

# Title of Manuscript: Acylated Iridoids with Cytotoxicity from *Valeriana jatamansi*

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Zheng-sheng Huang, Run-hui Liu, Xi-ke Xu, Wei-dong Zhang\*, Hui Wang\*

## Supporting Information Available

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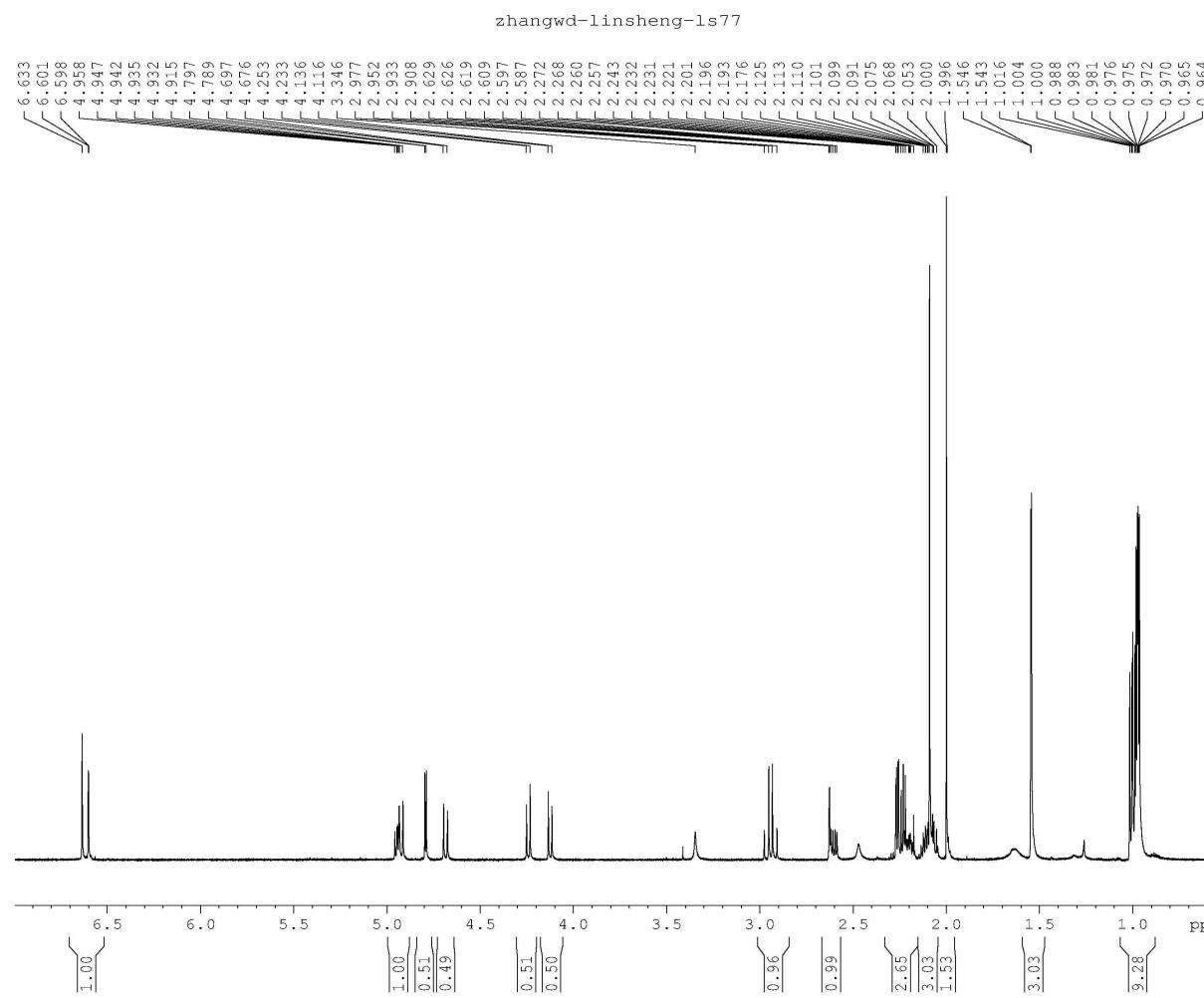
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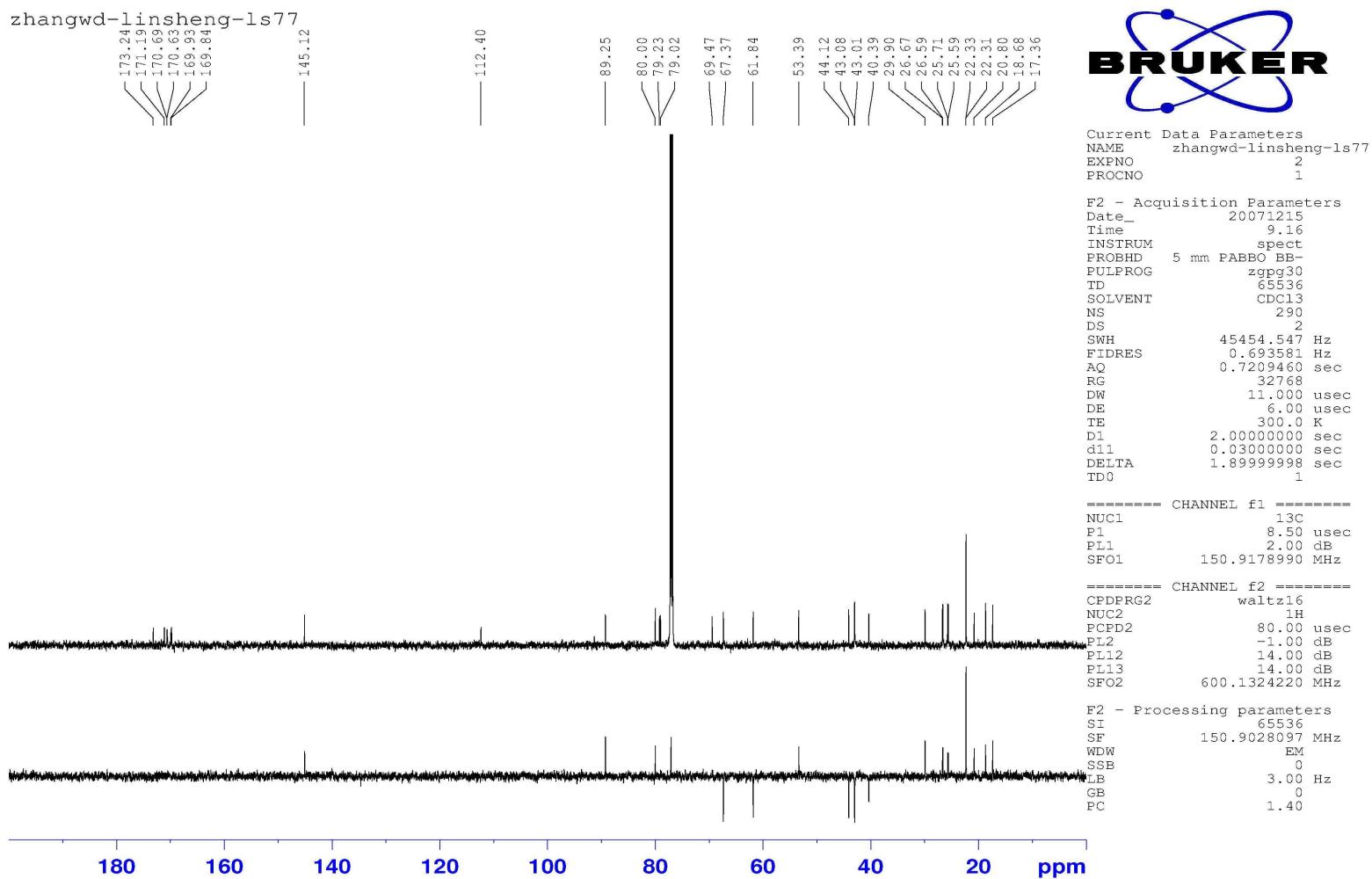
