

S1 File. The MS and NMR spectra of WS010117.

Fig. S1-1 Mass spectrum of WS010117 obtained by ESI-MS. (A) EMS spectrum. (B) MS² spectrum

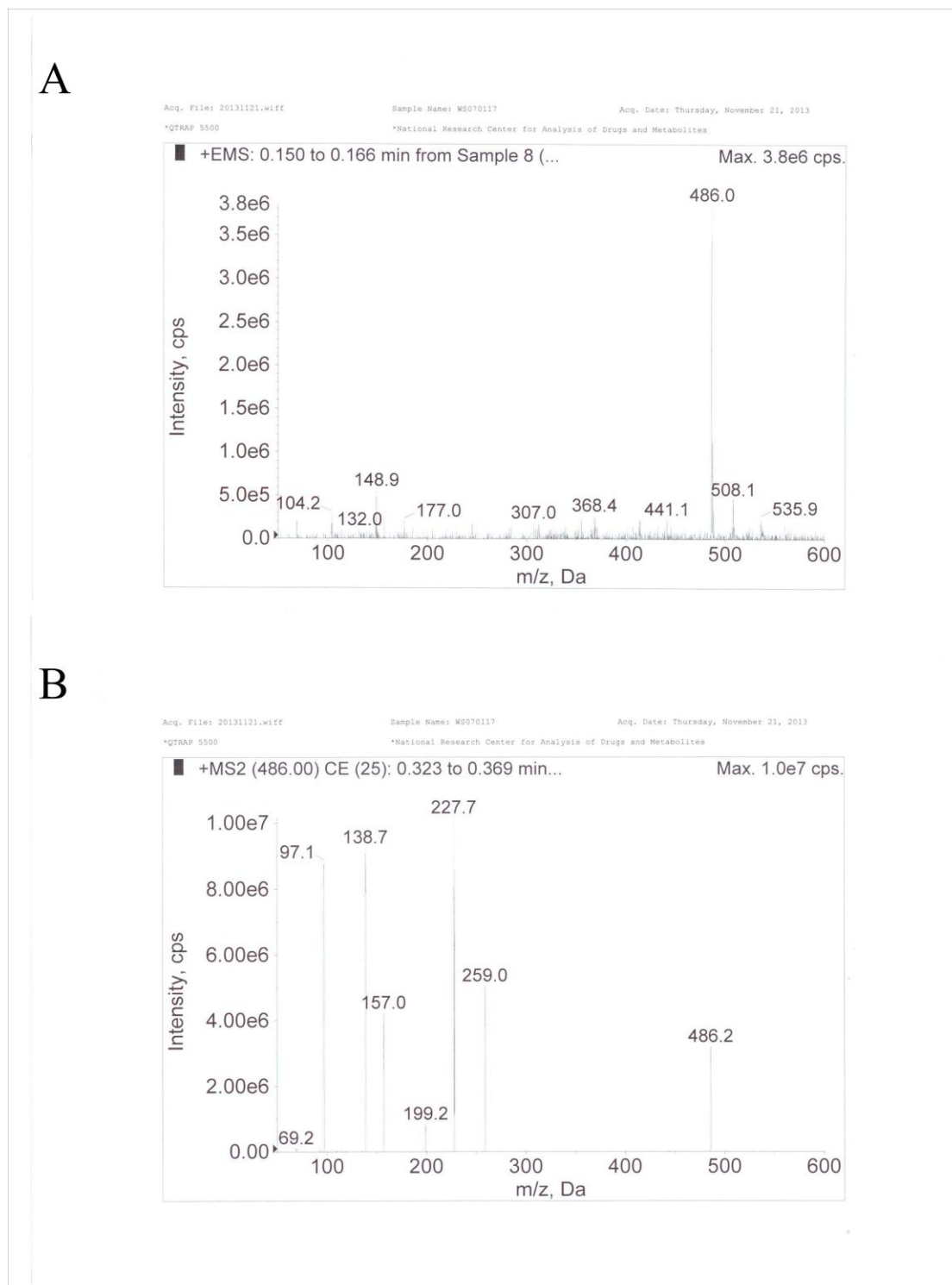


Fig. S1-2 ^1H NMR spectrum of WS010117 (500 MHz, DMSO, 25 $^\circ\text{C}$).

