Discovery of Dual Target Inhibitors against Cyclooxygenases and Leukotriene A_4 Hydrolyase

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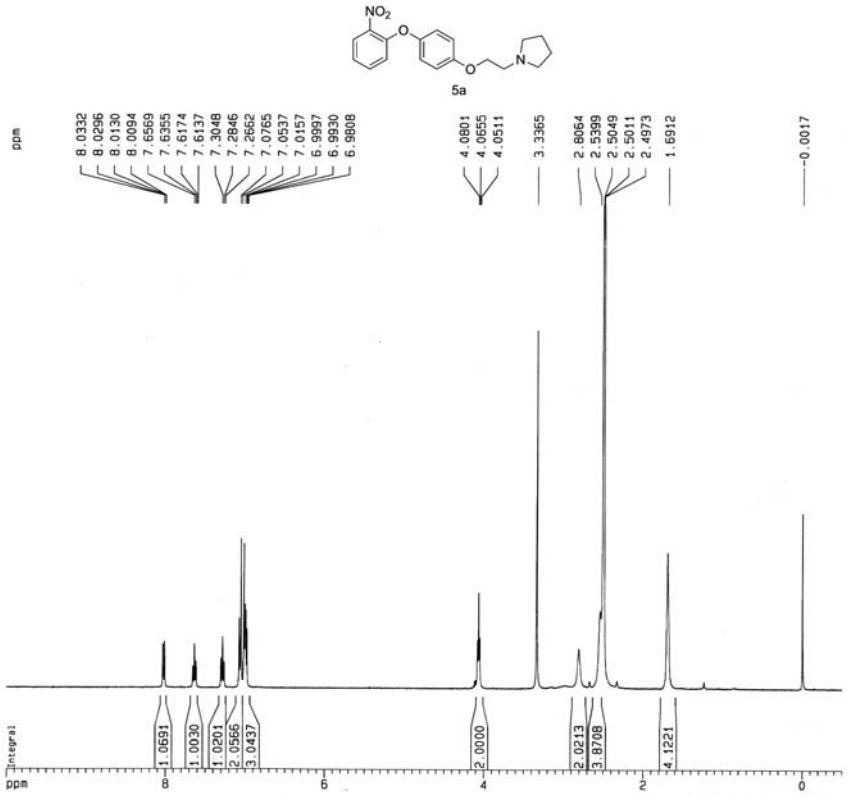
Supporting Information

Elemental analyses data of all the compounds; scanned spectrum of the ^{1}H NMR and ^{13}C NMR data, and high-resolution mass spectra of representative compounds.

Table A ^{1}H NMR and elemental analyses data of all the title compounds

Compd	^{1}H NMR (DMSO) δ	Formula	% Anal. found (% calcd)
5z	7.26 (2H, d) , 7.08 (2H, d), 7.17-6.95 (5H, m), 4.06 (2H, t), 2.82 (2H, t), 2.57 (4H, m), 1.70 (4H, m).	$C_{18}H_{21}NO_2$	C76.34(76.29), H7.41(7.47), N4.91(4.94)
5a	8.02 (1H, d) , 7.64 (1H, t), 7.29 (1H, t), 7.07-6.98 (5H, m), 4.06 (2H, t), 2.80 (2H, t), 2.53 (4H, m), 1.70 (4H, m)	$C_{18}H_{20}N_2O_4 \cdot 0.3H_2O$	C64.88(65.84), H6.15(6.14), N8.17(8.53)
5b	7.92 (1H, m), 7.64 (1H, m), 7.60 (1H, m), 7.43 (1H, m), 7.11 (2H, m), 7.05 (2H, m), 4.09(2H, t), 2.81(2H, t), 2.54(4H, m), 1.69(4H, m)	$C_{18}H_{20}N_2O_4 \cdot 0.4H_2O$	C64.30(65.84), H6.36(6.14), N8.65(8.53)
5c	8.20 (2H, m), 7.00 (4H, m), 6.82 (2H, m), 4.08 (2H, t), 2.74 (2H, t), 2.66 (4H, m), 1.74 (4H, s)	$C_{18}H_{20}N_2O_4$	C65.48(65.84), H6.17(6.14), N8.49(8.53)
5d	8.88 (1H, d), 8.45 (1H, m), 7.24 (2H, m), 7.11 (3H, m), 4.22 (2H, t), 3.24 (2H, t), 2.99 (4H, m), 1.84 (4H, m)	$C_{18}H_{19}N_3O_6 \cdot 0.4H_2O$	C56.69(57.90), H5.40(5.13), N11.13(11.25)
5e	8.12 (1H, d), 7.82 (1H, t), 7.07 (3H, m), 6.97 (3H, m), 4.08 (2H, t), 2.85 (2H, t), 2.59 (4H, s), 1.71 (4H, s)	$C_{17}H_{20}N_2O_2 \cdot 0.5\ H_2O$	C69.80(71.81), H7.11(7.09), N9.41(9.85)
5f	8.42 (2H, d), 7.02 (4H, m), 6.82 (2H, d), 4.08 (2H, t), 2.76 (2H, t), 2.65 (4H, m), 1.73 (4H, s)	$C_{17}H_{20}N_2O_2 \cdot 0.3H_2O$	C70.54(71.81), H7.15(7.09), N9.73(9.85)
5g	7.90 (1H, d), 7.64 (1H, t), 7.29 (1H, t), 7.11 (2H, d), 7.11 (2H, d), 7.03 (2H, d), 6.88 (1H, d), 4.07 (2H, t), 3.36 (3H, s), 2.79 (2H, t), 2.51 (4H, m), 1.69 (4H, m)	$C_{19}H_{23}NO_4S$	C63.01(63.13), H6.42(6.41), N3.91(3.88)
5h	7.96 (1H, s), 7.63 (2H, d), 7.34 (1H, m), 7.11-7.02 (4H, m), 4.08 (2H, t), 3.22 (3H, s), 2.81 (2H, t), 2.54 (4H, m), 1.69 (4H, m)	$C_{19}H_{23}NO_4S$	C62.94(63.13), H6.45(6.41), N3.94(3.88)
5i	7.88 (2H, d), 7.11-7.02 (6H, m), 4.08 (2H, t), 3.36 (3H, s), 2.80 (2H, t), 1.69 (4H, s)	$C_{19}H_{23}NO_4S$	C63.11(63.13), H6.47(6.41), N3.92(3.88)
5j	8.55 (1H, d), 8.11 (1H, d), 7.20 (2H, m), 7.12-7.06 (3H, m), 4.10 (2H, t), 3.30 (3H, s), 2.85 (2H, t), 2.58 (4H, m), 1.71 (4H, m)	$C_{19}H_{22}N_2O_6S$	C56.24(56.15), H5.23(5.46), N6.91(6.89)
5k	8.56 (1H, d), 8.40 (1H, d), 7.35 (1H, m), 7.13 (2H, d), 7.00 (2H, d), 4.08 (2H, t), 2.82 (2H, t), 2.53 (4H, m), 1.70 (4H, s)	$C_{16}H_{19}N_3O_2 \cdot 0.2H_2O$	C67.23(67.35), H6.87(6.71), N14.65(14.73)
5l	8.55 (1H, d), 8.39 (1H, t), 7.35 (1H, m), 7.13 (2H, d), 6.99 (2H, d), 4.08 (2H, t), 2.82 (2H, t), 1.70 (4H, s)	$C_{17}H_{19}N_3O_4$	C61.79(62.00), H5.84(5.81), N12.77(12.76)
5m	7.58 (1H, t), 7.42 (1H, d), 7.22-7.18 (2H, m), 7.08-7.00 (4H, m), 4.07 (2H, t), 2.79 (2H, t), 2.53 (4H, m), 1.69 (4H, m)	$C_{19}H_{20}F_3NO_2$	C65.14(64.95), H5.75(5.74), N4.24(3.99)