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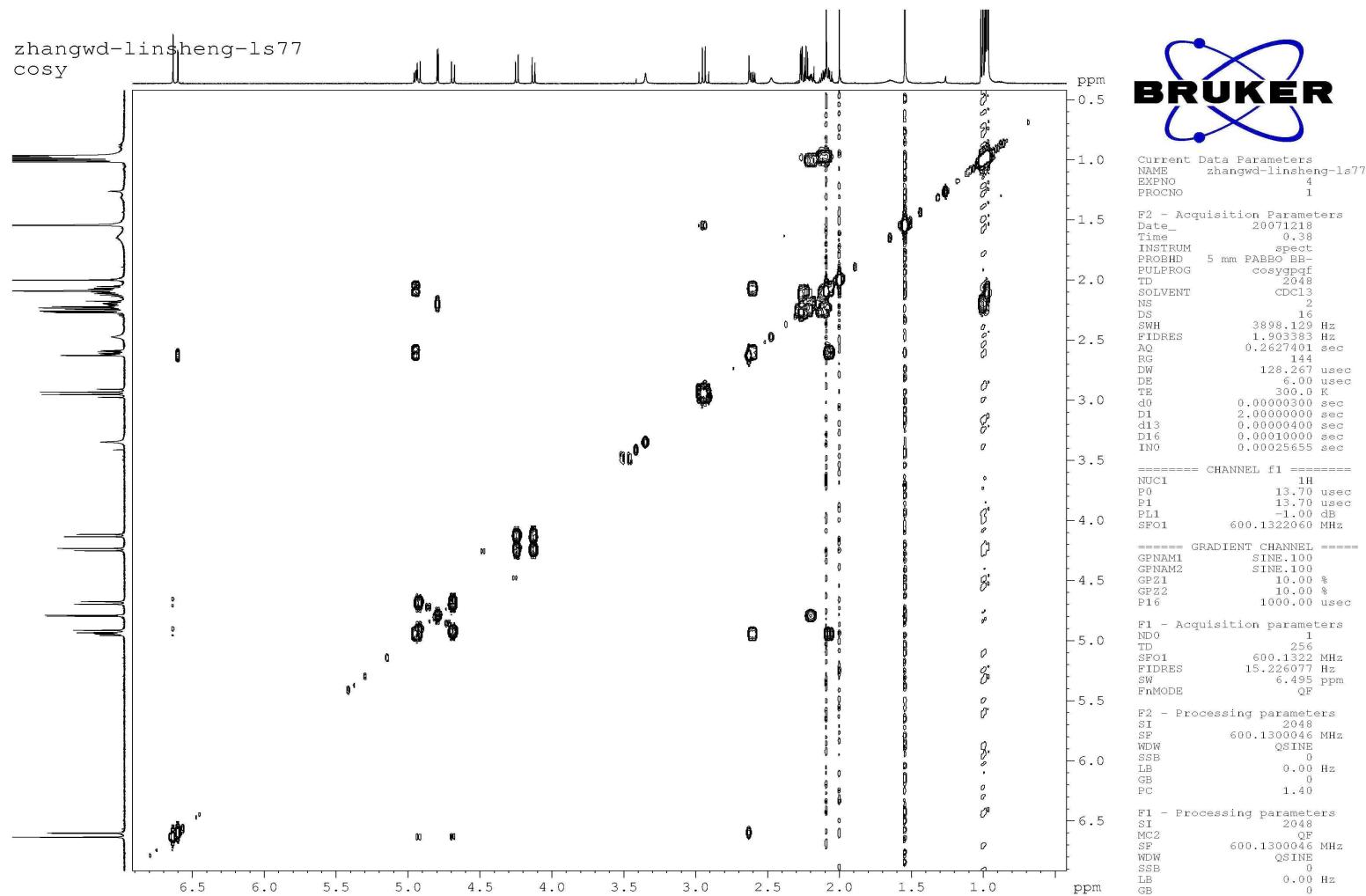
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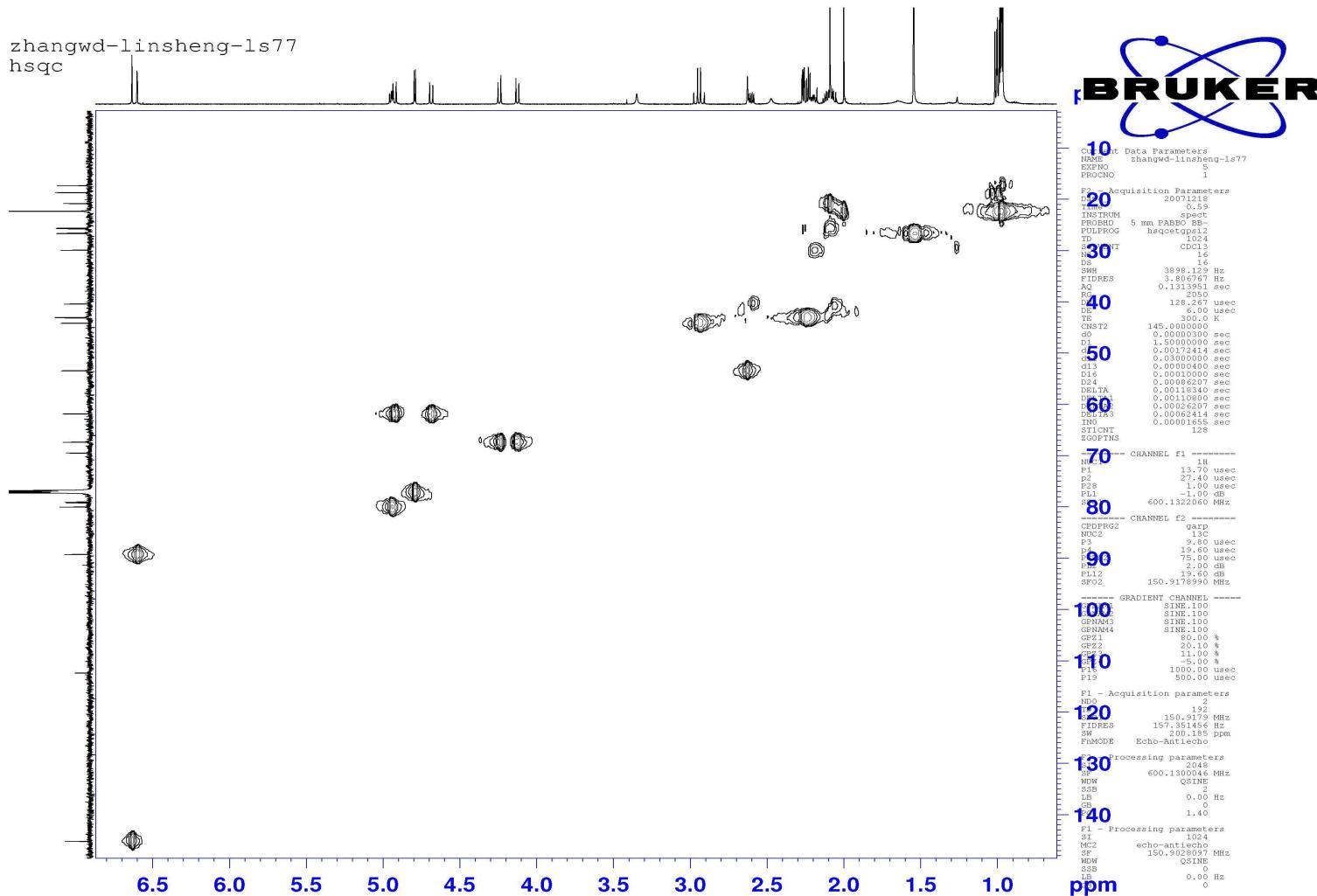
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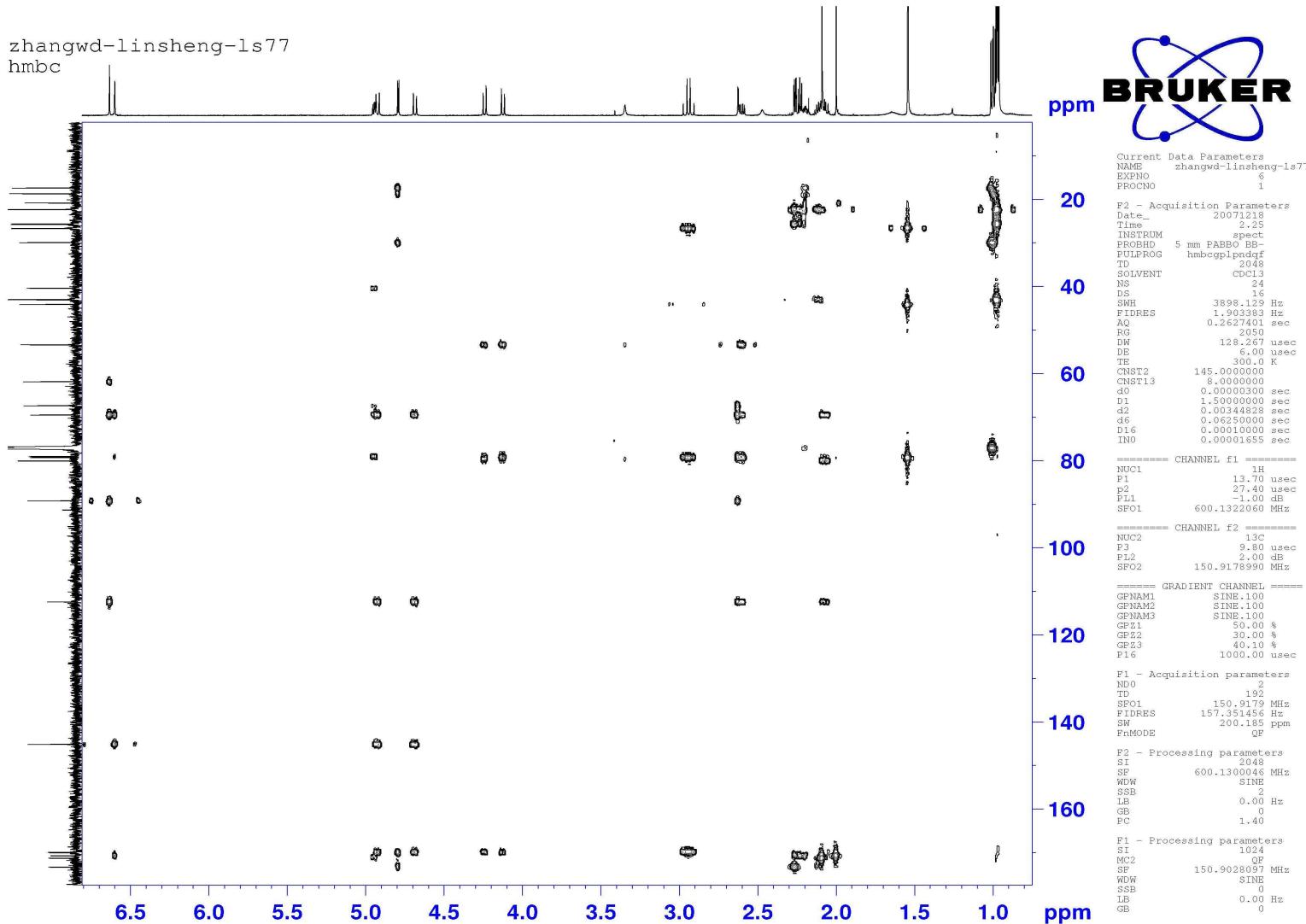
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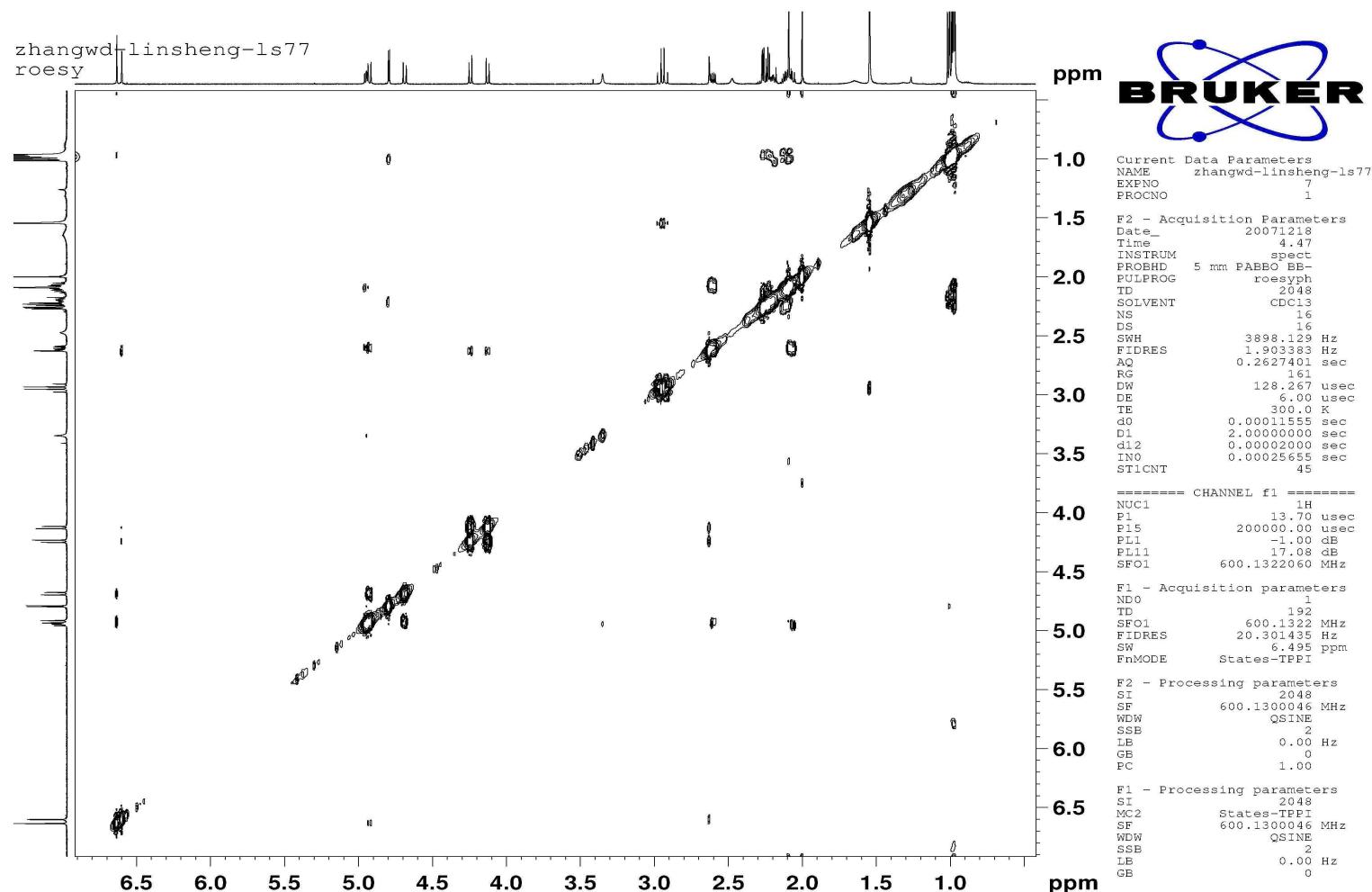
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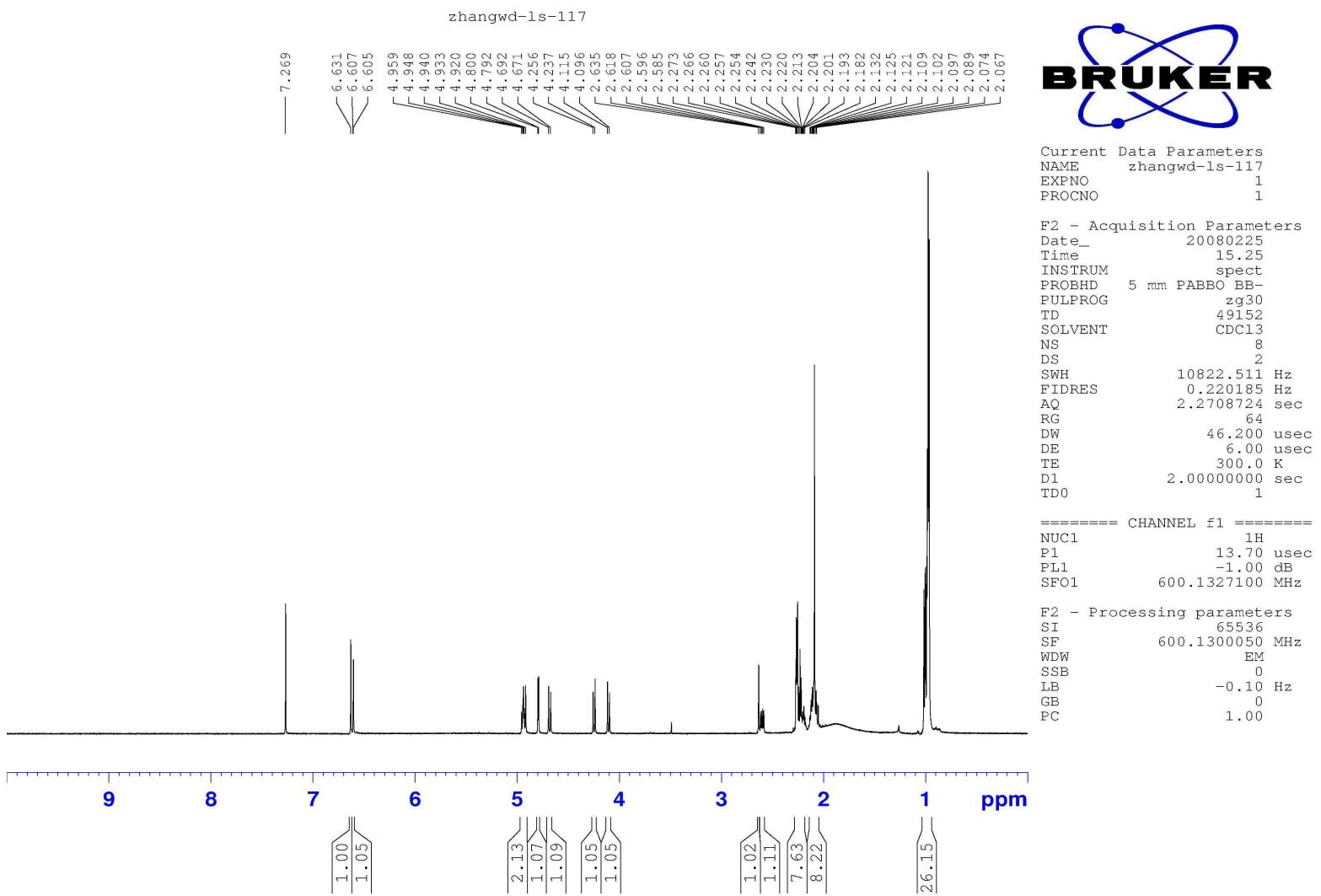
