

S5 File. The NMR spectra of M5.

Fig. S5-1 ^1H NMR spectrum of M5 (500 MHz, DMSO, 25 °C).

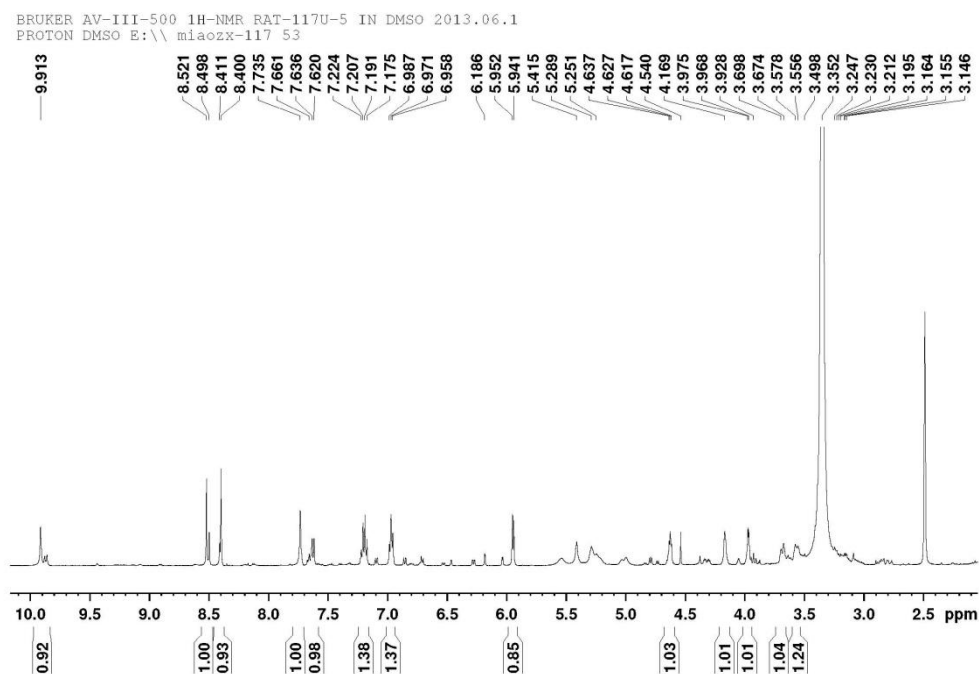


Fig. S5-2 ^1H NMR spectrum of M5 (500 MHz, DMSO, 25 °C).