5n	7.58 (1H, t), 7.42 (1H, d), 7.22-7.18 (2H, m), 7.08-7.00 (4H, m), 4.07 (2H, t), 2.80 (2H, t), 2.53 (4H, m), 1.69 (4H, m)	$C_{19}H_{20}F_3NO_2$	C65.24(64.95), H5.77(5.74), N4.03(3.99)
5o	7.69 (2H, d), 7.11-7.00 (6H, m), 4.08 (2H, t), 2.85 (2H, t), 2.58 (4H, m), 1.71 (4H, m)	$C_{19}H_{20}F_3NO_2$	C65.15(64.95), H5.73(5.74), N4.01(3.99)
5p	7.18 (2H, t), 6.96 (6H, m), 4.04 (2H, t), 2.77 (2H, t), 2.51 (4H, m), 1.68 (4H, m)	$C_{18}H_{20}FNO_2 \cdot 0.1H_2O$	C71.29(71.74), H6.78(6.69), N4.81(4.65)
5q	7.28 (2H, t), 7.06 (6H, m), 4.03 (2H, t), 2.78 (2H, t), 2.56 (4H, m), 1.68 (4H, m)	$C_{18}H_{20}ClNO_2$	C67.95(68.03), H6.32(6.34), N4.33(4.41)
5r	7.36 (2H, d), 7.26 (2H, d), 7.12 (2H, d), 7.04 (2H,d), 4.03 (2H, t), 2.78 (2H, t), 2.56 (4H, m), 1.71 (4H, m)	$C_{18}H_{20}BrNO_2$	C59.45(59.68), H5.66(5.56), N3.98(3.87)
6a	6.92-6.84 (5H, m), 6.79 (1H, d), 6.67 (1H, d), 6.50 (1H, t), 4.90 (2H, s), 4.00 (2H, t), 2.75 (2H, t), 2.49 (4H, m), 1.66 (4H, m)	$C_{18}H_{22}N_2O_2$	C72.35 (72.46), H7.31(7.43), N9.44(9.39)
6b	6.94 (5H, m), 6.24 (1H, d), 6.09-6.03 (2H, m), 5.16 (2H, s), 4.04 (3H, t), 2.80 (2H, t), 2.54 (4H, m), 1.69 (4H, m)	$C_{18}H_{22}N_2O_2$	C72.11(72.46), H7.60(7.43), N9.50(9.39)
6c	6.85 (2H, m), 6.34 (4H, d), 6.09 (2H, m), 5.26 (2H, s), 4.07 (3H, t), 2.85 (2H, t), 2.58 (4H, m), 1.70 (4H, m)	$C_{18}H_{22}N_2O_2$	C72.15(72.46), H7.56(7.43), N9.41(9.39)
7a	7.59 (1H, d) , 7.41 (1H, t), 7.13 (1H, t), 7.10-7.01 (4H, m), 6.76 (1H, d), 4.10 (2H, t), 3.54 (6H, s), 2.93 (2H, t), 2.64 (4H, m), 1.73 (4H, m)	$C_{20}H_{26}N_2O_6S_2 \cdot 0.1H_2O$	C52.54(52.85), H5.74(5.77), N6.17(6.16)
7b	7.43 (1H, m), 7.23 (1H, m), 7.11 (1H, m), 7.03 (1H, m), 6.97 (2H, m), 6.85 (2H, m), 4.11 (2H, t), 3.52 (6H, s), 2.86 (2H, t), 2.59 (4H, s), 1.72 (4H, m)	$C_{20}H_{26}N_2O_6S_2 \cdot 0.3H_2O$	C52.18(52.85), H5.77(5.77), N6.21(6.16)
8c	7.18 (2H, d), 6.96-6.91 (6H, m), 4.04 (3H, t), 2.93 (3H, s), 2.79 (2H, t), 2.53 (4H, m), 1.69 (4H, m)	$C_{19}H_{24}N_2O_4S \cdot 0.1H_2O$	C60.52(60.62), H7.35(7.44), N6.44(6.43)
13a	7.43 (1H, d) , 7.27 (1H, m), 7.11-6.98 (5H, m), 6.74 (1H, d), 4.05 (2H, t), 3.20 (3H, s), 3.05 (3H, s), 2.79 (2H, t), 2.52 (4H, m), 1.69 (4H, m)	$C_{20}H_{26}N_2O_4S$	C61.38(61.52), H6.76(6.71), N7.00(7.17)



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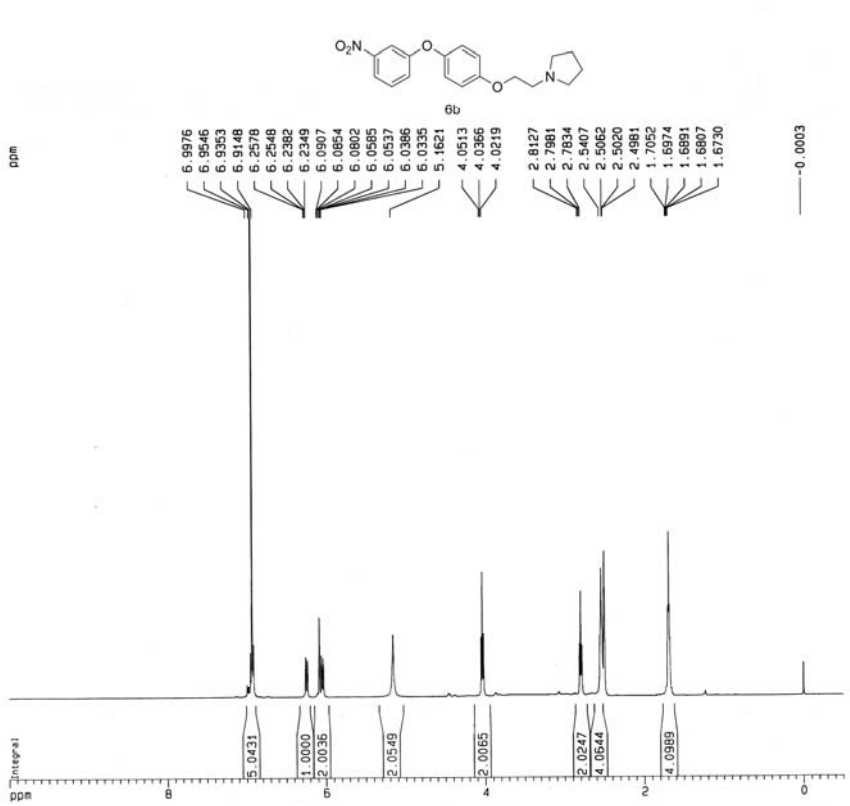

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NUCLEUS 1H

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1D NMR plot parameters
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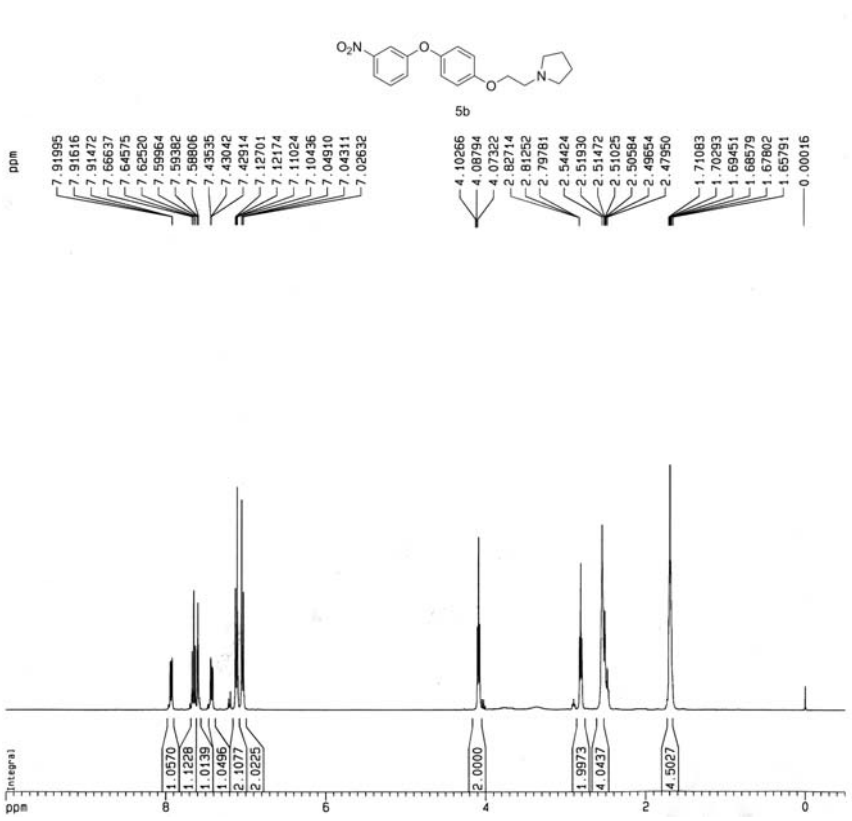


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F2 - Processing parameters
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1D NMR plot parameters
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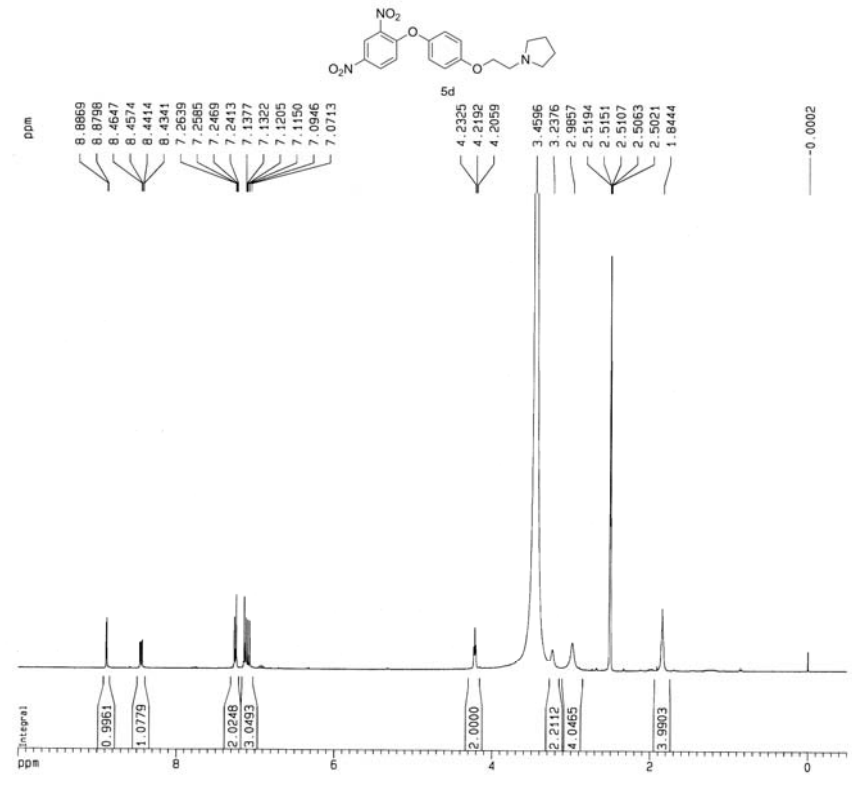