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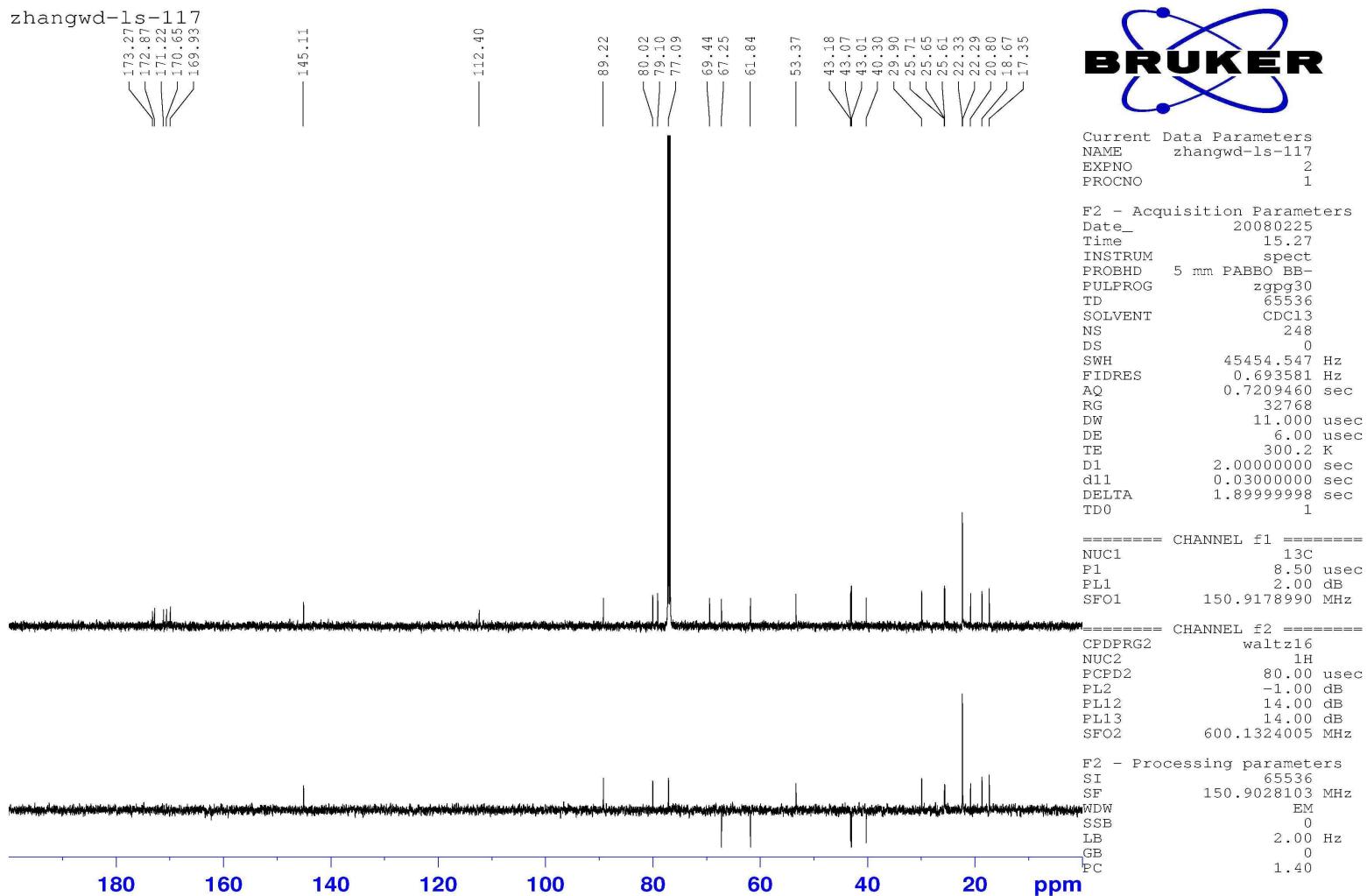
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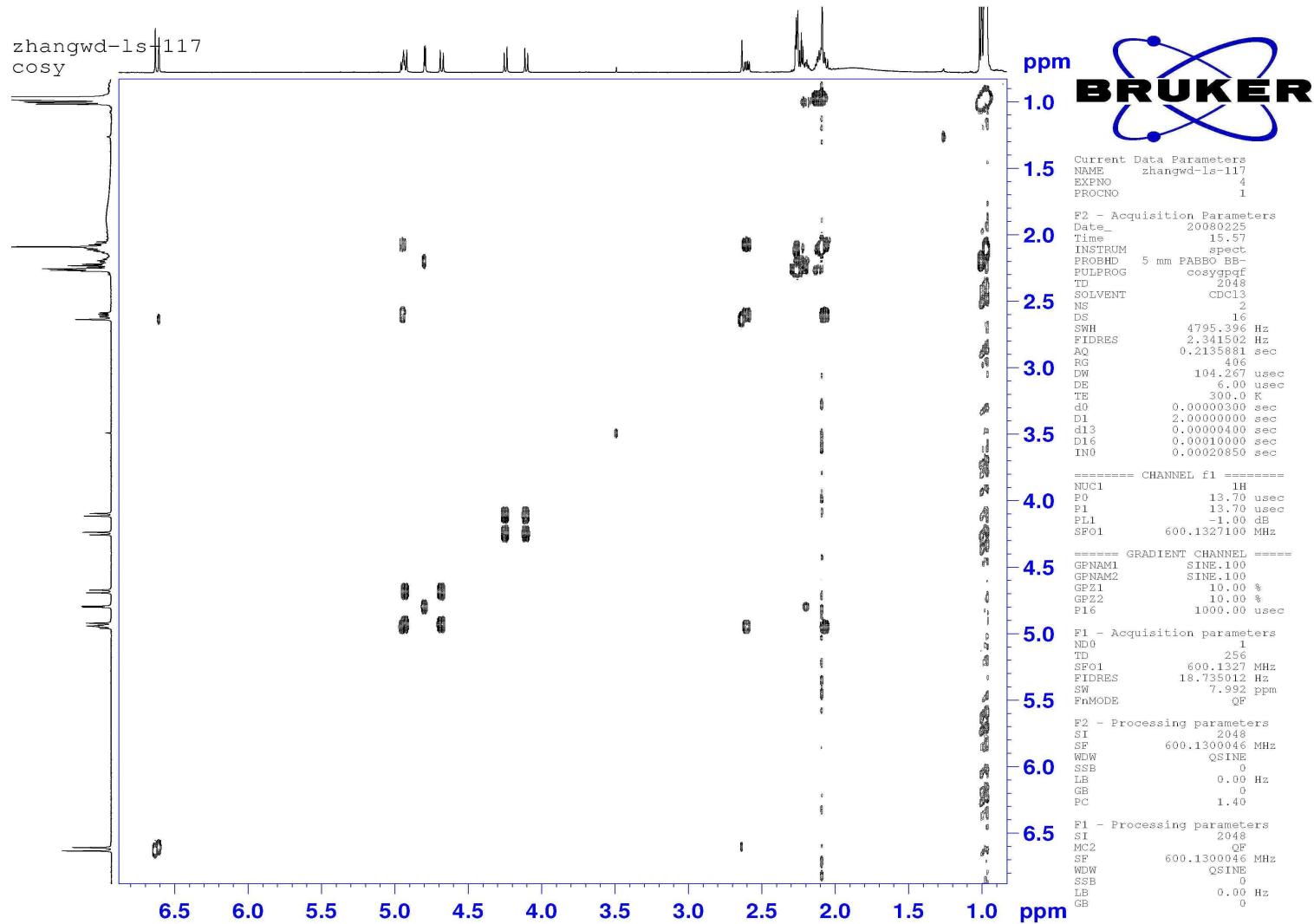
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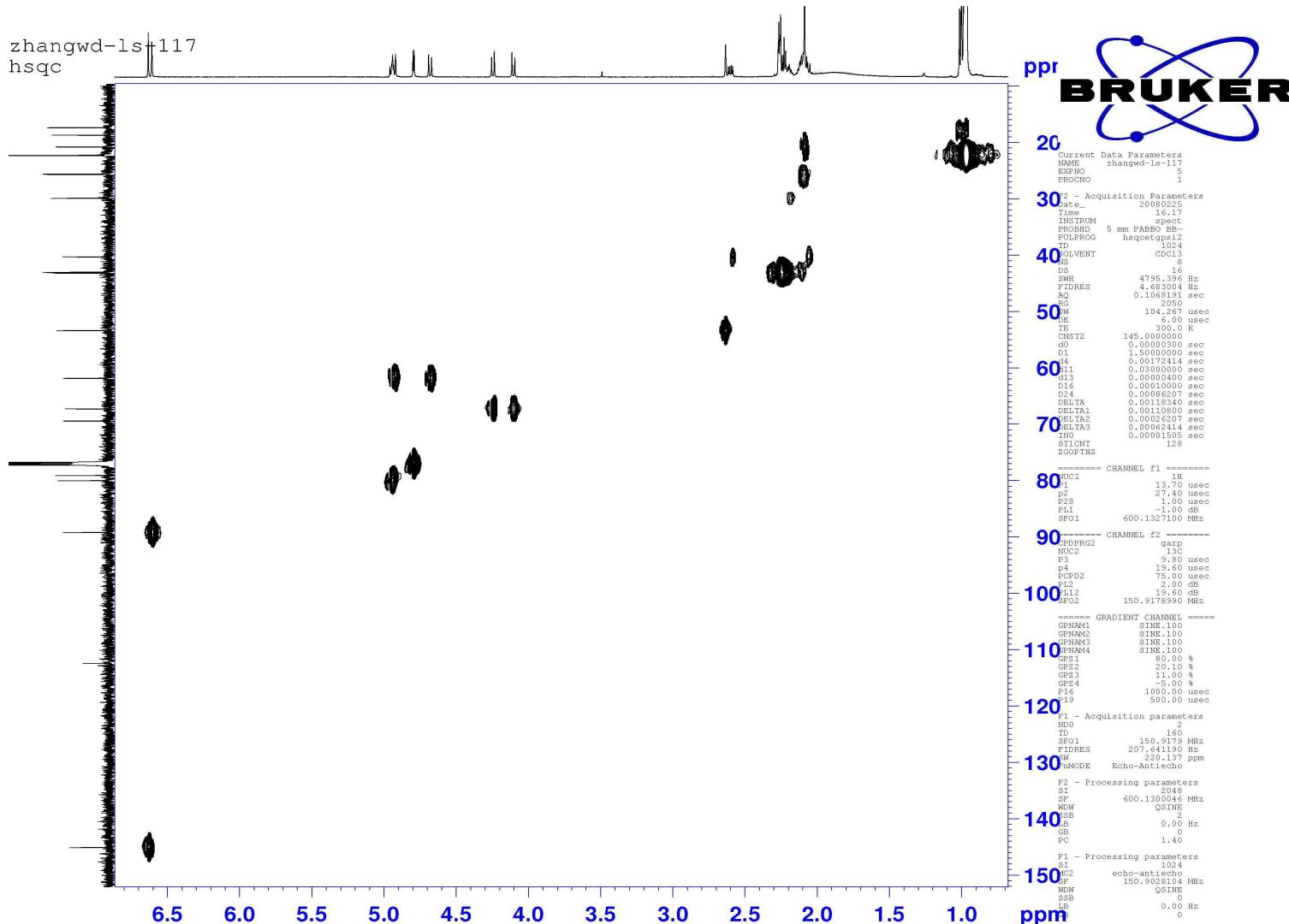
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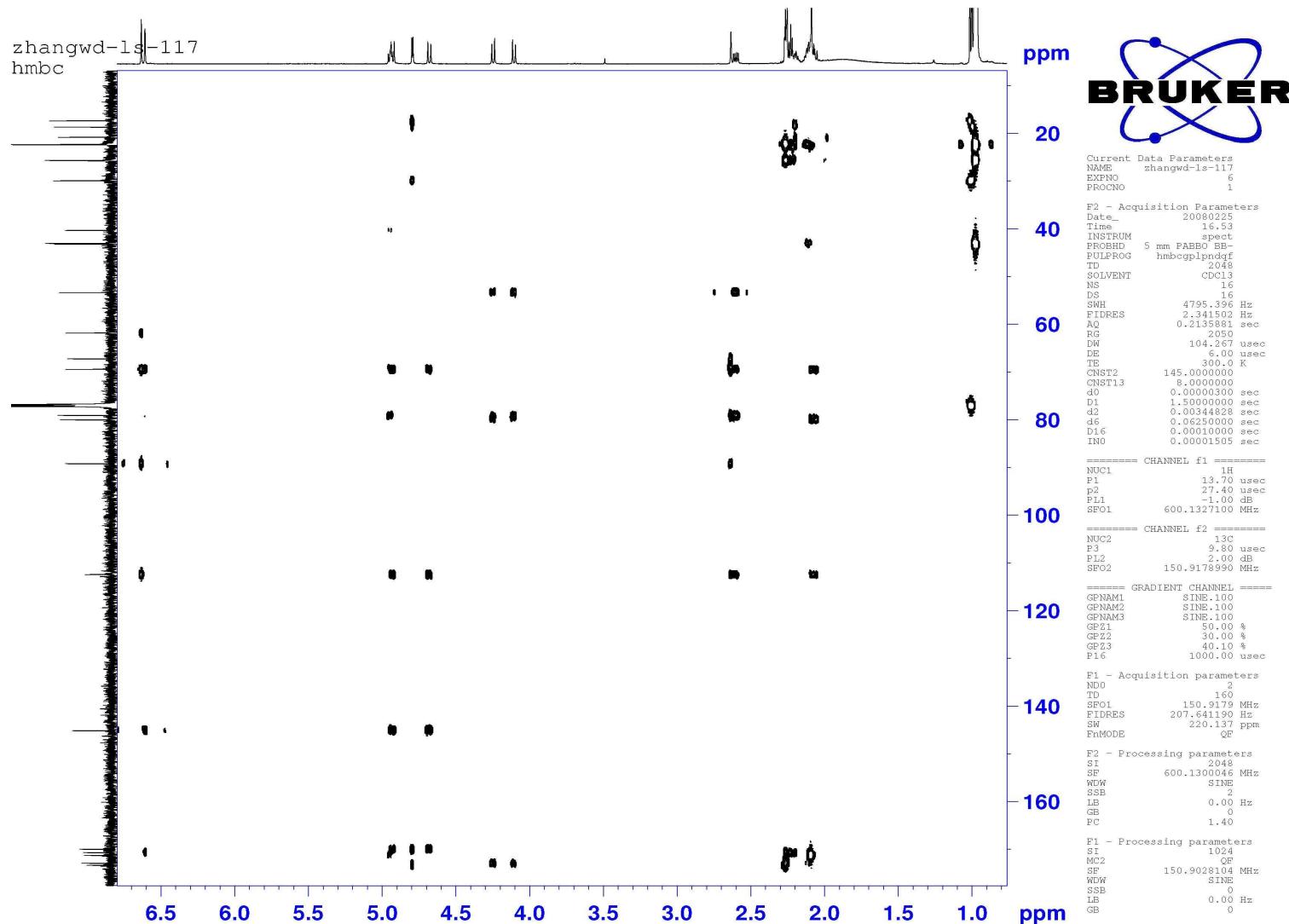
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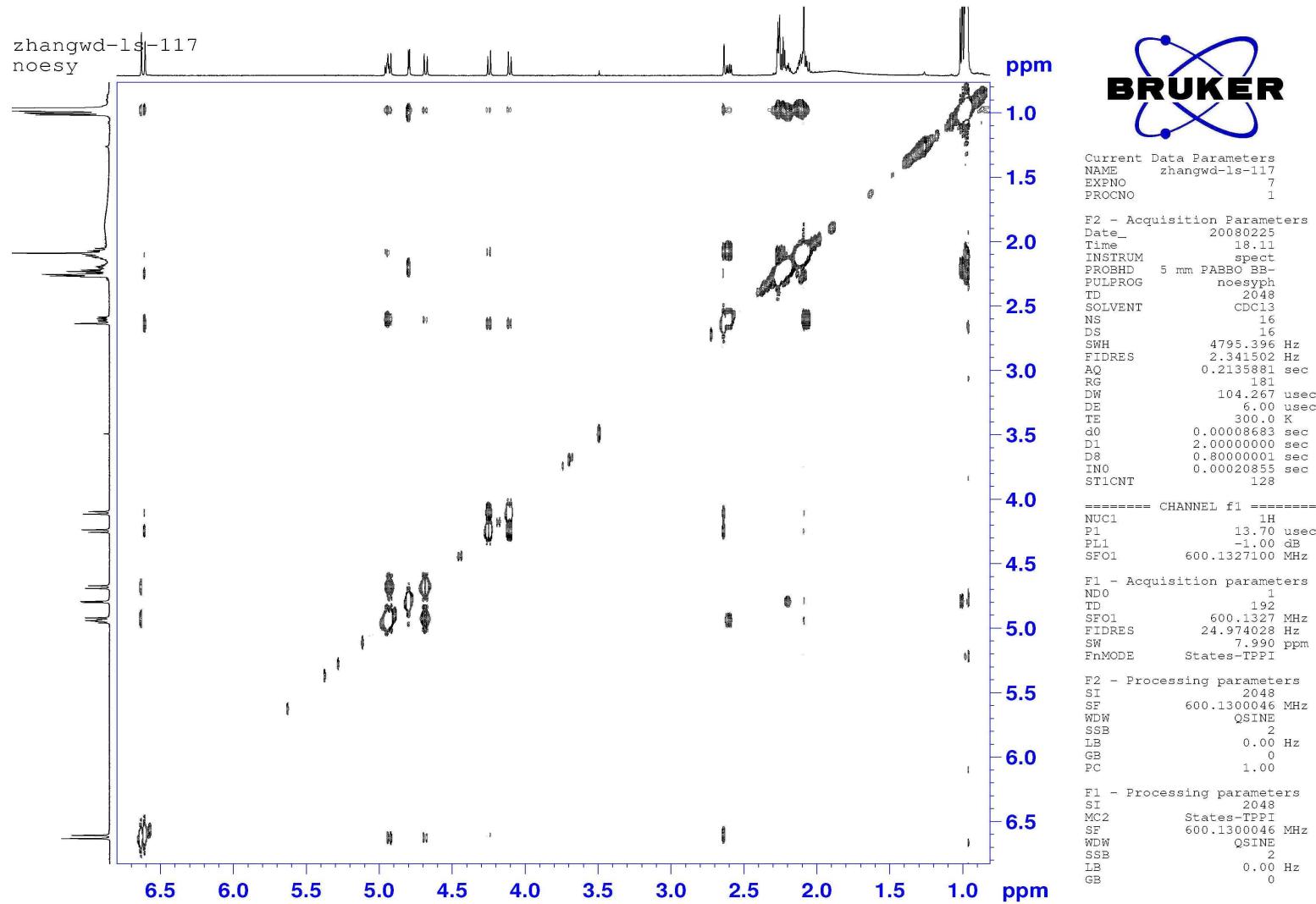