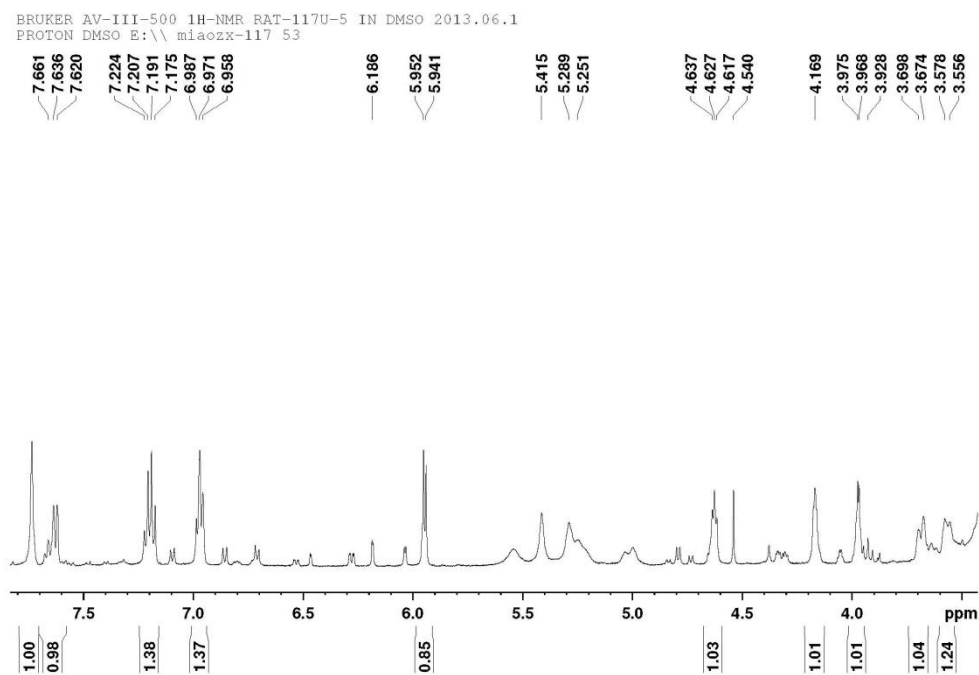


Fig. S5-3 ^{13}C NMR spectrum of M5 (500 MHz, DMSO, 25 °C).

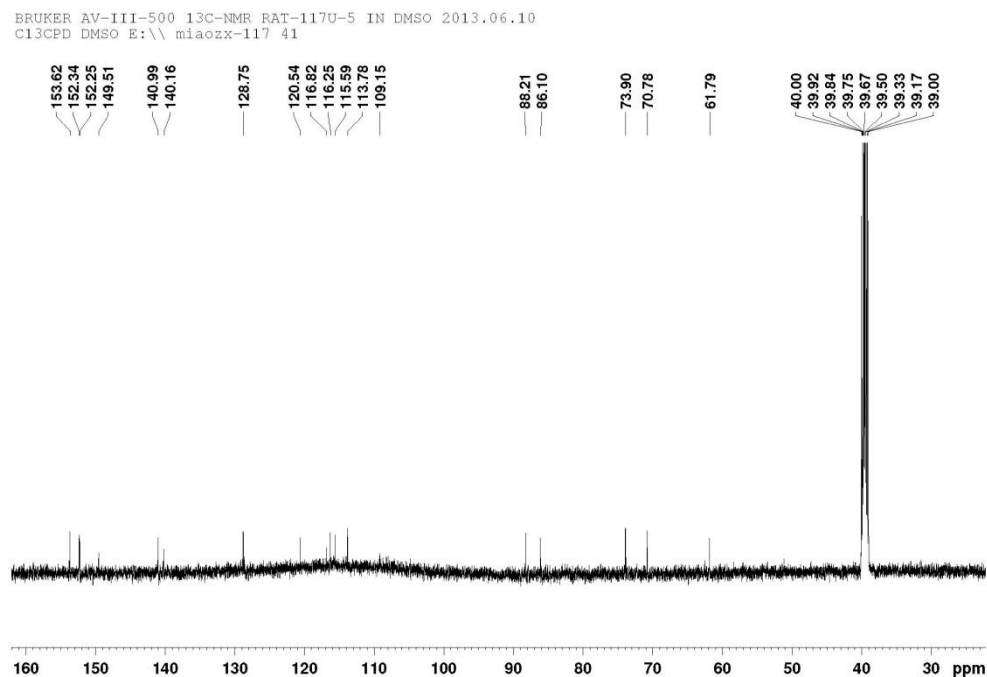


Fig. S5-4 COSY NMR spectrum of M5 (500 MHz, DMSO, 25 °C).