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1D NMR plot parameters
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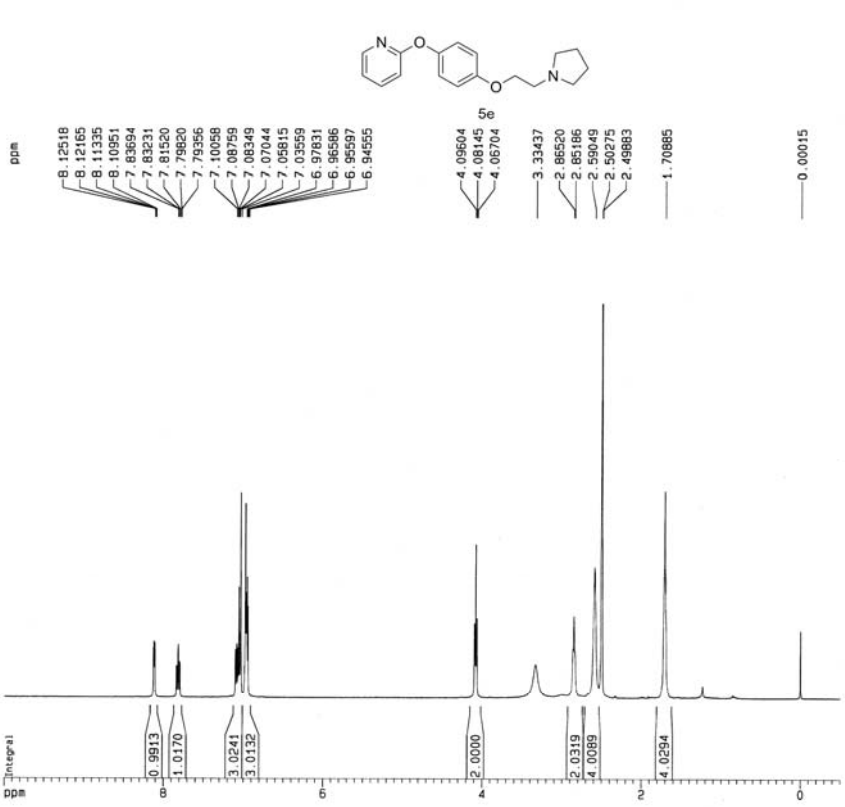

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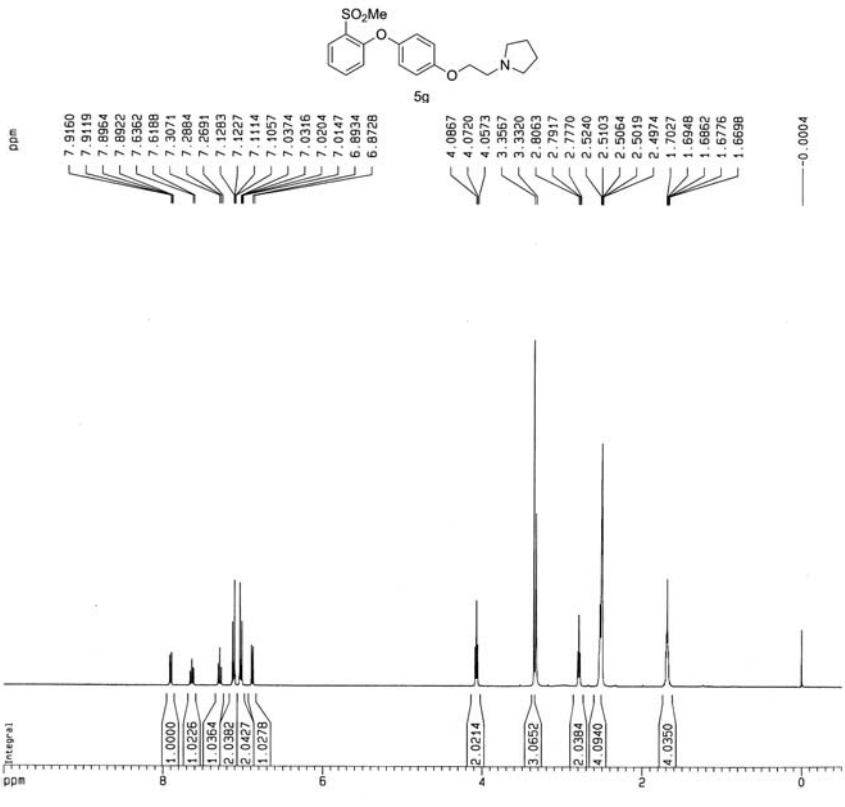

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PROCNO 1

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NUCLEUS 1H

F2 - Processing parameters
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1D NMR plot parameters
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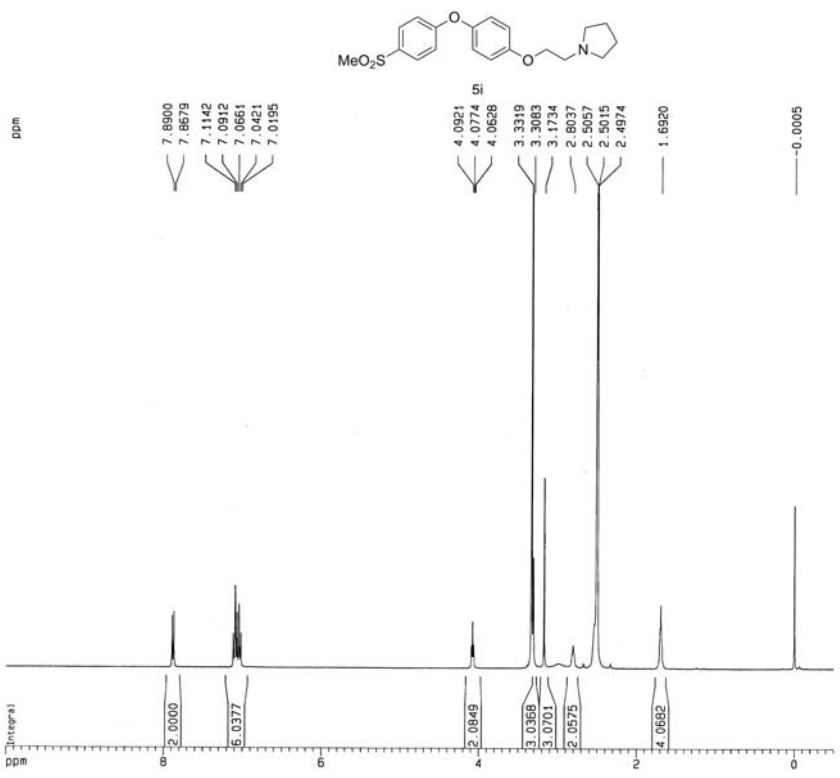


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1D NMR plot parameters
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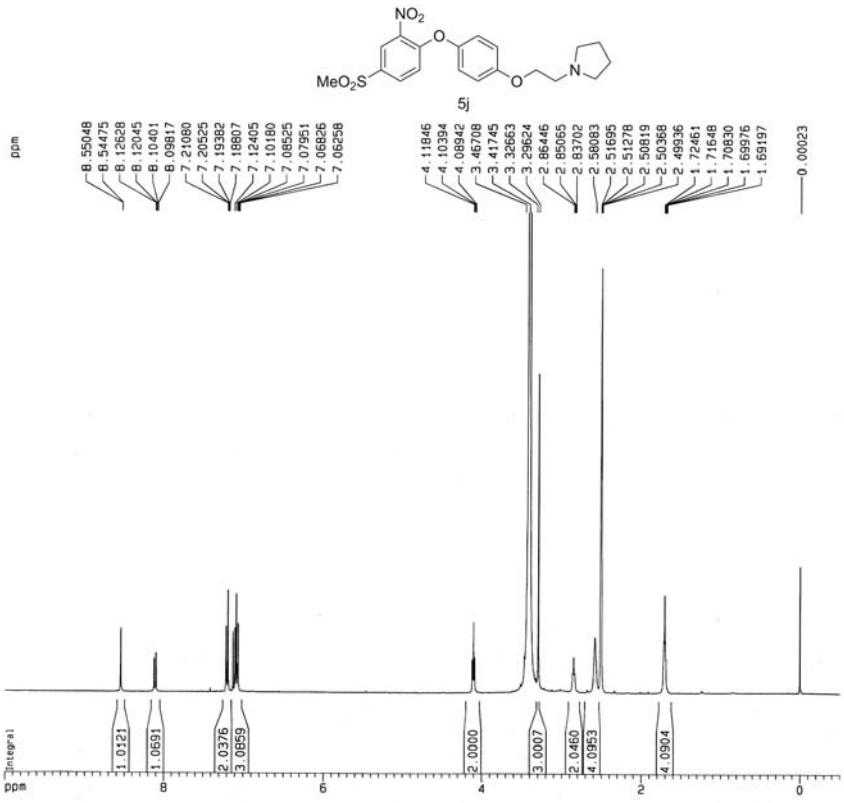


