

## S6 File. The NMR spectra of M6.

Fig. S6-1 <sup>1</sup>H NMR spectrum of M6 (500 MHz, DMSO, 25 °C).

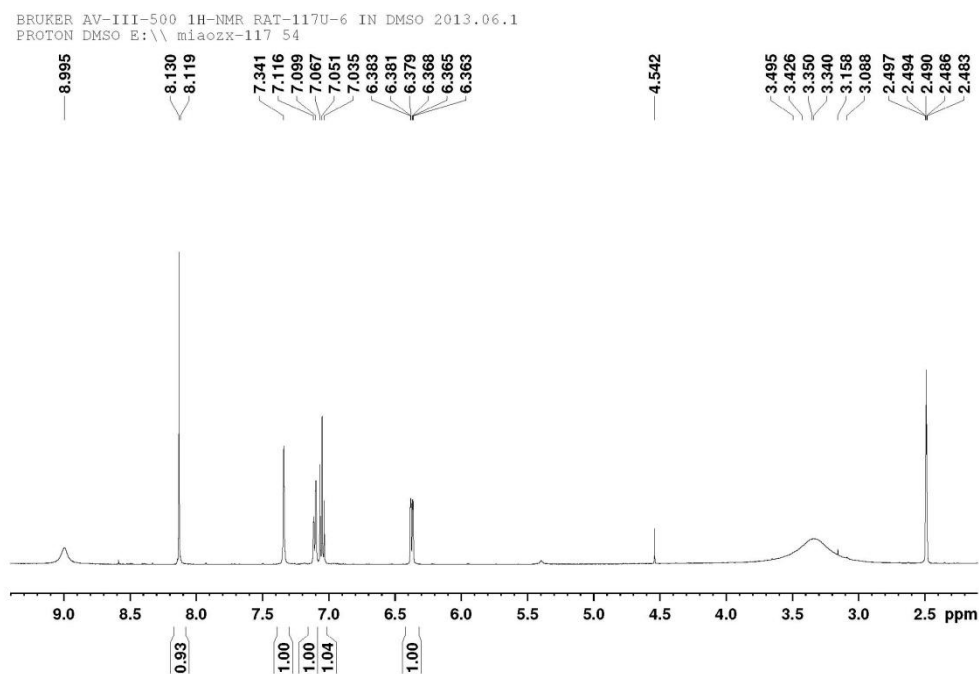
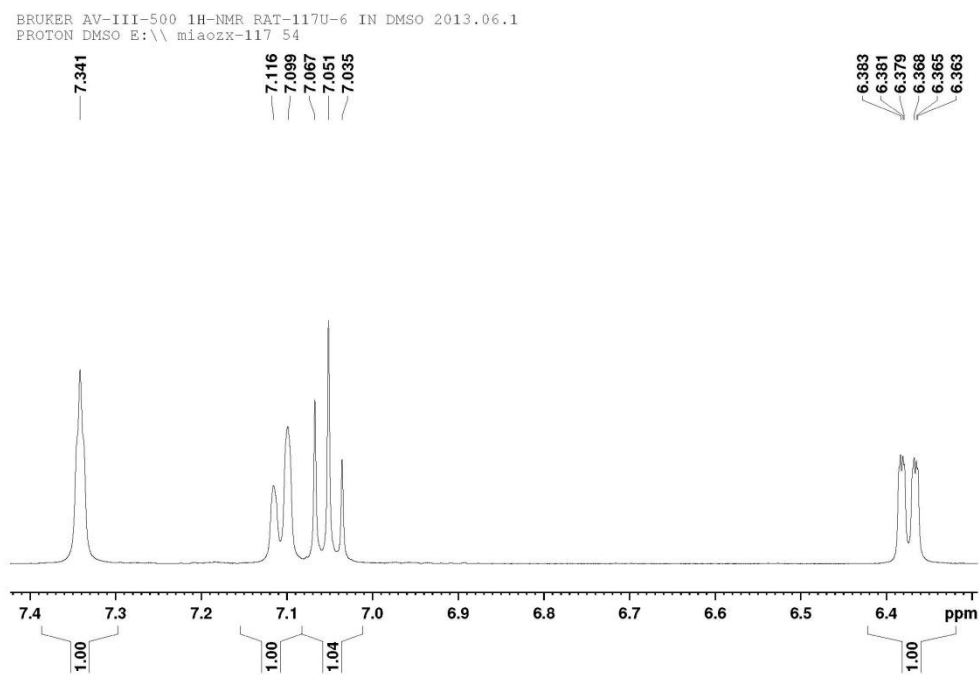
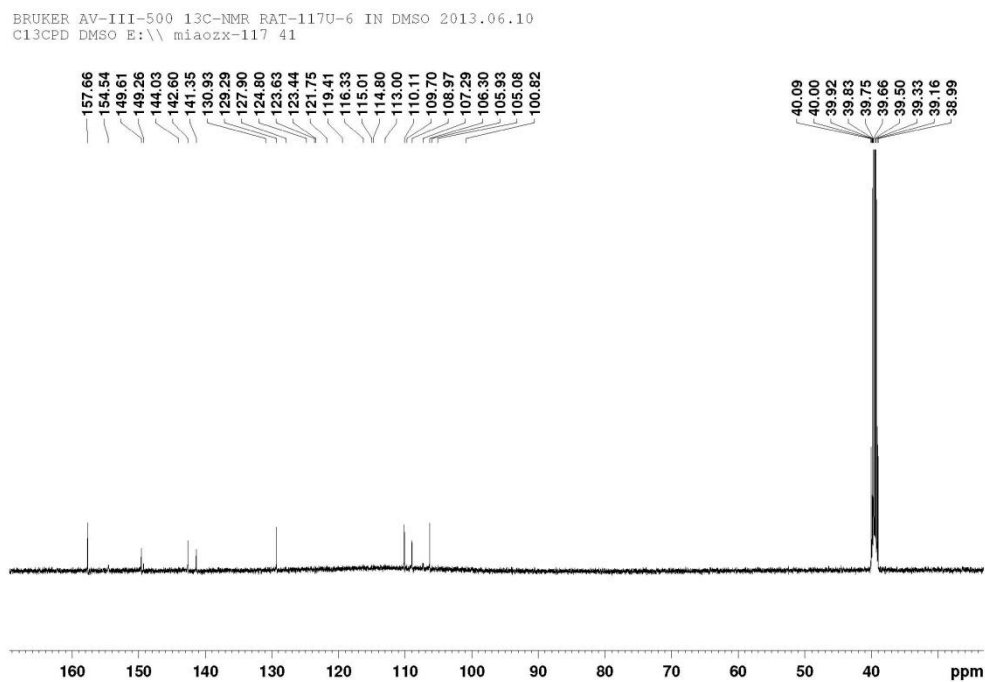