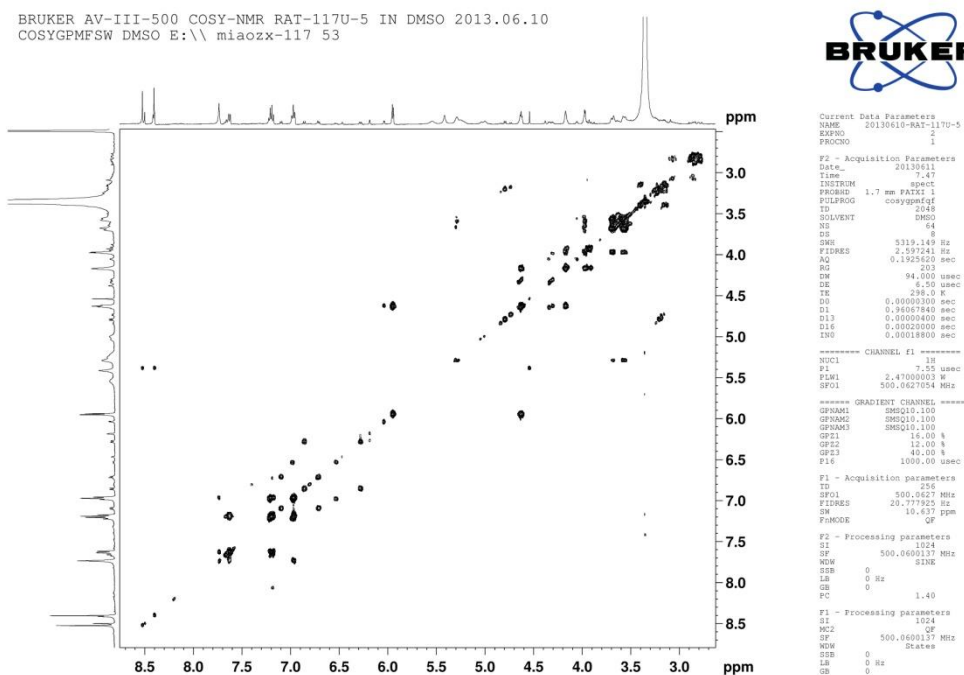
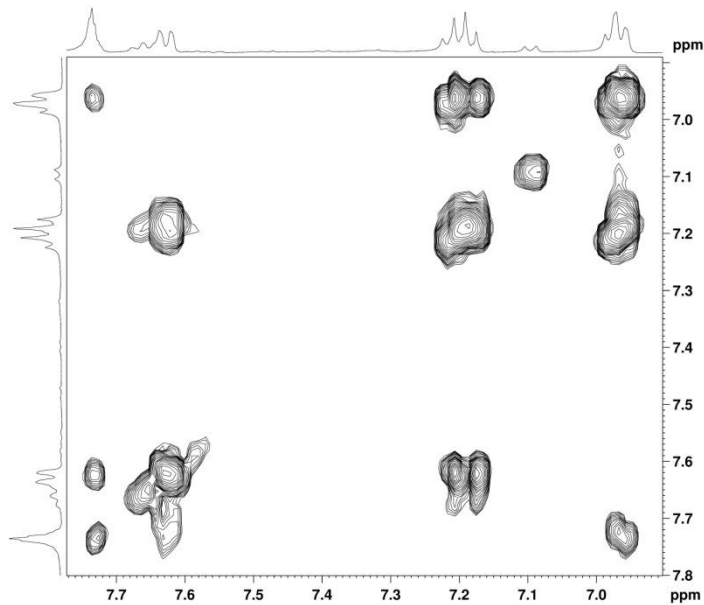


Fig. S5-5 COSY NMR spectrum of M5 (500 MHz, DMSO, 25 °C).

BRUKER AV-III-500 COSY-NMR RAT-117U-5 IN DMSO 2013.06.10
 COSYGMFSW DMSO E:\miaozx-117 53



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PROCNO   1

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PULPROG  cosygpmfsw
ID       2048
SOLVENT  DMSO
NS       64
DS       8
SWH      3319.149 Hz
FIDRES   2.597241 Hz
AQ       0.1925620 sec
RG       203
DM       94.000 usec
DE       6.50 usec
TE       298.0 K
D0       0.0000300 sec
D1       0.3600780 sec
D13      0.0000400 sec
D16      0.0002000 sec
IN0      0.0001800 sec

----- CHANNEL f1 -----
NUC1     1H
P1       7.25 usec
P1M1     2.47000003 W
SFO1     500.0627054 MHz