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F2 - Processing parameters
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1D NMR plot parameters
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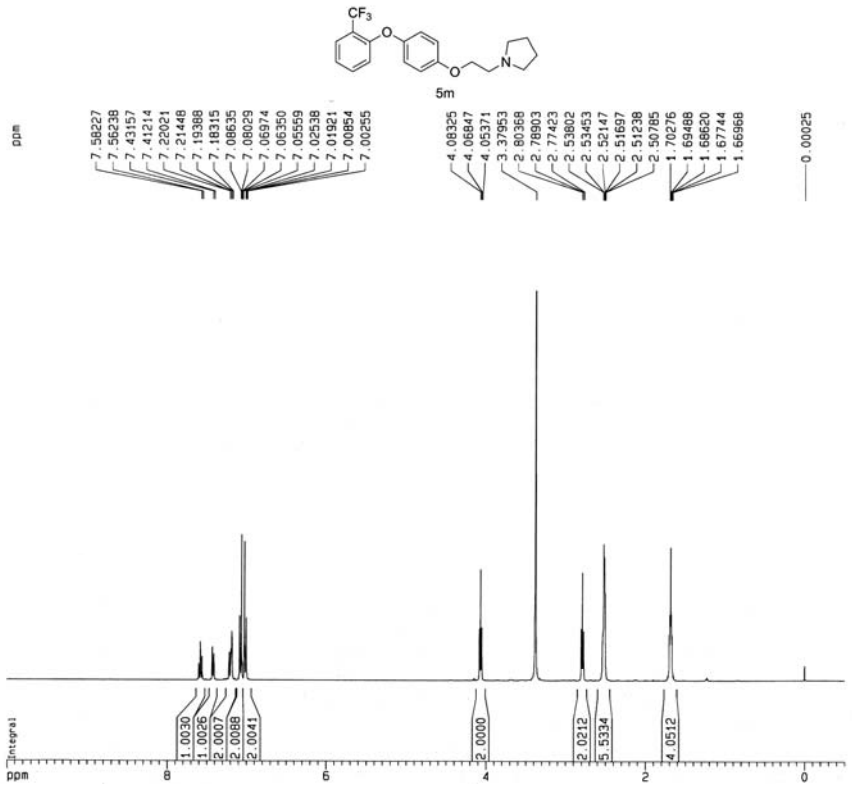


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PULPROG                zg
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RG                       715
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SFO1              400.1321971 MHz
NUCLEUS                  1H

F2 - Processing parameters
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WDW                       EM
SSB                        0
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GB                         0
PC                      4.00

1D NMR plot parameters
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F2P                   -0.500 ppm
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HZCM                210.06825 Hz/cm
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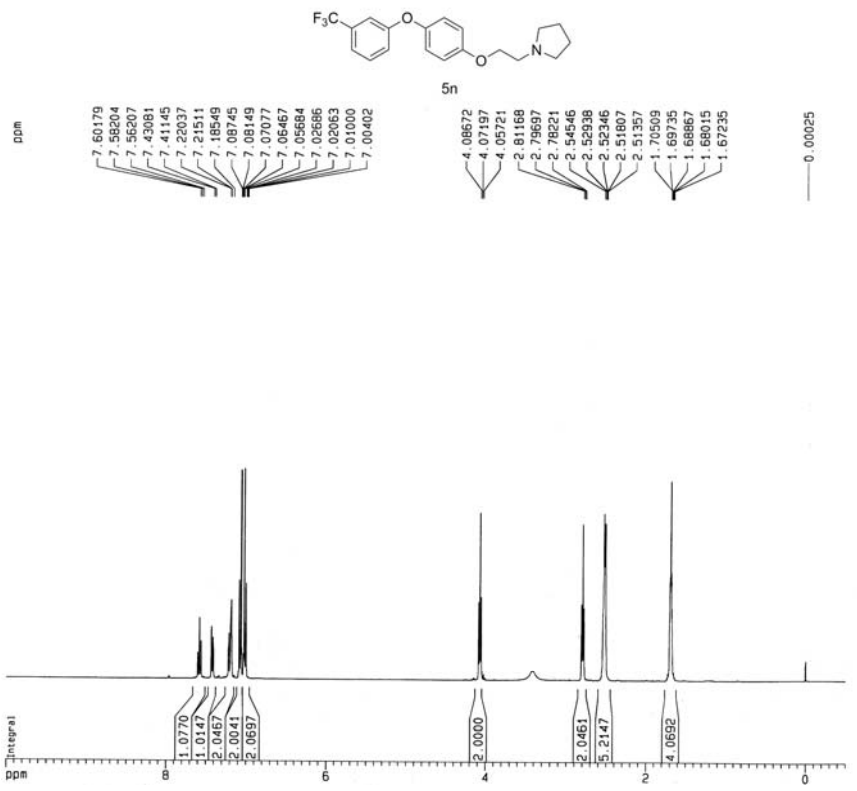


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PROCNO                     1

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TD                     32768
SOLVENT                DMSO
NS                        16
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FIDRES            0.186083 Hz
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RG                       715
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DE                  102.50 usec
TE                  300.0 K
D1                2.00000000 sec
P1                   3.00 usec
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SFO1              400.1321971 MHz
NUCLEUS                  1H