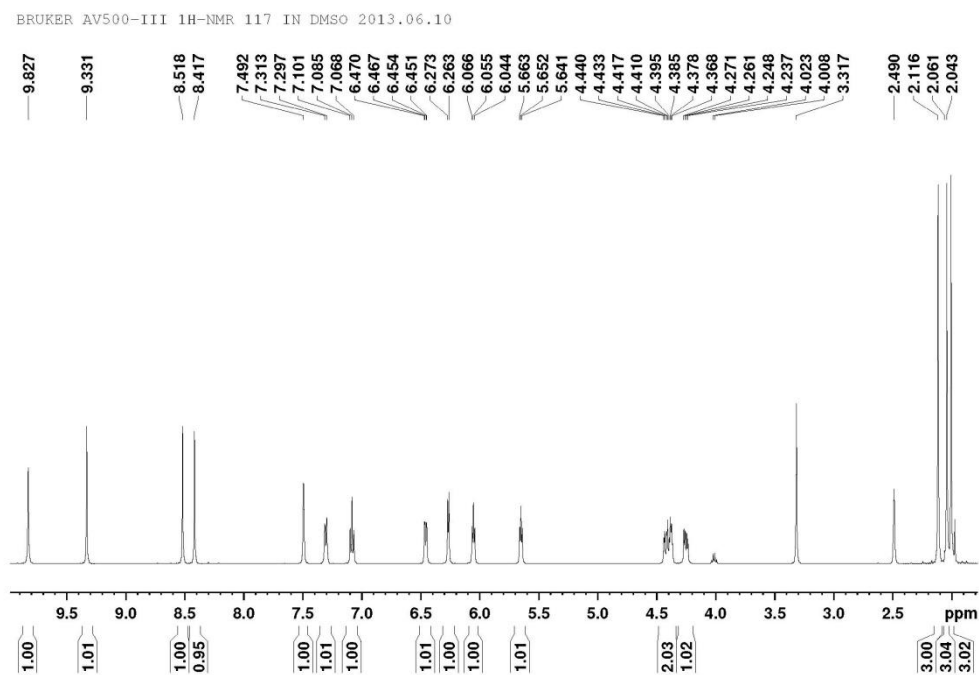


Fig. S1-3 ^{13}C NMR spectrum of WS010117 (500 MHz, DMSO, 25 $^\circ\text{C}$).

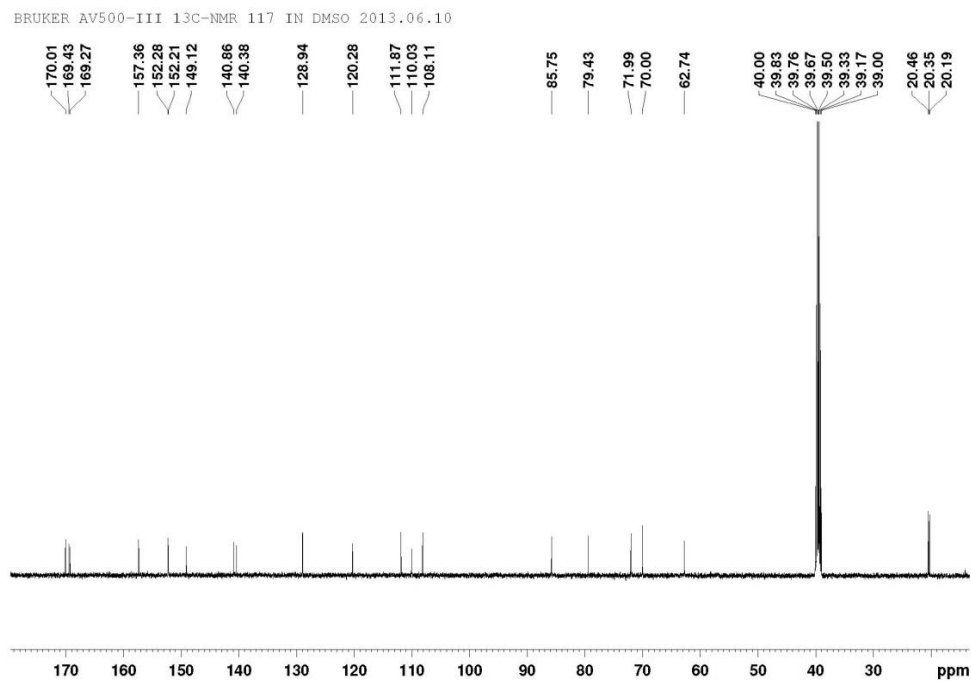


Fig. S1-4 DEPT NMR spectrum of WS010117 (500 MHz, DMSO, 25 °C).