----- GRADIENT CHANNEL -----
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GPM1M2   SMSQ10.100
GPM1M3   SMSQ10.100
OP1      18.00 %
OP2      12.00 %
OP3      40.00 %
P16      1000.00 usec

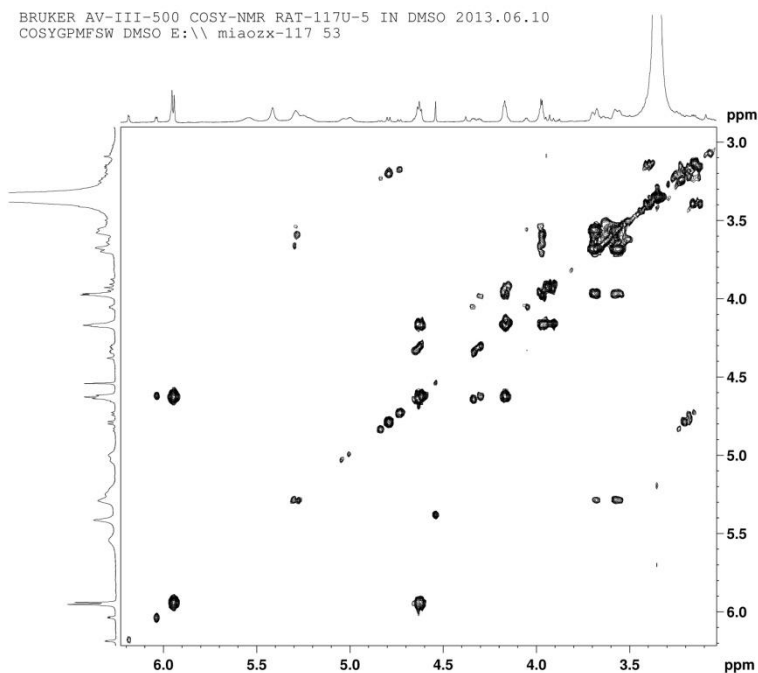
F1 - Acquisition parameters
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SFO1     500.0627 MHz
FIDRES   20.777925 Hz
SW       10.637 ppm
F0MODE   QF

F2 - Processing parameters
SI       1024
SF       500.0600137 MHz
WDW      SINC
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GB       0
PC       1.40

F1 - Processing parameters
SI       1024
SF       500.0600137 MHz
WDW      SINC
SSB      0 Hz
LB       0 Hz
GB       0
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Fig. S5-6 COSY NMR spectrum of M5 (500 MHz, DMSO, 25 °C).

BRUKER AV-III-500 COSY-NMR RAT-117U-5 IN DMSO 2013.06.10
 COSYGMFSW DMSO E:\miaozx-117 53



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EXPNO    1
PROCNO   1

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Time     7.47
INSTRUM  spect
PROBHD   1.7 mm PAXI 1
PULPROG  cosygpmfsw
ID       2048
SOLVENT  DMSO
NS       64
DS       8
SWH      3319.149 Hz
FIDRES   2.597241 Hz
AQ       0.1925620 sec
RG       203
DM       94.000 usec
DE       6.50 usec
TE       298.0 K
D0       0.0000300 sec
D1       0.3600780 sec
D13      0.0000400 sec
D16      0.0002000 sec
IN0      0.0001800 sec

----- CHANNEL f1 -----
NUC1     1H
P1       7.25 usec
P1M1     2.47000003 W
SFO1     500.0627054 MHz

----- GRADIENT CHANNEL -----
GPM1M1   SMSQ10.100
GPM1M2   SMSQ10.100
GPM1M3   SMSQ10.100
OP1      18.00 %
OP2      12.00 %
OP3      40.00 %
P16      1000.00 usec

F1 - Acquisition parameters
TD       256
SFO1     500.0627 MHz
FIDRES   20.777925 Hz
SW       10.637 ppm
F0MODE   QF

F2 - Processing parameters
SI       1024
SF       500.0600137 MHz
WDW      SINC
SSB      0 Hz
GB       0
PC       1.40

F1 - Processing parameters
SI       1024
SF       500.0600137 MHz
WDW      SINC
SSB      0 Hz
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Fig. S5-7 HSQC NMR spectrum of M5 (500 MHz, DMSO, 25 °C).

