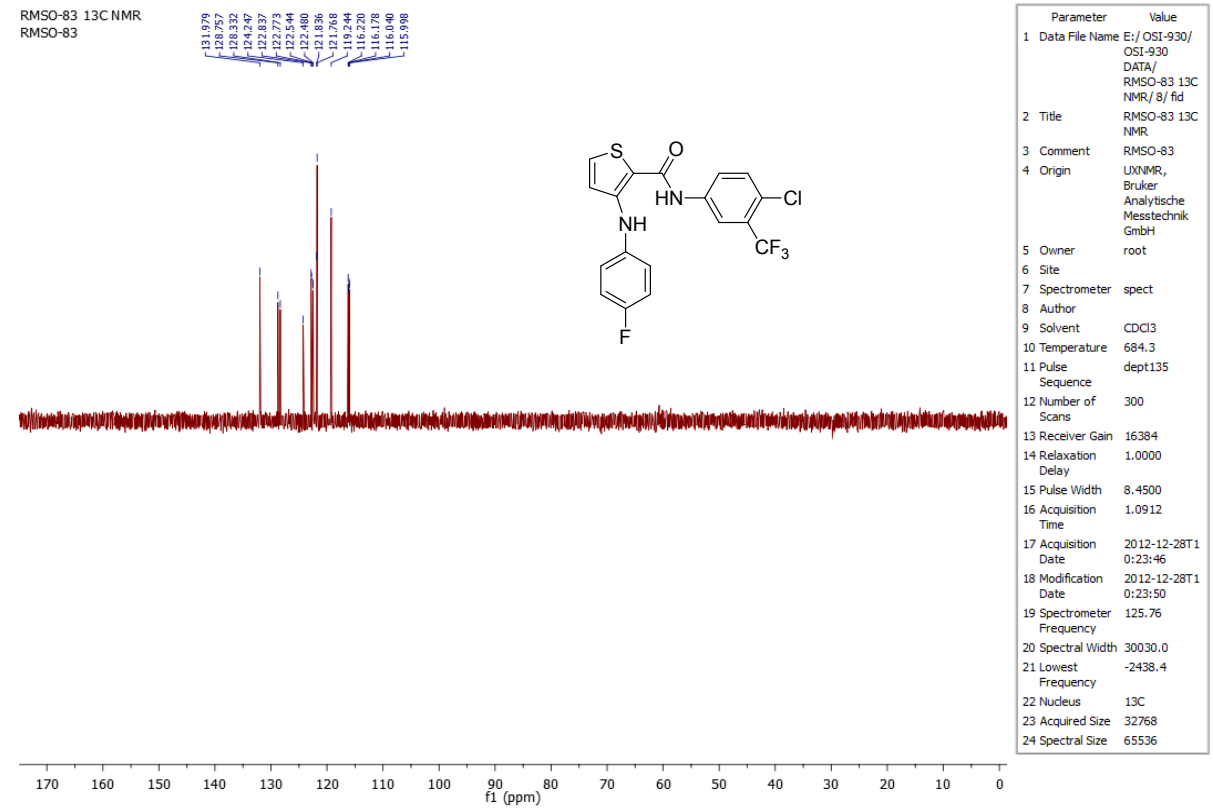
*N-(4-Chloro-3-(trifluoromethyl)phenyl)-3-((4-fluorophenyl)amino)thiophene-2-carboxamide (**1r**).*



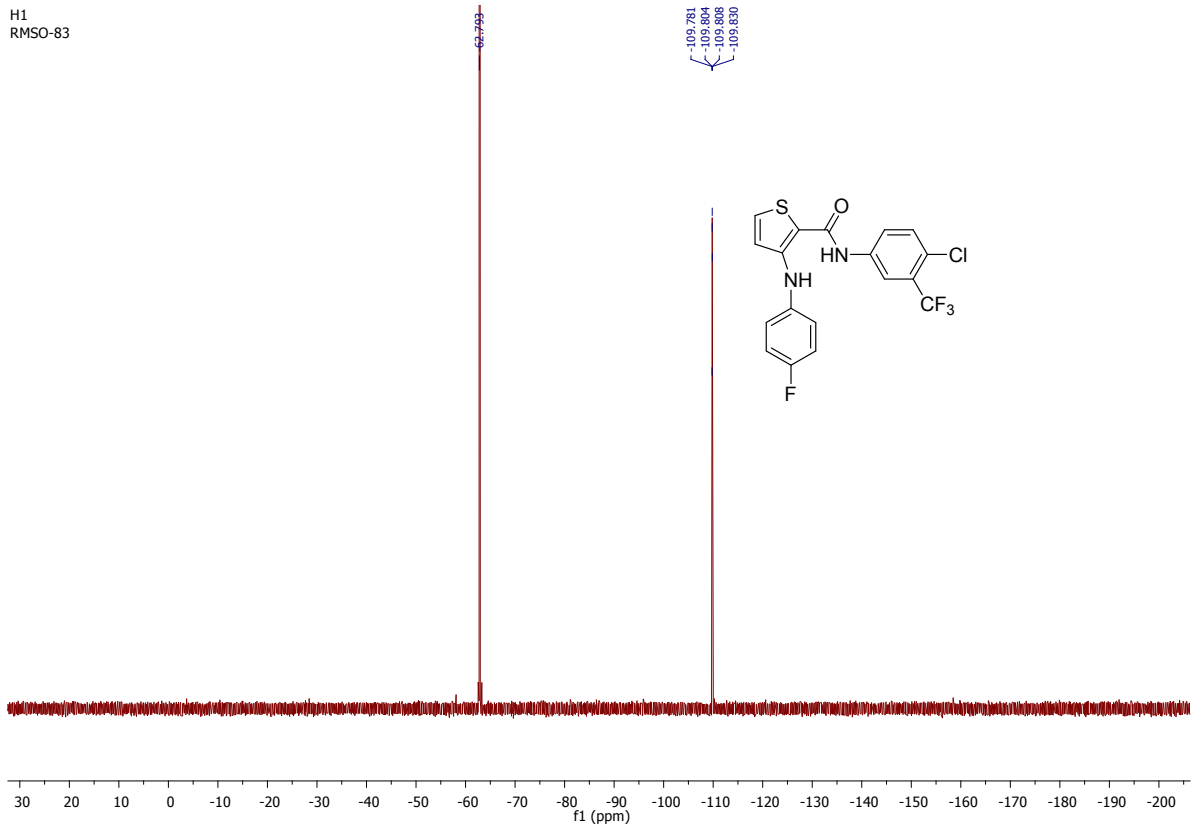
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-83/ fid
2	Title	OSI-930 DATA
3	Comment	RMSO-83
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	161
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2012-12-07T 14:43:26
18	Modification Date	2012-12-07T 14:43:28
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3133.5
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



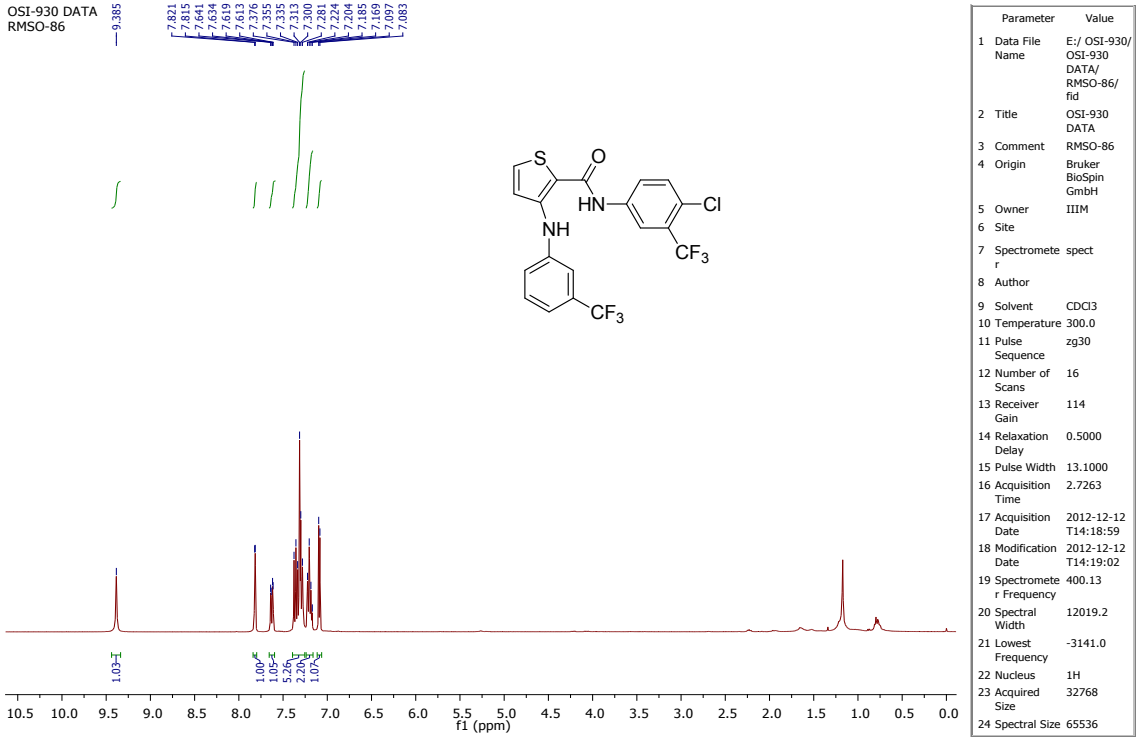
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-83 13C NMR/ 7/ fid
2	Title	RMSO-83 13C NMR
3	Comment	RMSO-83
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	683.7
11	Pulse Sequence	zgpg30
12	Number of Scans	600
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2012-12-28T 09:51:52
18	Modification Date	2012-12-28T 10:12:46
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3268.6
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



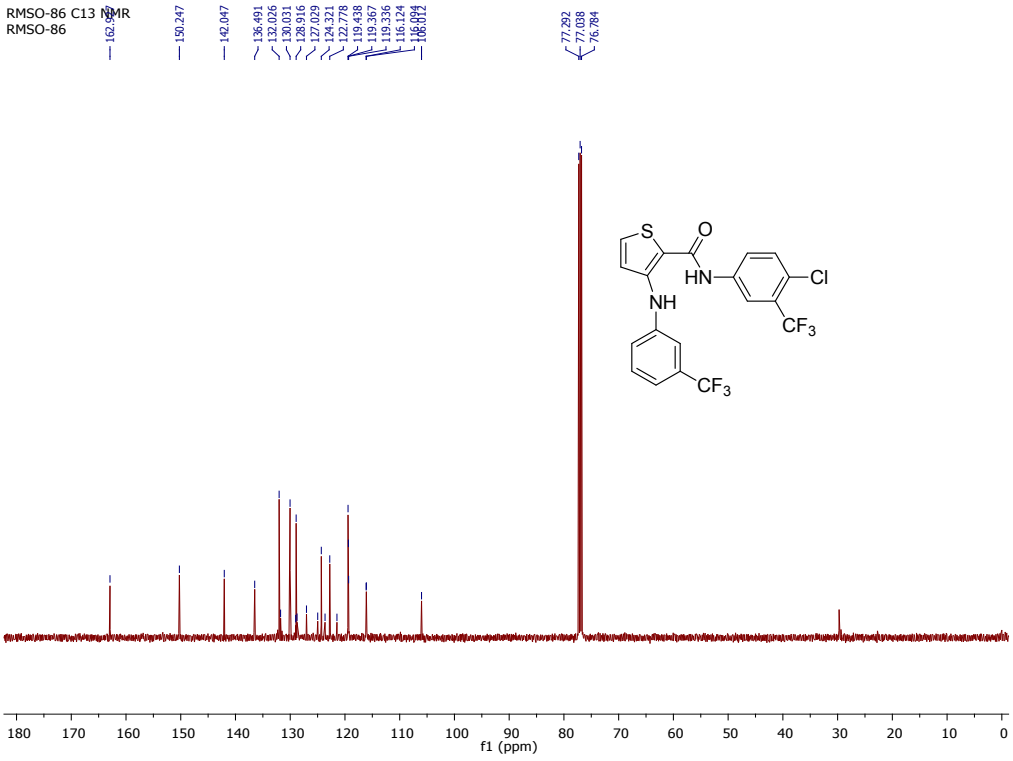
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-83 13C NMR/ 8/ fid
2	Title	RMSO-83 13C NMR
3	Comment	RMSO-83
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	684.3
11	Pulse Sequence	dept135
12	Number of Scans	300
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2012-12-28T10:23:46
18	Modification Date	2012-12-28T10:23:50
19	Spectrometer Frequency	125.76
20	Spectral Width	30030.0
21	Lowest Frequency	-2438.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



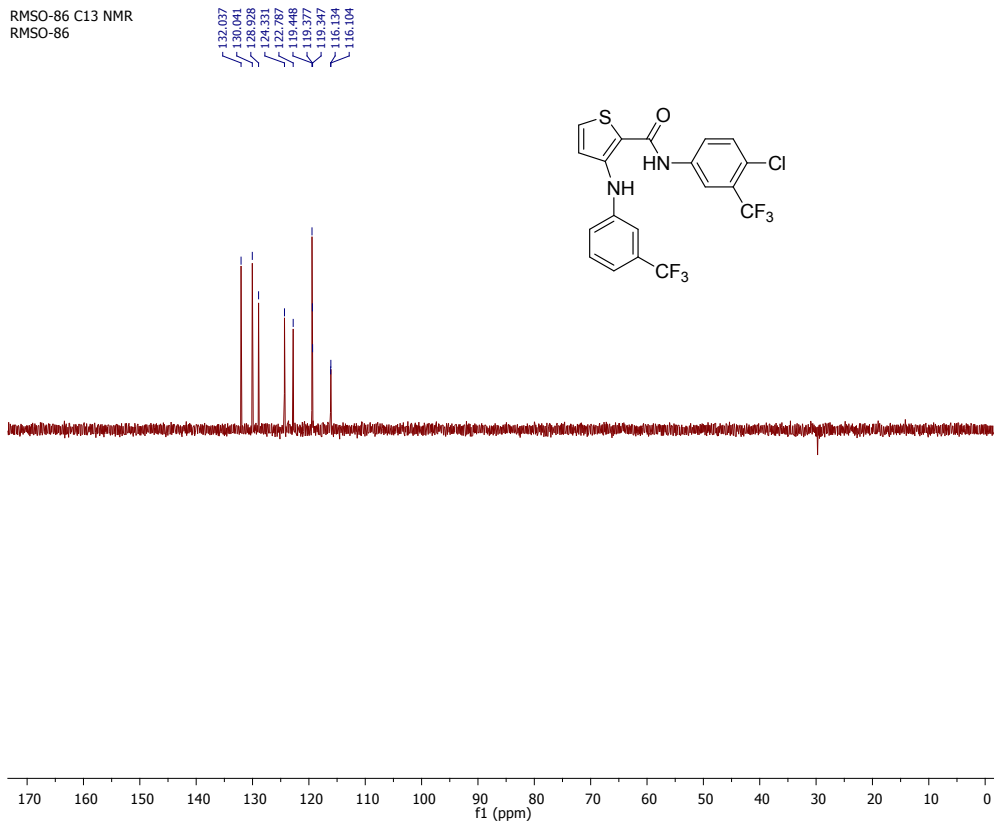
N-(4-Chloro-3-(trifluoromethyl)phenyl)-3-((3-(trifluoromethyl)phenyl)amino)thiophene-2-carboxamide (**1s**).