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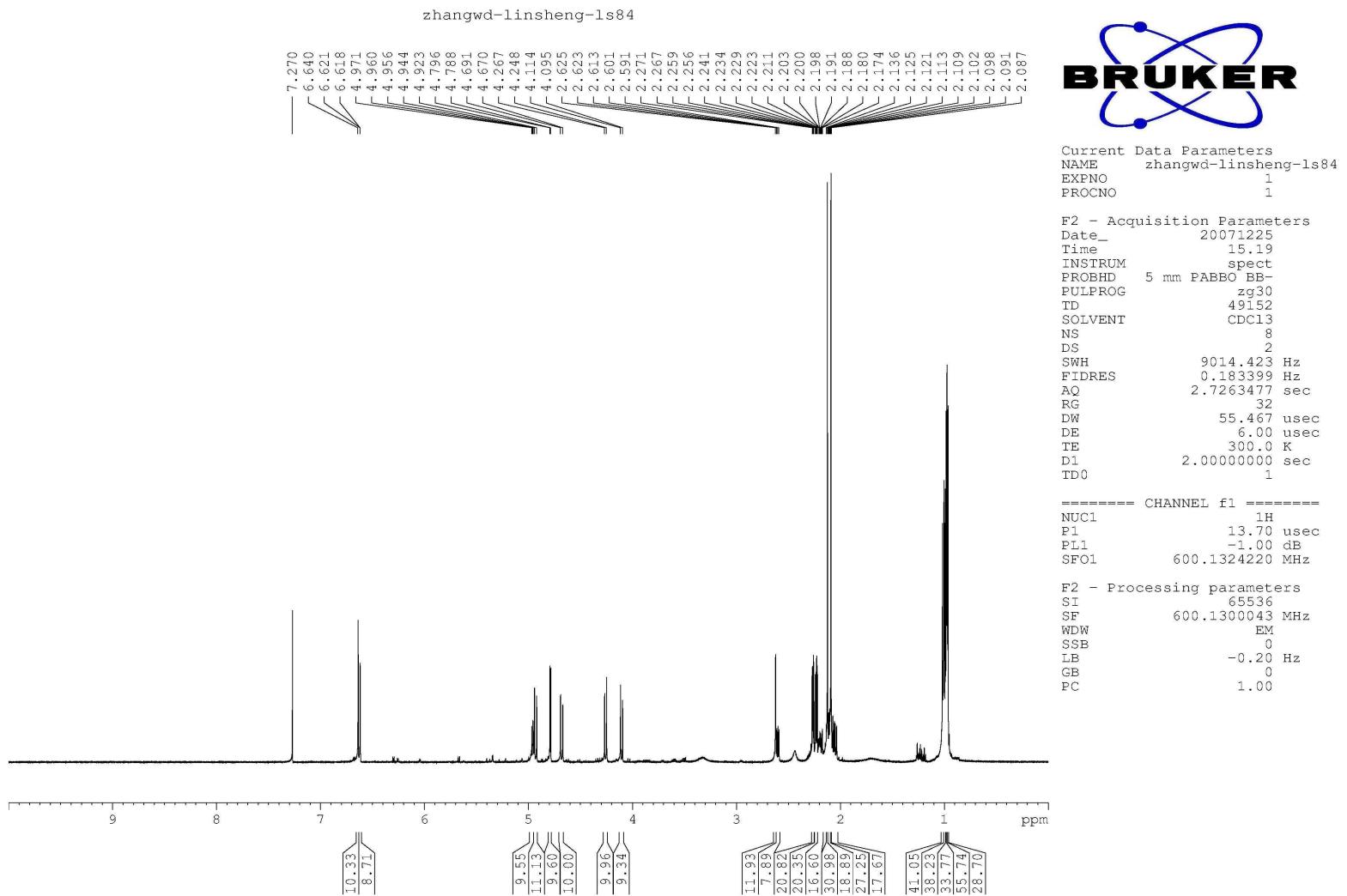
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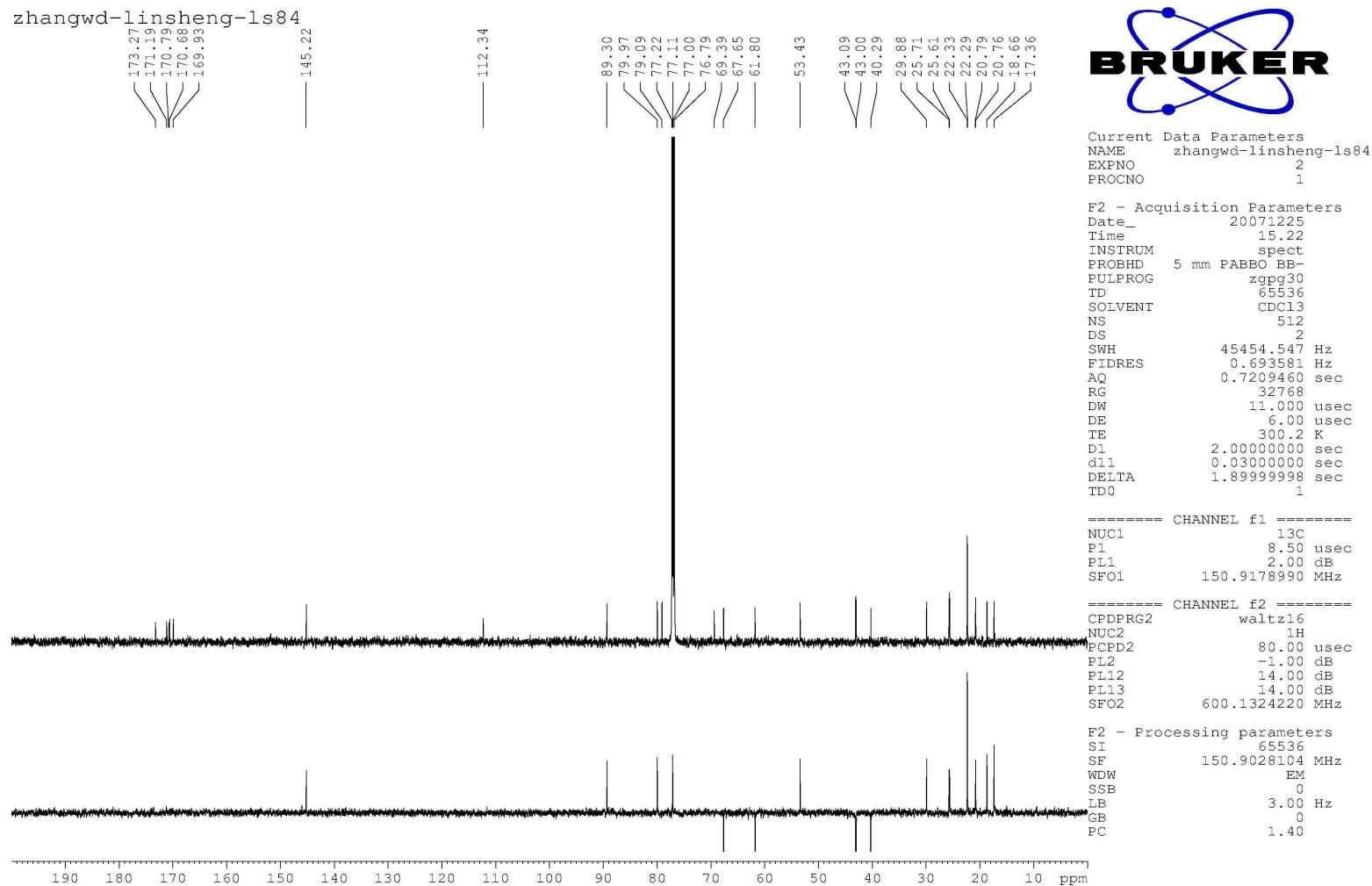
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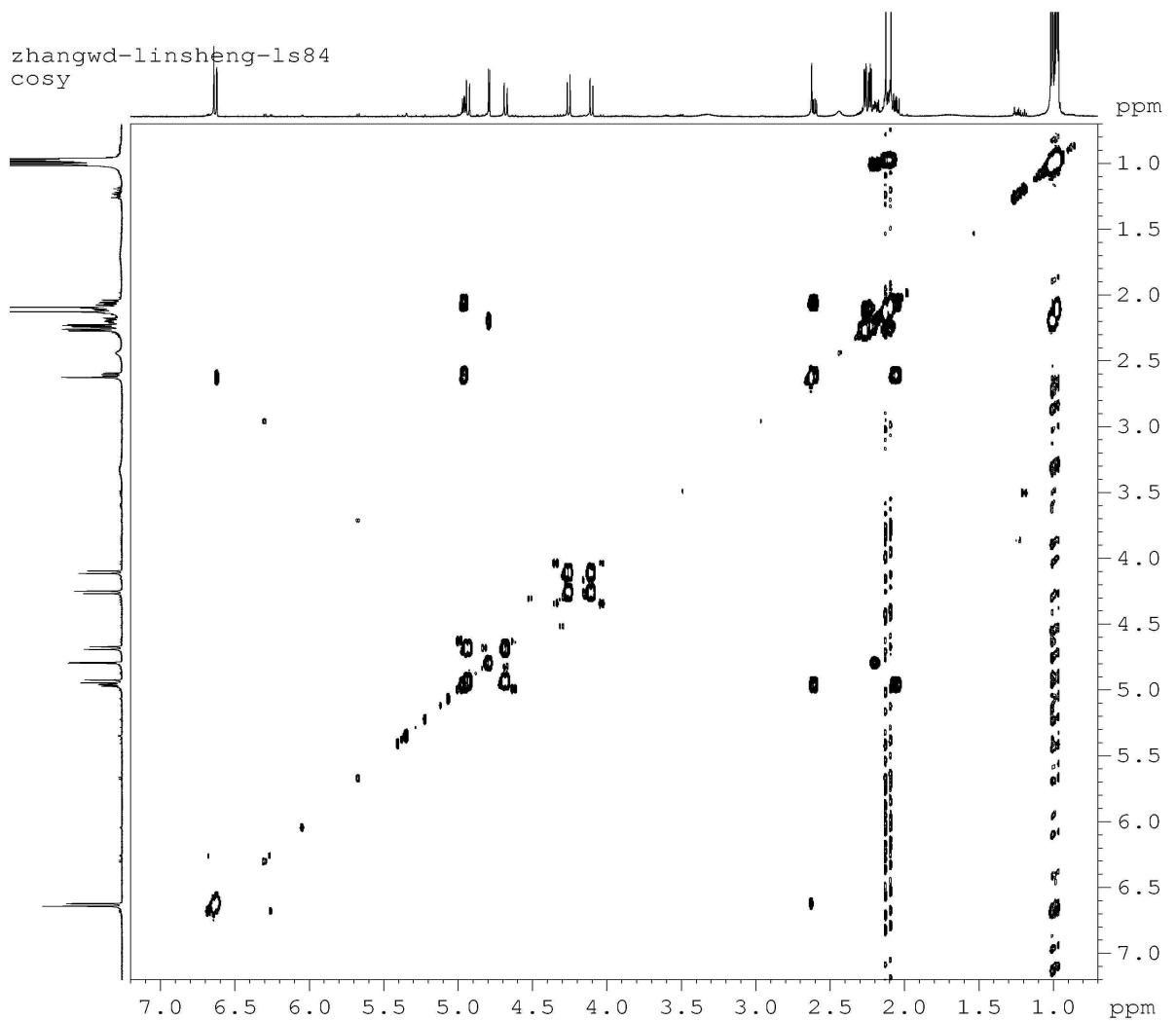
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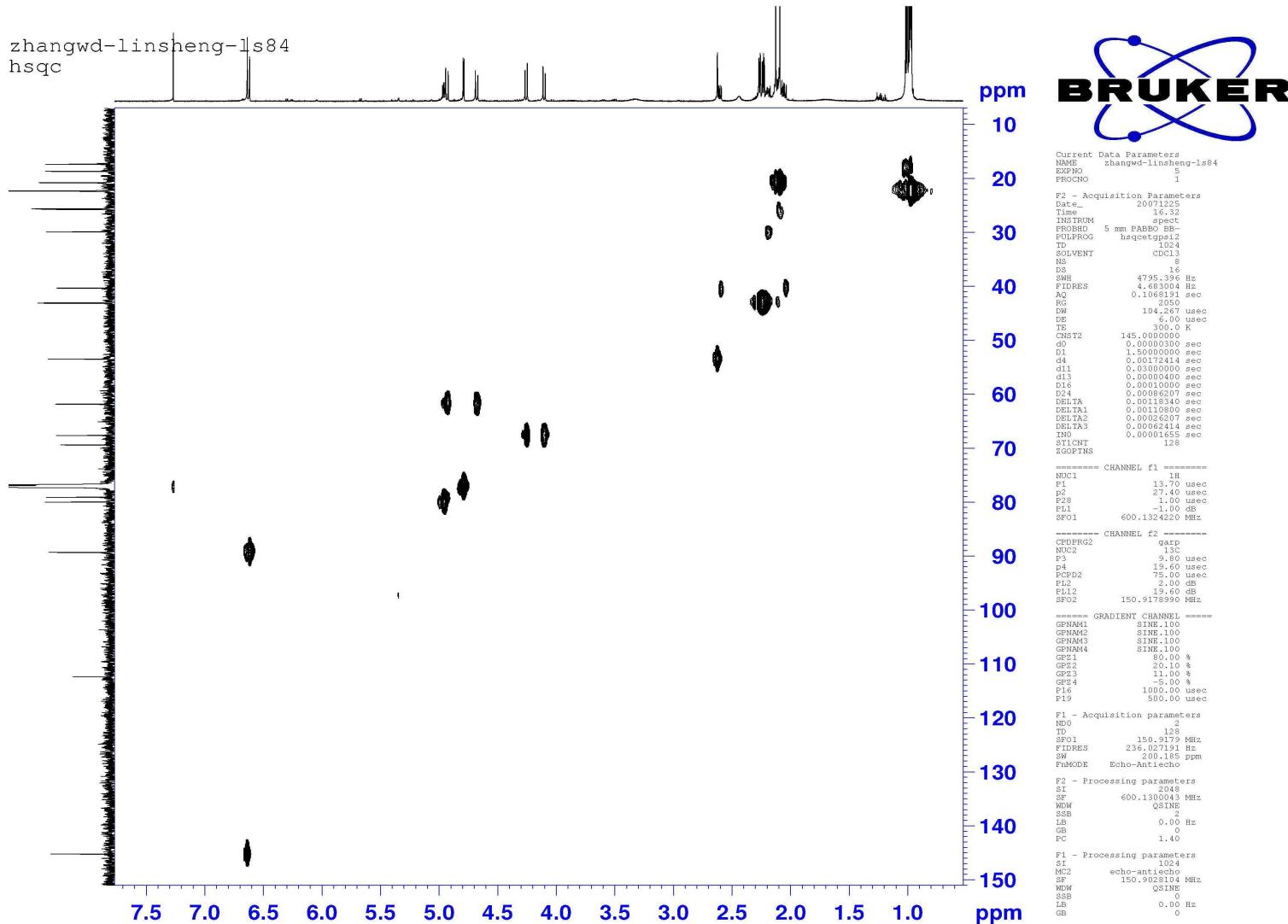
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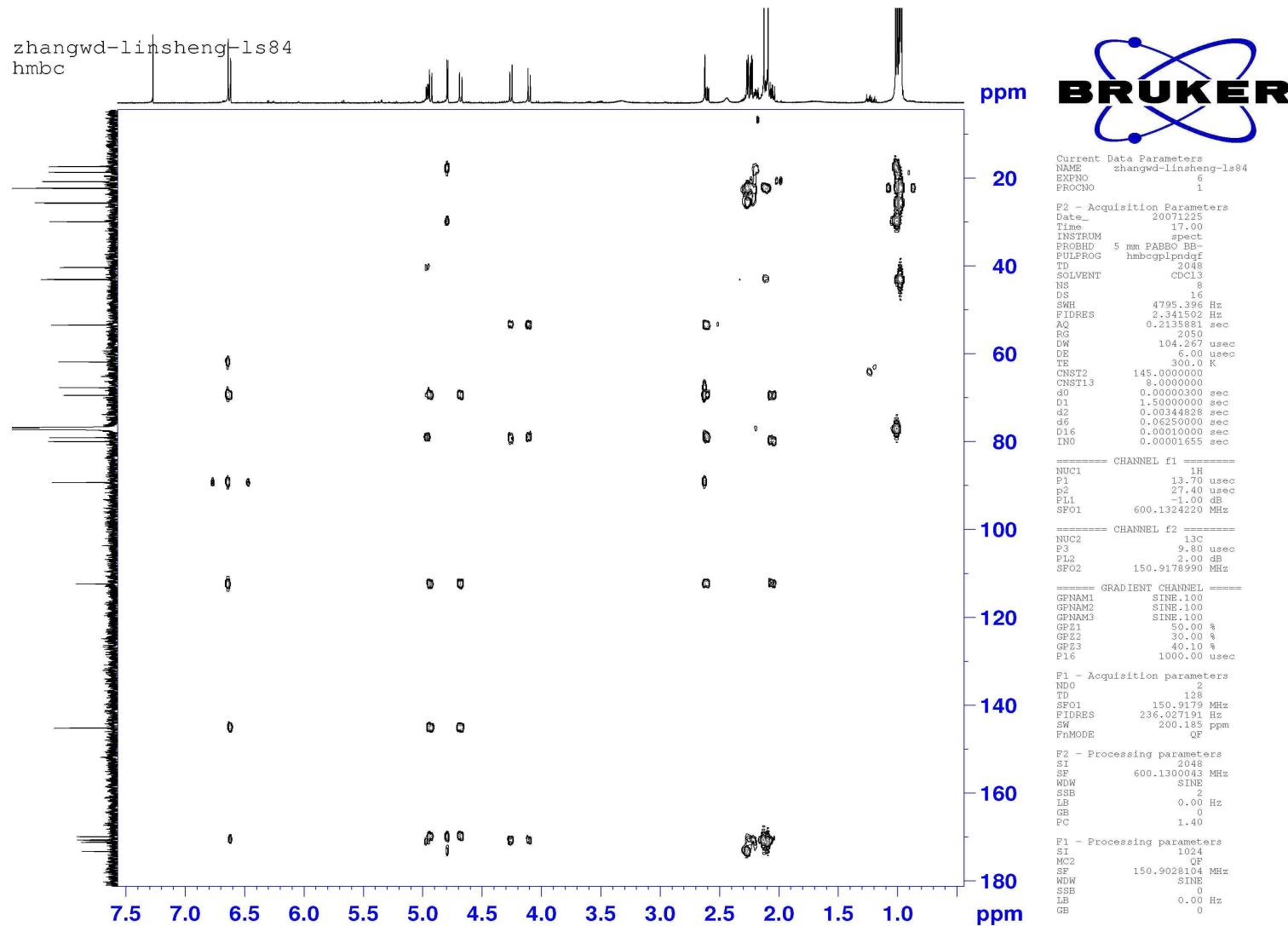