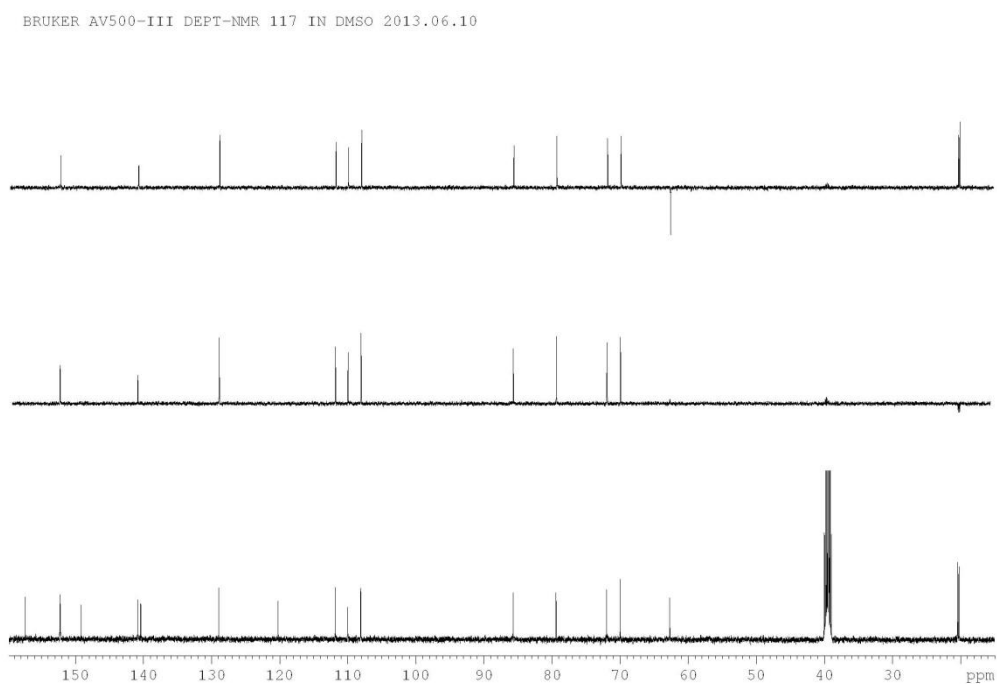


Fig. S1-5 COSY NMR spectrum of WS010117 (500 MHz, DMSO, 25 °C).