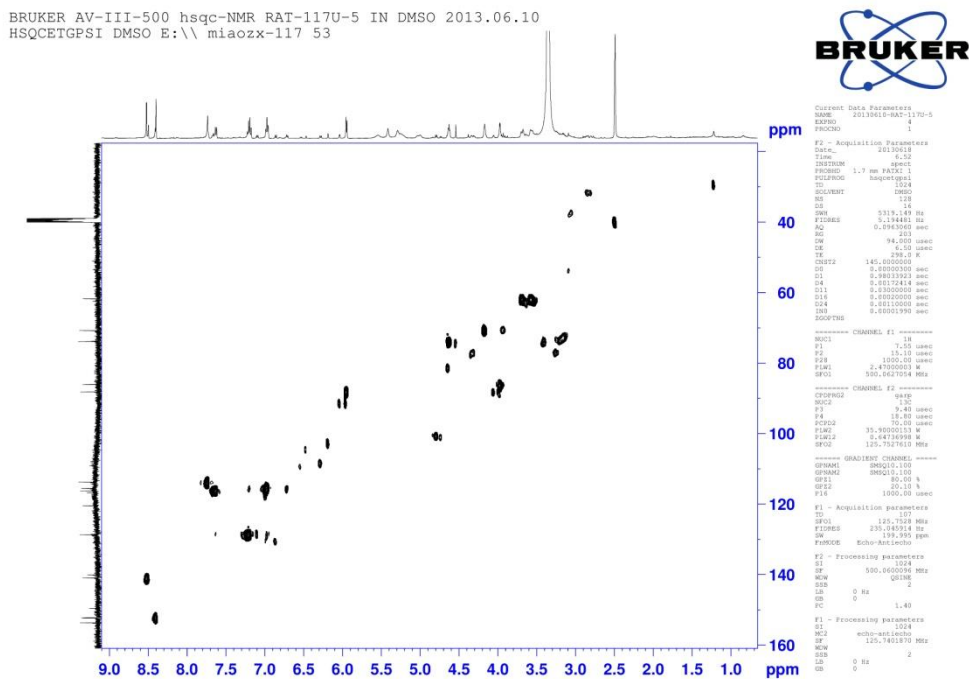


Fig. S5-8 HSQC NMR spectrum of M5 (500 MHz, DMSO, 25 °C).