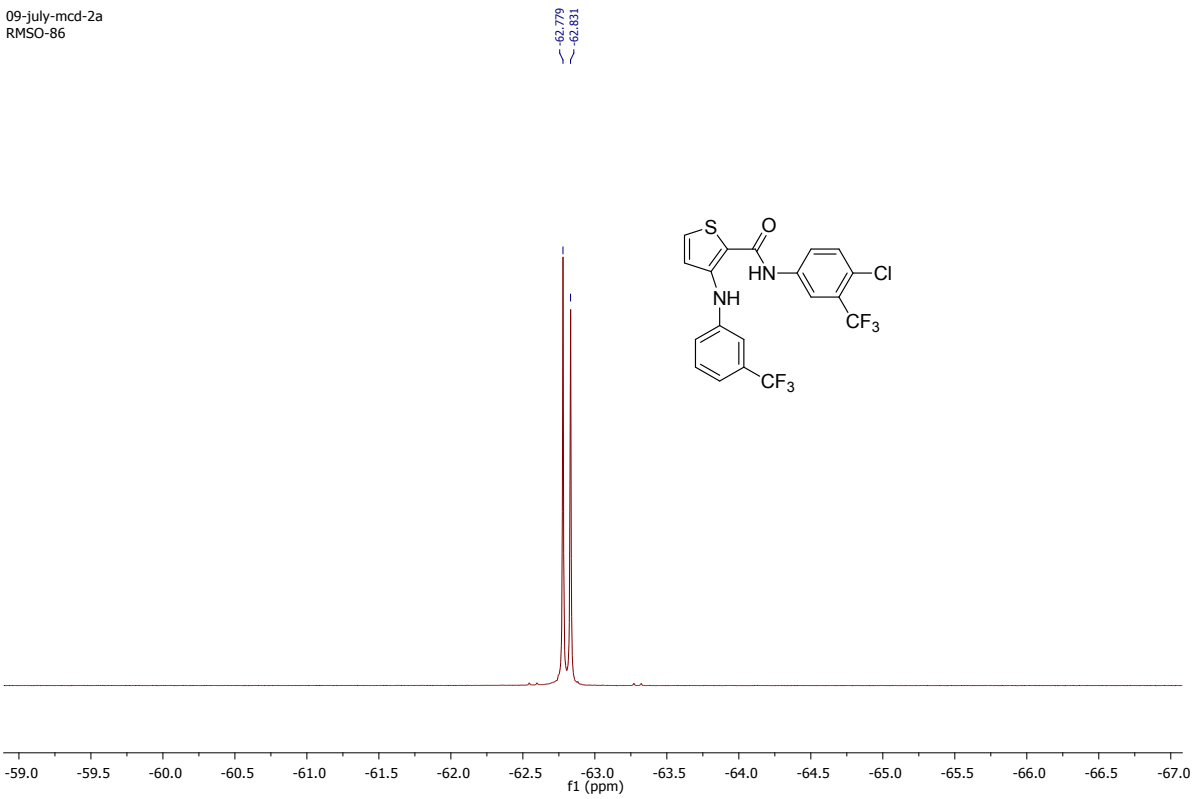
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-86/ fid
2	Title	OSI-930 DATA
3	Comment	RMSO-86
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	114
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2012-12-12 T14:18:59
18	Modification Date	2012-12-12 T14:19:02
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3141.0
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



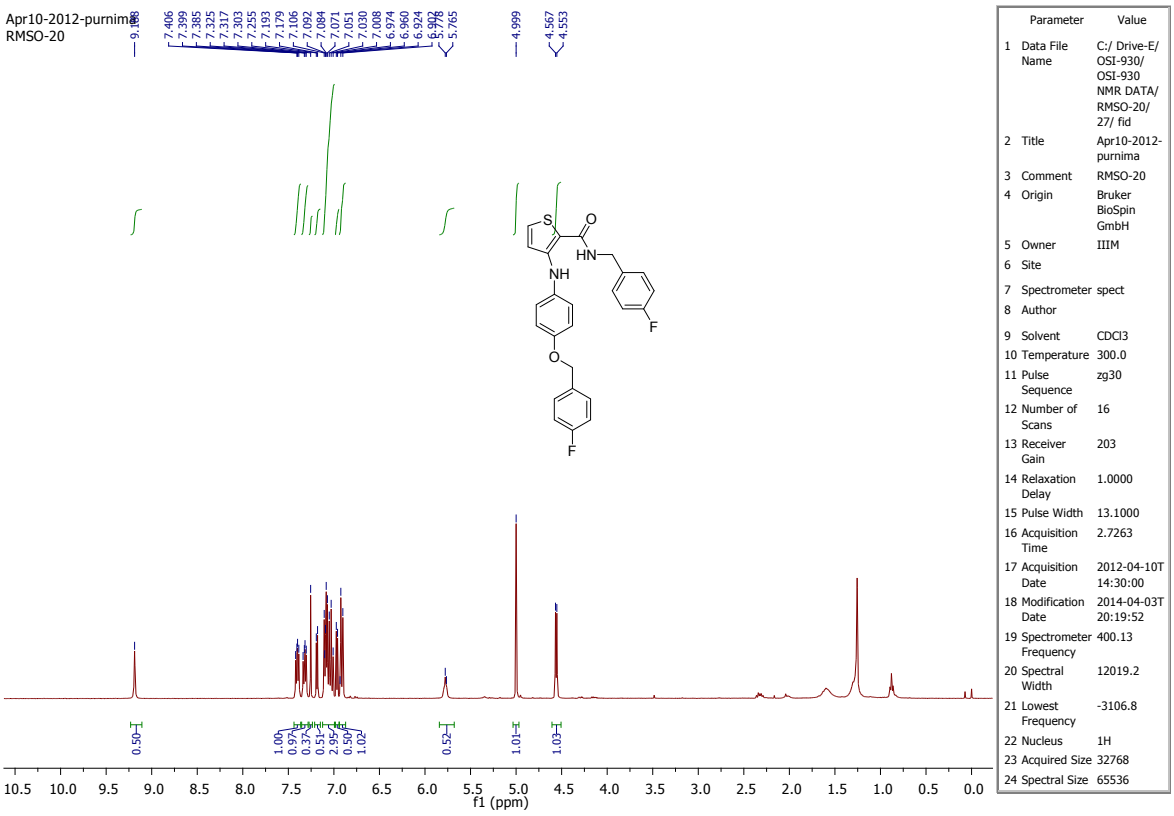
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-86 C13 NMR/ 5/ fid
2	Title	RMSO-86 C13 NMR
3	Comment	RMSO-86
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	683.5
11	Pulse Sequence	zgpg30
12	Number of Scans	400
13	Receiver Gain	1825
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0420
17	Acquisition Date	2012-12-28T 09:27:34
18	Modification Date	2012-12-28T 09:41:12
19	Spectrometer Frequency	125.76
20	Spectral Width	31446.5
21	Lowest Frequency	-3148.0
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



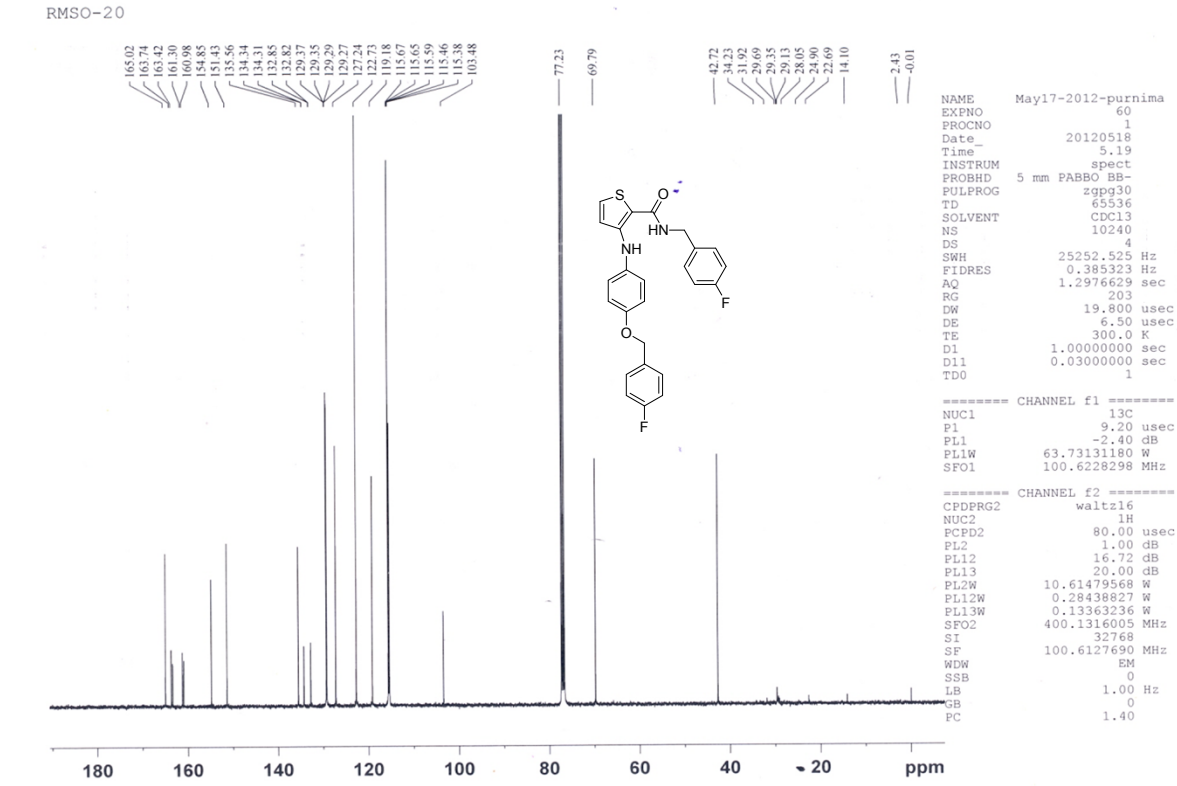
	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-86 C13 NMR/ 6/ fid
2	Title	RMSO-86 C13 NMR
3	Comment	RMSO-86
4	Origin	UXNMR, Bruker Analytische Messtechnik GmbH
5	Owner	root
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	683.6
11	Pulse Sequence	dept135
12	Number of Scans	200
13	Receiver Gain	16384
14	Relaxation Delay	1.0000
15	Pulse Width	8.4500
16	Acquisition Time	1.0912
17	Acquisition Date	2012-12-28T 09:46:11
18	Modification Date	2012-12-28T 09:48:42
19	Spectrometer Frequency	125.76
20	Spectral Width	30030.0
21	Lowest Frequency	-2438.4
22	Nucleus	13C
23	Acquired Size	32768
24	Spectral Size	65536



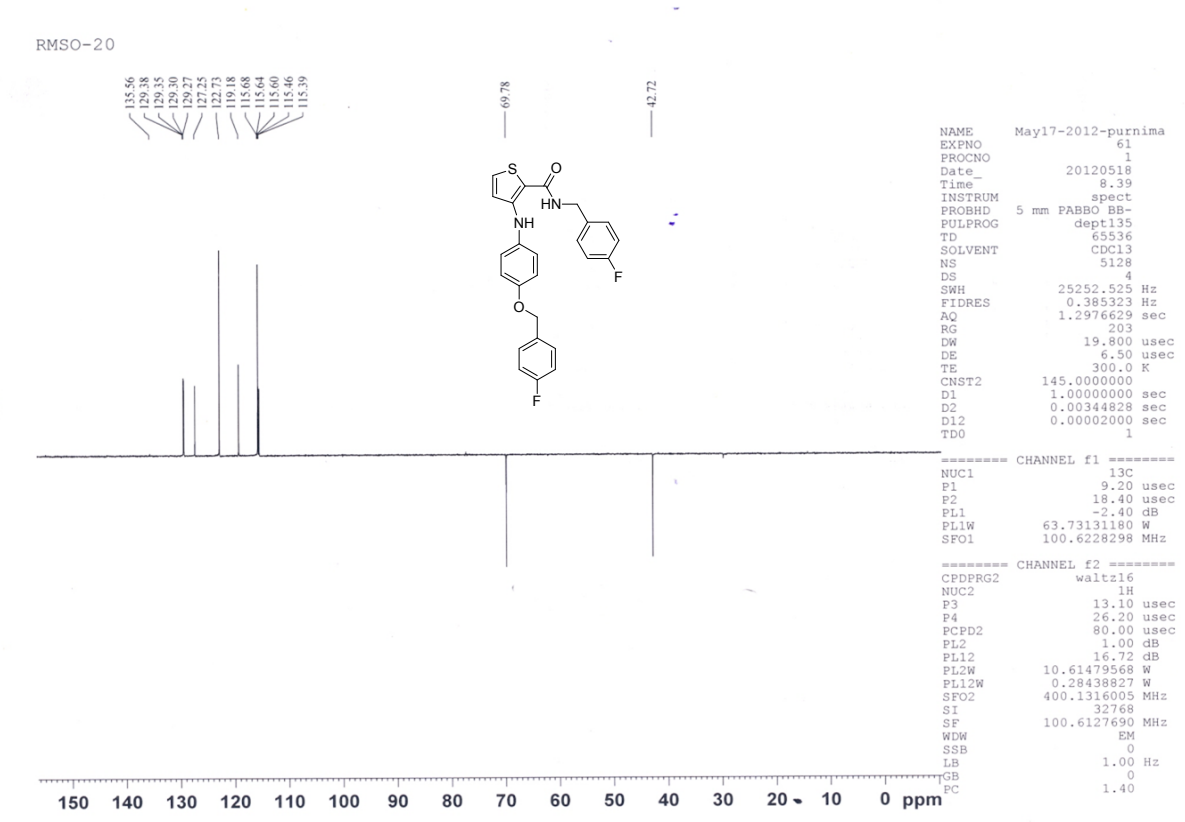
*N-(4-Fluorobenzyl)-3-((4-((4-fluorobenzyl)oxy)phenyl)amino)thiophene-2-carboxamide (**1t**).*

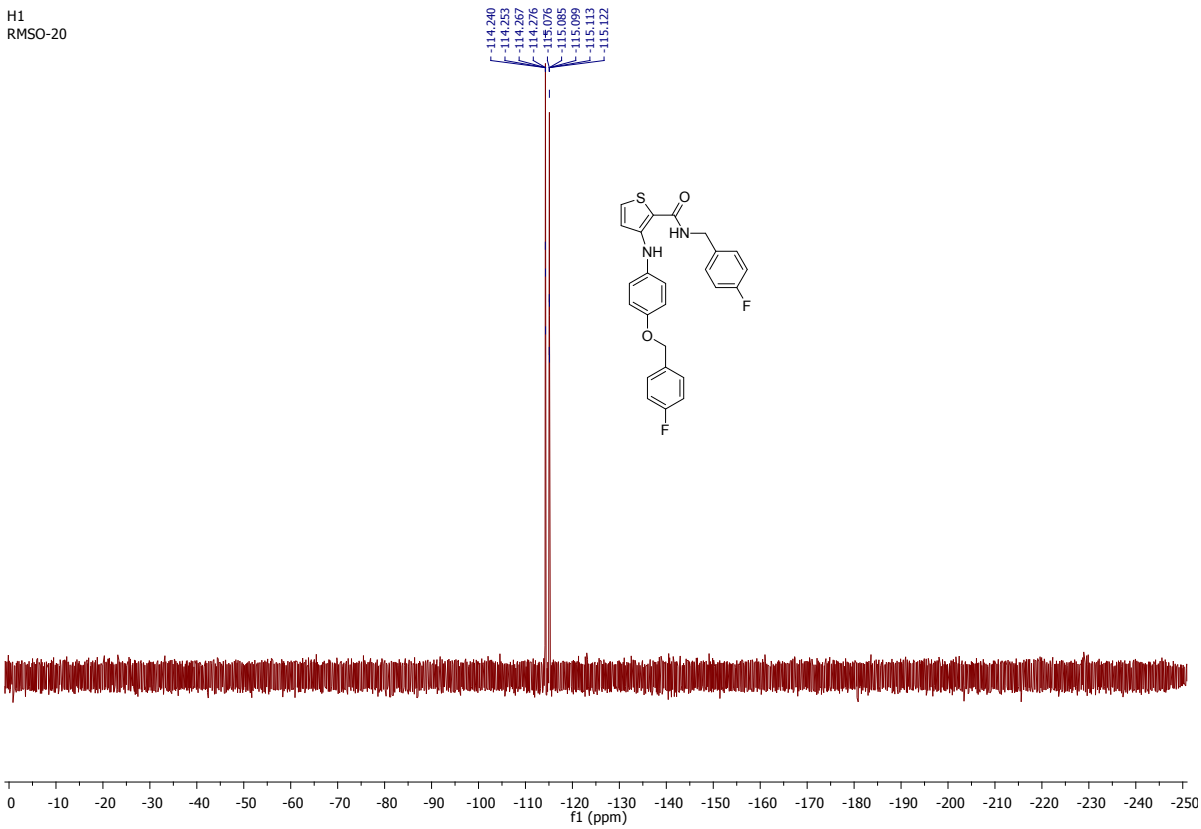


	Parameter	Value
1	Data File Name	C:/ Drive-E/ OSI-930/ OSI-930 NMR DATA/ RMSO-20/ 27/ fid
2	Title	Apr10-2012-purnima
3	Comment	RMSO-20
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	203
14	Relaxation Delay	1.0000
15	Pulse Width	13.1000
16	Acquisition Time	2.7263
17	Acquisition Date	2012-04-10T 14:30:00
18	Modification Date	2014-04-03T 20:19:52
19	Spectrometer Frequency	400.13
20	Spectral Width	12019.2
21	Lowest Frequency	-3106.8
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