F2 - Processing parameters
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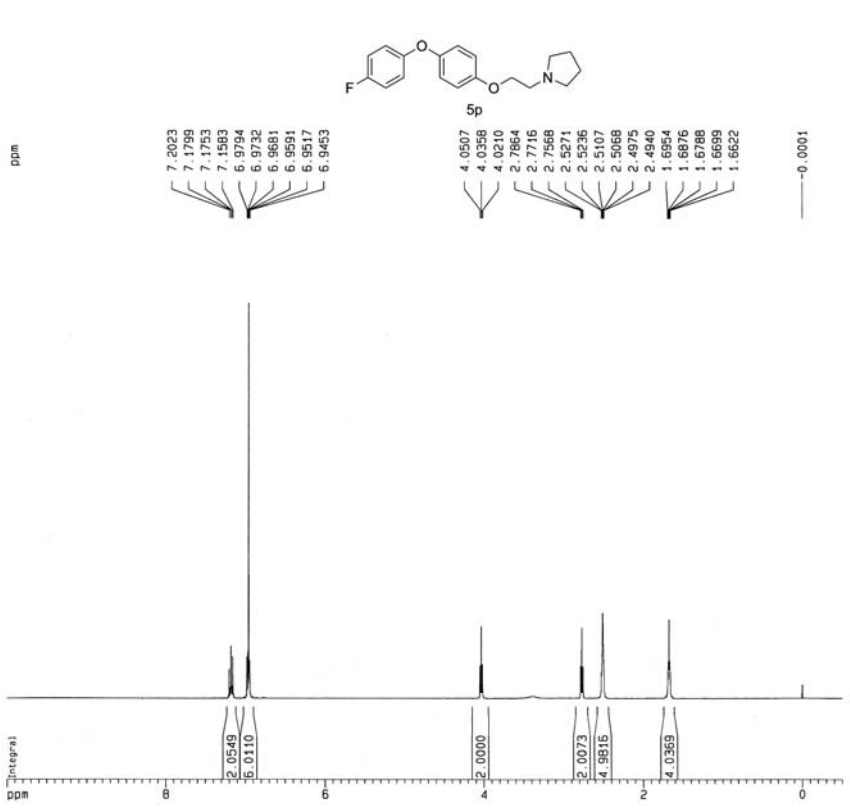
1D NMR plot parameters
CX                    20.00 cm
F1P                   10.000 ppm
F1                  4001.30 Hz
F2P                   -0.500 ppm
F2                  -200.07 Hz
PPMCM                 0.52500 ppm/cm
HZCM                210.06825 Hz/cm
```

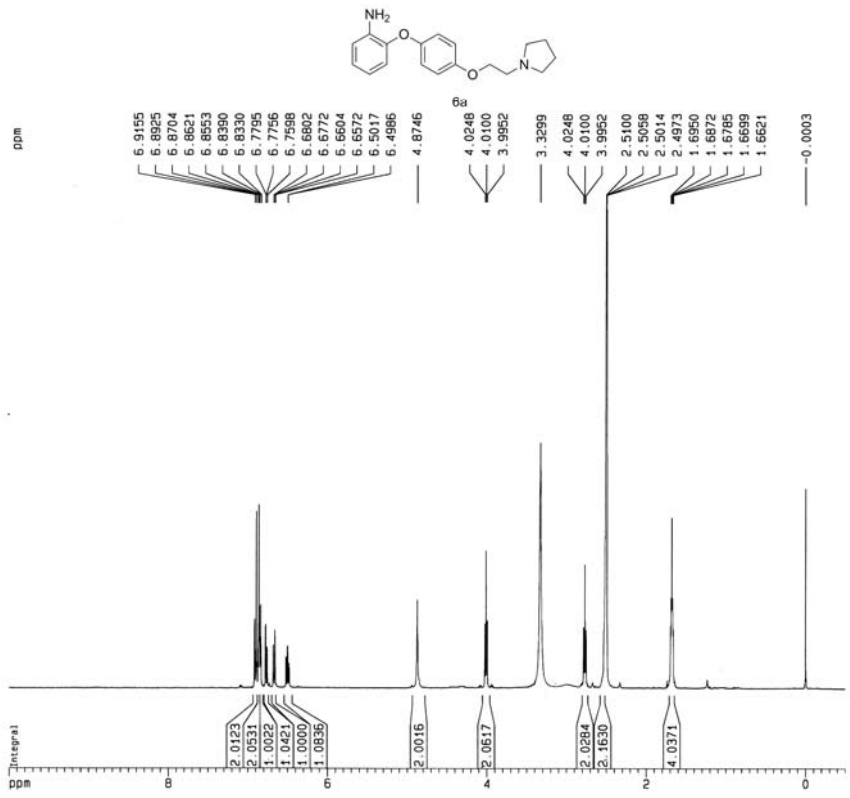


Current Data Parameters
NAME h02961
EXPNO 1
PROCNO 1

F2 - Acquisition Parameters
Date_ 20090904
Time 9.32
INSTRUM ARX400
PROBHD 5 mm Multinu
PULPROG zg
TD 32768
SOLVENT DMSO
NS 16
DS 0
SWH 6097.561 Hz
FIDRES 0.186083 Hz
AQ 2.6870260 sec
RG 715
DW 82.000 usec
DE 102.50 usec
TE 300.0 K
D1 2.00000000 sec
P1 3.00 usec
DE 102.50 usec
SFO1 400.1321971 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 16384
SF 400.1299999 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.52500 ppm/cm
HZCM 210.06825 Hz/cm



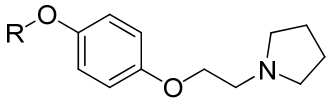
Current Data Parameters
NAME h02650
EXPNO 1
PROCNO 1

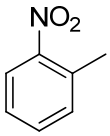
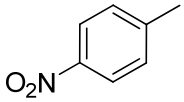
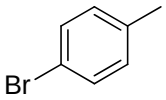
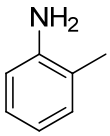
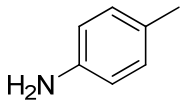
F2 - Acquisition Parameters
Date_ 20090714
Time 14.59
INSTRUM ARX400
PROBHD 5 mm Multinu
PULPROG zg
TD 32768
SOLVENT DMSO
NS 64
DS 0
SWH 6097.561 Hz
FIDRES 0.186083 Hz
AQ 2.6870260 sec
RG 2860
DW 82.000 usec
DE 102.50 usec
TE 300.0 K
D1 2.00000000 sec
P1 3.00 usec
DE 102.50 usec
SFO1 400.1321971 MHz
NUCLEUS 1H

F2 - Processing parameters
SI 16384
SF 400.1300029 MHz
WDW EM
SSB 0
LB 0.30 Hz
GB 0
PC 4.00

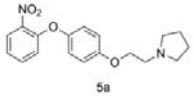
1D NMR plot parameters
CX 20.00 cm
F1P 10.000 ppm
F1 4001.30 Hz
F2P -0.500 ppm
F2 -200.07 Hz
PPMCM 0.52500 ppm/cm
HZCM 210.06825 Hz/cm

Table B ^{13}C NMR of representative compounds

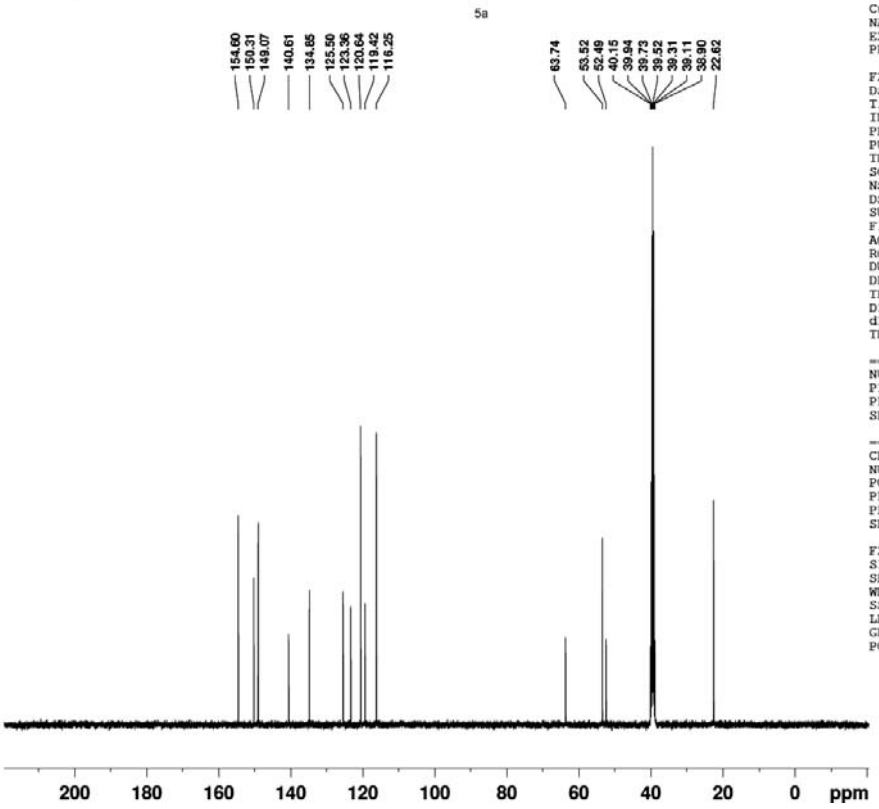


Compd	R	^{13}C NMR(DMSO) δ
5a		154.60, 150.31, 149.07, 140.61, 134.85, 125.50, 123.36, 120.64, 119.42, 116.25, 63.74, 53.52, 52.49, 22.62
5c		163.75, 156.04, 147.25, 141.84, 126.11, 121.88, 116.55, 115.96, 67.12, 54.28, 53.98, 23.14
5r		157.49, 155.17, 148.80, 132.54, 120.89, 119.22, 115.72, 114.00, 67.03, 54.27, 53.96, 23.12
6a		153.98, 150.78, 143.00, 140.04, 124.22, 118.95, 118.44, 116.24, 115.56, 115.36, 67.12, 54.39, 54.01, 23.14
6c		157.23, 154.20, 149.69, 144.89, 126.46, 124.80, 120.85, 116.17, 63.76, 53.57, 52.57, 22.60

O-NO2_13C



5a

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EXPNO                   5
PROCNO                  1

F2 - Acquisition Parameters
Date_              20110402
Time                 11.10
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgig
TD                  65536
SOLVENT              DMSO
NS                    512
DS                      4
SWH            24154.590 Hz
FIDRES         0.368570 Hz
AQ             1.3566452 sec
RG                   2048
DW                20.700 usec
DE                 6.00 usec
TE                299.2 K
D1             2.00000000 sec
d11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  10.00 usec
PL1                  1.00 dB
SFO1          100.6228303 MHz

======== CHANNEL f2 ========
CPDPRG2             garp4
NUC2                  1H
PCPD2             100.00 usec
PL12               17.00 dB
PL2                120.00 dB
SFO2          400.1316000 MHz

F2 - Processing parameters
SI                  65536
SF            100.6128164 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
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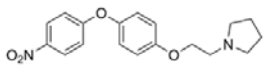
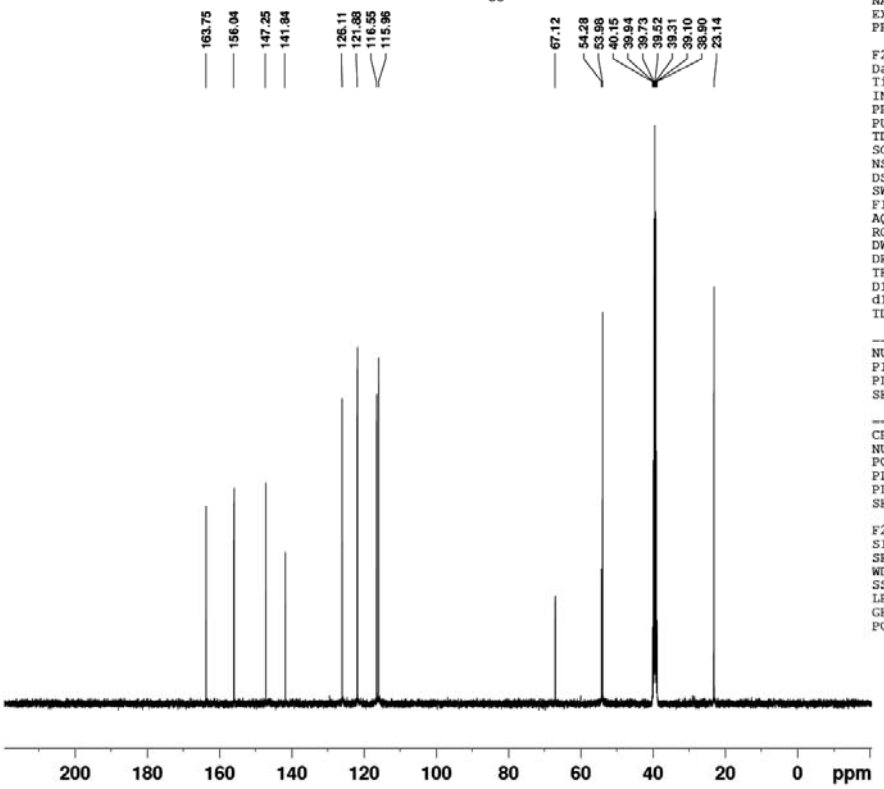
P-NO2 S2_13C



5c

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EXPNO                   7
PROCNO                  1

F2 - Acquisition Parameters
Date_              20110402
Time                 12.24
INSTRUM              spect
PROBHD   5 mm BBO BB-1H
PULPROG              zgig
TD                  65536
SOLVENT              DMSO
NS                    512
DS                      4
SWH            24154.590 Hz
FIDRES         0.368570 Hz
AQ             1.3566452 sec
RG                   2048
DW                20.700 usec
DE                 6.00 usec
TE                299.2 K
D1             2.00000000 sec
d11            0.03000000 sec
TD0                     1

======== CHANNEL f1 ========
NUC1                  13C
P1                  10.00 usec
PL1                  1.00 dB
SFO1          100.6228303 MHz

======== CHANNEL f2 ========