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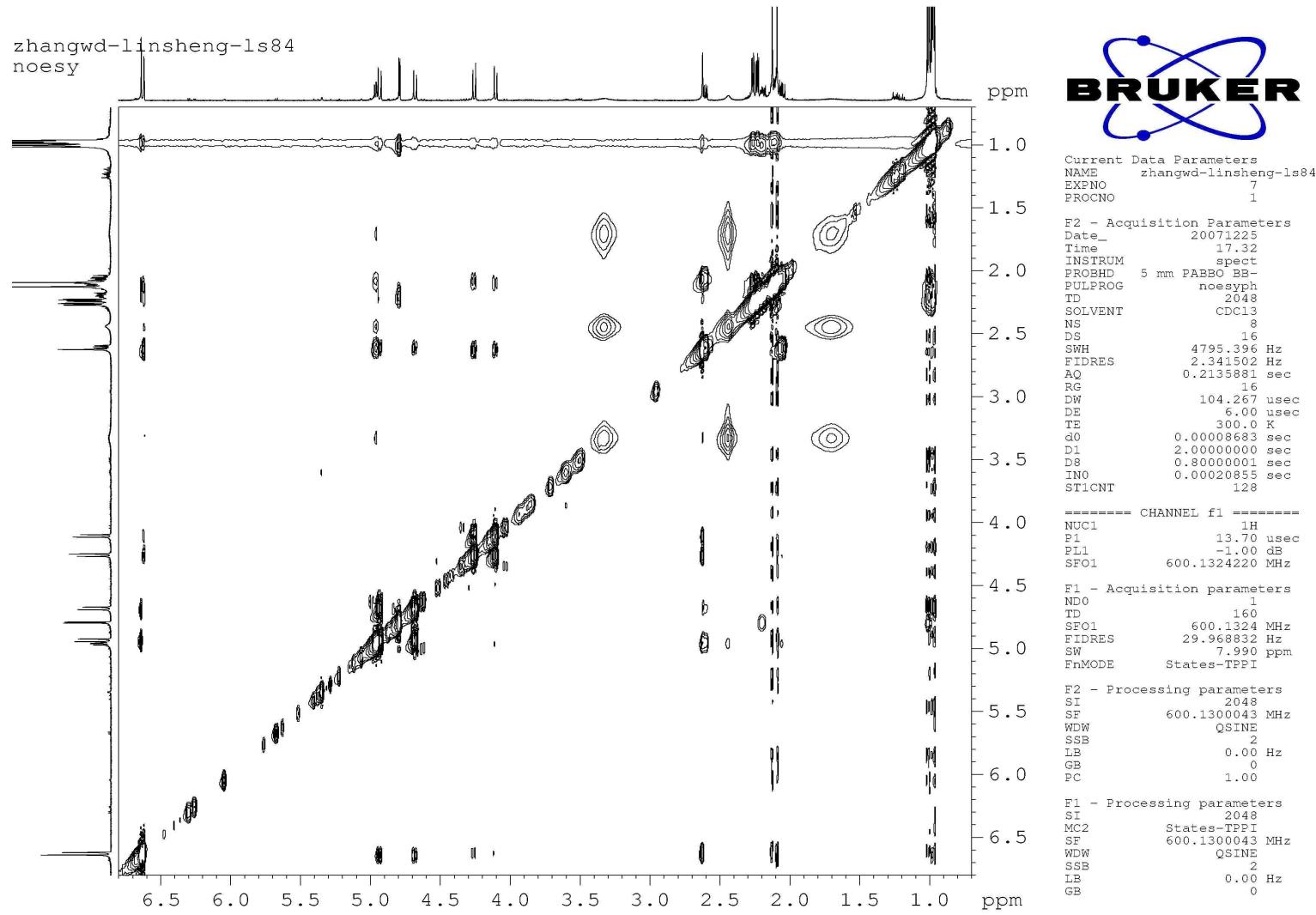
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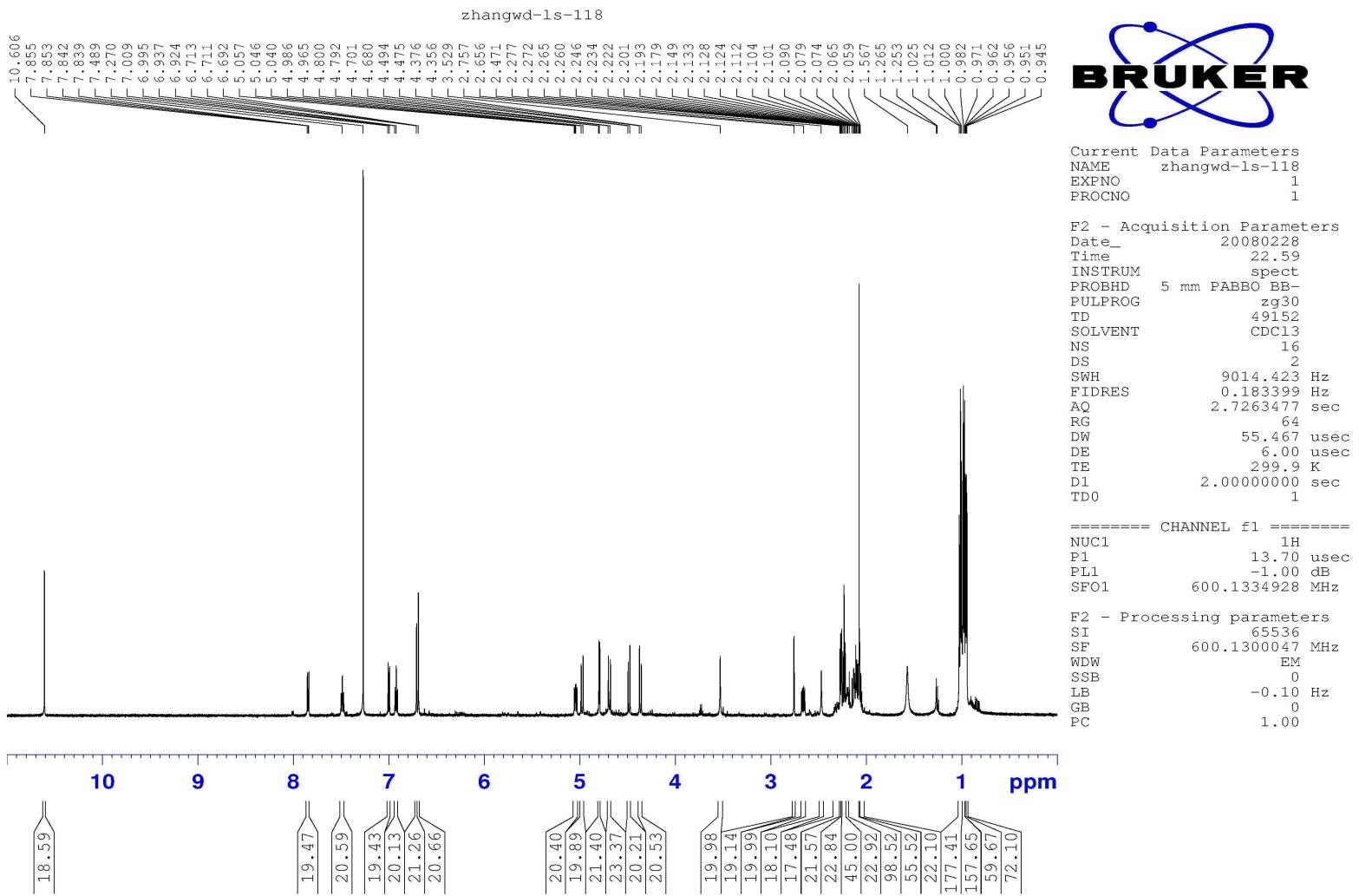
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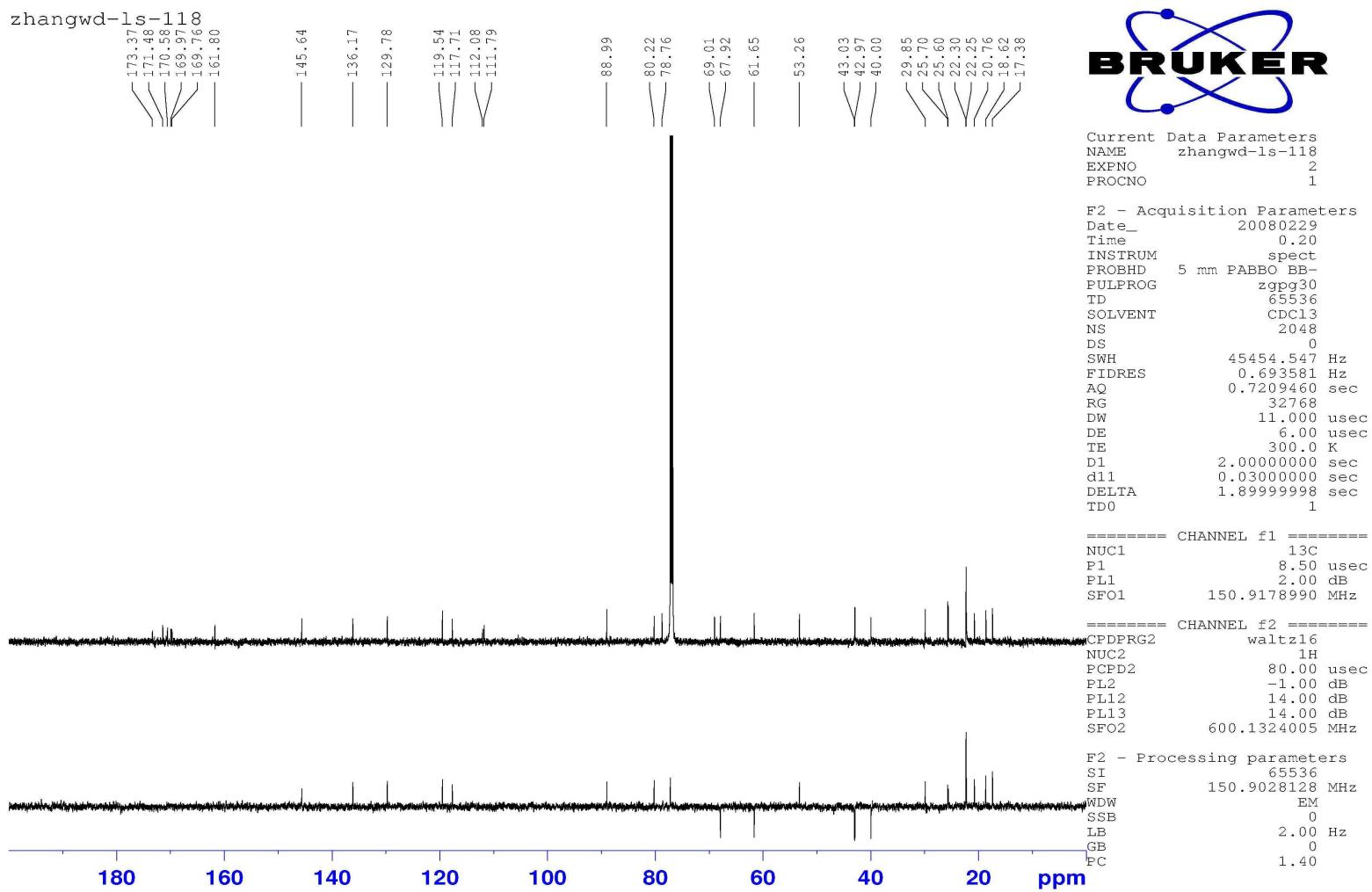
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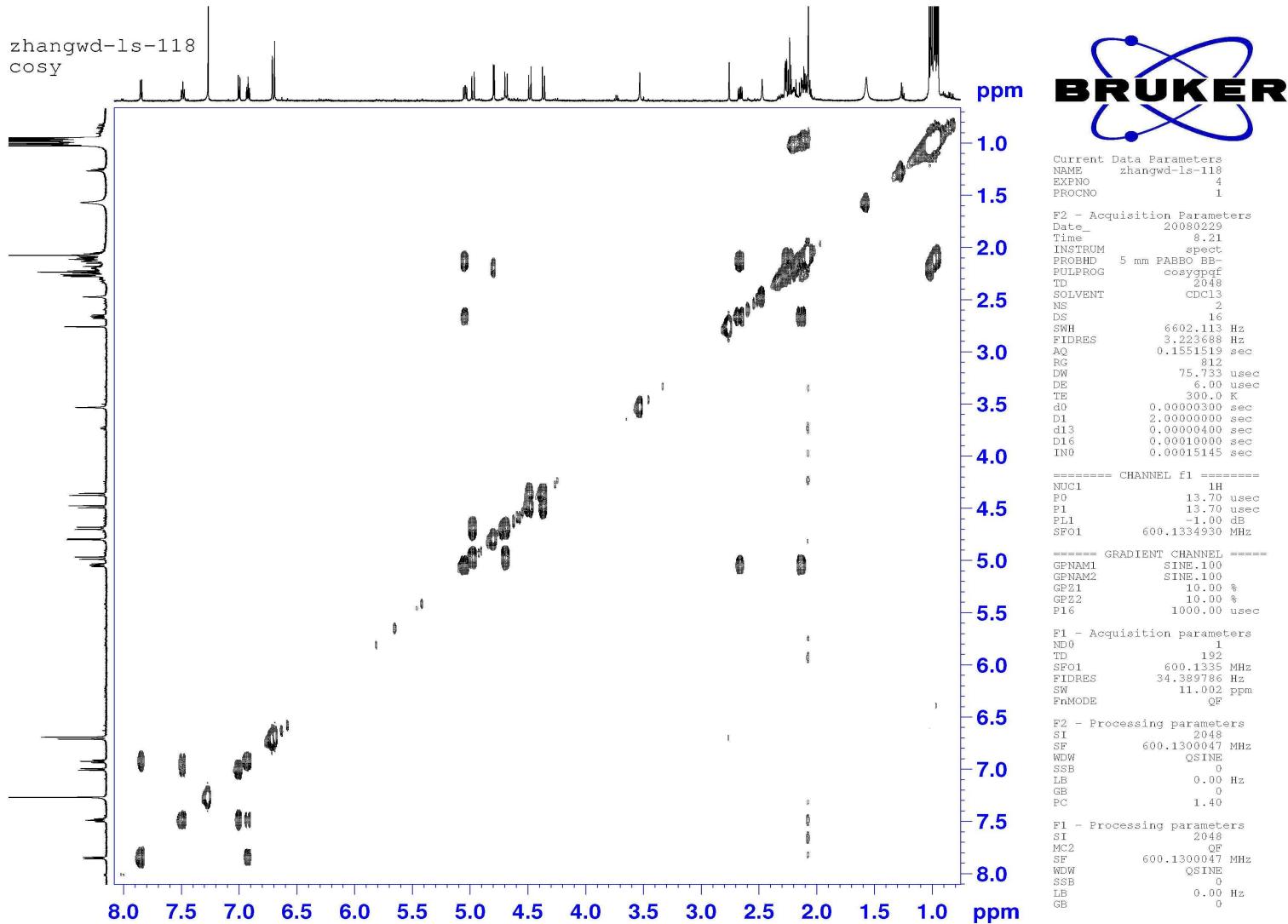
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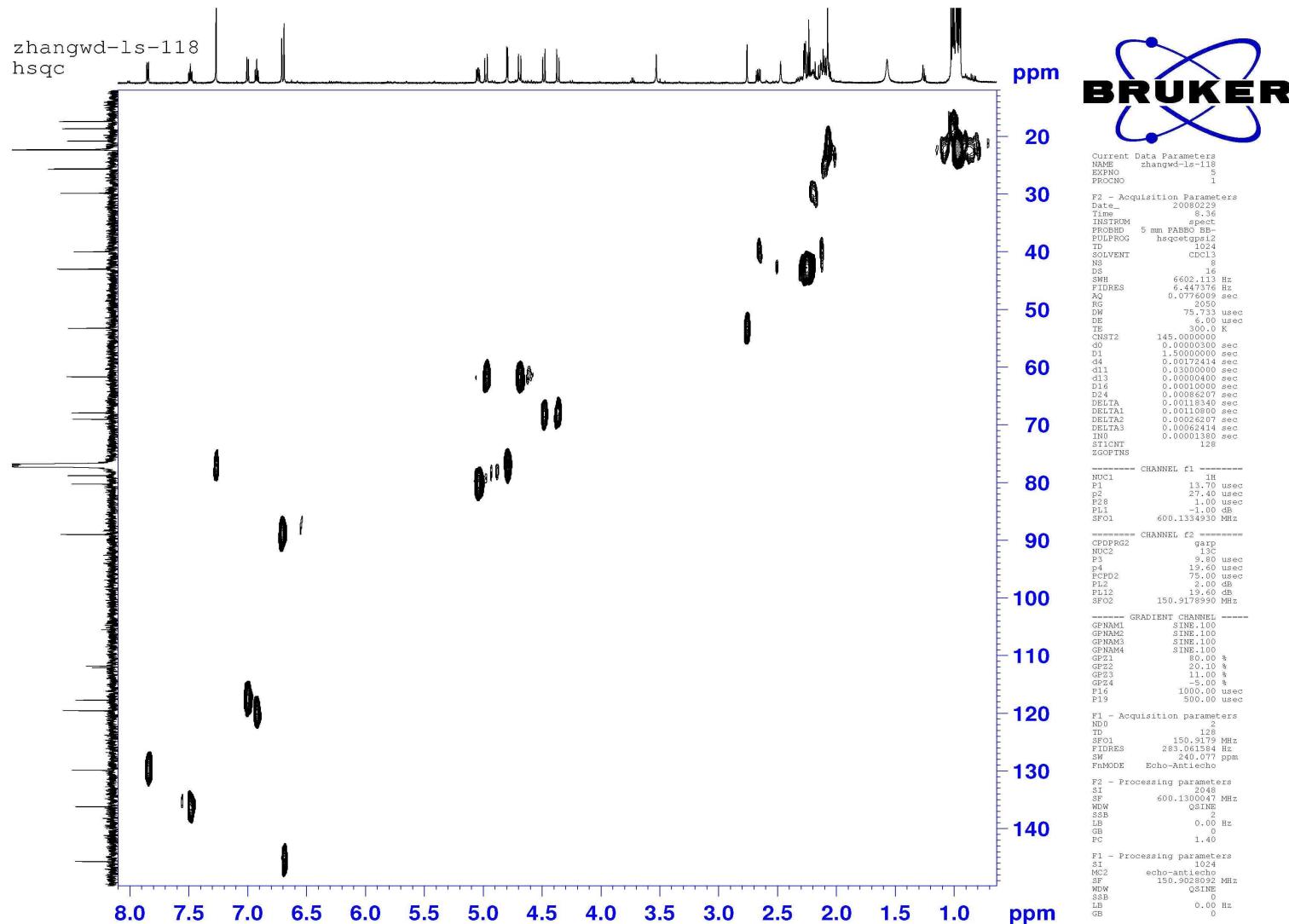