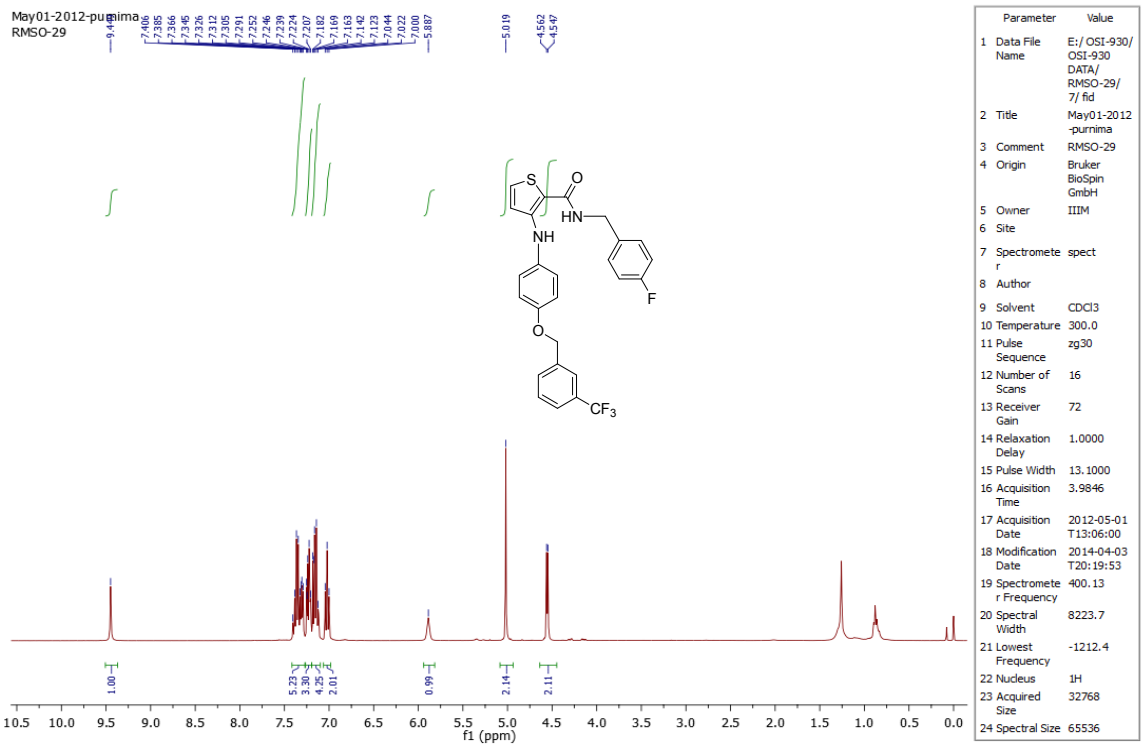


NAME	May17-2012-purnima
EXPNO	60
PROCNO	1
Date_	20120518
Time	5.19
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	10240
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	203
DW	19.800 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.20 usec
PL1	-2.40 dB
PL1W	63.73131180 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.72 dB
PL13	20.00 dB
PL2W	10.61479568 W
PL12W	0.28438827 W
PL13W	0.13363236 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127690 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

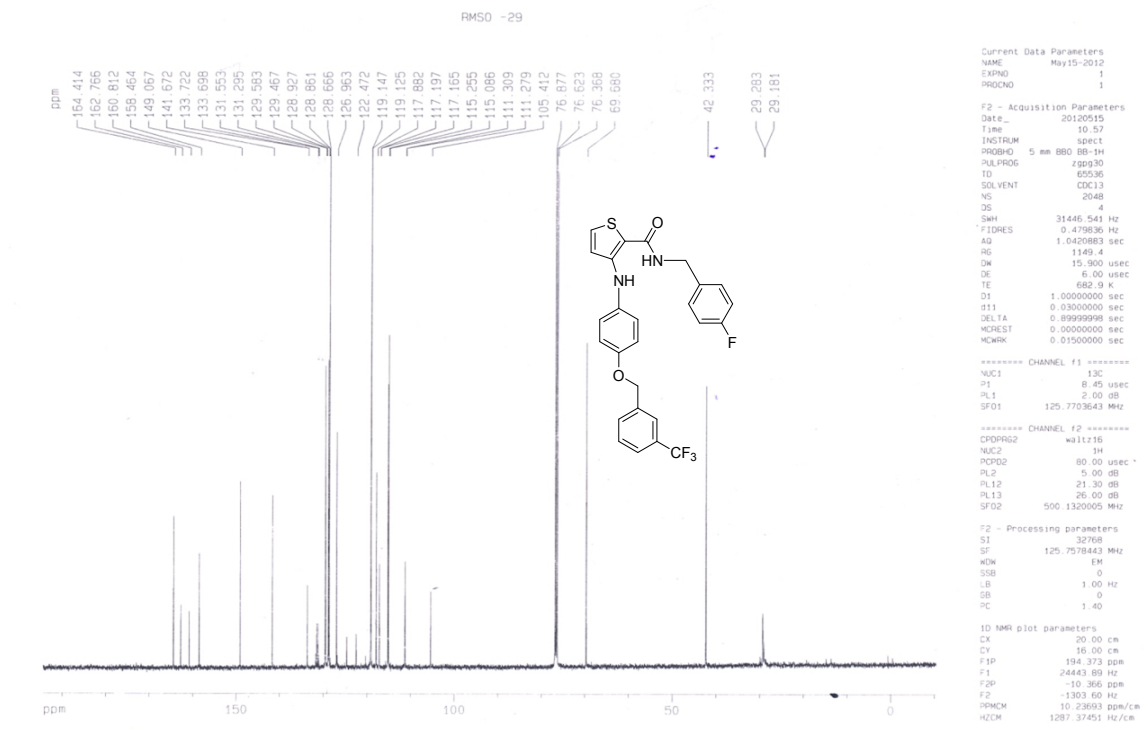

RMSO-20
135.56
129.38
129.35
129.30
129.27
127.25
122.73
119.18
115.68
115.64
115.60
115.46
115.39
69.78
42.72
S
O
HN
NH
F
O
F
NAME May17-2012-purnima
EXPNO 61
PROCNO 1
Date_ 20120518
Time 8.39
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 5128
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
======== CHANNEL f1 ========
NUC1 13C
P1 9.20 usec
P2 18.40 usec
PL1 -2.40 dB
PL1W 63.73131180 W
SFO1 100.6228298 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 13.10 usec
P4 26.20 usec
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.72 dB
PL2W 10.61479568 W
PL12W 0.28438827 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127690 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0 ppm


H1
RMSO-20
-114.240
-114.253
-114.267
-114.276
-115.076
-115.085
-115.099
-115.113
-115.122
S
O
HN
NH
F
O
F
0 -10 -20 -30 -40 -50 -60 -70 -80 -90 -100 -110 -120 -130 -140 -150 -160 -170 -180 -190 -200 -210 -220 -230 -240 -250
f1 (ppm)

N-(4-Fluorobenzyl)-3-((4-((3-(trifluoromethyl)benzyl)oxy)phenyl)amino)thiophene-2-carboxamide (**1u**).



	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-29/ 7/ fid
2	Title	May01-2012 -purnima
3	Comment	RMSO-29
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	72
14	Relaxation Delay	1.0000
15	Pulse Width	13.1000
16	Acquisition Time	3.9846
17	Acquisition Date	2012-05-01 T13:06:00
18	Modification Date	2014-04-03 T20:19:53
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-1212.4
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536



Current Data Parameters
NAME May15-2012
EXPNO 1
PROCNO 1

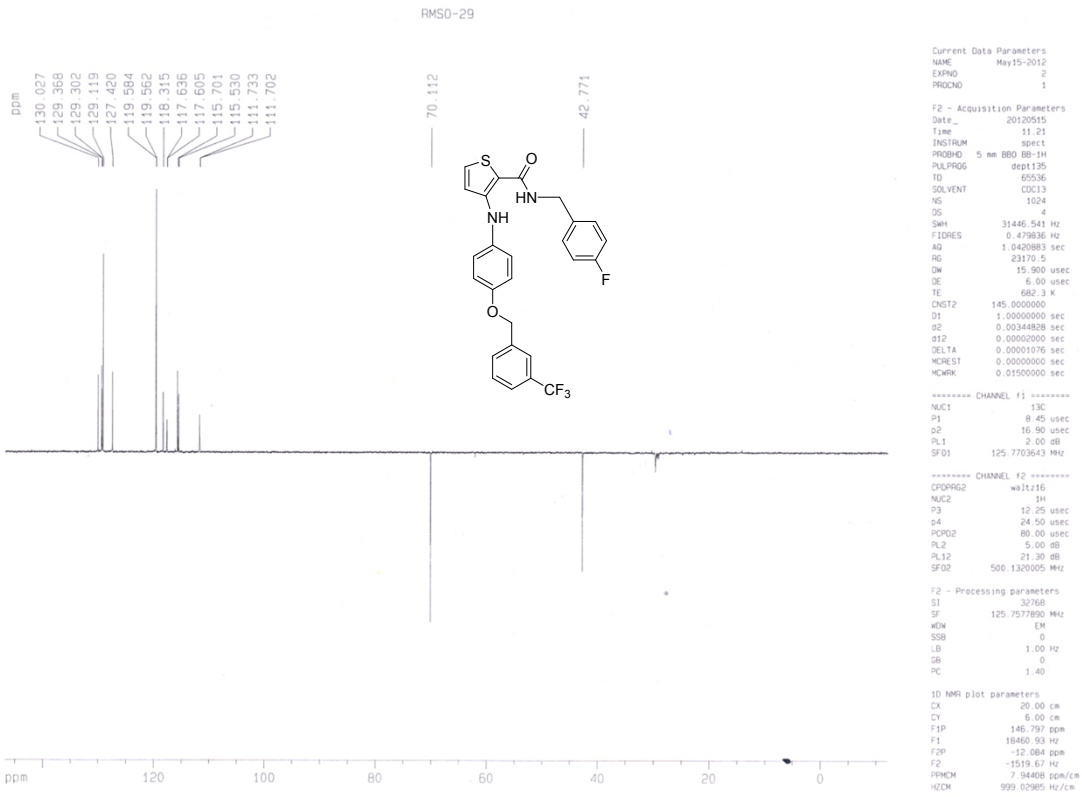
F2 - Acquisition Parameters
Date_ 20120515
Time 10.57
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2048
DS 4
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 1149.4
DW 15.900 usec
DE 6.00 usec
TE 682.9 K
D1 1.00000000 sec
d11 0.03000000 sec
DELTA 0.89999998 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec

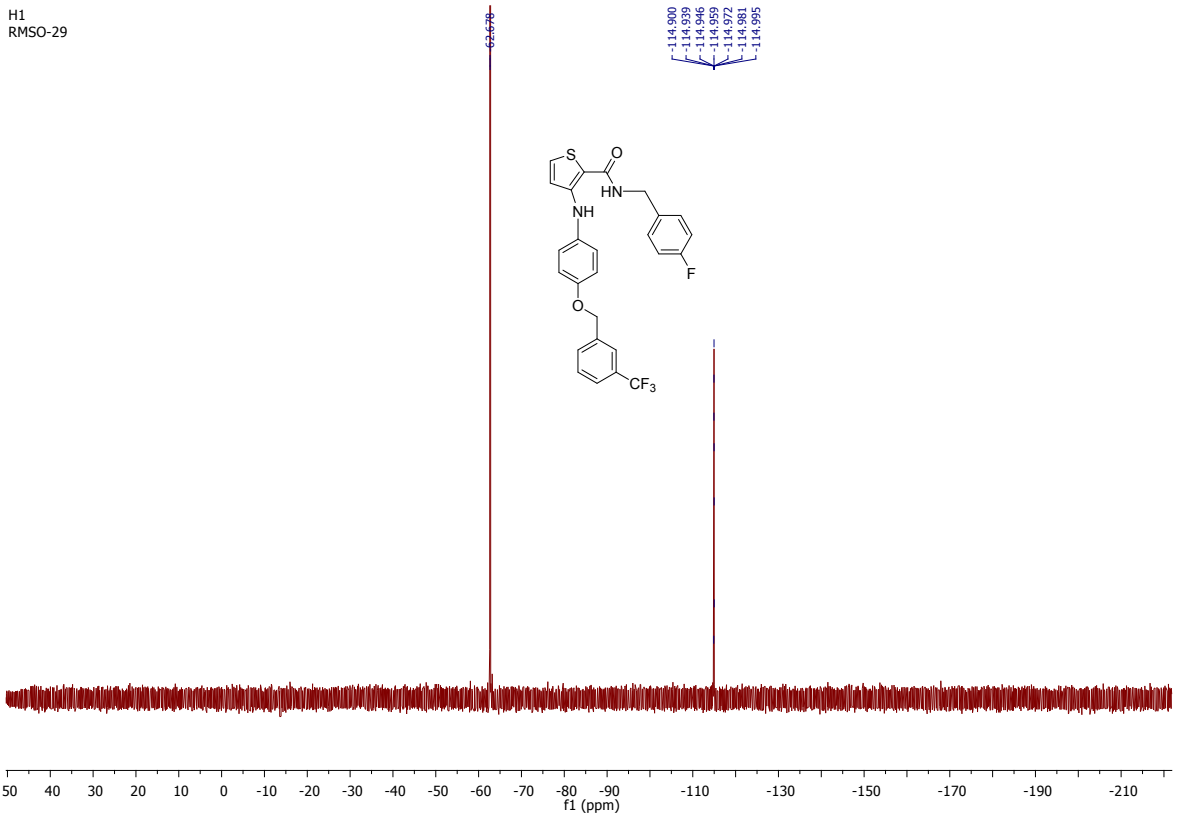
======== CHANNEL f1 ========
NUC1 13C
P1 8.45 usec
PL1 2.00 dB
SFO1 125.7703643 MHz

======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 5.00 dB
PL12 21.30 dB
PL13 26.00 dB
SFO2 500.1320005 MHz

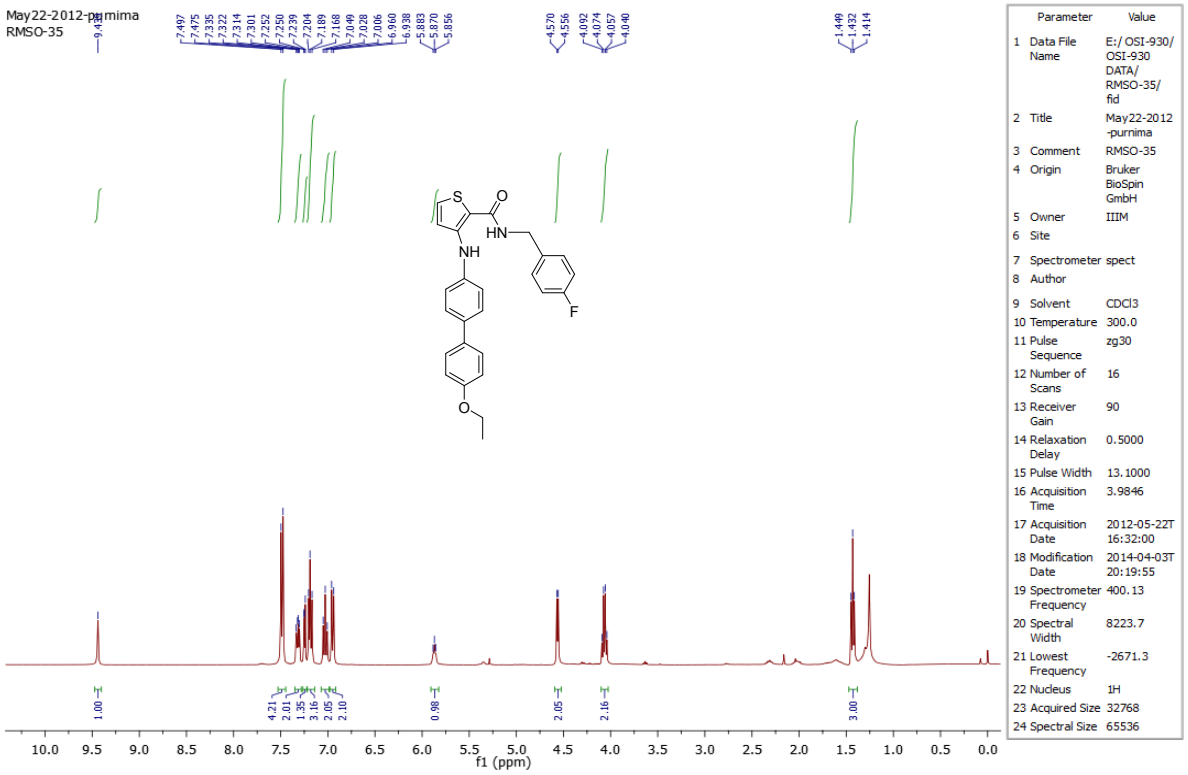
F2 - Processing parameters
SI 32768
SF 125.7578443 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