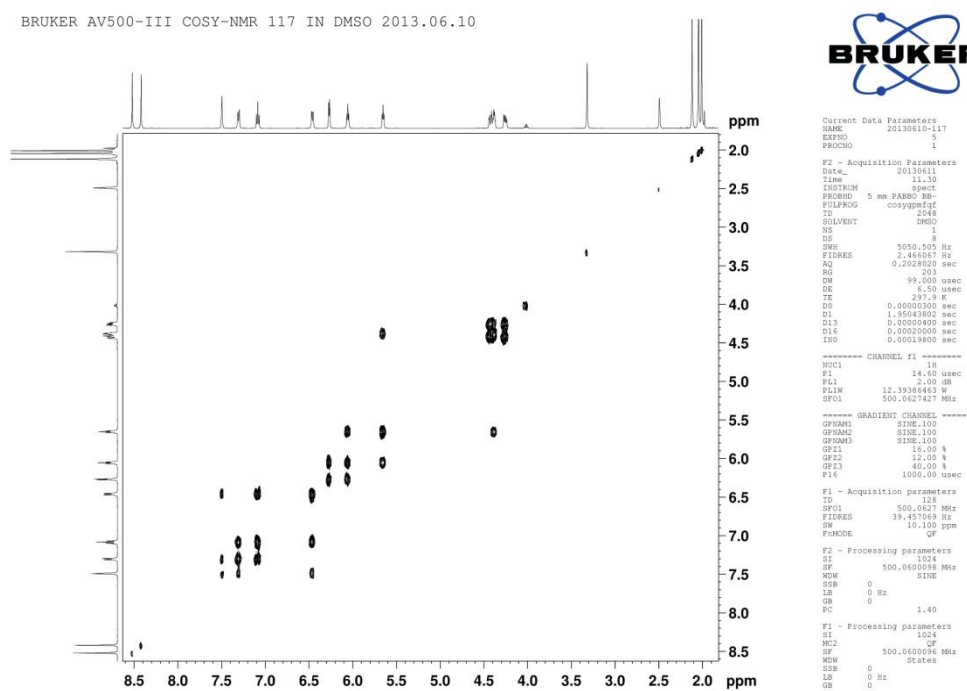
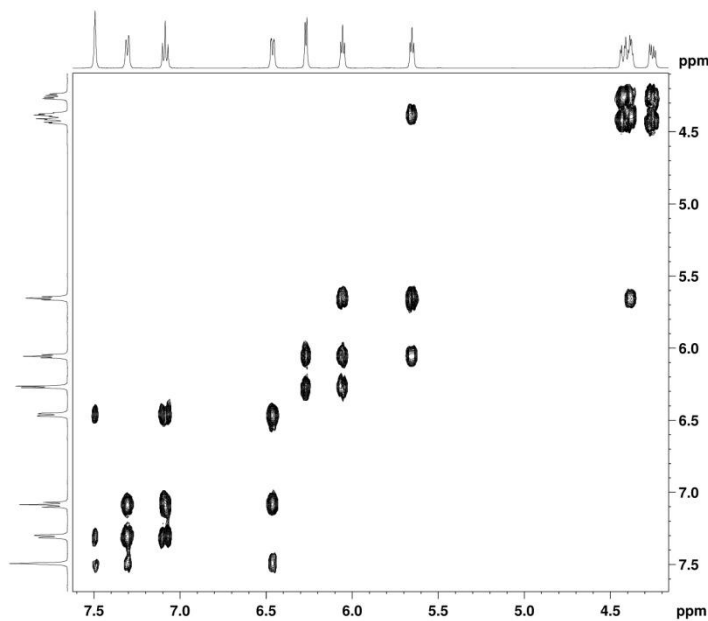


Fig. S1-6 COSY NMR spectrum of WS010117 (500 MHz, DMSO, 25 °C).

BRUKER AV500-III COSY-NMR 117 IN DMSO 2013.06.10



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Current Data Parameters
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PROCNO   1

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Time     11:30
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PROBHD   5 mm PABBO BB-
PULPROG  cosygmfzf9
TD        65536
SOLVENT  DMSO
NS        1
DS        4
SWH       5050.505 Hz
FIDRES   2.464067 Hz
AQ        0.2028020 sec
RG        203
DM        99.000 usec
DE        6.50 usec
TE        297.2 K
D0        0.0000300 sec
D1        1.30001900 sec
D13       0.0000400 sec
D14       0.0001000 sec
IN0       0.0001900 sec

----- CHANNEL f1 -----
NUC1      1H
P1        14.60 usec
PL1       2.00 dB
PL12      12.39386463 W
SFO1      500.0627427 MHz

----- GRADIENT CHANNEL -----
GPM1M1   SINE.100
GPM1M2   SINE.100
GPM1M3   SINE.100
GPF1     16.00 %
GPF2     12.00 %
GPF3     40.00 %
P14      1000.00 usec

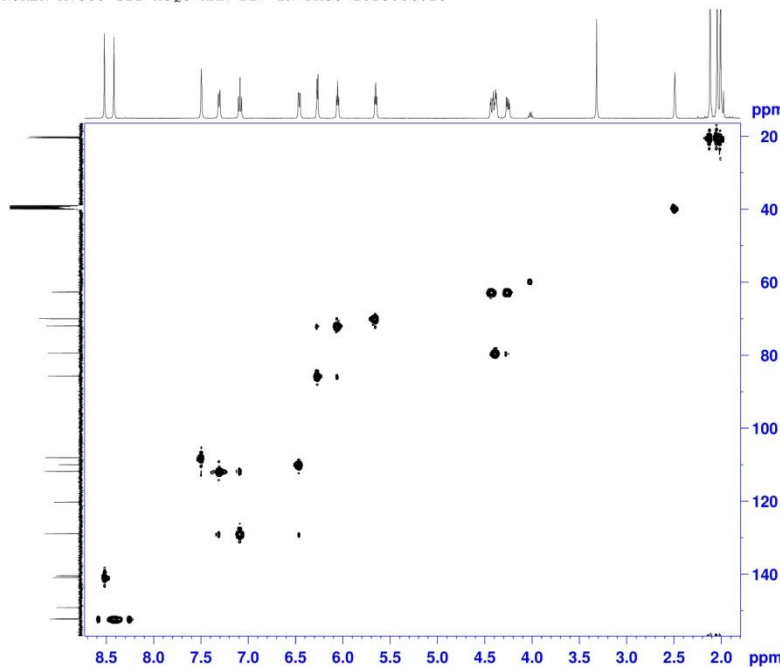
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SFO1     500.0627 MHz
FIDRES   39.457069 Hz
SW        10.100 ppm
F8MODE   QF