**S23. The  $^1\text{H}$  NMR Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate D (4)**

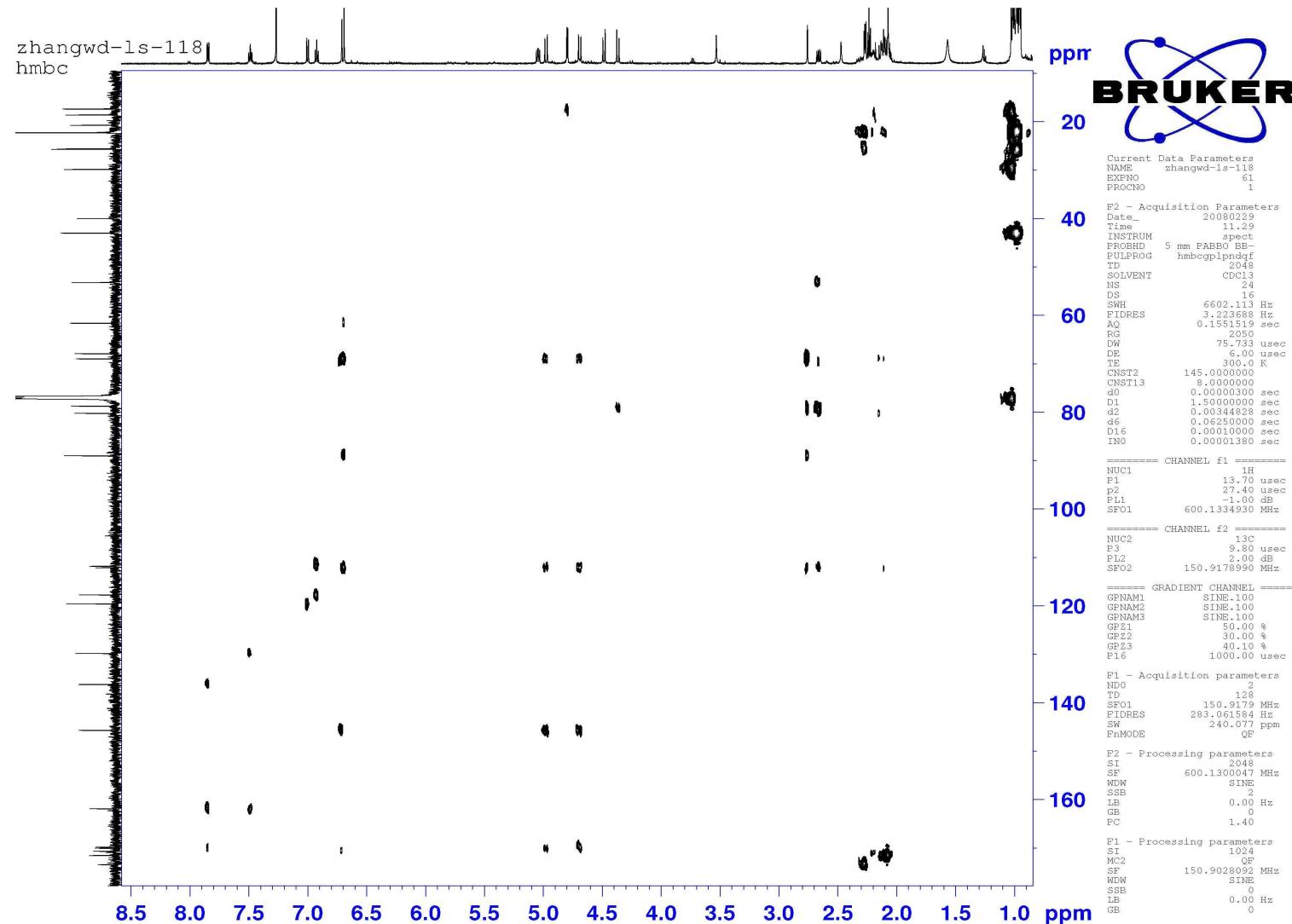


**S24. The  $^{13}\text{C}$  NMR and DEPT Spectra (150 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate D (4)**

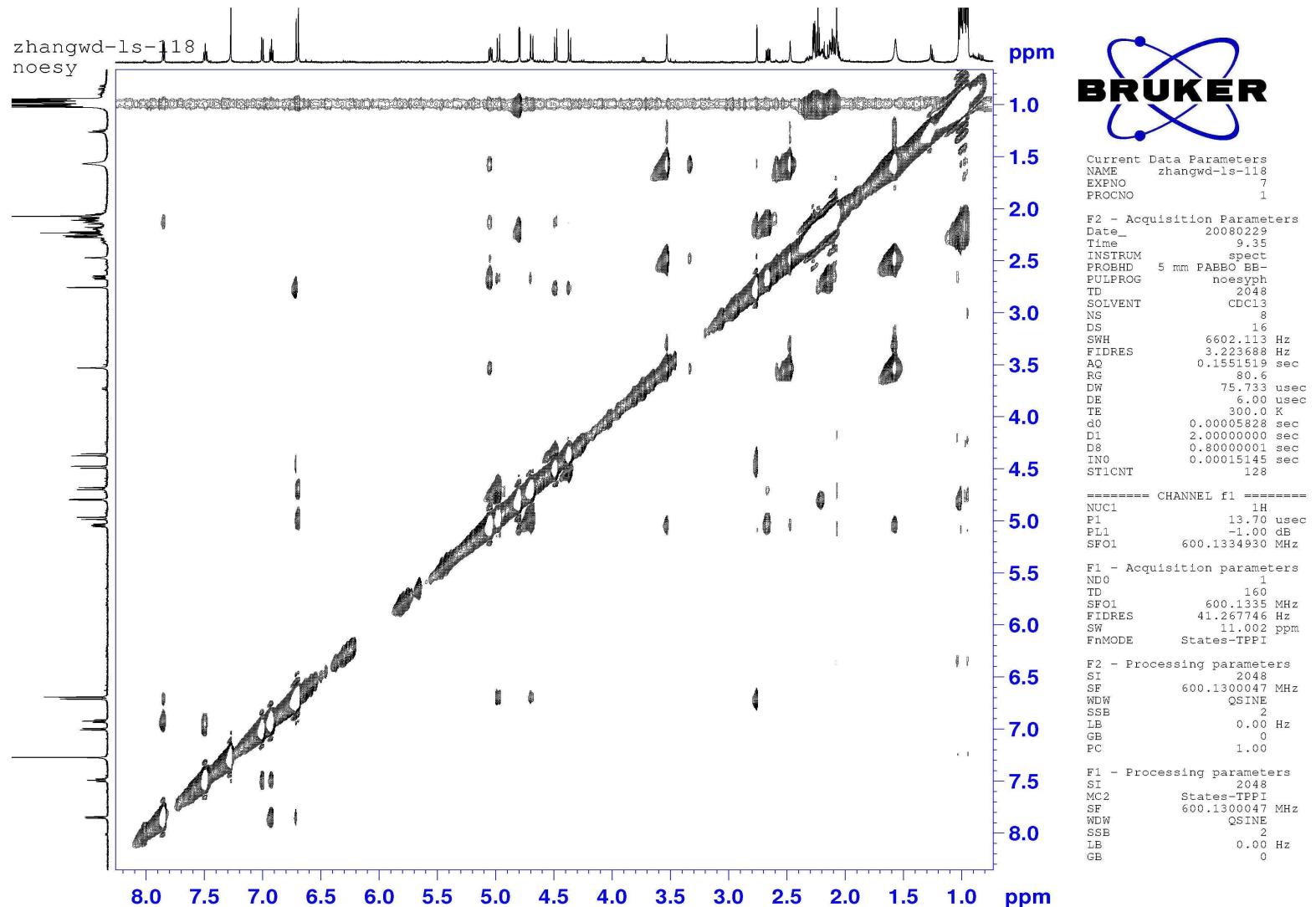




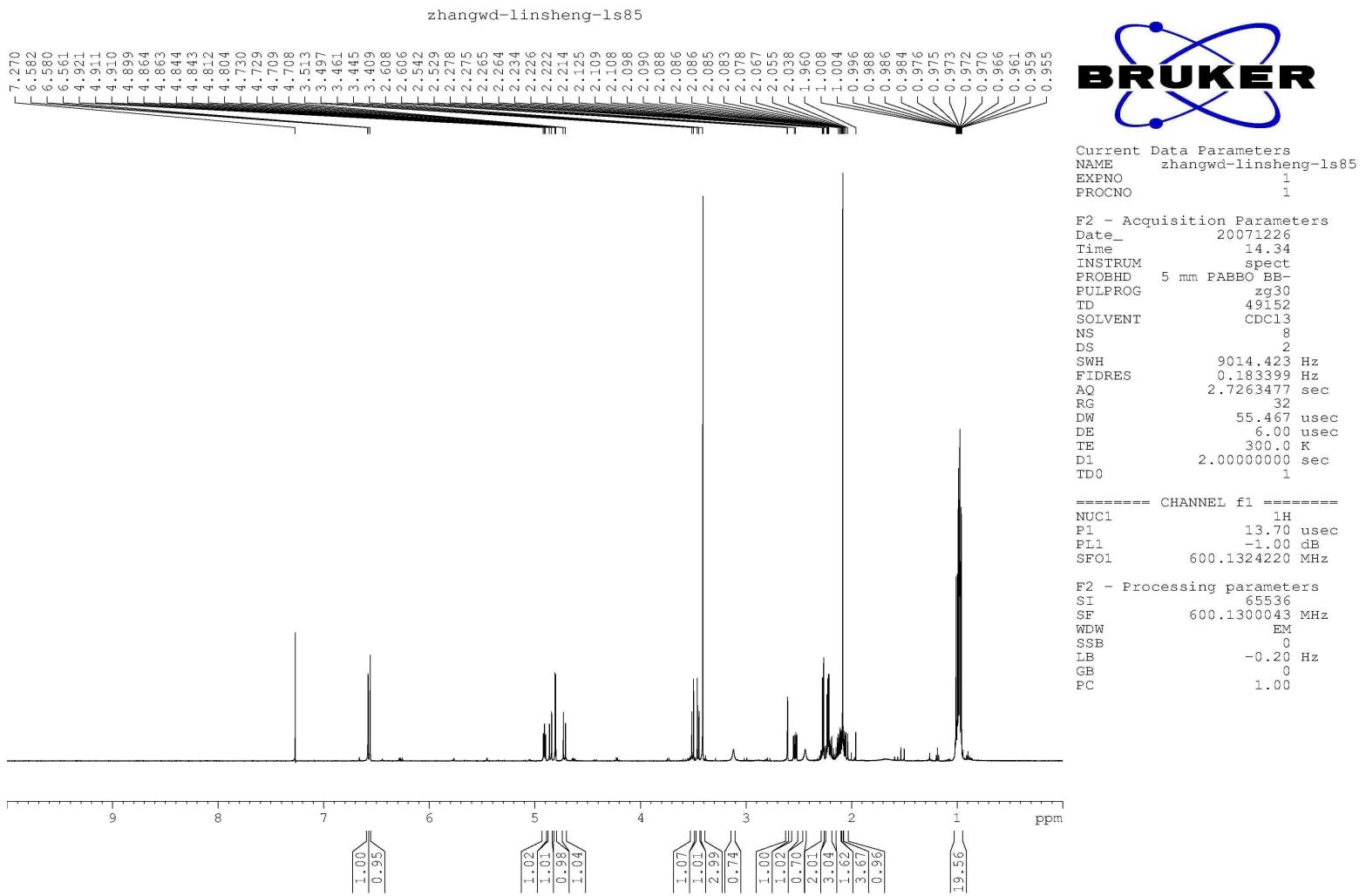
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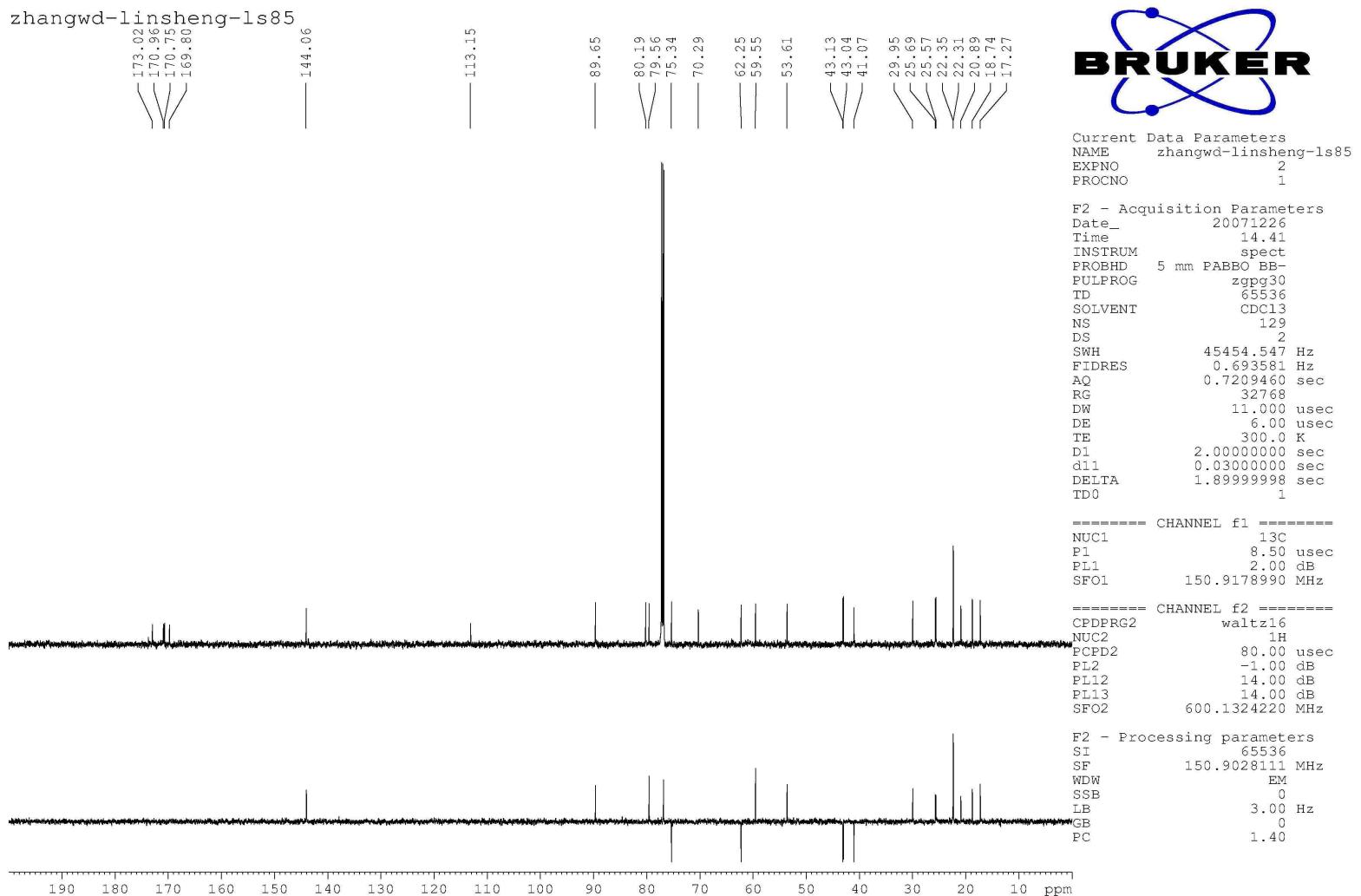
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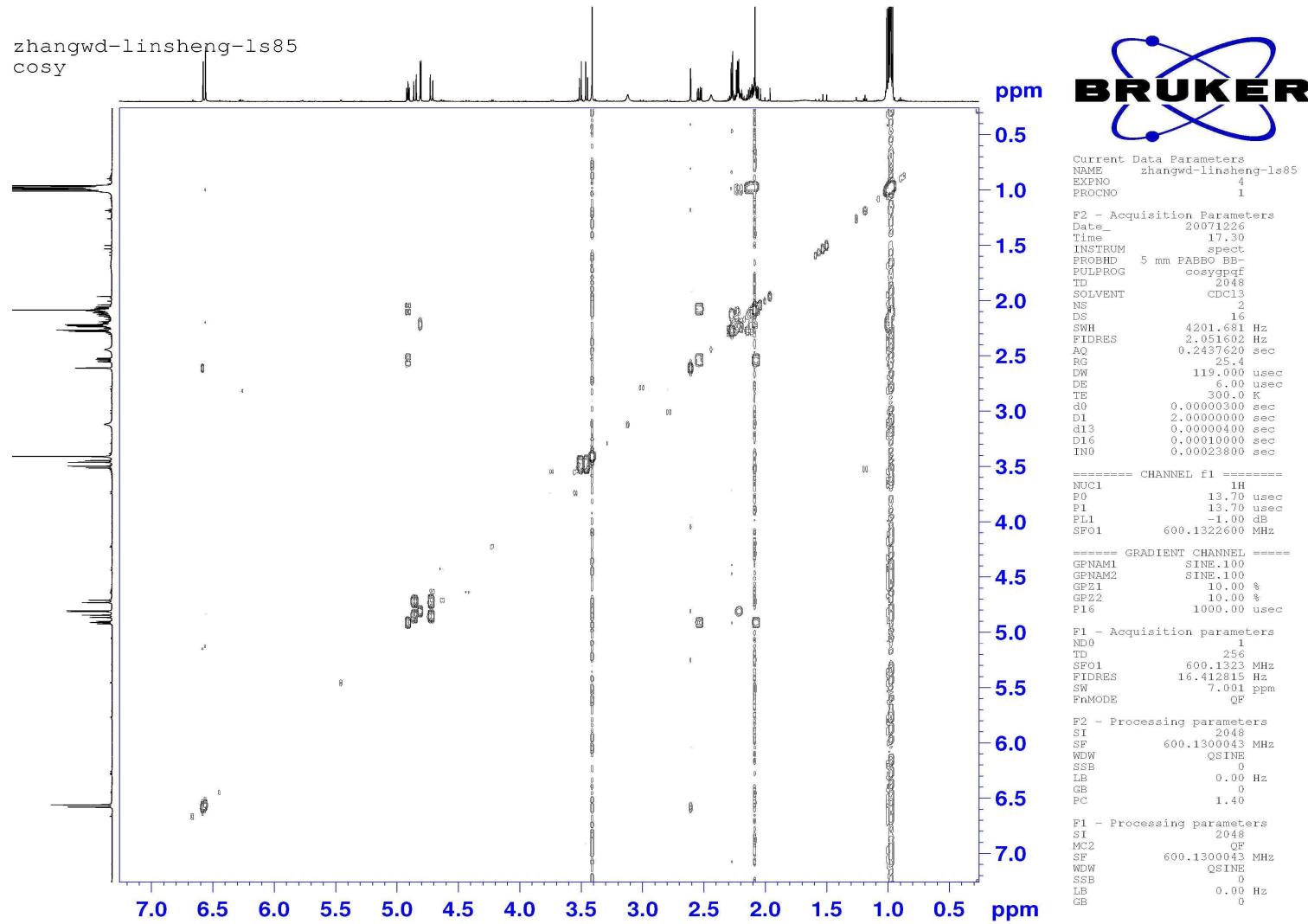
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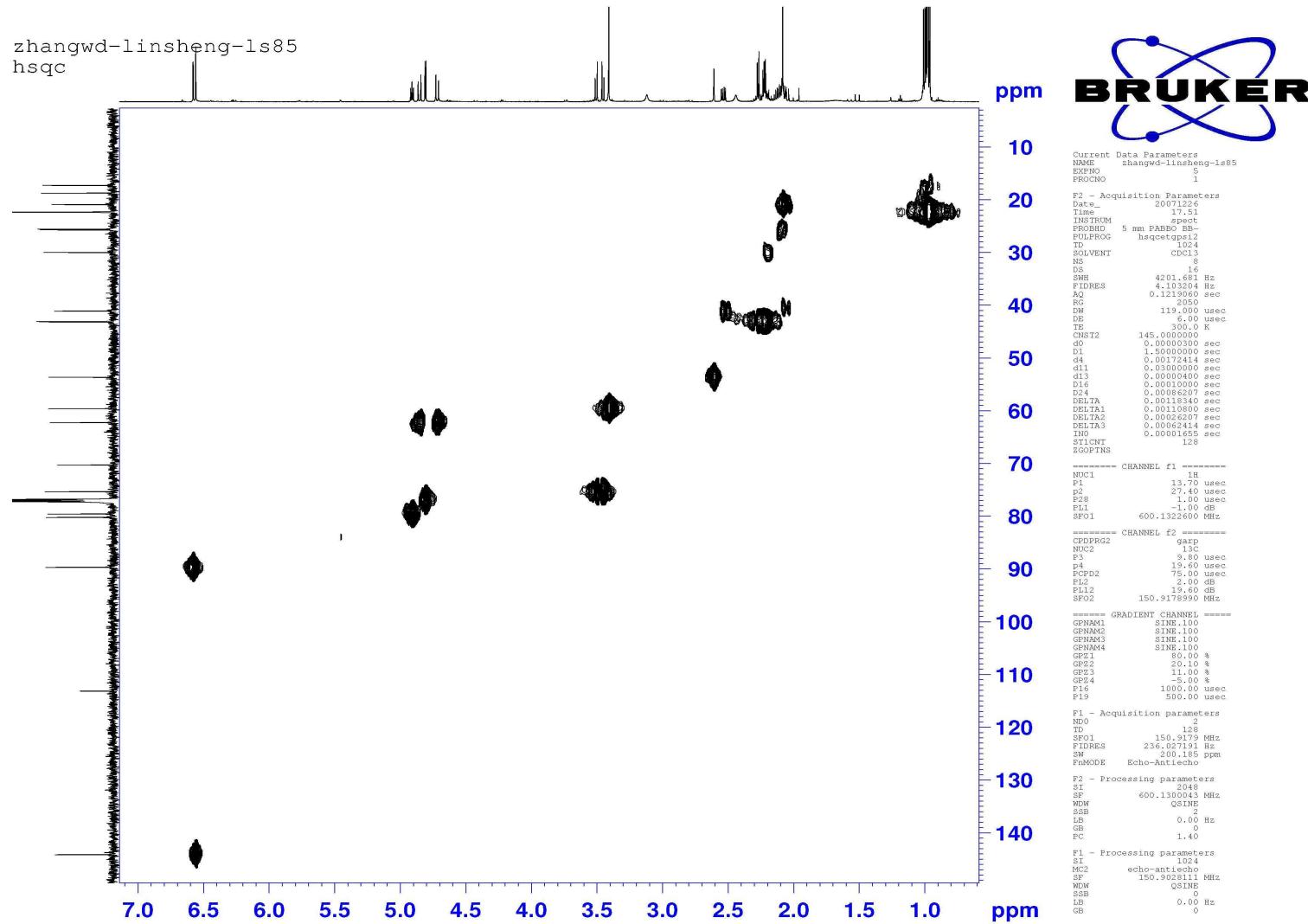
**S29. The <sup>1</sup>H NMR Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate E (5)**



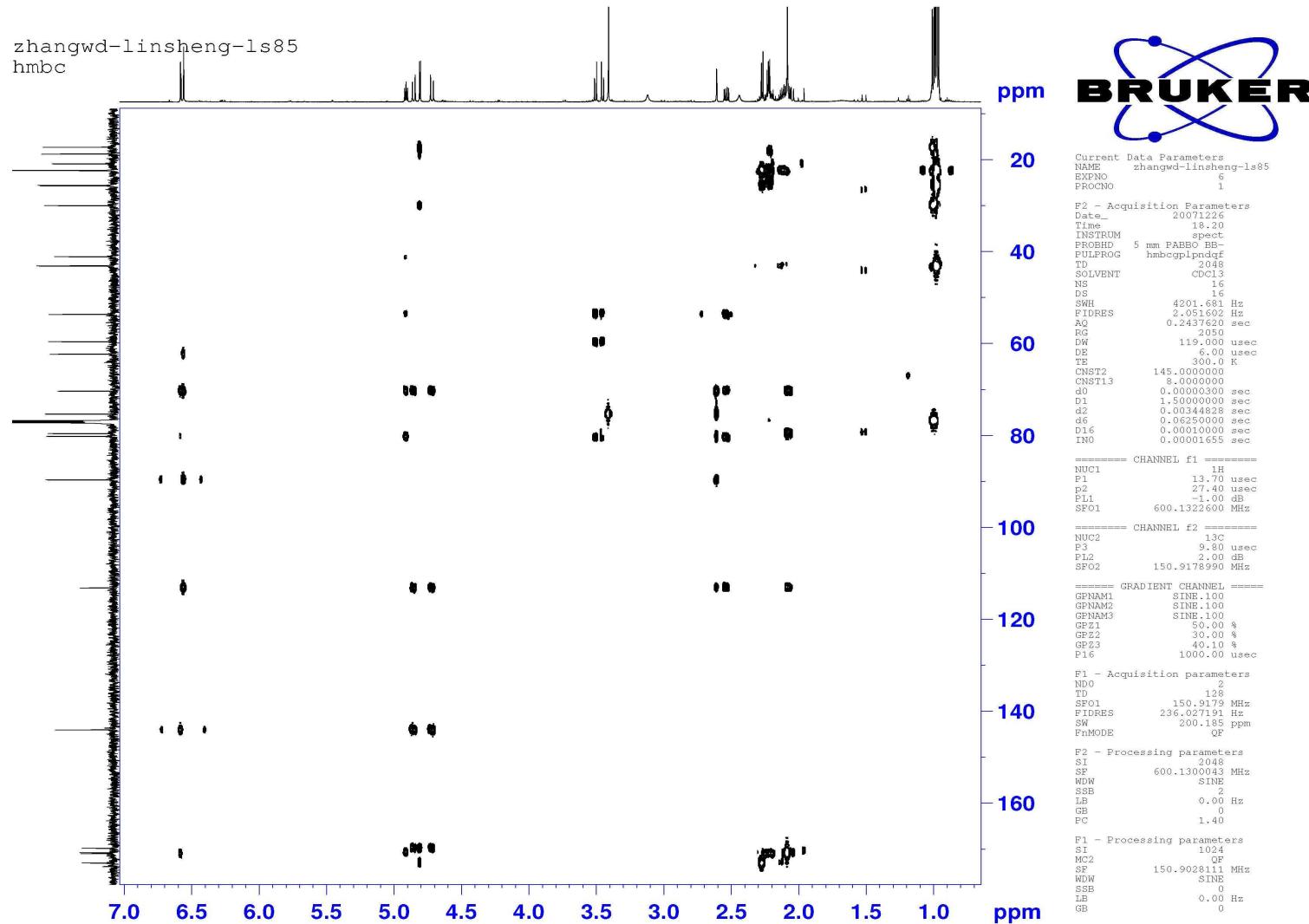
**S30. The  $^{13}\text{C}$  NMR and DEPT Spectra (150 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate E (5)**