1D NMR plot parameters
CX 20.00 cm
CY 16.00 cm
F1P 194.373 ppm
F1 24443.89 Hz
F2P -10.366 ppm
F2 -1303.60 Hz
PPMCM 10.23693 ppm/cm
HZCM 1287.37451 Hz/cm

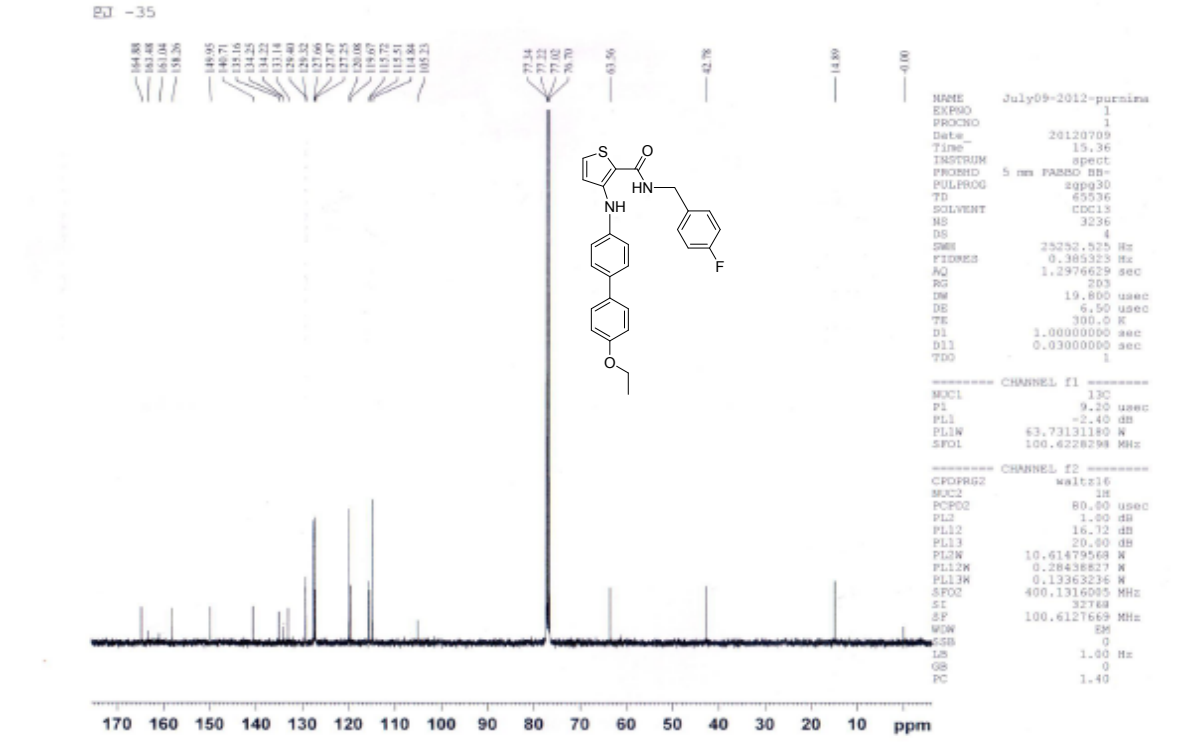

RMSO-29
ppm
130.027
129.368
129.302
129.119
127.420
119.584
119.562
118.315
117.636
117.605
115.701
115.530
111.733
111.702
70.112
42.771
S
O
HN
NH
F
O
CF3
ppm
120
100
80
60
40
20
0
Current Data Parameters
NAME May15-2012
EXPNO 2
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120515
Time 11.21
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 1024
DS 4
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 23170.5
DW 15.900 usec
DE 6.00 usec
TE 682.3 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
DELTA 0.00001076 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.45 usec
P2 16.90 usec
PL1 2.00 dB
SF01 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 12.25 usec
P4 24.50 usec
PCPD2 80.00 usec
PL2 5.00 dB
PL12 21.30 dB
SF02 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 146.797 ppm
F1 18460.93 Hz
F2P -12.084 ppm
F2 -1519.67 Hz
PPMCM 7.94408 ppm/cm
HZCM 999.02985 Hz/cm


H1
RMSO-29
-62.678
-114.900
-114.939
-114.946
-114.959
-114.972
-114.981
-114.995
S
O
HN
NH
F
O
CF3
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
f1 (ppm)

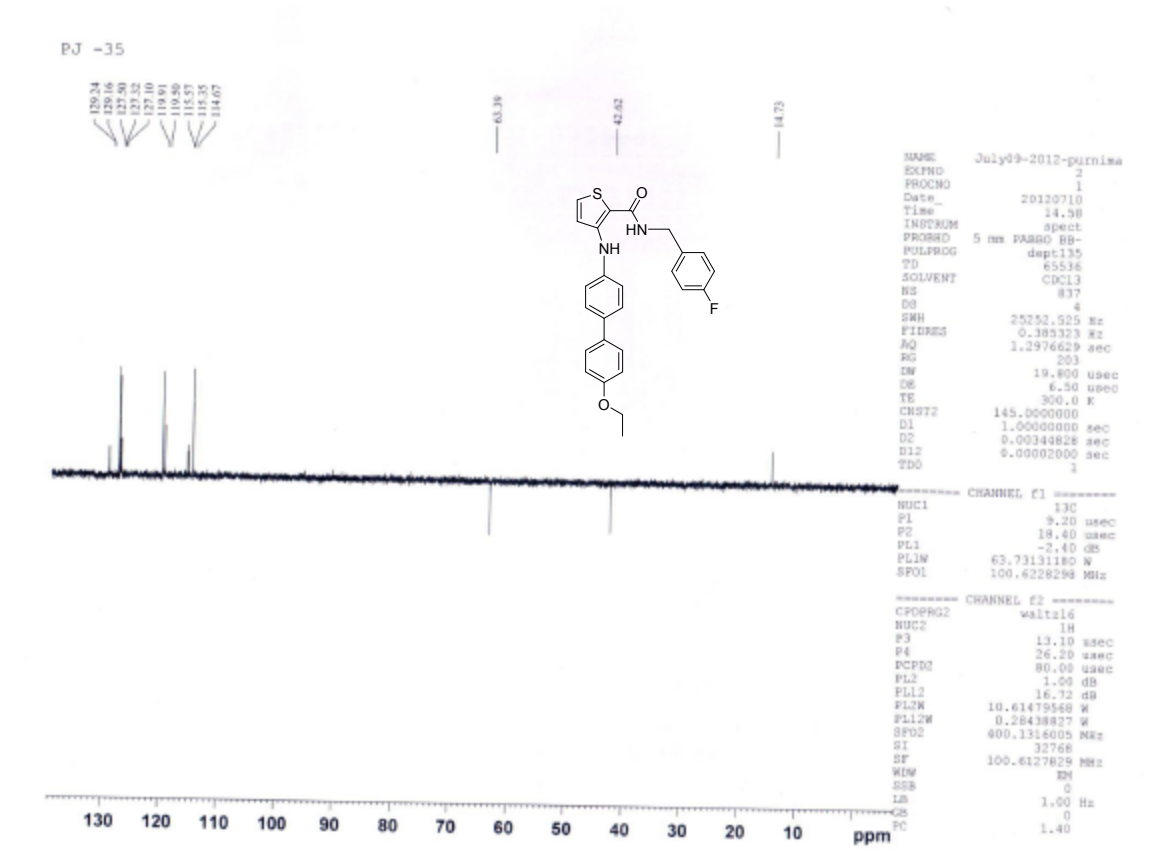
3-((4'-Ethoxy-[1,1'-biphenyl]-4-yl)amino)-N-(4-fluorobenzyl)thiophene-2-carboxamide (**1v**).

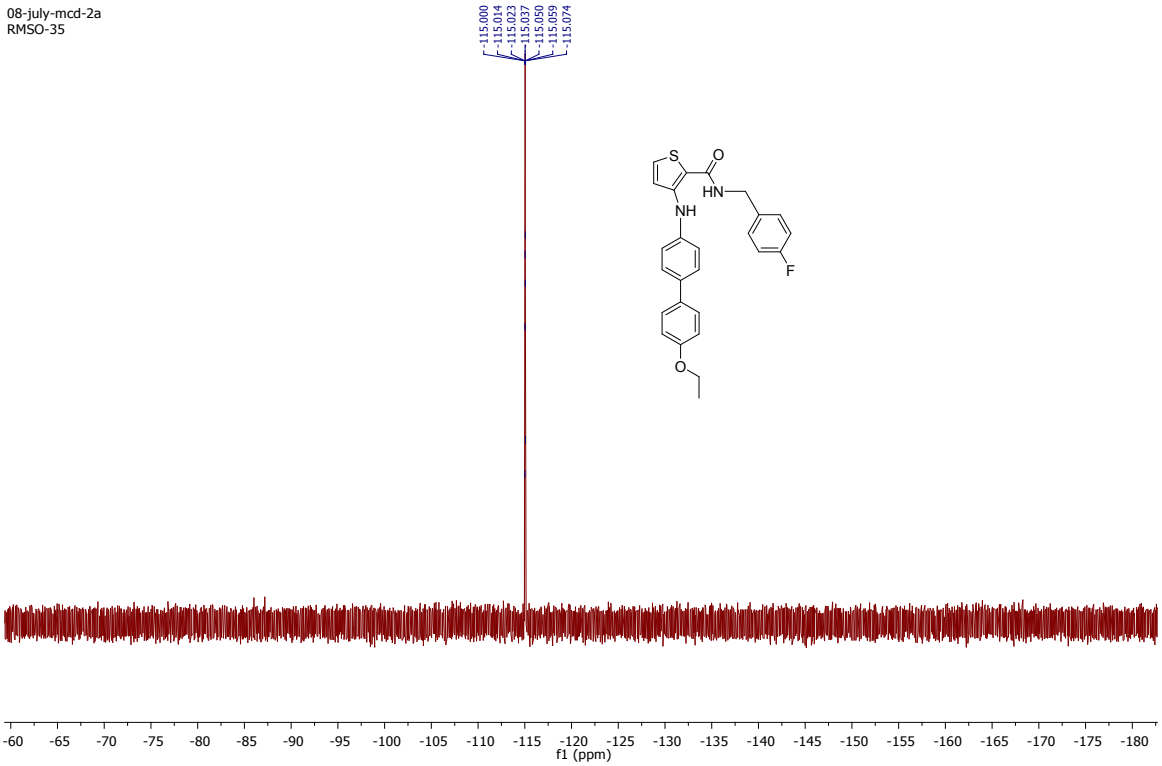


	Parameter	Value
1	Data File Name	E:/ OSI-930/ OSI-930 DATA/ RMSO-35/ fid
2	Title	May22-2012 -purnima
3	Comment	RMSO-35
4	Origin	Bruker BioSpin GmbH
5	Owner	IIIM
6	Site	
7	Spectrometer	spect
8	Author	
9	Solvent	CDCl3
10	Temperature	300.0
11	Pulse Sequence	zg30
12	Number of Scans	16
13	Receiver Gain	90
14	Relaxation Delay	0.5000
15	Pulse Width	13.1000
16	Acquisition Time	3.9846
17	Acquisition Date	2012-05-22T 16:32:00
18	Modification Date	2014-04-03T 20:19:55
19	Spectrometer Frequency	400.13
20	Spectral Width	8223.7
21	Lowest Frequency	-2671.3
22	Nucleus	1H
23	Acquired Size	32768
24	Spectral Size	65536