F2 - Processing parameters
SI        1024
SF        500.060098 MHz
WDW       SINE
SSB       0 Hz
GB        0
PC        1.40

F1 - Processing parameters
SI        1024
SF        500.060098 MHz
WDW       SINE
SSB       0 Hz
GB        0
PC        1.40
    
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Fig. S1-7 HSQC NMR spectrum of WS010117 (500 MHz, DMSO, 25 °C).

BRUKER AV500-III HSQC-NMR 117 IN DMSO 2013.06.10



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Current Data Parameters
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EXPNO    1
PROCNO   1

F2 - Acquisition Parameters
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Time     11:36
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PULPROG  hsqcgmfzf9
TD        65536
SOLVENT  DMSO
NS        4
DS        4
SWH       5050.505 Hz
FIDRES   4.920118 Hz
AQ        0.1014200 sec
RG        203
DM        99.000 usec
DE        6.50 usec
TE        297.2 K
D0        0.0000300 sec
D1        1.47501900 sec
D13       0.0017400 sec
D14       0.0000300 sec
D15       0.0000400 sec
D16       0.0001000 sec
D17       0.0011000 sec
IN0       0.0002400 sec

----- CHANNEL f1 -----
NUC1      1H
P1        14.60 usec
PL1       2.00 dB
PL12      12.39386463 W
SFO1      500.0627427 MHz

----- CHANNEL f2 -----
CPDPRG2  gcp2
NUC2      13C
P2        18.00 usec
PL2       19.00 usec
PL22      78.00 usec
PL23      0 Hz
PL24      0 Hz
PL25      0 Hz
PL26      0 Hz
PL27      0 Hz
PL28      0 Hz
PL29      0 Hz
PL2A      0 Hz
PL2B      0 Hz
PL2C      0 Hz
PL2D      0 Hz
PL2E      0 Hz
PL2F      0 Hz
PL2G      0 Hz
PL2H      0 Hz
PL2I      0 Hz
PL2J      0 Hz
PL2K      0 Hz
PL2L      0 Hz
PL2M      0 Hz
PL2N      0 Hz
PL2O      0 Hz
PL2P      0 Hz
PL2Q      0 Hz
PL2R      0 Hz
PL2S      0 Hz
PL2T      0 Hz
PL2U      0 Hz
PL2V      0 Hz
PL2W      0 Hz
PL2X      0 Hz
PL2Y      0 Hz
PL2Z      0 Hz
SFO2     125.7493653 MHz

----- GRADIENT CHANNEL -----
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GPM2M2   SINE.100
GPM2M3   SINE.100
GPF2     80.00 %
GPF3     20.00 %
P14      1000.00 usec

F1 - Acquisition parameters
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SFO1     500.0627 MHz
FIDRES   128.120 Hz
SW        162.21906 Hz
WDW       SINE
SSB       0 Hz
GB        0
PC        1.40

F2 - Processing parameters
SI        1024
SF        125.7402395 MHz
WDW       SINE
SSB       0 Hz
GB        0
PC        1.40

F1 - Processing parameters
SI        1024
SF        125.7402395 MHz
WDW       SINE
SSB       0 Hz
GB        0
PC        1.40
    
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Fig. S1-8 HSQC NMR spectrum of WS010117 (500 MHz, DMSO, 25 °C).