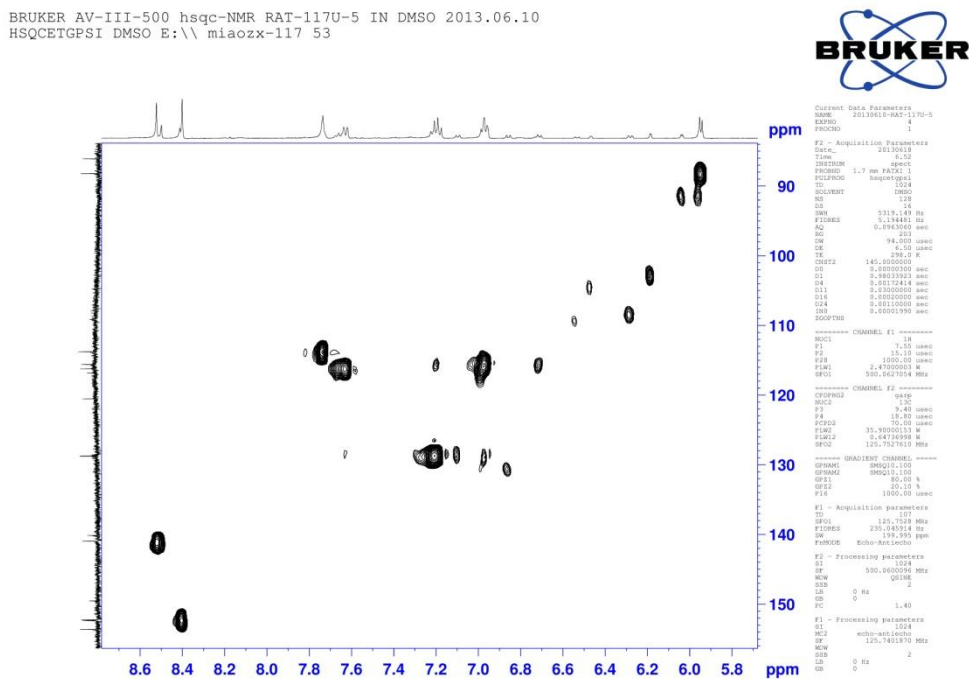


Fig. S5-9 HSQC NMR spectrum of M5 (500 MHz, DMSO, 25 °C).

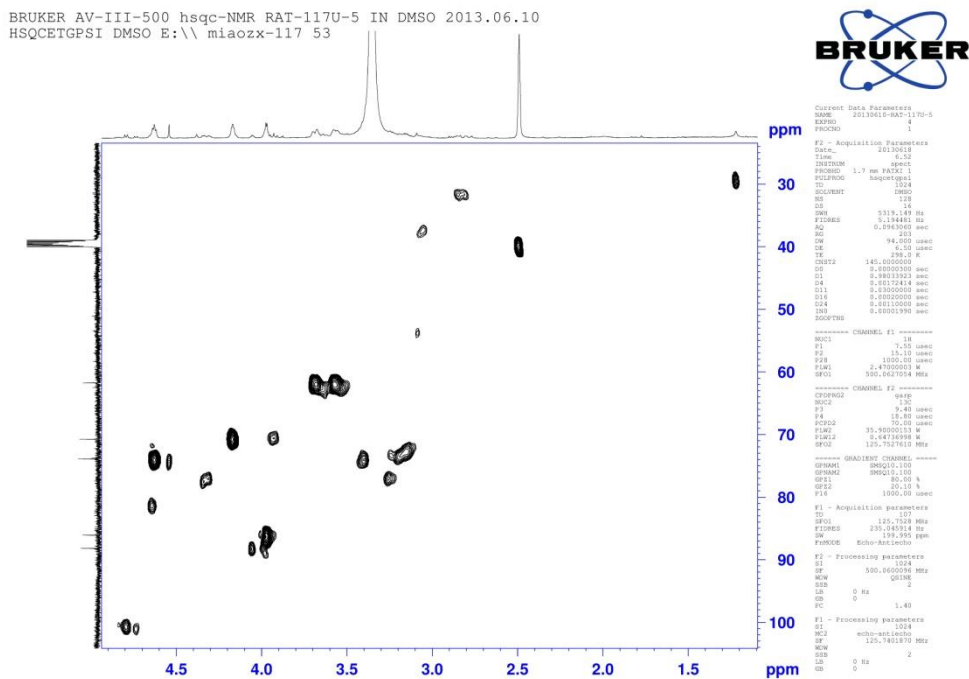


Fig. S5-10 HMBC NMR spectrum of M5 (500 MHz, DMSO, 25 °C).