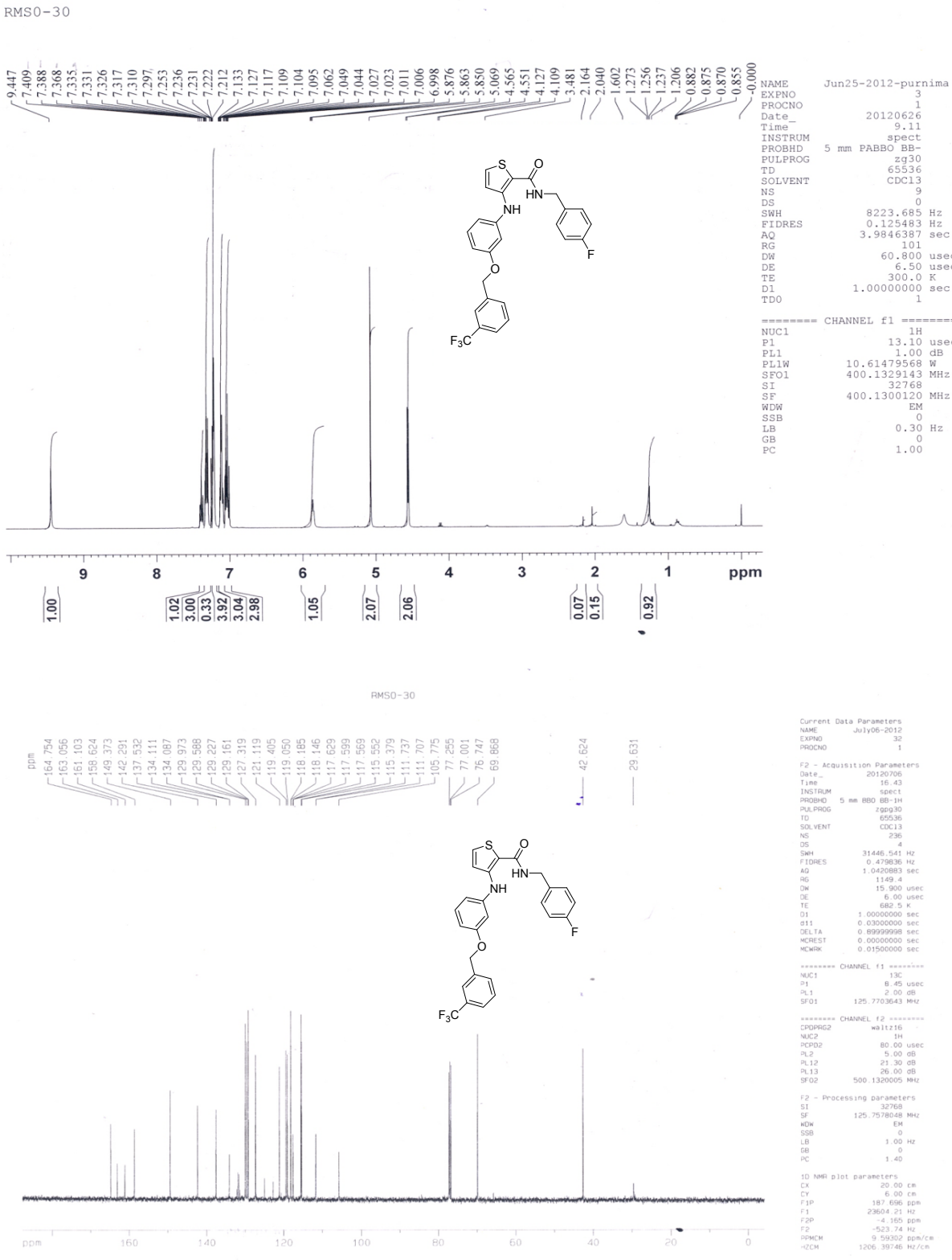


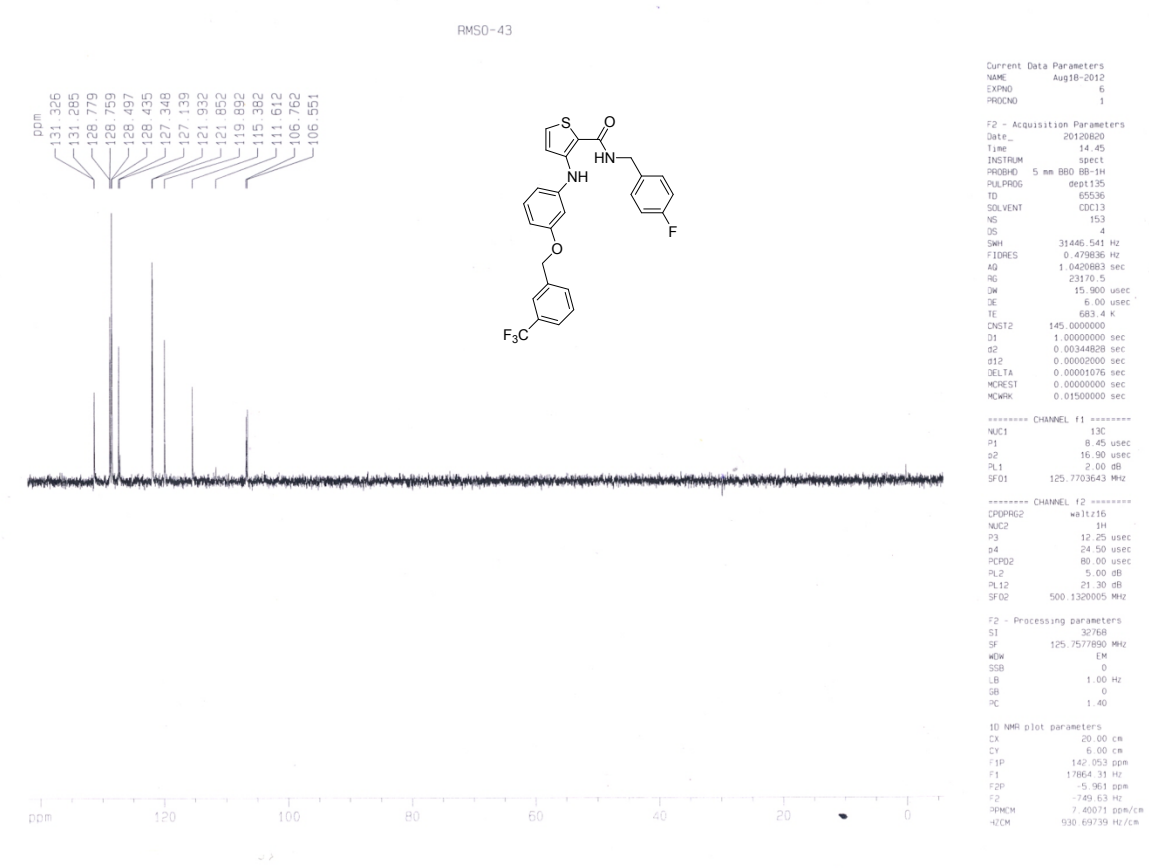
NAME	July09-2012-purnima
EXPNO	1
PROCNO	1
Date_	20120709
Time	15.36
INSTRUM	spect
PROBHD	5 mm PABBO BB-
PULPROG	zgpg30
TD	65536
SOLVENT	CDCl3
NS	3236
DS	4
SWH	25252.525 Hz
FIDRES	0.385323 Hz
AQ	1.2976629 sec
RG	203
DW	19.800 usec
DE	6.50 usec
TE	300.0 K
D1	1.00000000 sec
D11	0.03000000 sec
TD0	1
======== CHANNEL f1 ========	
NUC1	13C
P1	9.20 usec
PL1	-2.40 dB
PL1W	63.73131180 W
SFO1	100.6228298 MHz
======== CHANNEL f2 ========	
CPDPRG2	waltz16
NUC2	1H
PCPD2	80.00 usec
PL2	1.00 dB
PL12	16.72 dB
PL13	20.00 dB
PL2W	10.61479568 W
PL12W	0.28438827 W
PL13W	0.13363236 W
SFO2	400.1316005 MHz
SI	32768
SF	100.6127669 MHz
WDW	EM
SSB	0
LB	1.00 Hz
GB	0
PC	1.40

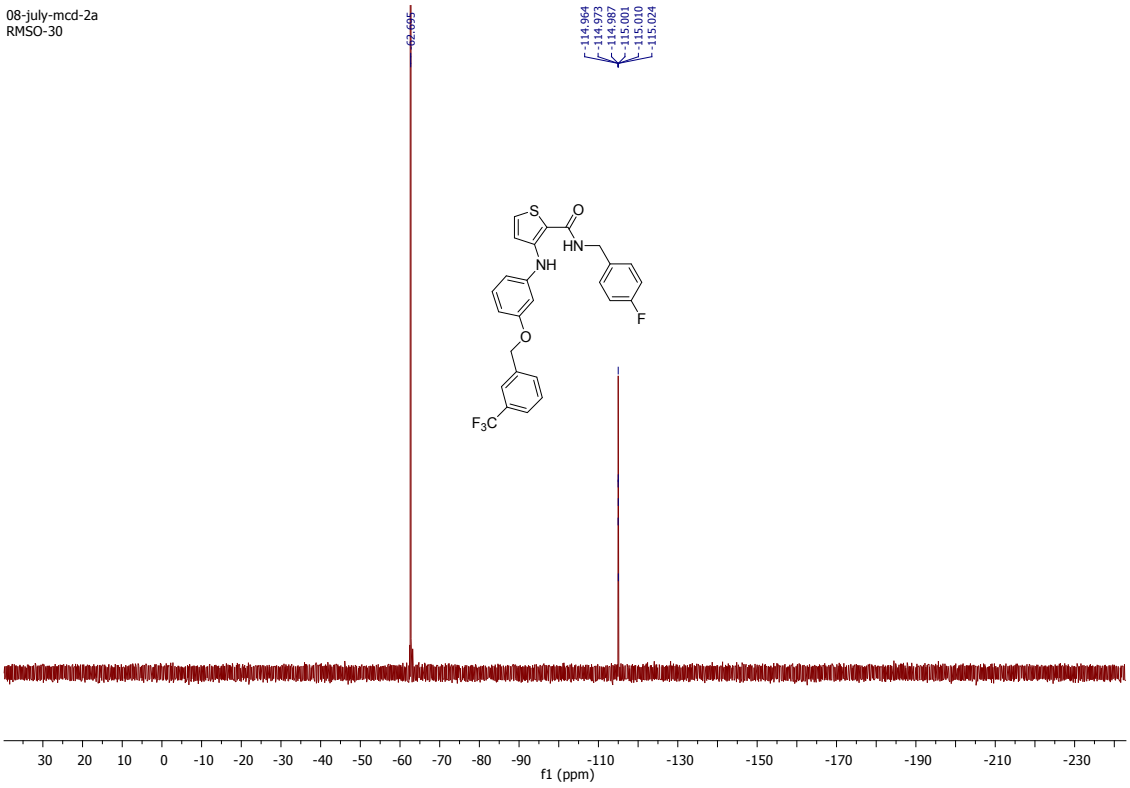

PJ -35
129.34
129.16
127.90
127.32
127.10
119.91
119.30
115.57
115.35
114.67
63.39
42.62
14.73
S
O
HN
NH
F
O
NAME July09-2012-purnima
EXPNO 2
PROCNO 1
Date_ 20120710
Time 14.58
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 837
DS 4
SWH 25252.525 Hz
FIDRES 0.385323 Hz
AQ 1.2976629 sec
RG 203
DW 19.800 usec
DE 6.50 usec
TE 300.0 K
CNST2 145.0000000
D1 1.00000000 sec
D2 0.00344828 sec
D12 0.00002000 sec
TD0 1
CHANNEL f1
NUC1 13C
P1 9.20 usec
P2 18.40 usec
PL1 -2.40 dB
PL1W 63.73131180 W
SFO1 100.6228298 MHz
CHANNEL f2
CPDPRG2 waltz16
NUC2 1H
P3 13.10 usec
P4 26.20 usec
PCPD2 80.00 usec
PL2 1.00 dB
PL12 16.72 dB
PL2W 10.61479568 W
PL12W 0.28438827 W
SFO2 400.1316005 MHz
SI 32768
SF 100.6127829 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
130 120 110 100 90 80 70 60 50 40 30 20 10 ppm


08-july-mcd-2a
RMSO-35
-115.000
-115.014
-115.023
-115.037
-115.050
-115.059
-115.074
S
O
HN
NH
F
O
-60 -65 -70 -75 -80 -85 -90 -95 -100 -105 -110 -115 -120 -125 -130 -135 -140 -145 -150 -155 -160 -165 -170 -175 -180
f1 (ppm)

N-(4-Fluorobenzyl)-3-((3-((3-(trifluoromethyl)benzyl)oxy)phenyl)amino)thiophene-2-carboxamide (**1w**).




RMSO-43
ppm
131.326
131.285
128.779
128.759
128.497
128.435
127.348
127.139
121.932
121.852
119.892
115.382
111.612
106.762
106.551
S
O
HN
NH
O
F
F3C
ppm
120
100
80
60
40
20
0
Current Data Parameters
NAME Aug18-2012
EXPNO 6
PROCNO 1
F2 - Acquisition Parameters
Date_ 20120820
Time 14.45
INSTRUM spect
PROBHD 5 mm BBO BB-1H
PULPROG dept135
TD 65536
SOLVENT CDCl3
NS 153
DS 4
SWH 31446.541 Hz
FIDRES 0.479836 Hz
AQ 1.0420883 sec
RG 23170.5
DW 15.900 usec
DE 6.00 usec
TE 683.4 K
CNST2 145.0000000
D1 1.00000000 sec
d2 0.00344828 sec
d12 0.00002000 sec
DELTA 0.00001076 sec
MCREST 0.00000000 sec
MCWRK 0.01500000 sec
======== CHANNEL f1 ========
NUC1 13C
P1 8.45 usec
p2 16.90 usec
PL1 2.00 dB
SF01 125.7703643 MHz
======== CHANNEL f2 ========
CPDPRG2 waltz16
NUC2 1H
P3 12.25 usec
p4 24.50 usec
PCPD2 80.00 usec
PL2 5.00 dB
PL12 21.30 dB
SF02 500.1320005 MHz
F2 - Processing parameters
SI 32768
SF 125.7577890 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40
1D NMR plot parameters
CX 20.00 cm
CY 6.00 cm
F1P 142.053 ppm
F1 17864.31 Hz
F2P -5.961 ppm
F2 -749.63 Hz
PPMCM 7.40071 ppm/cm
HZCM 930.69739 Hz/cm


08-july-mcd-2a
RMSO-30
-62.695
-114.964
-114.973
-114.987
-115.001
-115.010
-115.024
S
O
HN
NH
O
F
F3C
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-80
-90
-110
-130
-150
-170
-190
-210
-230
f1 (ppm)

S2. HPLC data of 1a-w.

Method-A: Shimadzu LC 10-AT; isocratic flow (water: acetonitrile (10: 90), 0.4 ml/min; Column: RP-18 (Merck, 5 µ, 4 × 250 mm), temp 30 °C, run time: 45 min.

Method-B: Shimadzu LC-6AD; isocratic flow Water: Methanol (30: 70), 1 ml/min, Column: Inertsil C8 (3.5 µ, 4.6 × 250 mm), run time: 30 min.

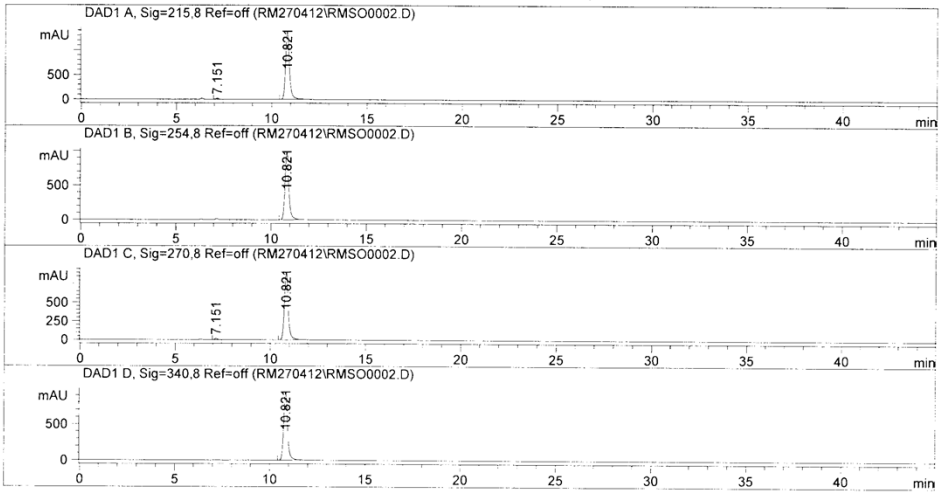
Code	Method	tR (min)	Purity (%)
1a	A	10.82	100.0
1b	A	9.19	100.0
1c	A	12.91	100.0
1d	A	13.20	97.2
1e	B	9.73	99.7
1f	B	5.07	99.0
1g	B	16.44	99.6
1h	B	10.36	100.0
1i	B	12.35	100.0
1j	B	19.88	97.2
1k	B	9.99	96.7
1l	B	7.62	98.9
1m	B	4.91	98.1
1n	B	9.64	98.8
1o	B	11.92	99.2
1p	B	5.10	93.1
1q	B	23.67	99.0
1s	B	18.06	99.6
1t	B	8.34	100
1u	B	9.59	100
1v	B	5.14	100

HPLC scan copies:

3-((4-((4-Fluorobenzyl)oxy)phenyl)amino)-N-(4-(trifluoromethoxy)phenyl)thiophene-2-carboxamide (**1a**).

Data File C:\HPCHEM\1\DATA\RM270412\RMSO0002.D Sample Name: RMSO-11

Injection Date : 4/27/2012 5:21:59 PM Seq. Line : 2
Sample Name : RMSO-11 Vial : 1
Acq. Operator : Vikram Bhardwaj Inj : 1
Inj Volume : 5 µl
Method : C:\HPCHEM\1\METHODS\VIK.M
Last changed : 4/27/2012 4:31:57 PM by Vikram Bhardwaj



Area Percent Report

Sorted By : Signal
Multiplier : 1.0000
Dilution : 1.0000

Signal 1: DAD1 A, Sig=215,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.151	PBA	0.1424	249.06676	26.81124	1.2119
2	10.821	PBA	0.2227	2.03022e4	1387.28345	98.7881
Totals :				2.05513e4	1414.09468	

Signal 2: DAD1 B, Sig=254,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.821	BBA	0.2186	1.42749e4	987.69446	100.0000
Totals :				1.42749e4	987.69446	

Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=270,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.151	PBA	0.1423	192.51022	20.72971	1.4399
2	10.821	BBA	0.2186	1.31774e4	912.06769	98.5601
Totals :				1.33699e4	932.79740	

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=340,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	10.821	BBA	0.2193	1.37755e4	949.19098	100.0000
Totals :				1.37755e4	949.19098	

Results obtained with enhanced integrator!