CPDPRG2             garp4
NUC2                  1H
PCPD2             100.00 usec
PL12               17.00 dB
PL2                120.00 dB
SFO2          400.1316000 MHz

F2 - Processing parameters
SI                  65536
SF            100.6128167 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   1.40
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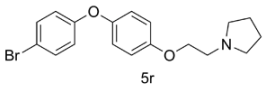
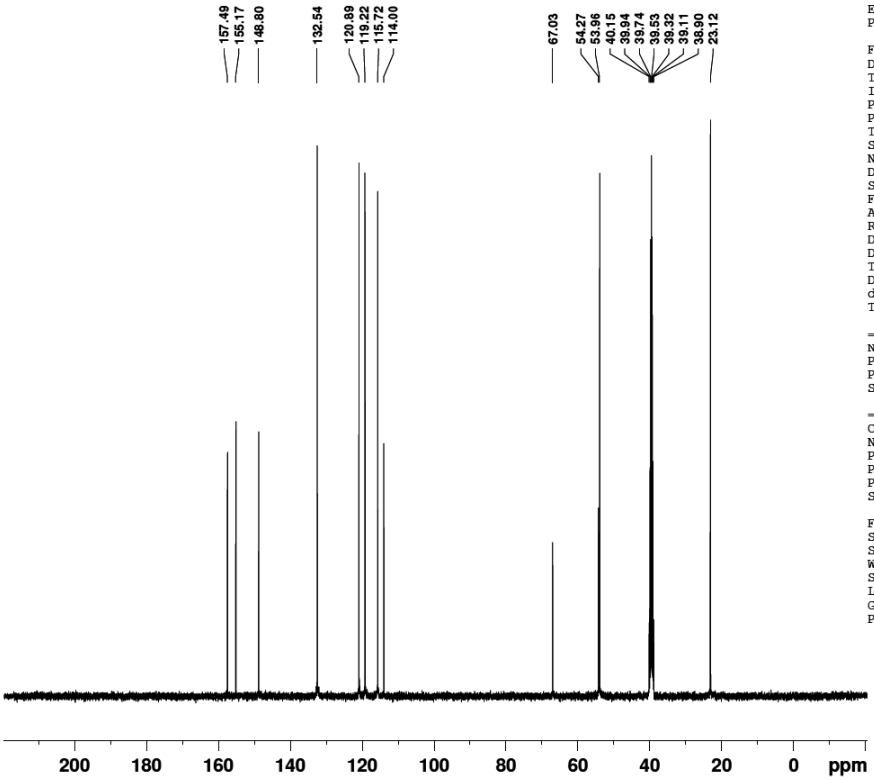
P-Br_13C



5r

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NAME      13C_040111_chem
EXPNO                   3
PROCNO                  1

F2 - Acquisition Parameters
Date_           20110402
Time               9.58
INSTRUM           spect
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PULPROG            zgig
TD                65536
SOLVENT             DMSO
NS                   512
DS                     4
SWH          24154.590 Hz
FIDRES        0.368570 Hz
AQ            1.3566452 sec
RG                  2048
DW                20.700 usec
DE                 6.00 usec
TE                299.3 K
D1           2.00000000 sec
d11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                  10.00 usec
PL1                  1.00 dB
SFO1         100.6228303 MHz

======== CHANNEL f2 ========
CPDPRG2             garp4
NUC2                   1H
PCPD2             100.00 usec
PL12               17.00 dB
PL2                120.00 dB
SFO2         400.1316000 MHz

F2 - Processing parameters
SI                    65536
SF           100.6128181 MHz
WDW                     EM
SSB                      0
LB                    1.00 Hz
GB                       0
PC                    1.40
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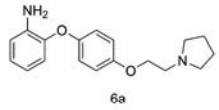
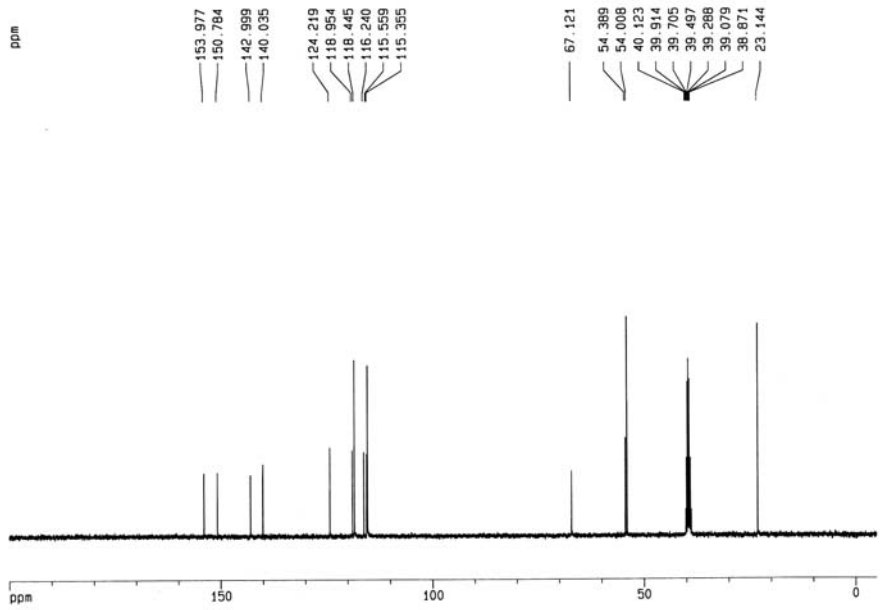


6a

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EXPNO                  1
PROCNO                 1

F2 - Acquisition Parameters
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Time               7.15
INSTRUM          ARX400
PROBHD    5 mm Multinu
PULPROG            zgdc
TD                32768
SOLVENT            DMSO
NS                  110
DS                    2
SWH          27777.777 Hz
FIDRES        0.847710 Hz
AQ            0.5898240 sec
RG                 1024
DW                18.000 usec
DE                25.71 usec
TE                300.0 K
D12          0.00002000 sec
DL5               24.00 dB
CPDPRG             waltz16
P31               100.00 usec
D1           2.00000000 sec
P1                 2.50 usec
DE                25.71 usec
SFO1         100.6233680 MHz
NUCLEUS               13C
D11          0.03000000 sec

F2 - Processing parameters
SI                 32768
SF           100.6120156 MHz
WDW                    EM
SSB                     0
LB                   1.00 Hz
GB                      0
PC                   0.50

1D NMR plot parameters
CX                  20.00 cm
F1P               200.000 ppm
F1              20122.56 Hz
F2P                -5.000 ppm
F2               -503.06 Hz
PPMCM             10.25000 ppm/cm
HZCM           1031.28149 Hz/cm
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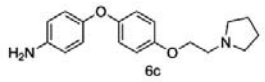
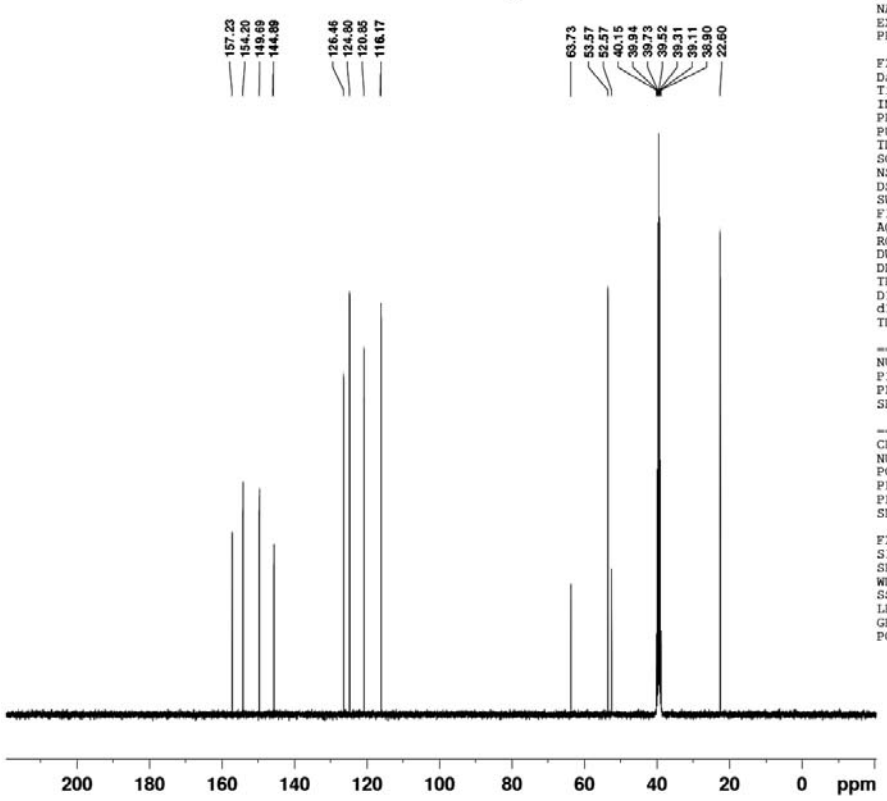
P-NH2_13C



6c

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NAME      13C_040111_chem
EXPNO                   4
PROCNO                  1

F2 - Acquisition Parameters
Date_            20110402
Time                10.36
INSTRUM             spect
PROBHD   5 mm BBO BB-1H
PULPROG             zgig
TD                 65536
SOLVENT             DMSO
NS                   512
DS                     4
SWH            24154.590 Hz
FIDRES         0.368570 Hz
AQ             1.3566452 sec
RG                  2048
DW                20.700 usec
DE                 6.00 usec
TE                299.2 K
D1           2.00000000 sec
d11          0.03000000 sec
TD0                    1

======== CHANNEL f1 ========
NUC1                  13C
P1                 10.00 usec
PL1                 1.00 dB
SFO1         100.6228303 MHz

======== CHANNEL f2 ========
CPDPRG2             garp4
NUC2                  1H
PCPD2             100.00 usec
PL12               17.00 dB
PL2                120.00 dB
SFO2         400.1316000 MHz

F2 - Processing parameters
SI                 65536
SF           100.6128166 MHz
WDW                   EM
SSB                    0
LB                  1.00 Hz
GB                     0
PC                  1.40
```