Fig. S6-2 <sup>1</sup>H NMR spectrum of M6 (500 MHz, DMSO, 25 °C).



**Fig. S6-3**  $^{13}\text{C}$  NMR spectrum of M6 (500 MHz, DMSO, 25 °C).



**Fig. S6-4** COSY NMR spectrum of M6 (500 MHz, DMSO, 25 °C).

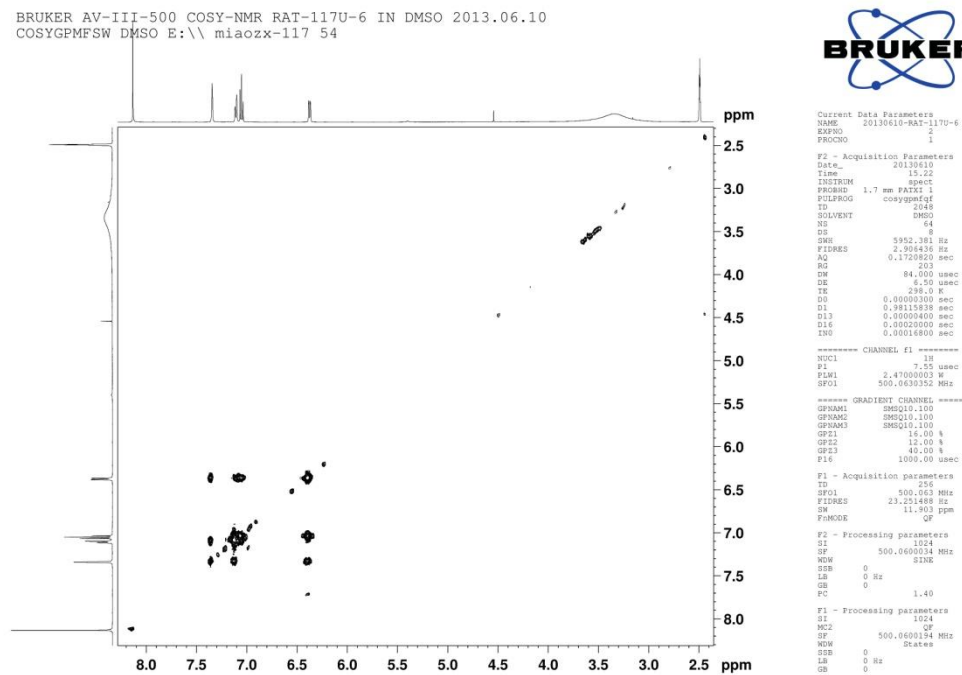
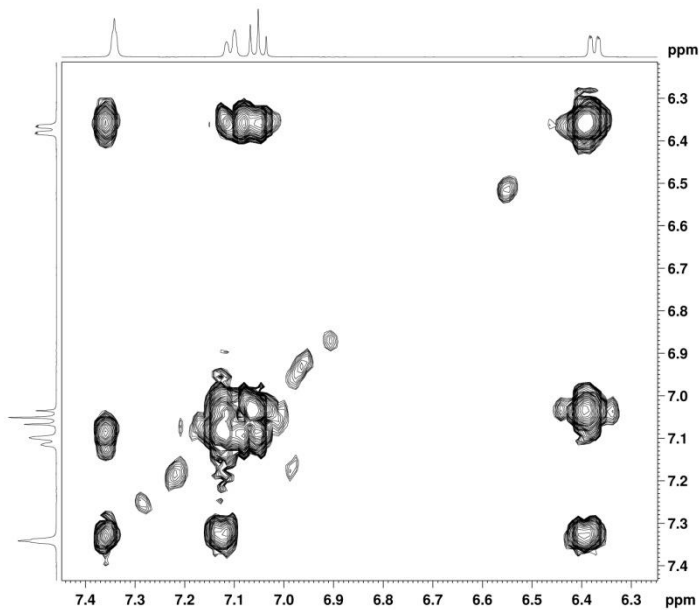