*** End of Report ***

*3-(Quinolin-3-ylamino)-N-(4-(trifluoromethoxy)phenyl)thiophene-2-carboxamide (**1b**).*

Data File C:\HPCHEM\1\DATA\NPC\RM000008.D Sample Name: RMSO-14

```
==========================================================================
Injection Date  : 4/30/2012 4:15:36 PM
Sample Name     : RMSO-14                          Vial :   2
Acq. Operator   : Vikram Bhardwaj
                                                   Inj Volume : 5 µl
Method          : C:\HPCHEM\1\METHODS\VIK.M
Last changed    : 4/30/2012 2:12:06 PM by Vikram Bhardwaj
                  (modified after loading)
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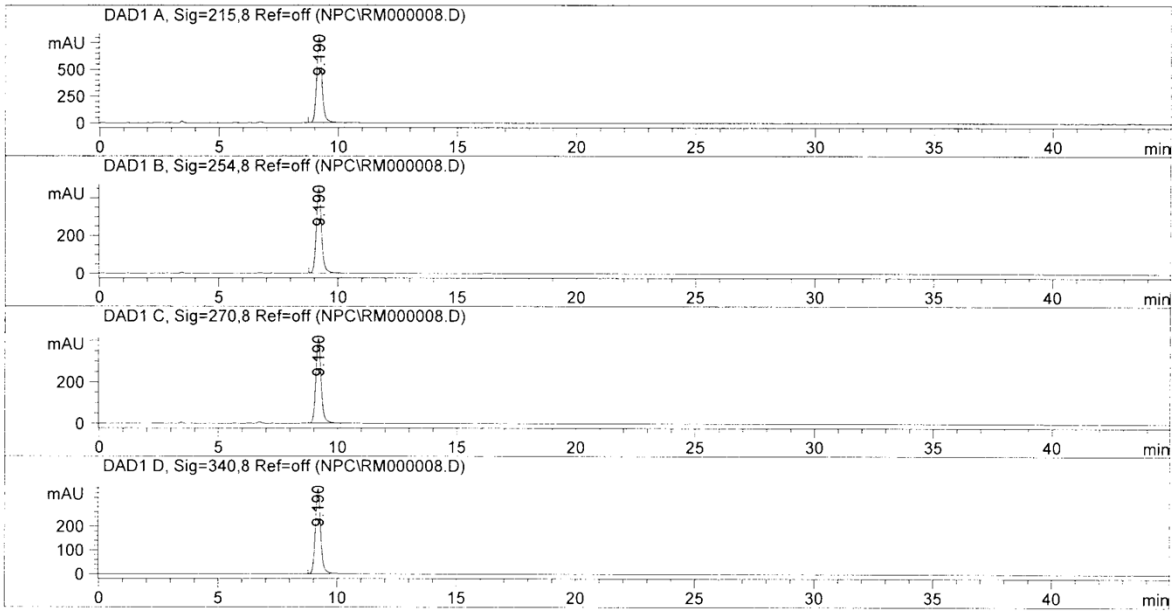



```
==========================================================================
                        Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000


Signal 1: DAD1 A, Sig=215,8 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------
   1   9.190 BBA   0.2365 1.22938e4   794.78577 100.0000

Totals :                  1.22938e4   794.78577

 Results obtained with enhanced integrator!
```

Signal 2: DAD1 B, Sig=254,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.190	BBA	0.2360	6951.86279	450.69421	100.0000
Totals :				6951.86279	450.69421	

Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=270,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.190	BBA	0.2360	6317.55078	409.56714	100.0000
Totals :				6317.55078	409.56714	

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=340,8 Ref=off

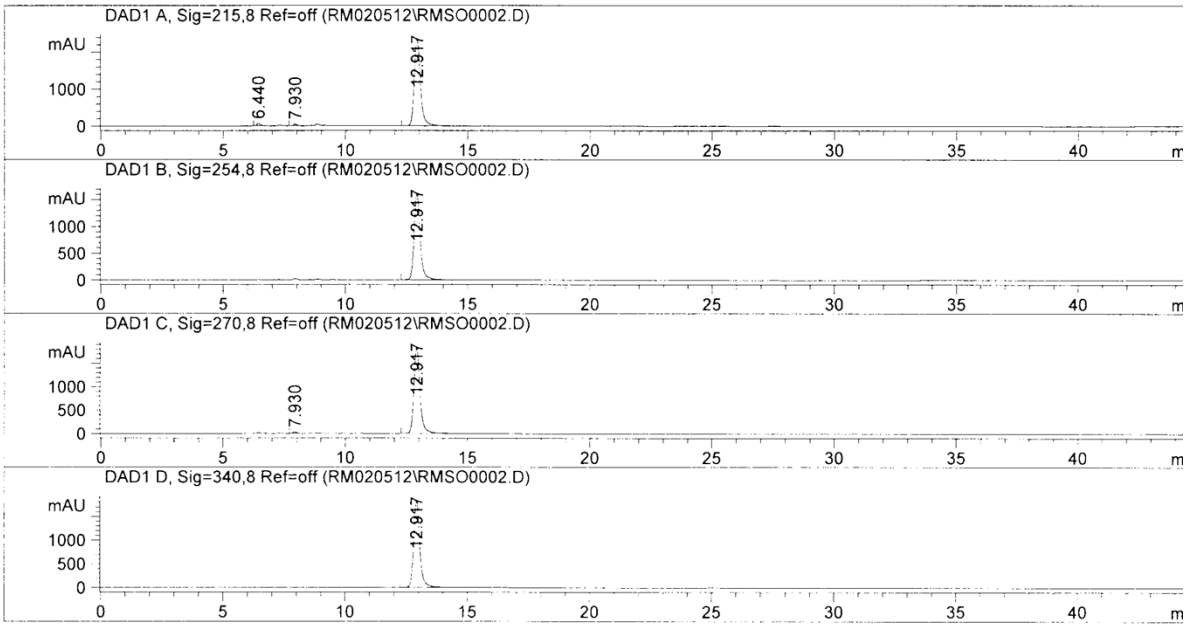
Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.190	PBA	0.2357	5511.81592	357.77042	100.0000
Totals :				5511.81592	357.77042	

Results obtained with enhanced integrator!

*** End of Report ***

*N-(4-(Trifluoromethoxy)phenyl)-3-((4-((3-(trifluoromethyl)benzyl)oxy)phenyl)amino)thiophene-2-carboxamide (**1c**).*

```
==========================================================================
Injection Date  : 5/2/2012 6:03:12 PM            Seq. Line :   2
Sample Name     : RMSO-27                             Vial :   1
Acq. Operator   : Vikram Bhardwaj                      Inj :   1
                                                 Inj Volume : 5 µl
Method          : C:\HPCHEM\1\METHODS\VIK.M
Last changed    : 5/2/2012 5:14:02 PM by Vikram Bhardwaj
```




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

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000


Signal 1: DAD1 A, Sig=215,8 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.440 BBA   0.1533  741.37158   71.29202   1.7167
   2   7.930 BB    0.1573  547.03418   53.48403   1.2667
   3  12.917 BBA   0.2681 4.18970e4  2371.92480  97.0166

Totals :                  4.31854e4  2496.70085

 Results obtained with enhanced integrator!
```

Signal 2: DAD1 B, Sig=254,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.917	PBA	0.2642	2.82265e4	1628.65881	100.0000
Totals :				2.82265e4	1628.65881	

Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=270,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	7.930	PB	0.1577	389.88022	37.99956	1.1965
2	12.917	PBA	0.2646	3.21951e4	1854.11304	98.8035
Totals :				3.25850e4	1892.11260	

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=340,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	12.917	PBA	0.2666	3.24318e4	1849.15161	100.0000
Totals :				3.24318e4	1849.15161	

Results obtained with enhanced integrator!

*** End of Report ***

*N-(4-(Trifluoromethoxy)phenyl)-3-((3-((3-(trifluoromethyl)benzyl)oxy)phenyl)amino)thiophene-2-carboxamide (**1d**).*

```
==========================================================================
Injection Date  : 5/2/2012 6:49:56 PM            Seq. Line :   3
Sample Name     : RMSO-28                            Vial :   2
Acq. Operator   : Vikram Bhardwaj                     Inj :   1
                                                 Inj Volume : 5 µl
Method          : C:\HPCHEM\1\METHODS\VIK.M
Last changed    : 5/2/2012 5:14:02 PM by Vikram Bhardwaj
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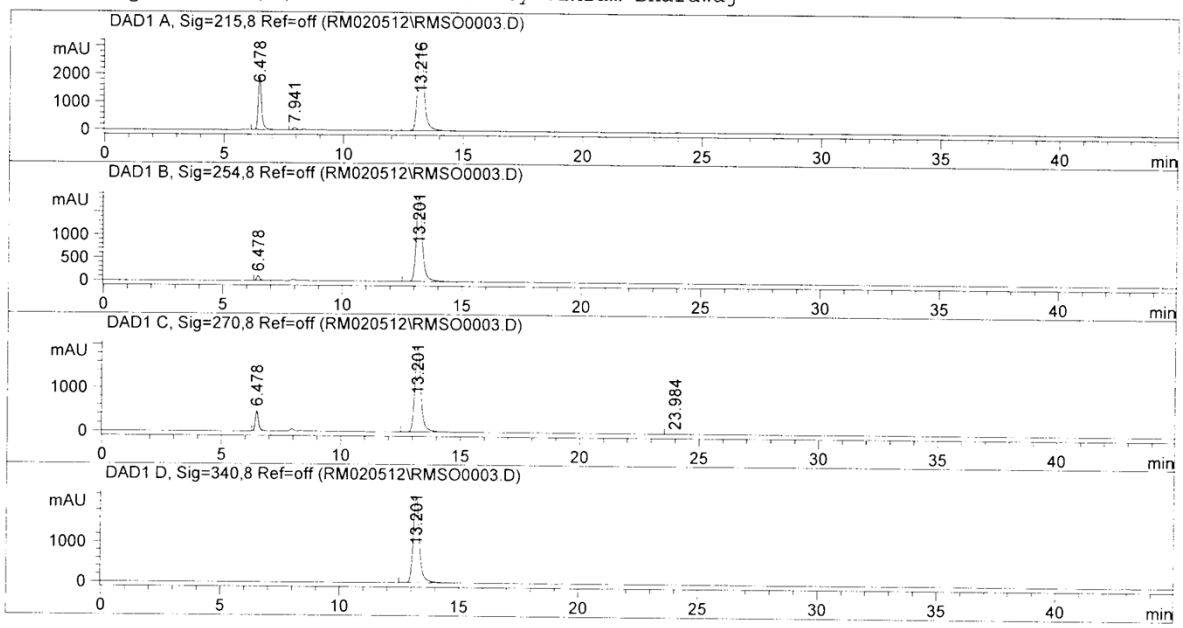



```
==========================================================================
                          Area Percent Report
==========================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000