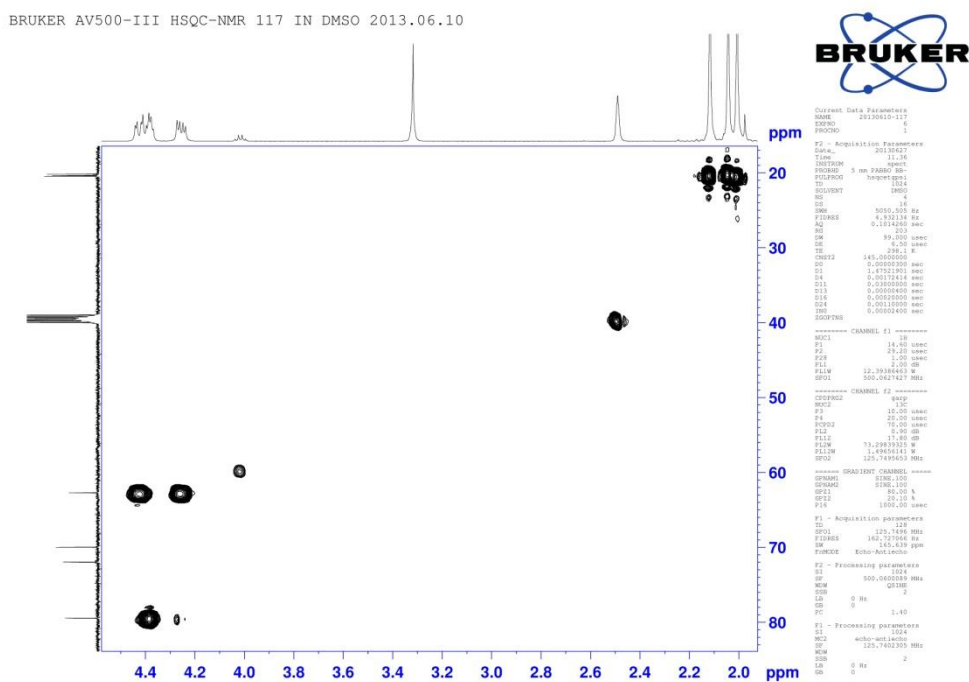


Fig. S1-9 HSQC NMR spectrum of WS010117 (500 MHz, DMSO, 25 °C).

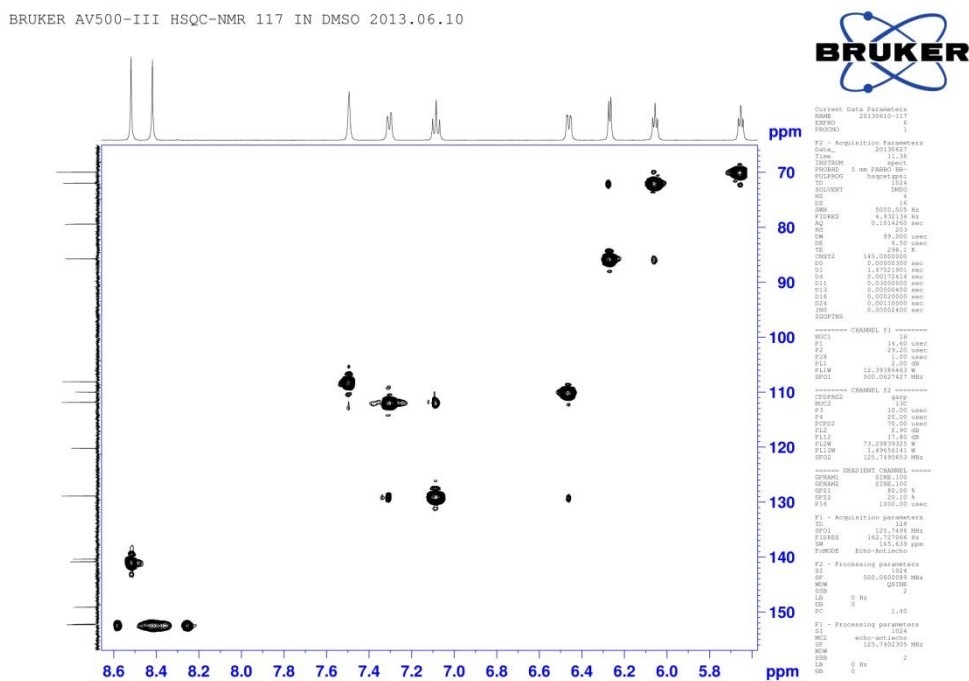


Fig. S1-10 HMBC NMR spectrum of WS010117 (500 MHz, DMSO, 25 °C).