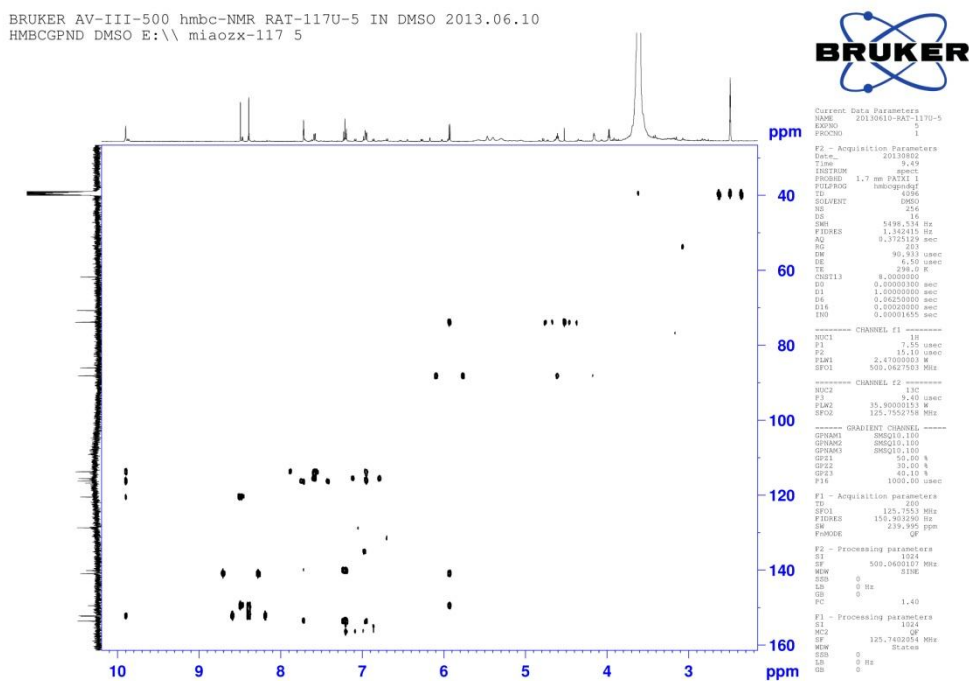


Fig. S5-11 HMBC NMR spectrum of M5 (500 MHz, DMSO, 25 °C).

BRUKER AV-III-500 hmbc-NMR RAT-117U-5 IN DMSO 2013.06.10
 HMBGPNDDMSO E:\miaozx-117 5

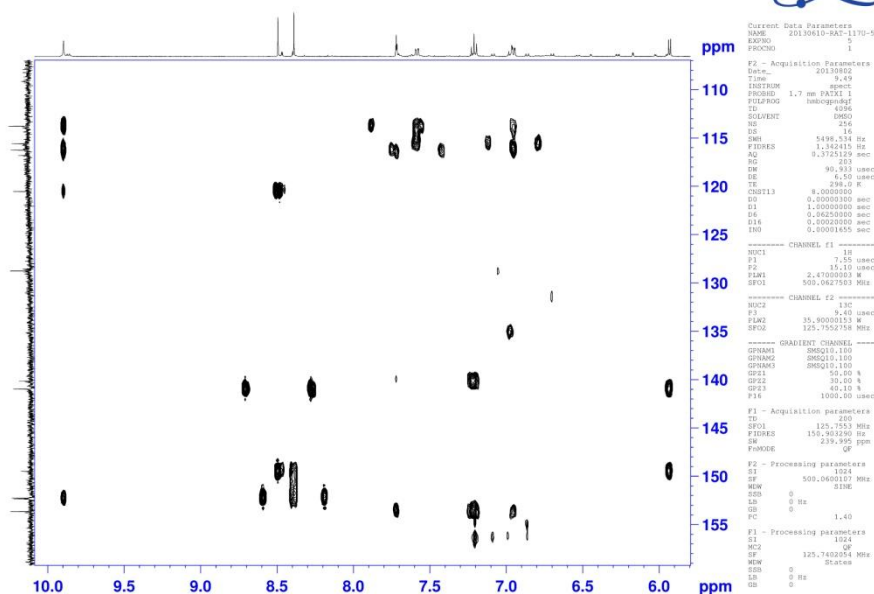


Fig. S5-12 HMBC NMR spectrum of M5 (500 MHz, DMSO, 25 °C).

BRUKER AV-III-500 hmbc-NMR RAT-117U-5 IN DMSO 2013.06.10
 HMBGPNDDMSO E:\miaozx-117 5