Fig. S6-5 COSY NMR spectrum of M6 (500 MHz, DMSO, 25 °C).

BRUKER AV-III-500 COSY-NMR RAT-117U-6 IN DMSO 2013.06.10  
 COSYGMFSW DMSO E:\miaozx-117 54



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Current Data Parameters
NAME      20130610-RAT-117U-6
EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
Date_    20130610
Time     15.22
INSTRUM spect
PROBHD   1.7 mm PATEX 1
PULPROG cosygpmfsw
TD        65536
SOLVENT  DMSO
NS        64
DS        8
SWH       5352.361 Hz
FIDRES   2.988436 Hz
AQ        0.173020 sec
RG        203
SWH       84.000 usec
DE        236.0 Hz
TE        298.0 K
D0        0.0000000 sec
D1        0.0011589 sec
D11       0.0000400 sec
D16       0.0002000 sec
DNO       0.0011800 sec

----- CHANNEL f1 -----
NUC1      1H
P1        7.50 usec
P1M1     2.4700003 Hz
SFO1     500.0600302 MHz

----- GRADIENT CHANNEL -----
GPM1M1   SMSQ10.100
GPM1M2   SMSQ10.100
GPM1M3   SMSQ10.100
GPM1M4   SMSQ10.100
GPM1M5   12.00 Hz
GPM1M6   40.00 Hz
P16      1000.00 usec

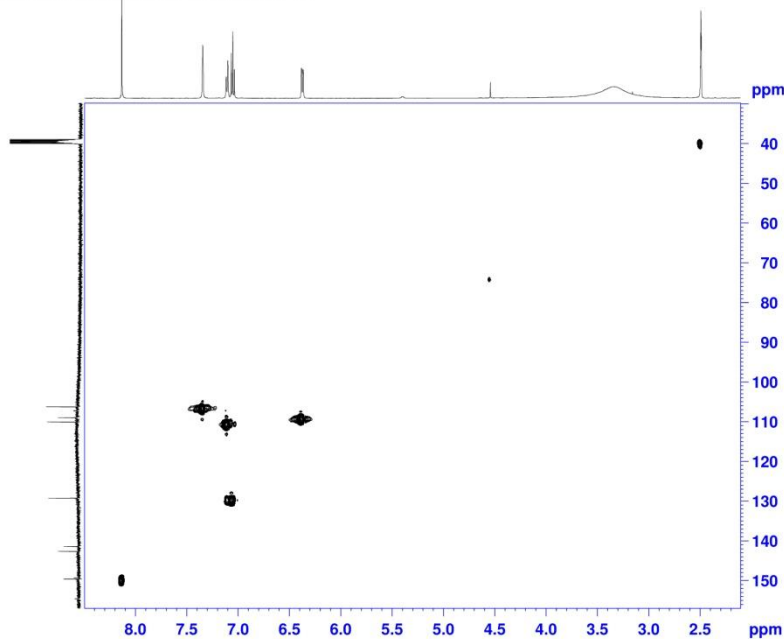
F1 - Acquisition parameters
TD        65536
SFO1     500.063 MHz
FIDRES   23.231468 Hz
SWH      11.403 ppm
F2MODE   QF

F2 - Processing parameters
SI        1024
SF        500.0600304 MHz
WDW       0 Hz
SSB       0
GB        0
PC        1.40

F1 - Processing parameters
SI        1024
SF        500.060194 MHz
WDW       States
SSB       0 Hz
LB        0 Hz
GB        0
    