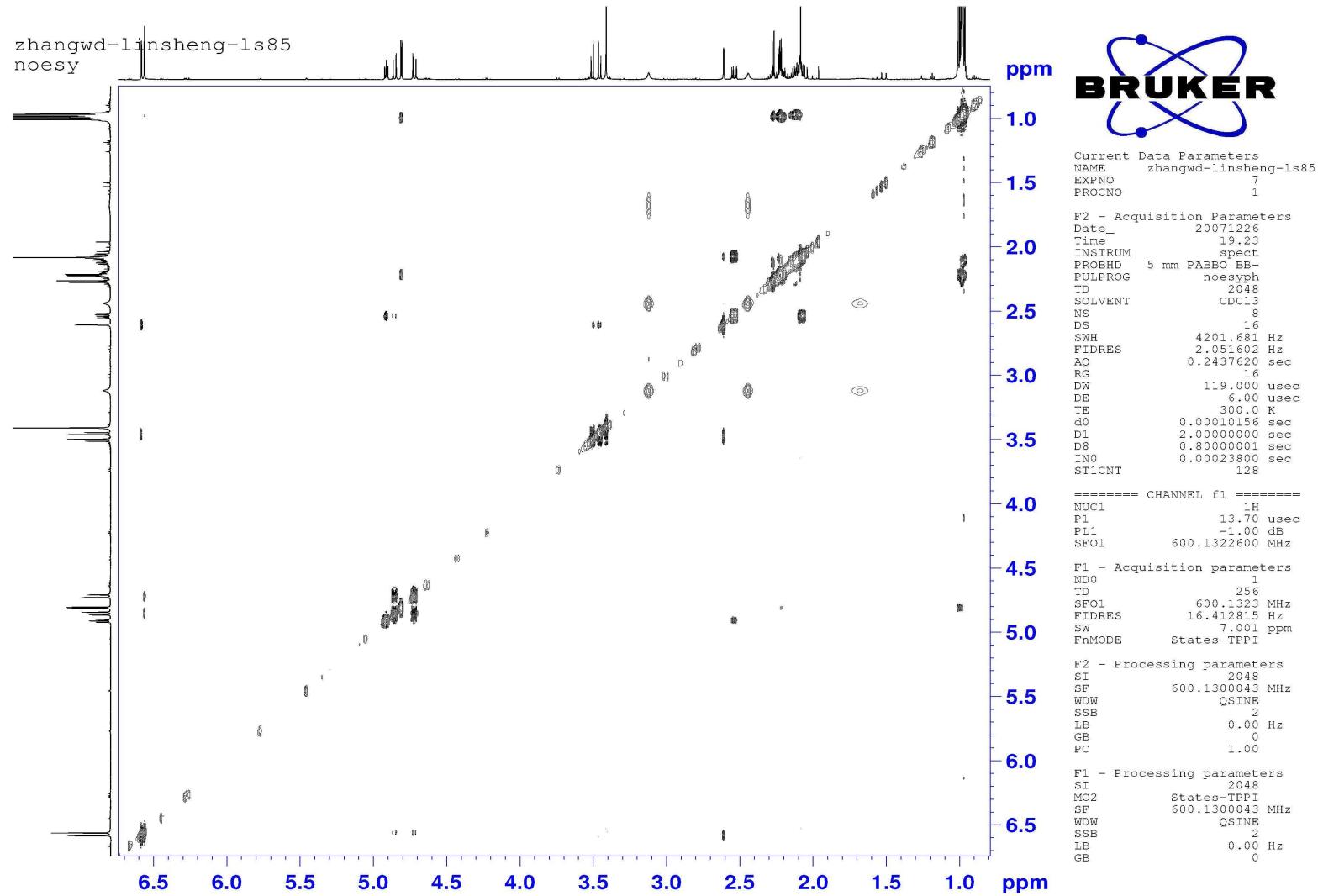
**S31. The  $^1\text{H}$ - $^1\text{HCOSY}$  Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate E (5)**



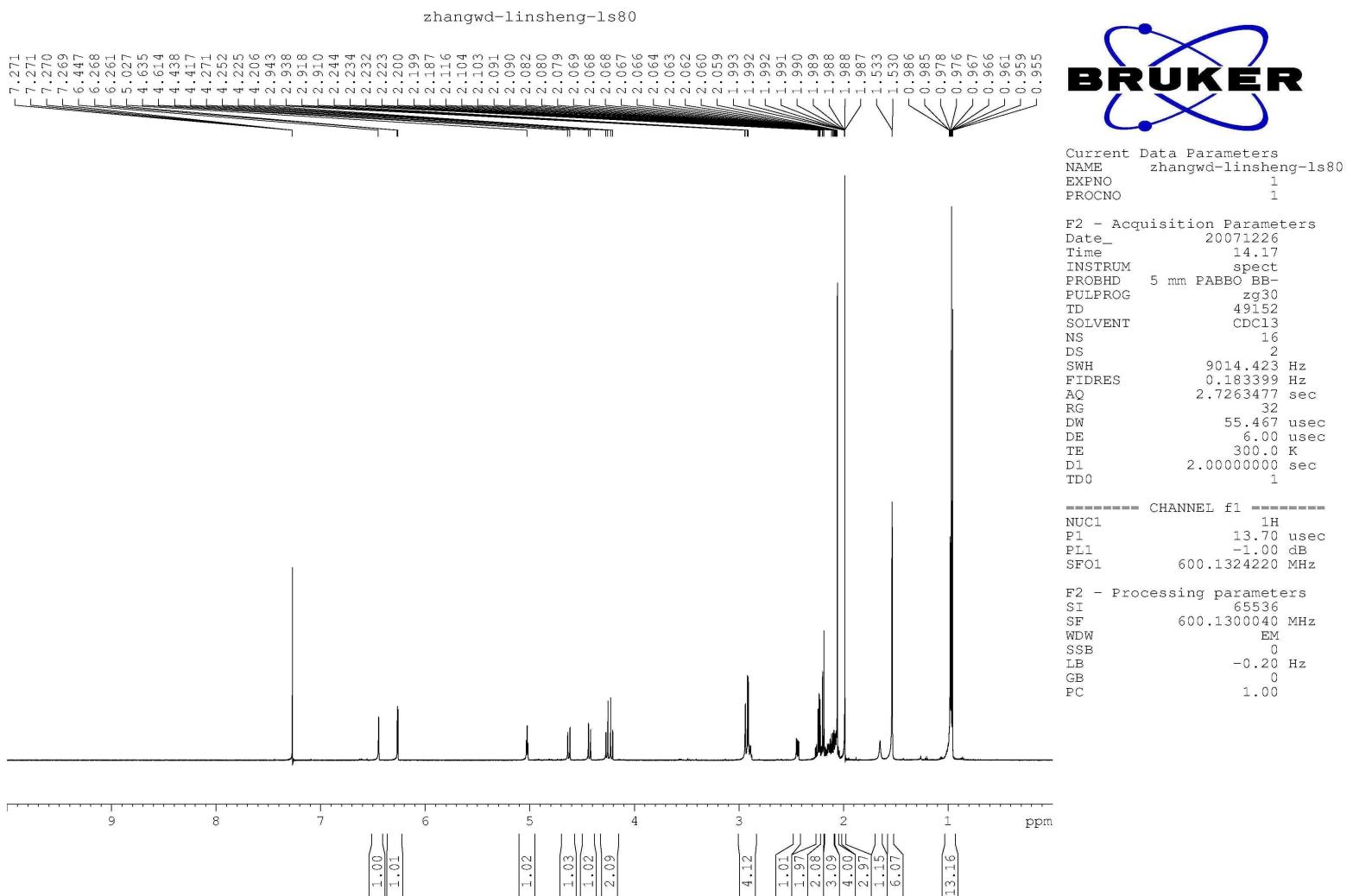
S32. The HSQC Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate E (5)



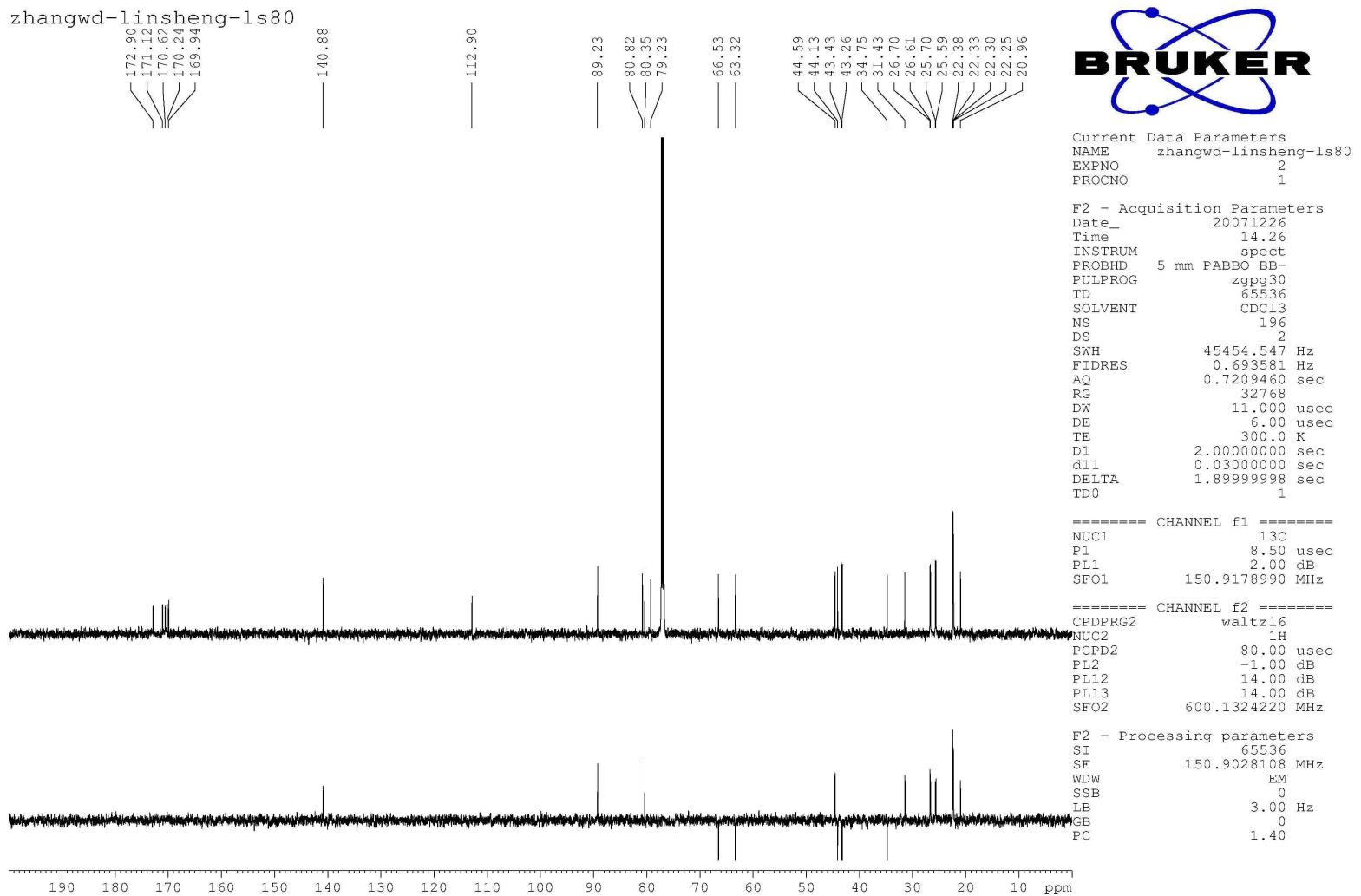
**S33. The HMBC Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate E (5)**



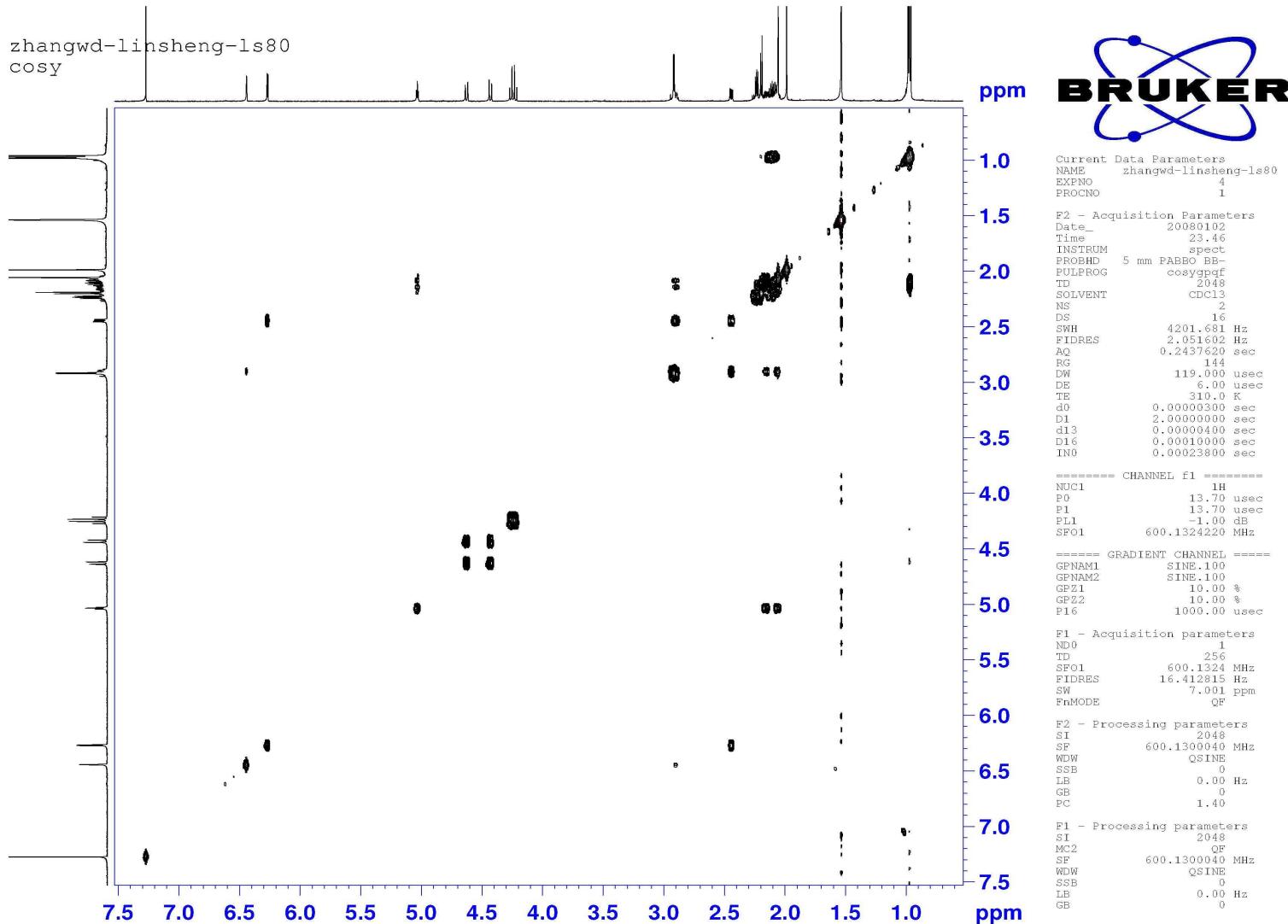
**S34. The NOESY Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate E (5)**



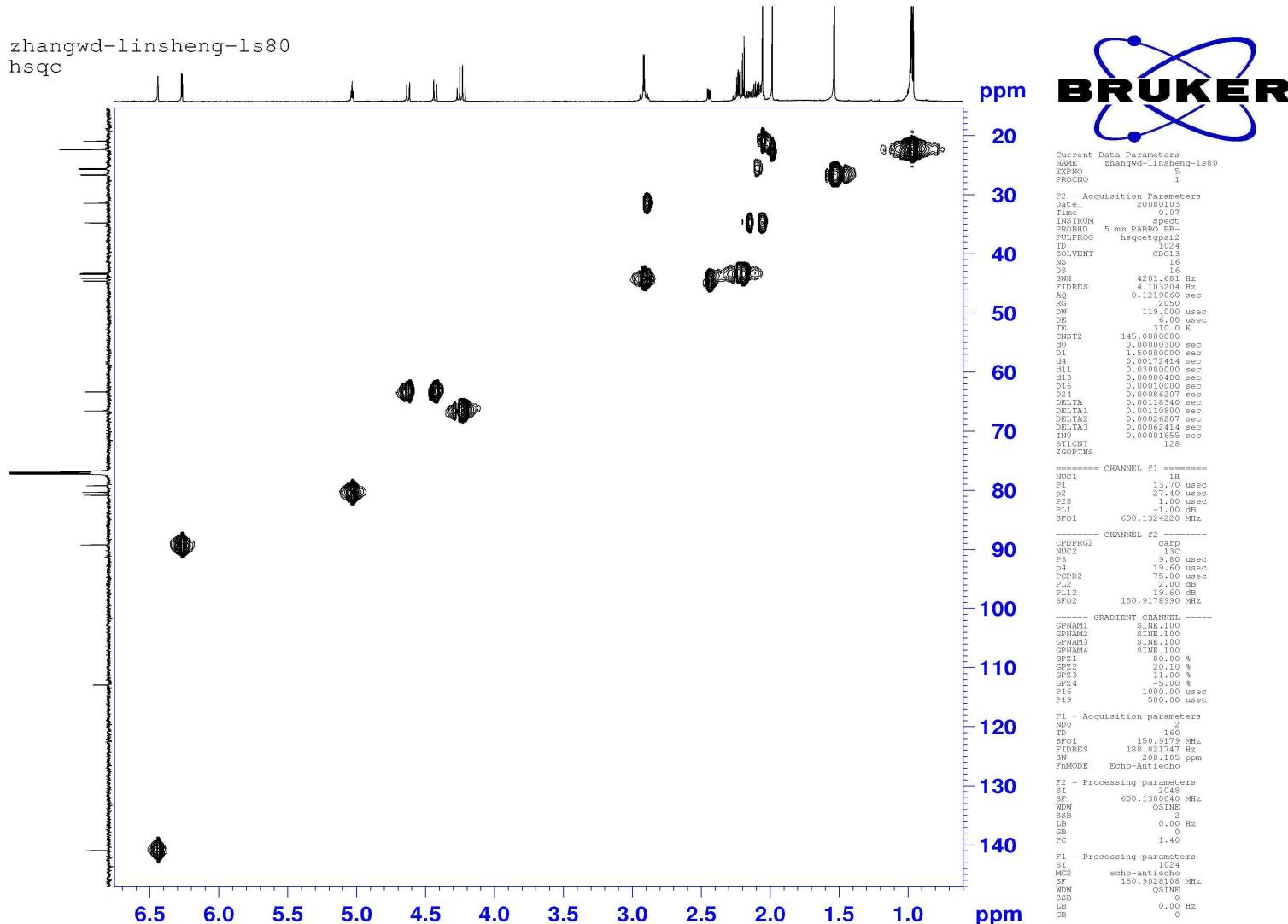
**S35. The  $^1\text{H}$  NMR Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate F (6)**