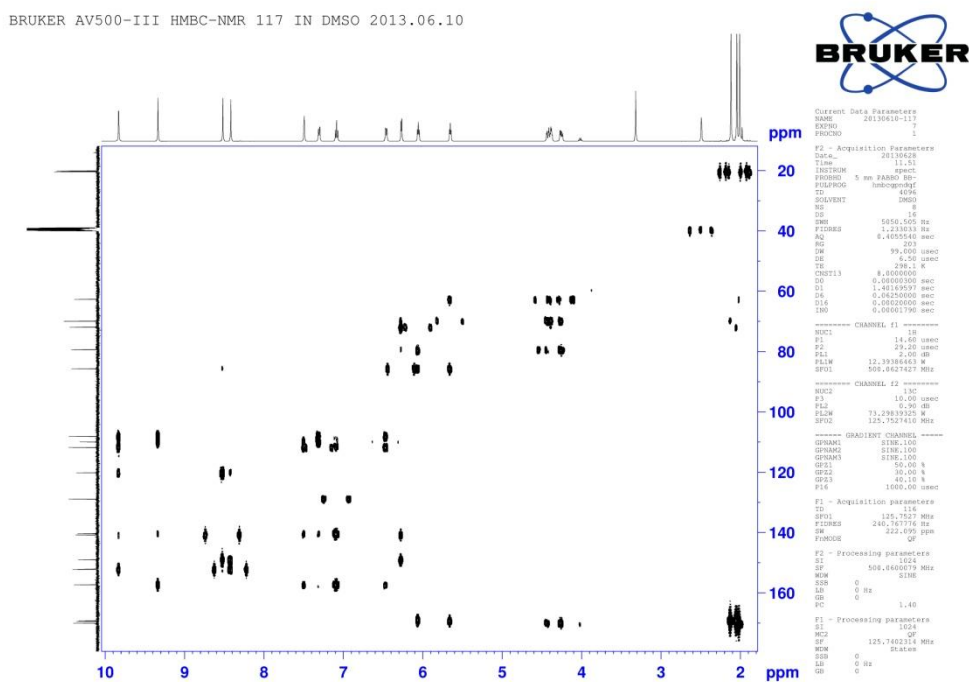


Fig. S1-11 HMBC NMR spectrum of WS010117 (500 MHz, DMSO, 25 °C).

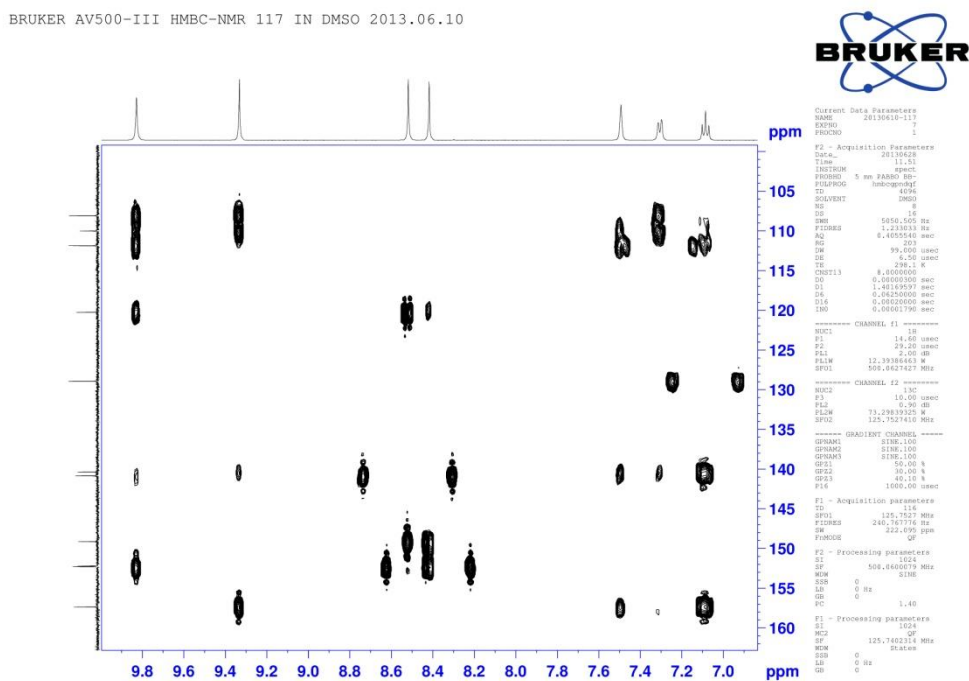


Fig. S1-12 HMBC NMR spectrum of WS010117 (500 MHz, DMSO, 25 °C).

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