```

Fig. S6-6 HSQC NMR spectrum of M6 (500 MHz, DMSO, 25 °C).

BRUKER AV-III-500 hsqc-NMR RAT-117U-6 IN DMSO 2013.06.10  
 HSQCETGPSI DMSO E:\miaozx-117 54



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Current Data Parameters
NAME      20130610-RAT-117U-6
EXPNO    4
PROCNO   1

F2 - Acquisition Parameters
Date_    20130610
Time     1.49
INSTRUM spect
PROBHD   1.7 mm PATEX 1
PULPROG hsqcetgps1
TD        65536
SOLVENT  DMSO
NS        128
DS        8
SWH       5352.361 Hz
FIDRES   5.412870 Hz
AQ        0.0000000 sec
RG        203
SWH       84.000 usec
DE        236.0 Hz
TE        298.0 K
D0        0.0000000 sec
D1        0.0000000 sec
D11       0.0017414 sec
D16       0.0000000 sec
DNO       0.0011800 sec
DNO2     0.0001999 sec
SFOPTM5  0.0001999 sec

----- CHANNEL f1 -----
NUC1      13C
P1        7.10 usec
P1M1     13.10 usec
P2M1     150.00 usec
P1M2     2.4700003 Hz
SFO1     100.6260302 MHz

----- CHANNEL f2 -----
CPDPRG2  gddp
NUC2      1H
P2        7.50 usec
P2M2     15.00 usec
P2M3     70.00 usec
P2M4     35.9000003 Hz
P2M5     5.6476998 Hz
SFO2     125.7637610 MHz

----- GRADIENT CHANNEL -----
GPM1M1   SMSQ10.100
GPM1M2   SMSQ10.100
GPM1M3   80.00 Hz
GPM1M4   20.10 Hz
P16      1000.00 usec

F1 - Acquisition parameters
TD        65536
SFO1     125.763 MHz
FIDRES   196.485088 Hz
SWH      193.959 ppm
F2MODE   Echo-Antiecho

F2 - Processing parameters
SI        1024
SF        500.0600000 MHz
WDW       0 Hz
SSB       0
GB        0
PC        1.40

F1 - Processing parameters
SI        1024
SF        125.7601810 MHz
WDW       0 Hz
SSB       0 Hz
LB        0 Hz
GB        0
    
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Fig. S6-7 HMBC NMR spectrum of M6 (500 MHz, DMSO, 25 °C).

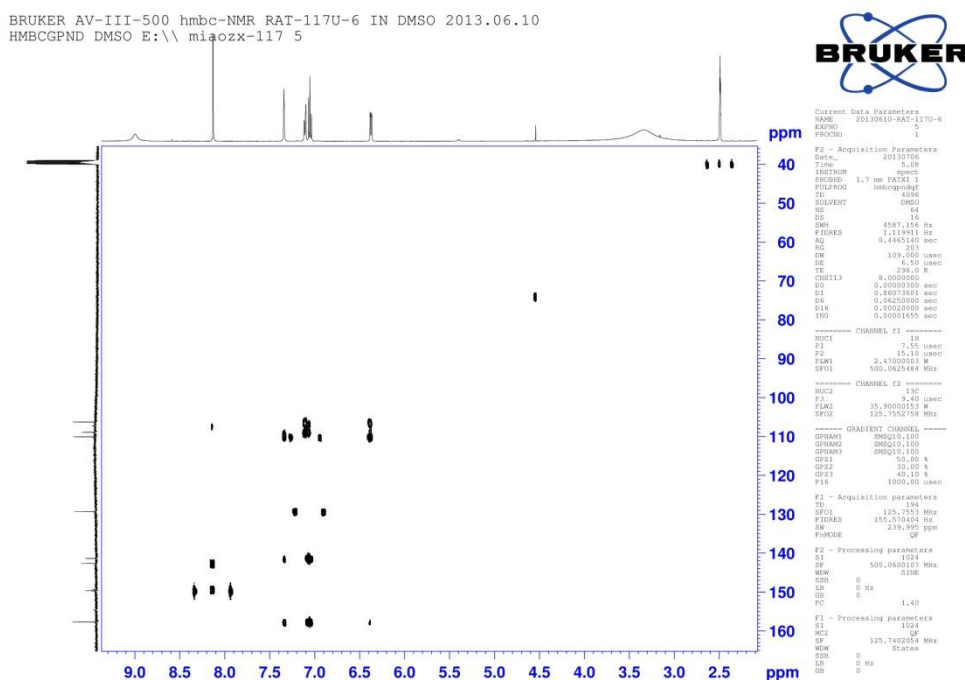


Fig. S6-8 HMBC NMR spectrum of M6 (500 MHz, DMSO, 25 °C).