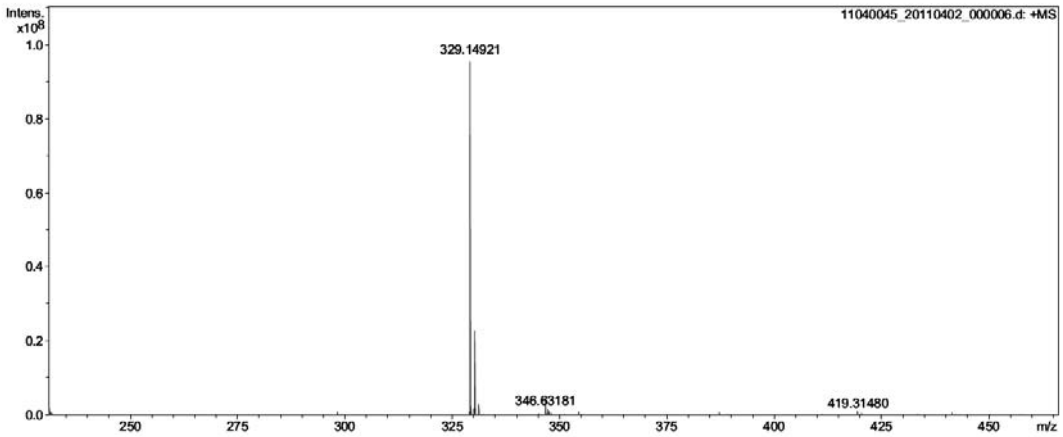
Table C HRMS of some compounds

Compd	Formula	calcd ([M+H]$^+$)	found ([M+H]$^+$)
5a	$C_{18}H_{20}N_2O_4$	329.1496	329.1492
5c	$C_{18}H_{20}N_2O_4$	329.1496	329.1491
5h	$C_{19}H_{23}NO_4S$	362.1420	362.1415
5i	$C_{19}H_{23}NO_4S$	362.1420	362.1418
5r	$C_{18}H_{20}BrNO_2$	362.0750	362.0746
6c	$C_{18}H_{22}N_2O_2$	299.1754	299.1747
7a	$C_{20}H_{26}N_2O_6S_2$	455.1305	455.1304
8c	$C_{19}H_{24}N_2O_4S$	377.1529	377.1528
13a	$C_{20}H_{26}N_2O_4S$	391.1686	391.1685

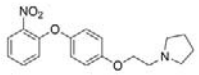
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name	11040045_20110402_000006.d	Acquisition Date	4/2/2011 11:36:10 AM
Sample	o-NO2	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
329.14921	1	C 18 H 21 N 2 O 4	100.00	329.14958	0.4	1.1	18.9	9.5	even	ok

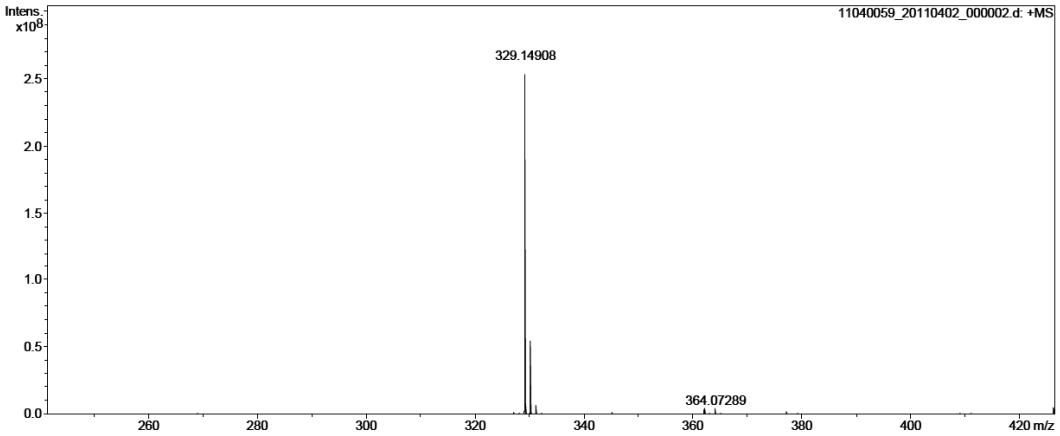


5a

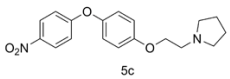
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name	11040059_20110402_000002.d	Acquisition Date	4/2/2011 4:25:27 PM
Sample	p-NO2	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
329.14908	1	C 18 H 21 N 2 O 4	100.00	329.14958	0.5	1.5	3.8	9.5	even	ok

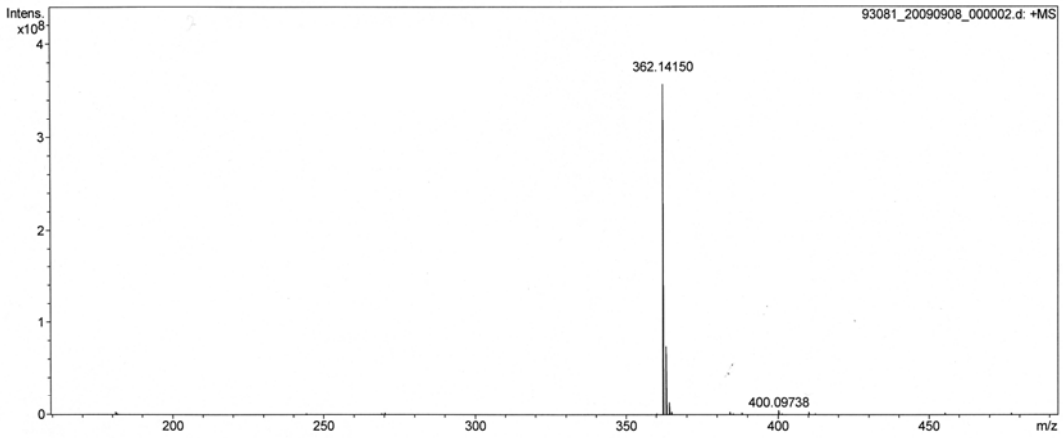


5c

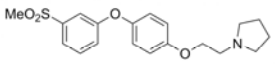
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name	93081_20090908_000002.d	Acquisition Date	9/8/2009 5:53:14 PM
Sample	80	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
362.14150	1	C 19 H 24 N O 4 S	100.00	362.14206	0.6	1.5	20.5	8.5	even	ok



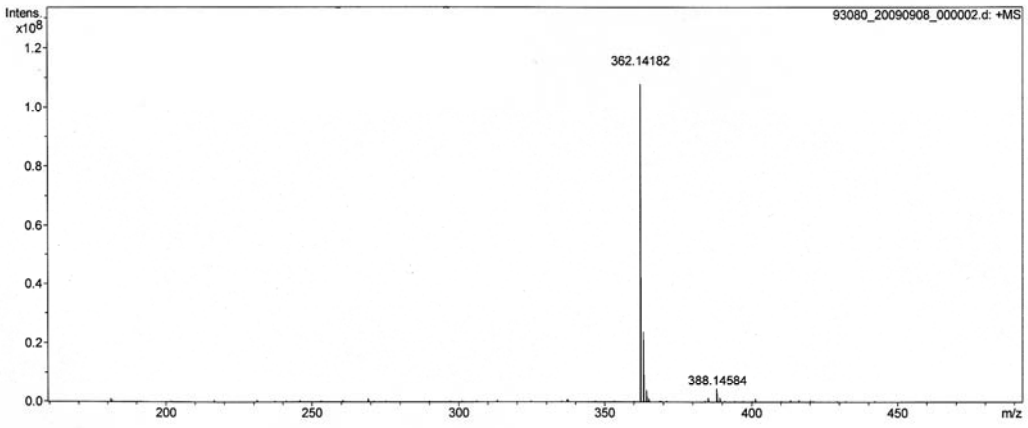
5h

Bruker Compass DataAnalysis 4.0 printed: 9/8/2009 5:54:04 PM Page 1 of 1

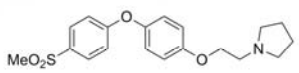
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name	93080_20090908_000002.d	Acquisition Date	9/8/2009 5:49:58 PM
Sample	CZ-LC-70	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
362.14182	1	C 19 H 24 N O 4 S	100.00	362.14206	0.2	0.7	19.6	8.5	even	ok