Signal 1: DAD1 A, Sig=215,8 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   6.478 PBA   0.1485 1.85812e4  1893.67615  23.2856
   2   7.941 PB    0.1525  819.66077   83.50230   1.0272
   3  13.216 BBA   0.3042 6.03961e4  3060.24976  75.6872
```

Signal 2: DAD1 B, Sig=254,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.478	BBA	0.1418	943.09802	100.23803	2.7669
2	13.201	PBA	0.2693	3.31413e4	1865.07751	97.2331
Totals :				3.40844e4	1965.31554	

Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=270,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	6.478	BB	0.1406	4357.50342	468.31680	11.0300
2	13.201	PBA	0.2695	3.50368e4	1970.33972	88.6876
3	23.984	BBA	0.4051	111.55297	3.97816	0.2824
Totals :				3.95059e4	2442.63468	

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=340,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	13.201	PBA	0.2759	3.90696e4	2151.32568	100.0000
Totals :				3.90696e4	2151.32568	

Results obtained with enhanced integrator!

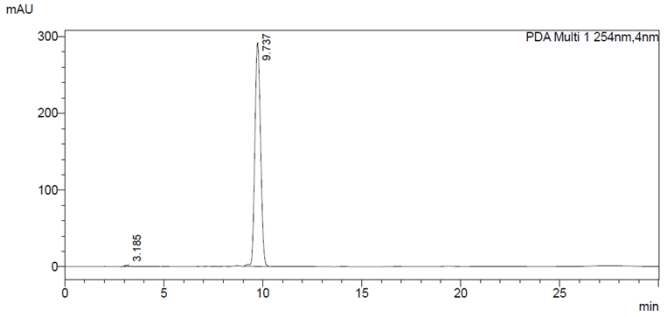
*** End of Report ***

*3-((3-Fluoro-[1,1'-biphenyl]-4-yl)amino)-N-(4-(trifluoromethoxy)phenyl)thiophene-2-carboxamide (**1e**).*

<Sample Information>

Sample Name	: RMSO-43		
Sample ID	: RMSO-43		
Data Filename	: RMSO-43.lcd		
Method Filename	: ramesh_iso_70-MeOH.lcm		
Batch Filename	: RAJNI KHELLIN NEW BATCH.lcb		
Vial #	: 1-2	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 12-09-2014 13:57:52	Acquired by	: System Administrator
Date Processed	: 12-09-2014 14:28:00	Processed by	: System Administrator

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

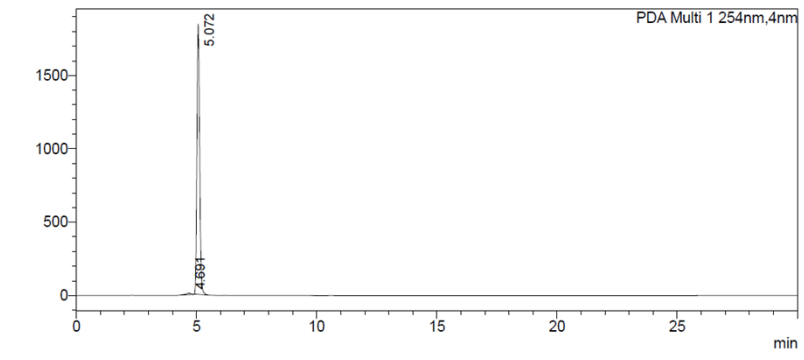
Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	3.185	14155	2001	2.965	3.243	0.243
2	9.737	5816760	291901	9.088	10.315	99.757
Total		5830915	293902			100.000

*3-((2,3-Dihydrobenzo[b][1,4]dioxin-6-yl)amino)-N-(4-(trifluoromethoxy)phenyl)thiophene-2-carboxamide (**1f**).*

<Sample Information>

Sample Name	: RMSO-44		
Sample ID	: RMSO-44		
Data Filename	: RMSO-44R.lcd		
Method Filename	: ramesh_iso_70-MeOH.lcm		
Batch Filename	: RAJNI KHELLIN NEW BATCH.lcb		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 5 uL		
Date Acquired	: 13-09-2014 15:13:59	Acquired by	: System Administrator
Date Processed	: 13-09-2014 15:44:06	Processed by	: System Administrator

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

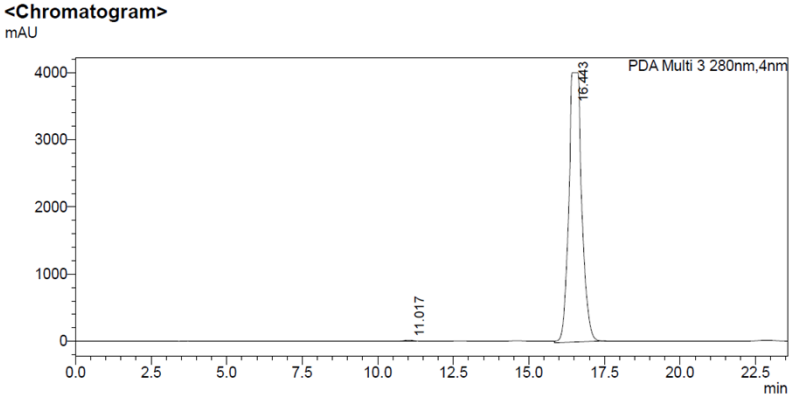
Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.691	135010	8876	4.373	4.885	0.931
2	5.072	14364000	1839424	4.885	5.461	99.069
Total		14499011	1848301			100.000

*3-((3-Bromo-5-fluorophenyl)amino)-N-(4-(trifluoromethoxy)phenyl)thiophene-2-carboxamide (**1g**).*

<Sample Information>

Sample Name	: RMSO-74		
Sample ID	: RMSO-74		
Data Filename	: RMSO-74.lcd		
Method Filename	: ramesh_iso_70-MeOH.lcm		
Batch Filename	: RAJNI KHELLIN NEW BATCH.lcb		
Vial #	: 1-5	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 12-09-2014 19:10:27	Acquired by	: System Administrator
Date Processed	: 12-09-2014 19:34:03	Processed by	: System Administrator

<Chromatogram>



<Peak Table>

PDA Ch3 280nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	11.017	461733	19575	10.549	11.275	0.383
2	16.443	120017268	4012610	15.851	17.557	99.617
Total		120479001	4032185			100.000

*3-((4-Fluorophenyl)amino)-N-(4-(trifluoromethoxy)phenyl)thiophene-2-carboxamide (**1h**).*

<Sample Information>

Sample Name	: RMSO-82		
Sample ID	: RMSO-82		
Data Filename	: RMSO-82.lcd		
Method Filename	: ramesh_iso_70-MeOH.lcm		
Batch Filename	: RAJNI KHELLIN NEW BATCH.lcb		
Vial #	: 1-4	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 12-09-2014 18:39:56	Acquired by	: System Administrator
Date Processed	: 12-09-2014 19:10:03	Processed by	: System Administrator

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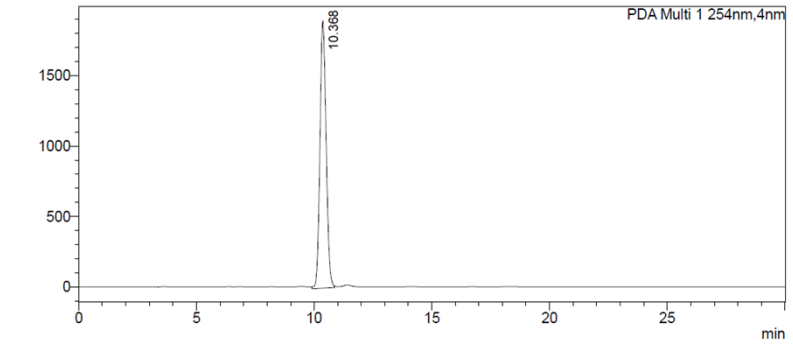


<Peak Table>

PDA Ch1 254nm

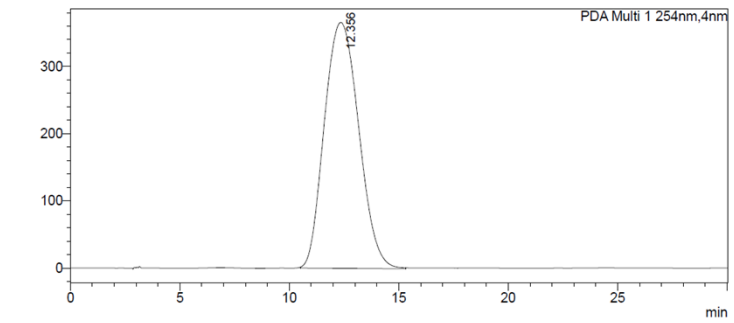
Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	10.368	34680411	1897650	9.909	10.869	100.000
Total		34680411	1897650			100.000

*N-(4-(Trifluoromethoxy)phenyl)-3-((3-(trifluoromethyl)phenyl)amino)thiophene-2-carboxamide (**1i**).*

<Sample Information>

Sample Name	: RMSO-84		
Sample ID	: RMSO-84		
Data Filename	: RMSO-84.lcd		
Method Filename	: ramesh_iso_70-MeOH.lcm		
Batch Filename	: RAJNI KHELLIN NEW BATCH.lcb		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 12-09-2014 13:24:20	Acquired by	: System Administrator
Date Processed	: 12-09-2014 13:54:28	Processed by	: System Administrator

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	12.356	40145989	366066	10.528	15.307	100.000
Total		40145989	366066			100.000

*N-(4-Fluorophenyl)-3-((4-((3-(trifluoromethyl)benzyl)oxy)phenyl)amino)thiophene-2-carboxamide (**1j**).*

<Sample Information>

Sample Name	: RMSO-63		
Sample ID	: RMSO-63		
Data Filename	: RMSO-63.lcd		
Method Filename	: ramesh_iso_70-MeOH.lcm		
Batch Filename	: RAJNI KHELLIN NEW BATCH.lcb		
Vial #	: 1-4	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 12-09-2014 14:58:58	Acquired by	: System Administrator
Date Processed	: 12-09-2014 15:29:05	Processed by	: System Administrator

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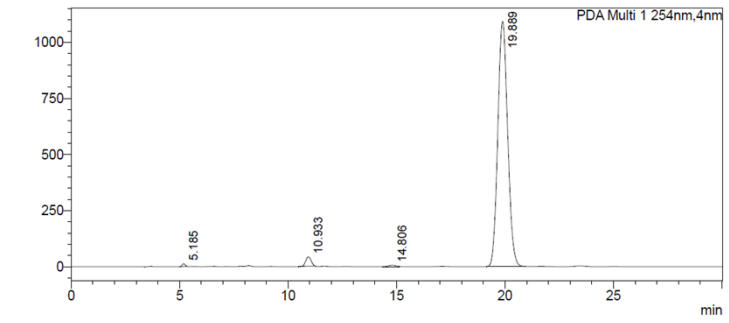

<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	5.185	116338	12850	5.013	5.333	0.328
2	10.933	699929	41303	10.485	11.264	1.973
3	14.806	145559	6212	14.325	15.115	0.410
4	19.889	34504941	1092754	19.136	20.949	97.288
Total		35466767	1153118			100.000

*3-((4-((4-Fluorobenzyl)oxy)phenyl)amino)-N-(4-fluorophenyl)thiophene-2-carboxamide (**1k**).*

<Sample Information>

Sample Name	: RMSO-64		
Sample ID	: RMSO-64		
Data Filename	: RMSO-64.lcd		
Method Filename	: ramesh_iso_70-MeOH.lcm		
Batch Filename	: RAJNI KHELLIN NEW BATCH.lcb		
Vial #	: 1-3	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 12-09-2014 18:09:23	Acquired by	: System Administrator
Date Processed	: 12-09-2014 18:39:31	Processed by	: System Administrator

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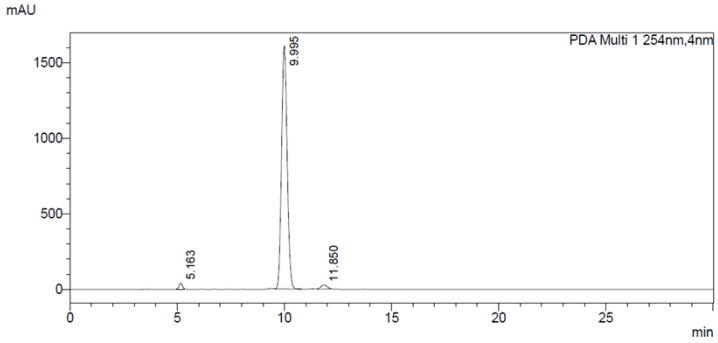


<Peak Table>

PDA Ch1 254nm

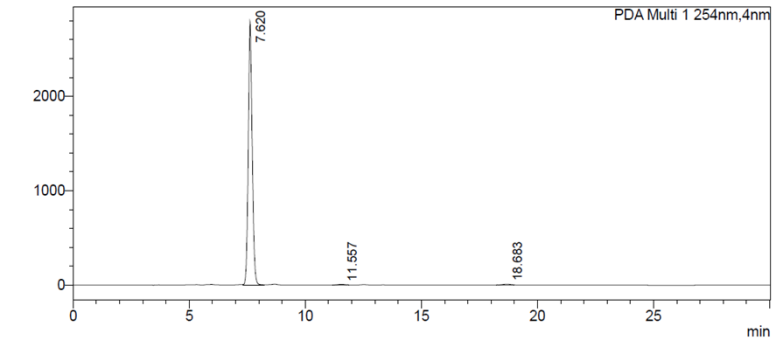
Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	5.163	434536	41907	4.981	5.312	1.433
2	9.995	29343126	1606736	9.525	10.763	96.775
3	11.850	543445	27428	11.552	12.160	1.792
Total		30321108	1676071			100.000

*3-(Benzo[d][1,3]dioxol-5-ylamino)-N-(4-fluorophenyl)thiophene-2-carboxamide (**1l**).*

<Sample Information>

Sample Name	: RMSO-66		
Sample ID	: RMSO-66		
Data Filename	: RMSO-66.lcd		
Method Filename	: ramesh_iso_70-MeOH.lcm		
Batch Filename	: RAJNI KHELLIN NEW BATCH.lcb		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 12 uL		
Date Acquired	: 12-09-2014 17:08:19	Acquired by	: System Administrator
Date Processed	: 12-09-2014 17:38:26	Processed by	: System Administrator

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

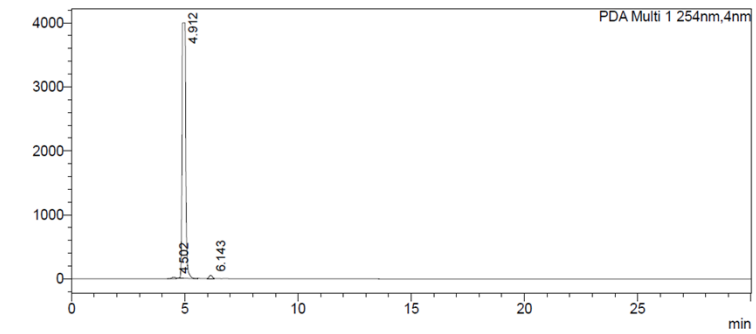
Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	7.620	32569905	2789735	7.296	8.235	98.939
2	11.557	149731	6863	11.168	11.861	0.455
3	18.683	199378	8166	18.240	18.987	0.606
Total		32919014	2804764			100.000

*3-((2,3-Dihydrobenzo[b][1,4]dioxin-6-yl)amino)-N-(4-fluorophenyl)thiophene-2-carboxamide (**1m**).*

<Sample Information>

Sample Name	: RMSO-71		
Sample ID	: RMSO-71		
Data Filename	: RMSO-71.lcd		
Method Filename	: ramesh_iso_70-MeOH.lcm		
Batch Filename	: RAJNI KHELLIN NEW BATCH.lcb		
Vial #	: 1-2	Sample Type	: Unknown
Injection Volume	: 12 uL		
Date Acquired	: 13-09-2014 12:45:29	Acquired by	: System Administrator
Date Processed	: 13-09-2014 13:15:35	Processed by	: System Administrator

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

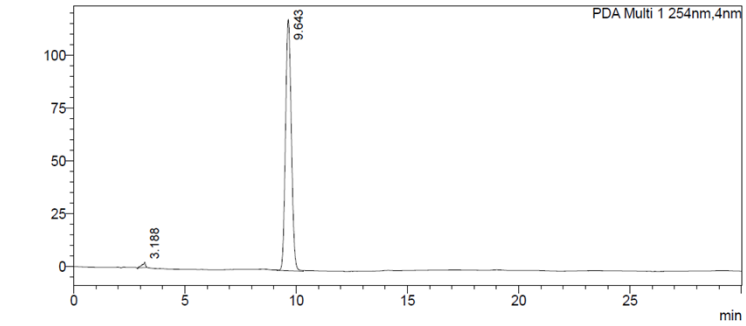
Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.502	254788	22256	4.245	4.608	0.566
2	4.912	44189655	3990988	4.704	5.557	98.137
3	6.143	584088	58054	5.984	6.315	1.297
Total		45028531	4071297			100.000

*3-((3-Fluoro-[1,1'-biphenyl]-4-yl)amino)-N-(4-fluorophenyl)thiophene-2-carboxamide (**1n**).*

<Sample Information>

Sample Name	: RMSO-68		
Sample ID	: RMSO-68		
Data Filename	: RMSO-68.lcd		
Method Filename	: rameshi_iso_60-MeOH.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 12-09-2014 12:41:31	Acquired by	: System Administrator
Date Processed	: 12-09-2014 13:11:38	Processed by	: System Administrator

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	3.188	24417	2446	2.912	3.253	1.115
2	9.643	2164672	118807	9.152	10.325	98.885
Total		2189088	121252			100.000

*3-((3-Bromo-5-fluorophenyl)amino)-N-(4-fluorophenyl)thiophene-2-carboxamide (**1o**).*

<Sample Information>

Sample Name	: RMSO-78		
Sample ID	: RMSO-78		
Data Filename	: RMSO-78.lcd		
Method Filename	: ramesh_iso_70-MeOH.lcm		
Batch Filename	: RAJNI KHELLIN NEW BATCH.lcb		
Vial #	: 1-2	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 12-09-2014 17:38:51	Acquired by	: System Administrator
Date Processed	: 12-09-2014 18:08:59	Processed by	: System Administrator

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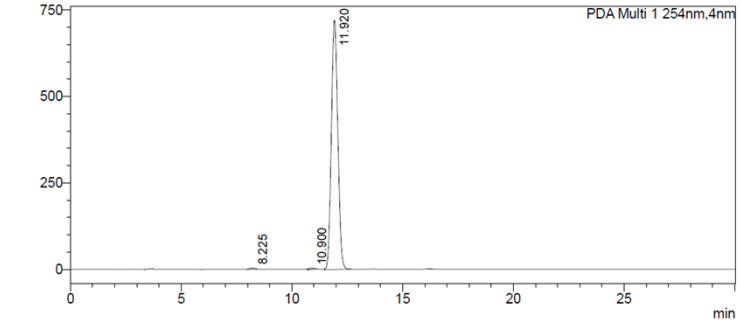


<Peak Table>

PDA Ch1 254nm

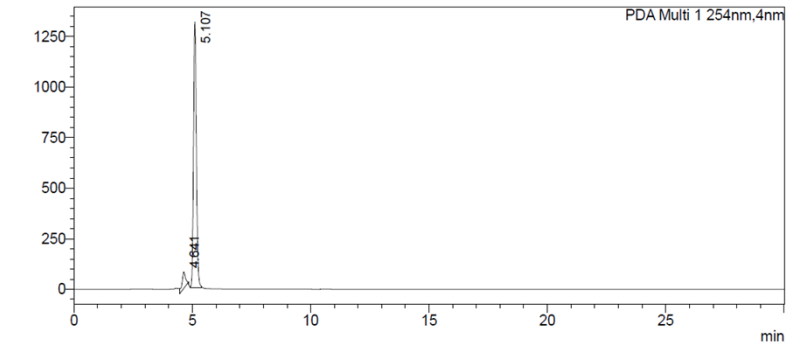
Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	8.225	47193	3568	7.968	8.416	0.321
2	10.900	66050	3791	10.688	11.072	0.450
3	11.920	14568282	721361	11.456	12.672	99.229
Total		14681524	728721			100.000

*3-((4-((4-Fluorobenzyl)oxy)phenyl)amino)-N-(4-(trifluoromethyl)phenyl)thiophene-2-carboxamide (**1p**).*

<Sample Information>

Sample Name	: RMSO-18		
Sample ID	: RMSO-18		
Data Filename	: RMSO-18		
Method Filename	: ramesh_iso_70-MeOH.lcm		
Batch Filename	: RAJNI KHELLIN NEW BATCH.lcb		
Vial #	: 1-3	Sample Type	: Unknown
Injection Volume	: 15 uL		
Date Acquired	: 13-09-2014 13:15:59	Acquired by	: System Administrator
Date Processed	: 13-09-2014 13:46:06	Processed by	: System Administrator

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	4.641	816119	80365	4.459	4.832	6.802
2	5.107	11181376	1316877	4.907	5.387	93.198
Total		11997495	1397242			100.000

*3-((3-Bromo-5-fluorophenyl)amino)-N-(4-chloro-3-(trifluoromethyl)phenyl)thiophene-2-carboxamide (**1q**).*

<Sample Information>

Sample Name	: RMSO-77		
Sample ID	: RMSO-77		
Data Filename	: RMSO-77.lcd		
Method Filename	: ramesh_iso_70-MeOH.lcm		
Batch Filename	: RAJNI KHELLIN NEW BATCH.lcb		
Vial #	: 1-6	Sample Type	: Unknown
Injection Volume	: 20 uL		
Date Acquired	: 12-09-2014 16:00:01	Acquired by	: System Administrator
Date Processed	: 12-09-2014 16:30:08	Processed by	: System Administrator

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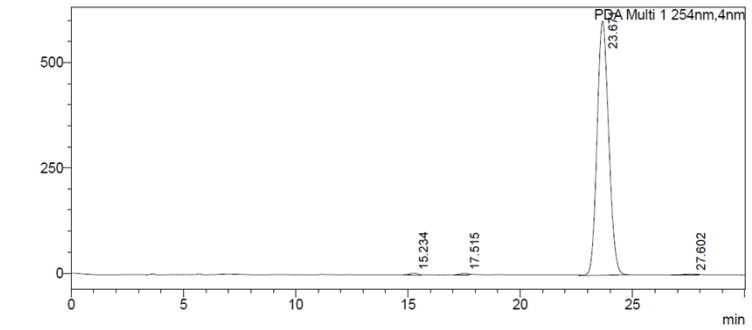


<Peak Table>

PDA Ch1 254nm

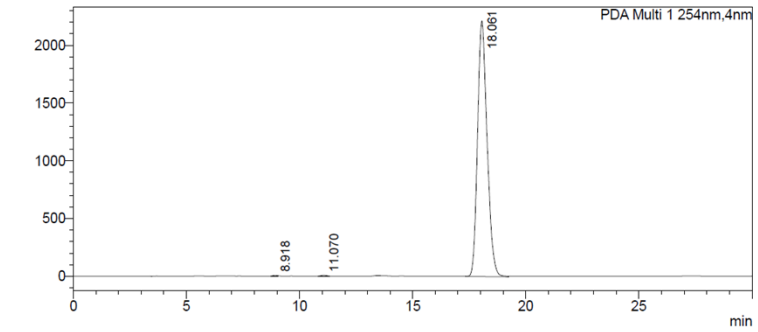
Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	15.234	104320	4339	14.795	15.573	0.476
2	17.515	62332	3098	17.067	17.707	0.285
3	23.671	21704369	603037	22.613	24.821	99.087
4	27.602	33391	1545	26.741	27.957	0.152
Total		21904412	612019			100.000

N-(4-Chloro-3-(trifluoromethyl)phenyl)-3-((3-(trifluoromethyl)phenyl)amino)thiophene-2-carboxamide (**1s**).

<Sample Information>

Sample Name	: RMSO-86		
Sample ID	: RMSO-86		
Data Filename	: RMSO-86.lcd		
Method Filename	: ramesh_iso_70-MeOH.lcm		
Batch Filename	:		
Vial #	: 1-1	Sample Type	: Unknown
Injection Volume	: 10 uL		
Date Acquired	: 12-09-2014 16:32:49	Acquired by	: System Administrator
Date Processed	: 12-09-2014 17:02:56	Processed by	: System Administrator

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	8.918	126795	8575	8.715	9.056	0.194
2	11.070	125263	7694	10.816	11.307	0.192
3	18.061	65011071	2212030	17.344	19.221	99.614
Total		65263130	2228299			100.000

*N-(4-Fluorobenzyl)-3-((4-((4-fluorobenzyl)oxy)phenyl)amino)thiophene-2-carboxamide (**1t**).*

```
==================================================================
Injection Date  : 4/27/2012 7:42:11 PM          Seq. Line :   5
Sample Name     : RMSO-20                            Vial :   4
Acq. Operator   : Vikram Bhardwaj                     Inj :   1
                                                 Inj Volume : 5 µl
Method          : C:\HPCHEM\1\METHODS\VIK.M
Last changed    : 4/27/2012 4:31:57 PM by Vikram Bhardwaj
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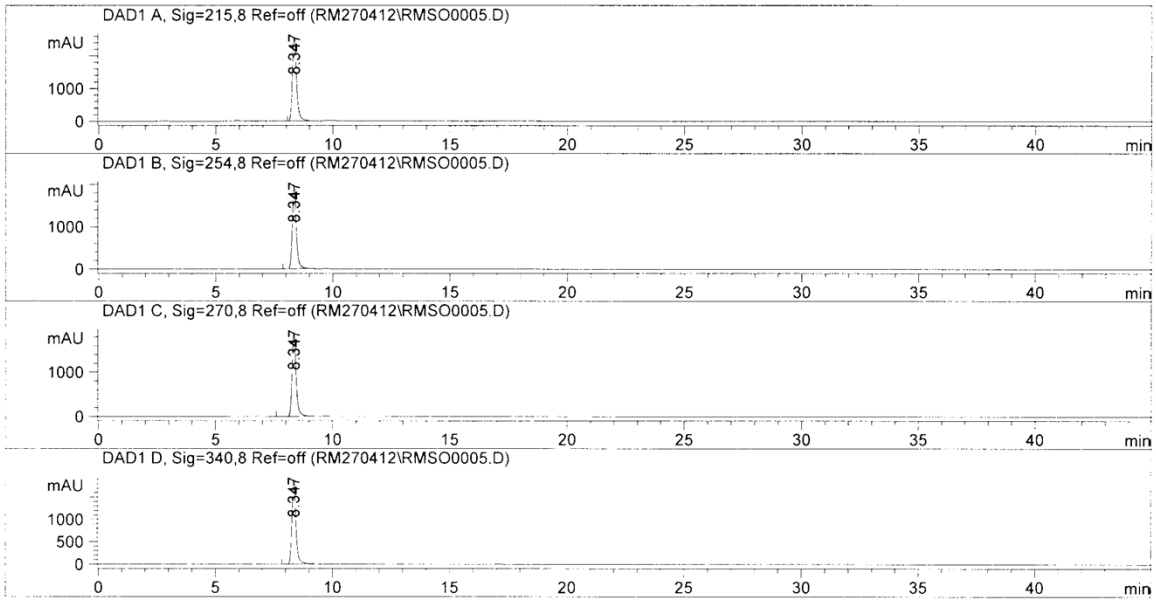


```
==================================================================
                      Area Percent Report
==================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000


Signal 1: DAD1 A, Sig=215,8 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]    [mAU*s]     [mAU]      %
----|-------|----|-------|----------|----------|--------|
   1   8.347 BB    0.1931 3.23580e4  2565.96948 100.0000

Totals :                  3.23580e4  2565.96948

 Results obtained with enhanced integrator!
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.347	PBA	0.1800	2.32982e4	1969.34448	100.0000
Totals :				2.32982e4	1969.34448	

Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=270,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.347	BB	0.1805	2.23989e4	1886.87854	100.0000
Totals :				2.23989e4	1886.87854	

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=340,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	8.347	PBA	0.1816	2.24881e4	1879.39197	100.0000
Totals :				2.24881e4	1879.39197	

Results obtained with enhanced integrator!

*** End of Report ***

N-(4-Fluorobenzyl)-3-((4-((3-(trifluoromethyl)benzyl)oxy)phenyl)amino)thiophene-2-carboxamide (**1u**).

```
======================================================================
Injection Date  : 5/2/2012 7:36:40 PM          Seq. Line :   4
Sample Name     : RMSO-29                           Vial :   3
Acq. Operator   : Vikram Bhardwaj                    Inj :   1
                                                Inj Volume : 5 µl
Method          : C:\HPCHEM\1\METHODS\VIK.M
Last changed    : 5/2/2012 5:14:02 PM by Vikram Bhardwaj
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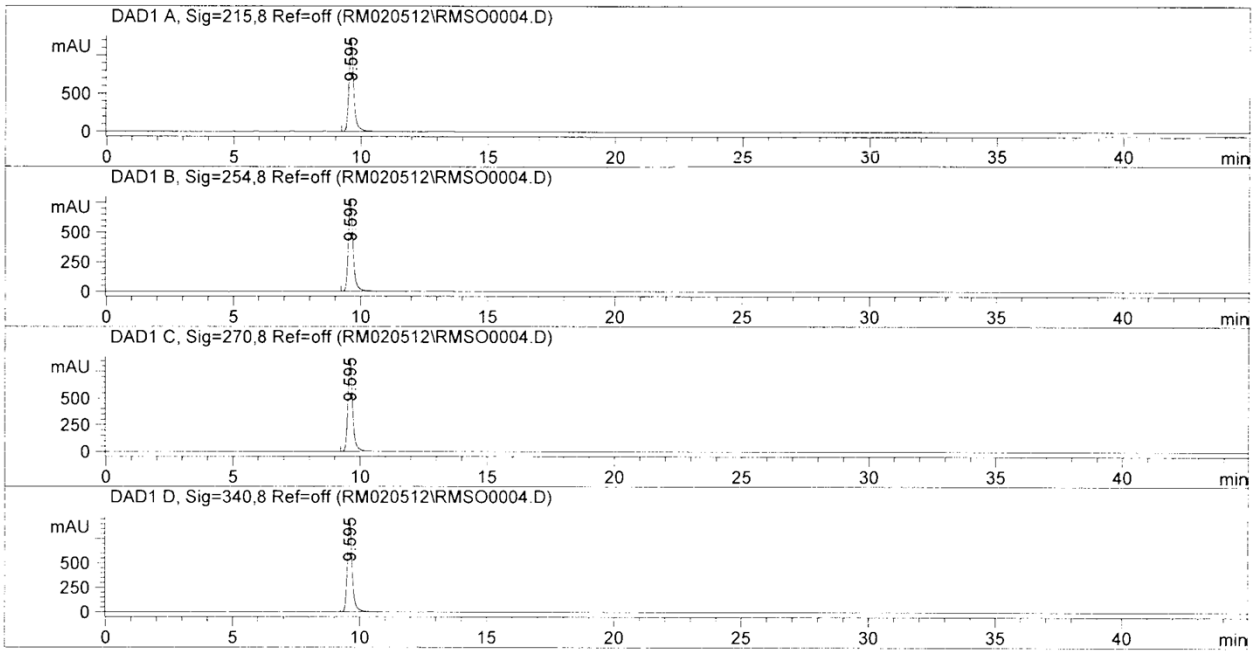



```
======================================================================
                        Area Percent Report
======================================================================

Sorted By             :      Signal
Multiplier            :      1.0000
Dilution              :      1.0000


Signal 1: DAD1 A, Sig=215,8 Ref=off

Peak RetTime Type  Width     Area      Height     Area
  #   [min]        [min]   [mAU*s]     [mAU]       %
----|-------|----|-------|----------|----------|--------|
   1   9.595 BBA   0.2042 1.59957e4  1194.60864 100.0000

Totals :                  1.59957e4  1194.60864
```

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.595	BBA	0.2003	1.00497e4	759.91925	100.0000
Totals :				1.00497e4	759.91925	

Results obtained with enhanced integrator!

Signal 3: DAD1 C, Sig=270,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.595	BBA	0.2026	1.12314e4	847.77570	100.0000
Totals :				1.12314e4	847.77570	

Results obtained with enhanced integrator!

Signal 4: DAD1 D, Sig=340,8 Ref=off

Peak #	RetTime [min]	Type	Width [min]	Area [mAU*s]	Height [mAU]	Area %
1	9.595	PBA	0.2029	1.23191e4	928.04987	100.0000
Totals :				1.23191e4	928.04987	

Results obtained with enhanced integrator!

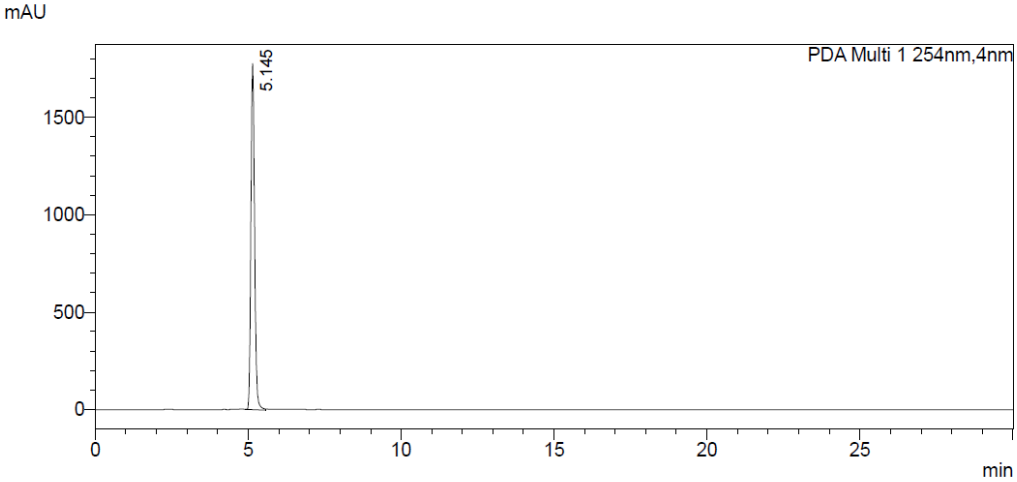
*** End of Report ***

3-((4'-Ethoxy-[1,1'-biphenyl]-4-yl)amino)-N-(4-fluorobenzyl)thiophene-2-carboxamide (**1v**).

<Sample Information>

Sample Name	: RMSO-35		
Sample ID	:RMSO-35		
Data Filename	: RMSO-35 R.lcd		
Method Filename	: ramesh_iso_80-MeOH.lcm		
Batch Filename	: RAJNI KHELLIN NEW BATCH.lcb		
Vial #	: 1-6	Sample Type	: Unknown
Injection Volume	: 15 uL		
Date Acquired	: 13-09-2014 14:40:17	Acquired by	: System Administrator
Date Processed	: 13-09-2014 15:10:25	Processed by	: System Administrator

<Chromatogram>



<Peak Table>

PDA Ch1 254nm

Peak#	Ret. Time	Area	Height	Peak Start	Peak End	Area%
1	5.145	14881309	1777005	4.917	5.579	100.000
Total		14881309	1777005			100.000

S3. Structures of thiophene-2-carboxamides **1a-w**

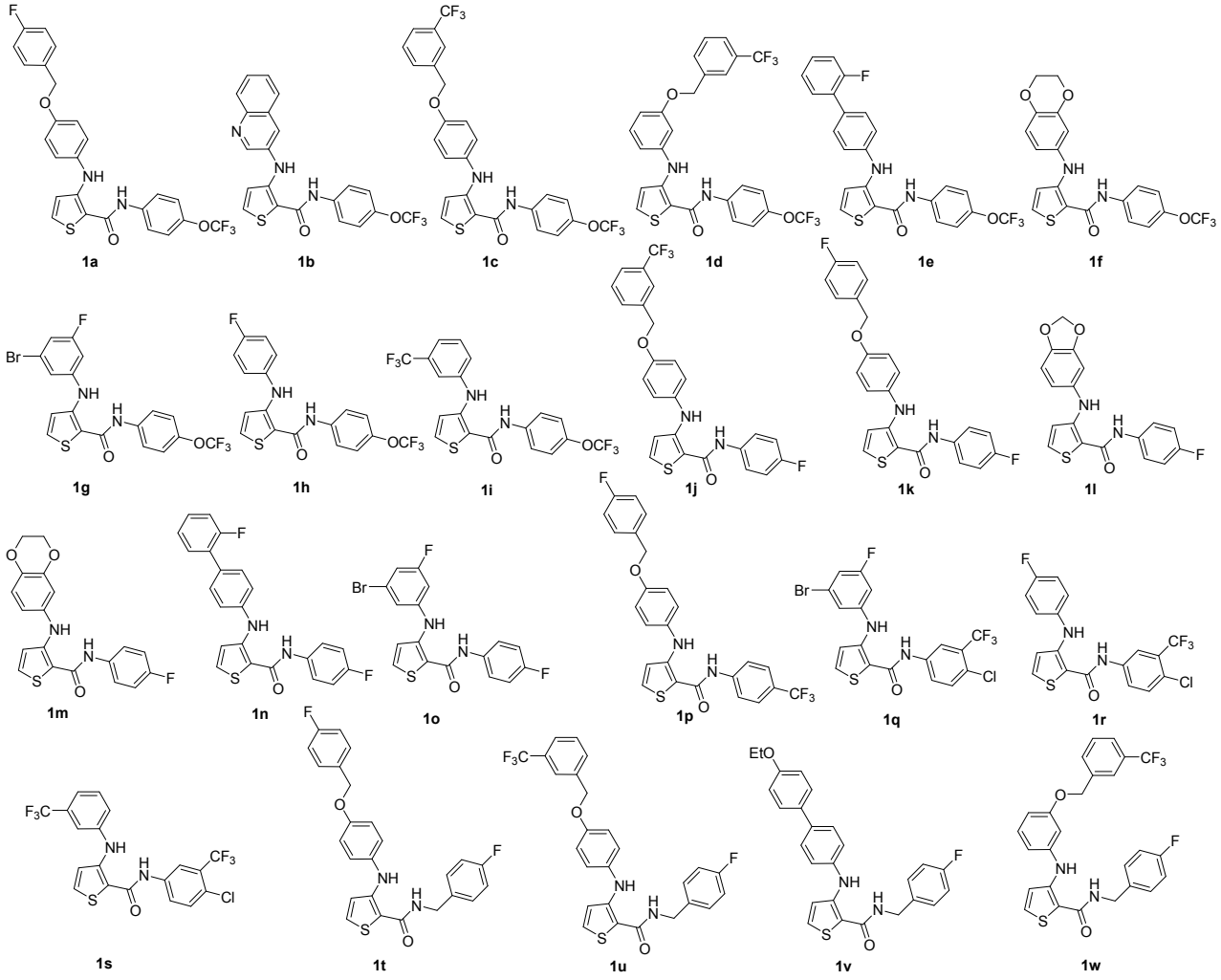


Figure S1. Structures of thiophene-2-carboxamides **1a-w**

S4. **MTT assay of combined treatment of doxorubicin with P-gp inhibitors 1l and 1m:**

MTT assay was performed to determine the cell viability. Cells were seeded in 96 well plates and exposed to different concentrations of synthesize molecules for 48 h. MTT dye (2.5 mg/ml in PBS) was added 4 hours priors to experiment termination. The plates were then centrifuged at 1500 RPM for 15 min and the supernatant was discarded, while the MTT formazan crystals were dissolved in 150 µL of DMSO. The OD measured at 570 nm with reference wavelength of 620 nm. For MTT assay of combined treatment of doxorubicin and P-gp inhibitors **1l** and **1m**, different concentrations of doxorubicin (ranging from 2.5 µM to 0.0097 µM along with 50 µM of P-gp inhibitors were used. Details are provided below.

Doxorubicin (µM)	**1l** or **1m** (µM)	Molar ratio of doxorubicin with P-gp inhibitors
2.5	50	1: 20
1.25	50	1: 40
0.625	50	1: 80
0.3125	50	1: 160
0.1562	50	1: 320
0.0781	50	1: 640
0.0390	50	1: 1282
0.0195	50	1: 2564
0.0097	50	1: 5154