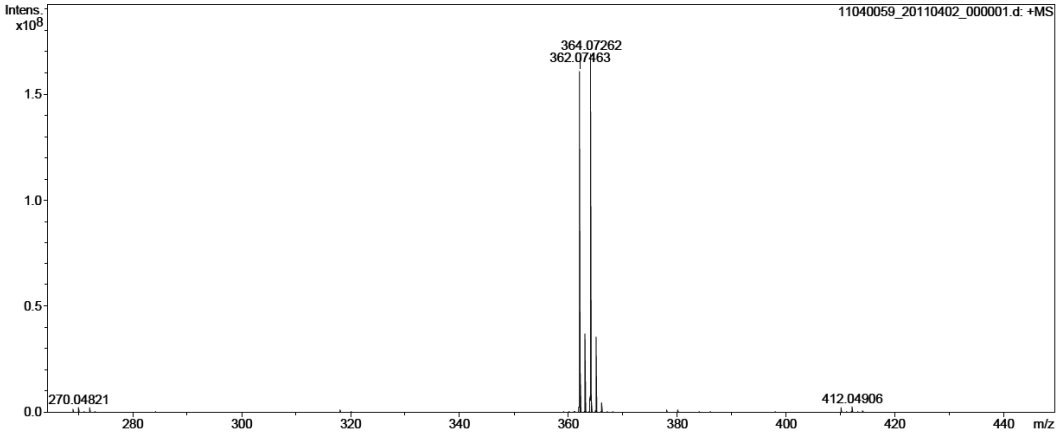
5i

Bruker Compass DataAnalysis 4.0 printed: 9/8/2009 5:50:58 PM Page 1 of 1

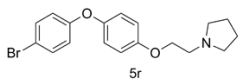
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name	11040059_20110402_000001.d	Acquisition Date	4/2/2011 4:23:48 PM
Sample	p-Br	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
362.07463	1	C 18 H 21 Br N O 2	100.00	362.07502	0.4	1.1	20.4	8.5	even	ok

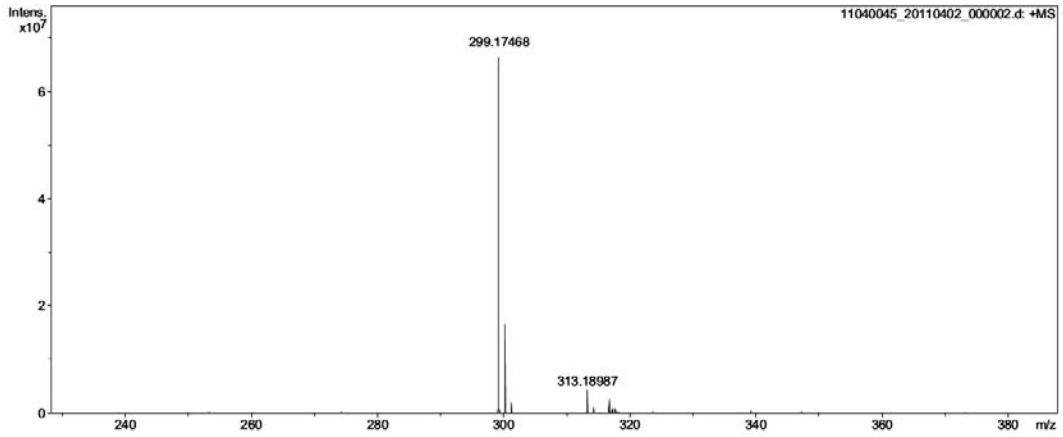


5r

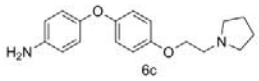
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name	11040045_20110402_000002.d	Acquisition Date	4/2/2011 11:21:28 AM
Sample	p-NH2	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
299.17468	1	C 18 H 23 N 2 O 2	100.00	299.17540	0.7	2.4	25.9	8.5	even	ok

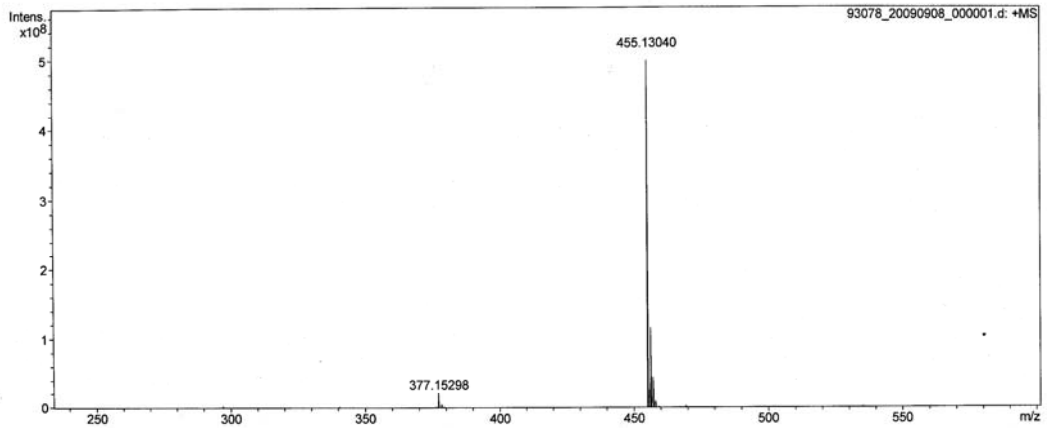


6c

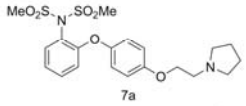
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name	93078_20090908_000001.d	Acquisition Date	9/8/2009 5:43:29 PM
Sample	57	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
377.15298	1	C 19 H 25 N 2 O 4 S	100.00	377.15295	-0.0	-0.1	22.3	8.5	even	ok
455.13040	1	C 20 H 27 N 2 O 6 S 2	100.00	455.13050	0.1	0.2	23.6	8.5	even	ok



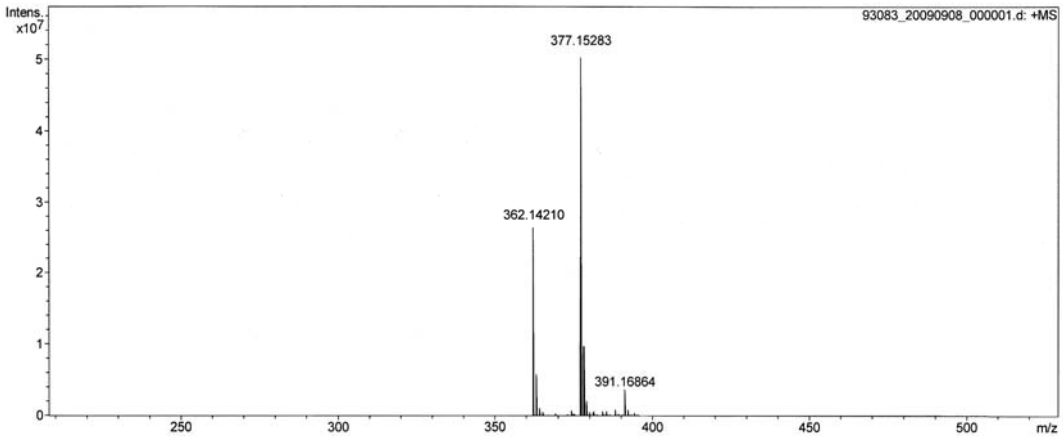
7a

Bruker Compass DataAnalysis 4.0 printed: 9/8/2009 5:45:09 PM Page 1 of 1

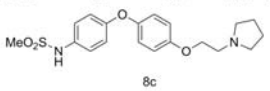
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name	93083_20090908_000001.d	Acquisition Date	9/8/2009 5:56:28 PM
Sample	74	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
377.15283	1	C 19 H 25 N 2 O 4 S	100.00	377.15295	0.1	0.3	21.9	8.5	even	ok



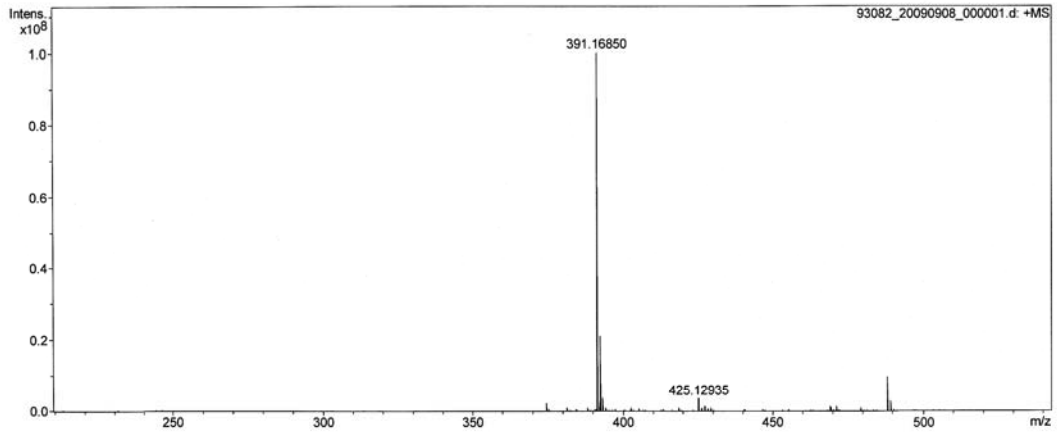
8c

Bruker Compass DataAnalysis 4.0 printed: 9/8/2009 5:58:05 PM Page 1 of 1

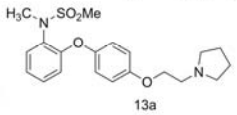
Peking University Mass Spectrometry Sample Analysis Report

Analysis Info

Analysis Name	93082_20090908_000001.d	Acquisition Date	9/8/2009 5:54:49 PM
Sample	20	Instrument	Bruker Apex IV FTMS
Comment	ESI Positive	Operator	Peking University



Meas. m/z	#	Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e⁻ Conf	N-Rule
391.16850	1	C 20 H 27 N 2 O 4 S	100.00	391.16860	0.1	0.3	23.2	8.5	even	ok



13a