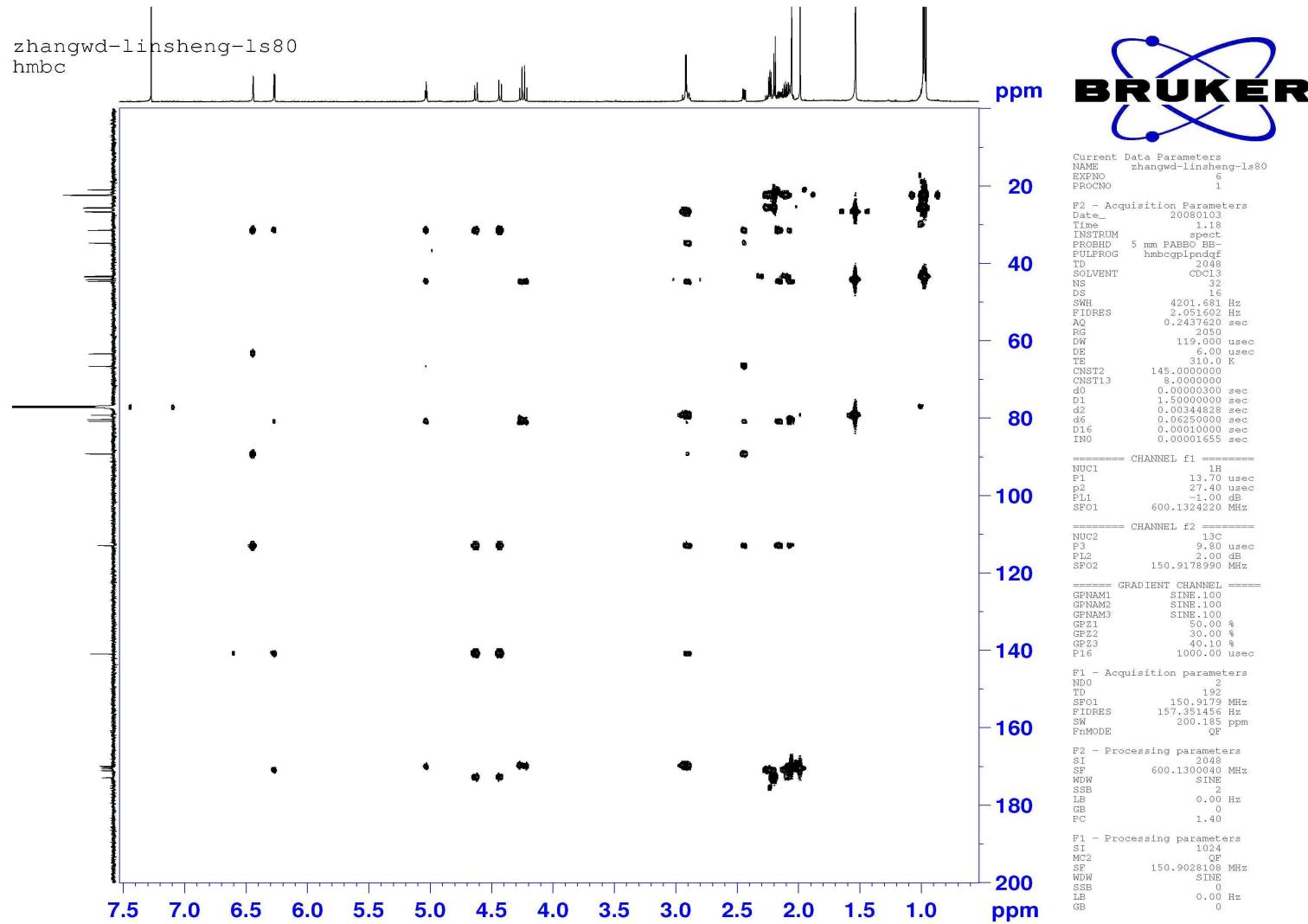
S36. The  $^{13}\text{C}$  NMR and DEPT Spectra (150 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate F (6)



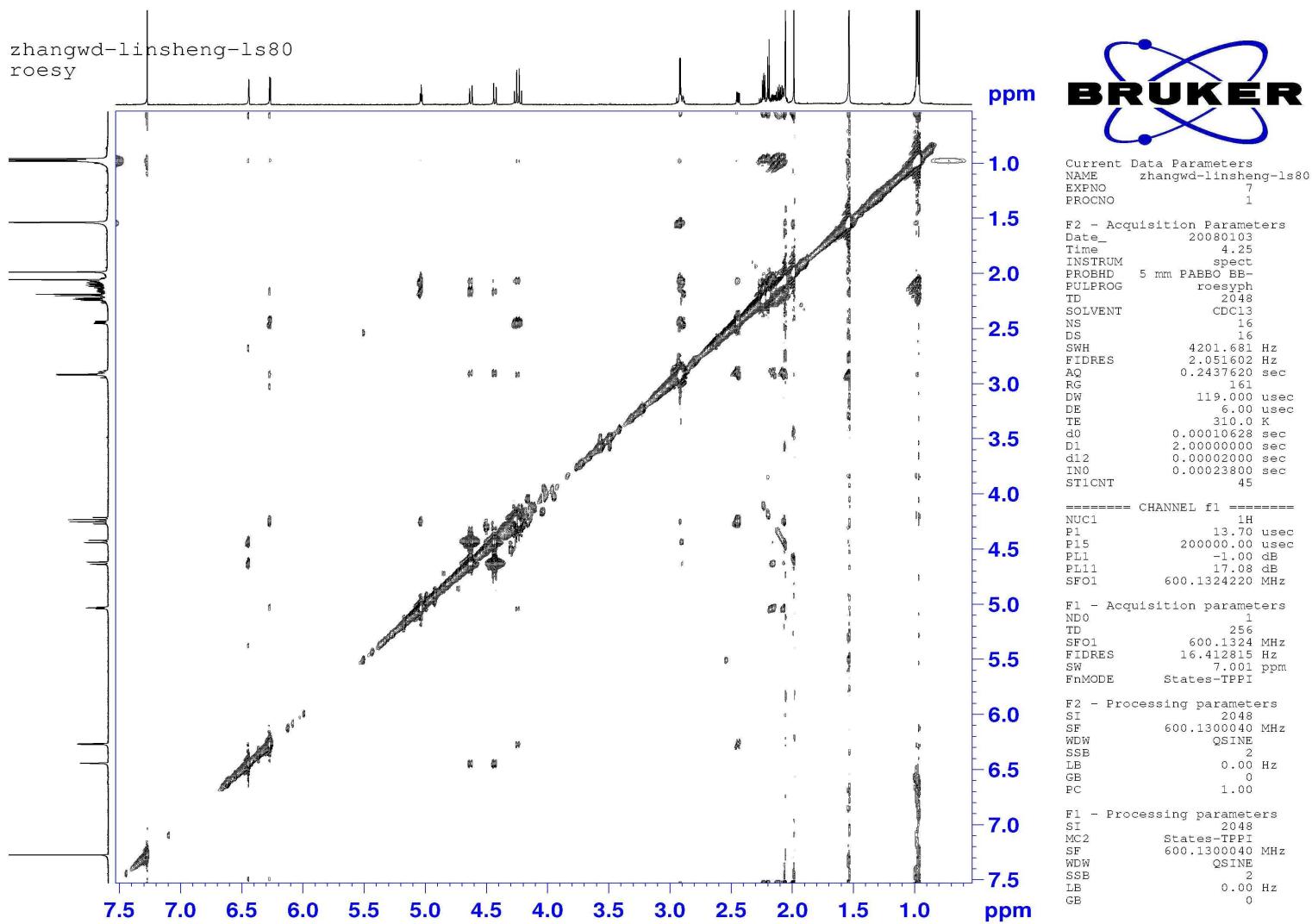
S37. The  $^1\text{H}$ - $^1\text{H}$ COSY Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate F (6)



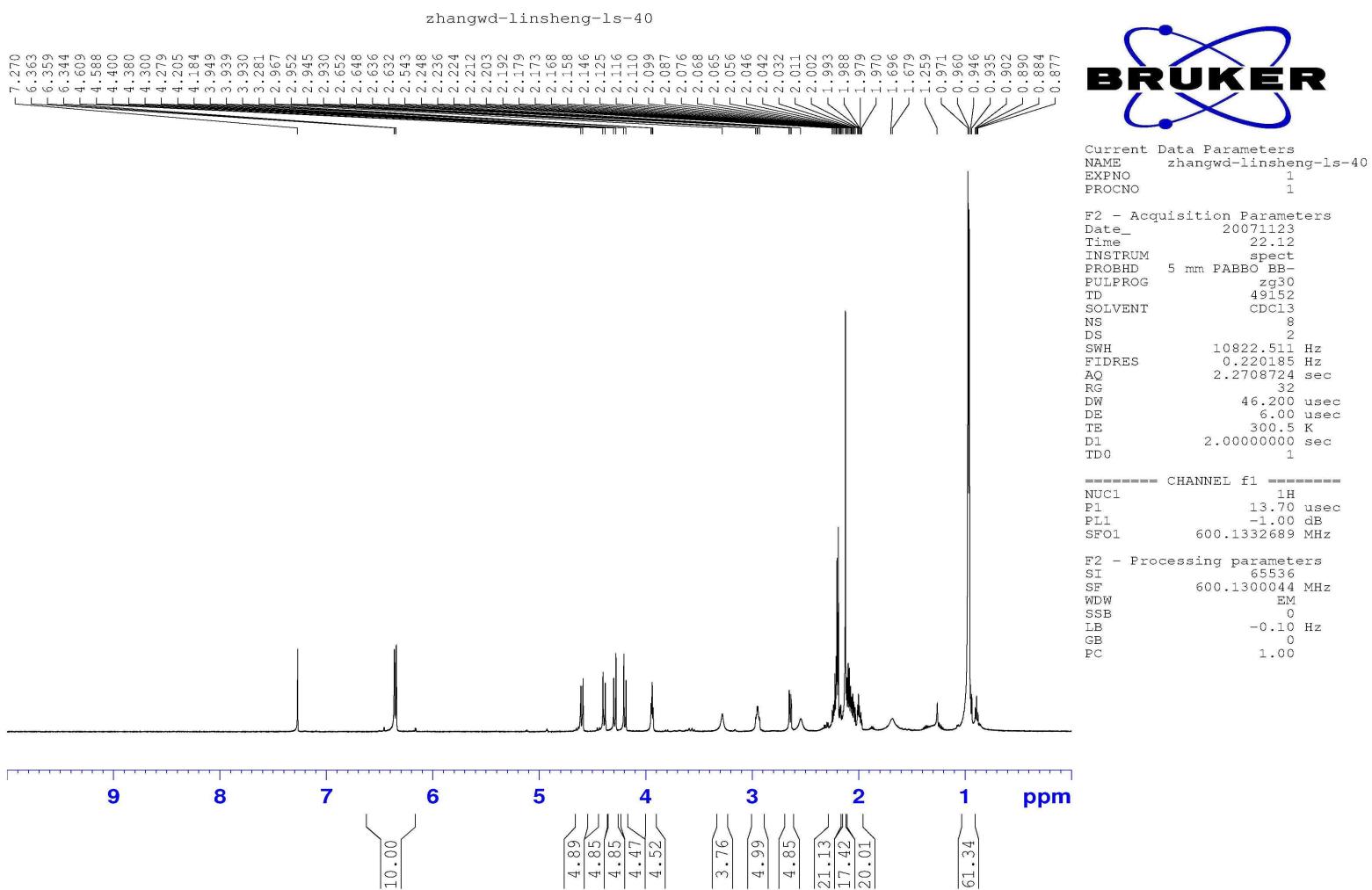
**S38. The HSQC Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate F (6)**



S39. The HMBC Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate F (6)

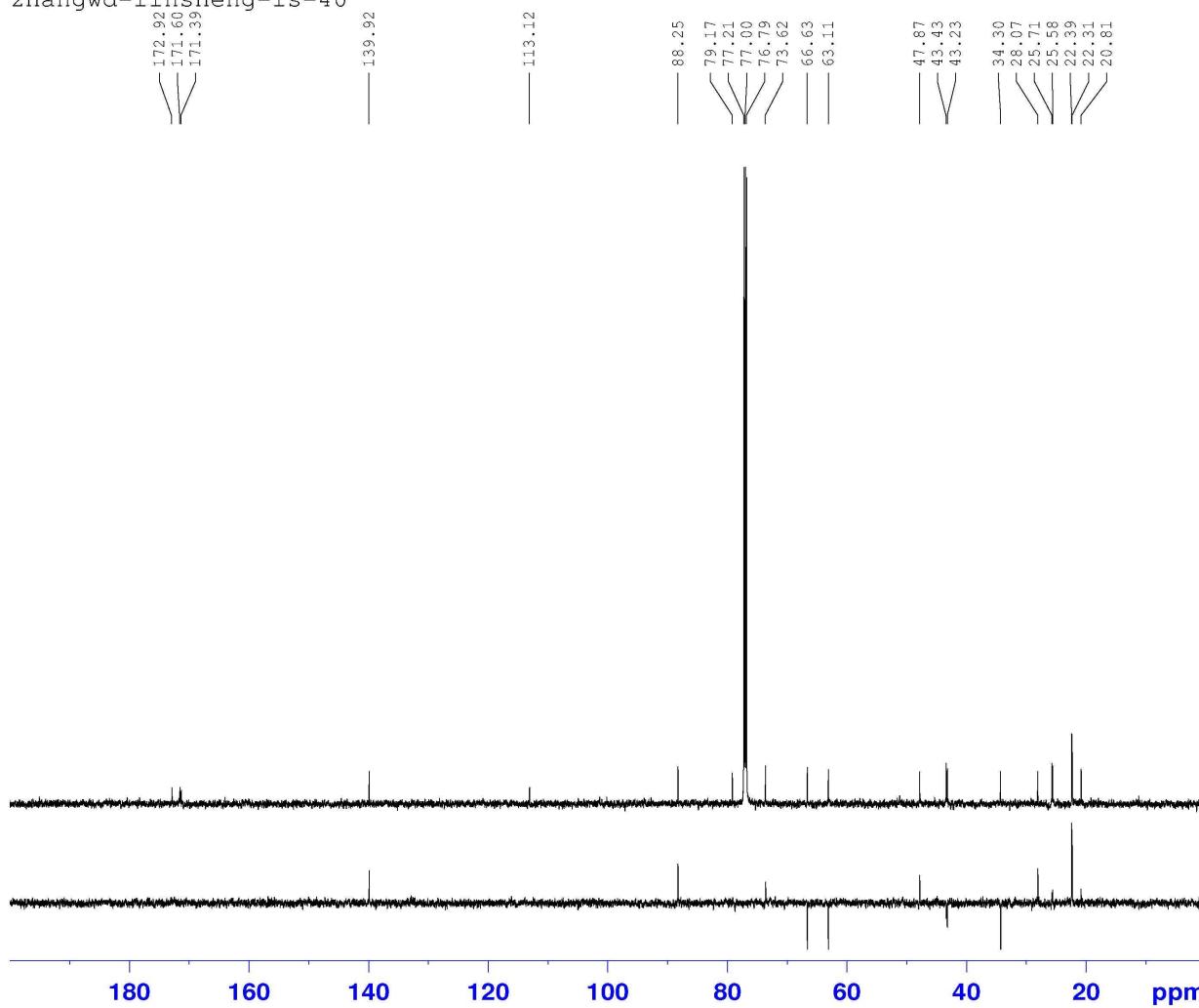


S40. The ROESY Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate F (**6**)



**S41. The  $^1\text{H}$  NMR Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate G (7)**

zhangwd-linsheng-ls-40



Current Data Parameters  
NAME zhangwd-linsheng-ls-40  
EXPNO 2  
PROCNO 1

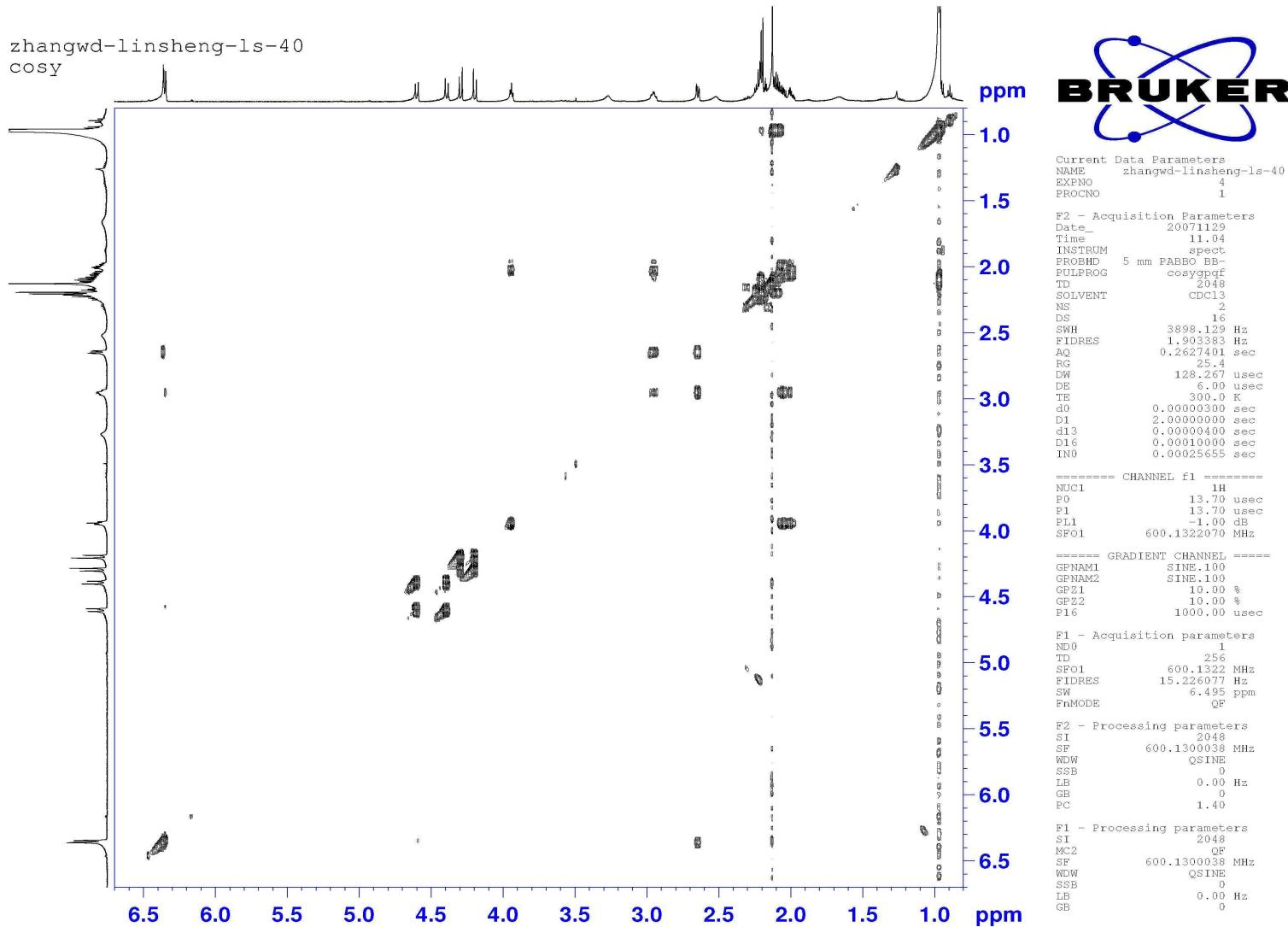
F2 - Acquisition Parameters  
Date\_ 20071123  
Time 22.25  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl<sub>3</sub>  
NS 278  
DS 2  
SWH 45454.547 Hz  
FIDRES 0.693581 Hz  
AQ 0.7209460 sec  
RG 32768  
DW 11.000 usec  
DE 6.00 usec  
TE 300.3 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.8999998 sec  
TD0 1

===== CHANNEL f1 ======  
NUC1 13C  
P1 8.50 usec  
PL1 2.00 dB  
SFO1 150.9149090 MHz

===== CHANNEL f2 ======  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.00 dB  
PL13 14.00 dB  
SFO2 600.1324005 MHz

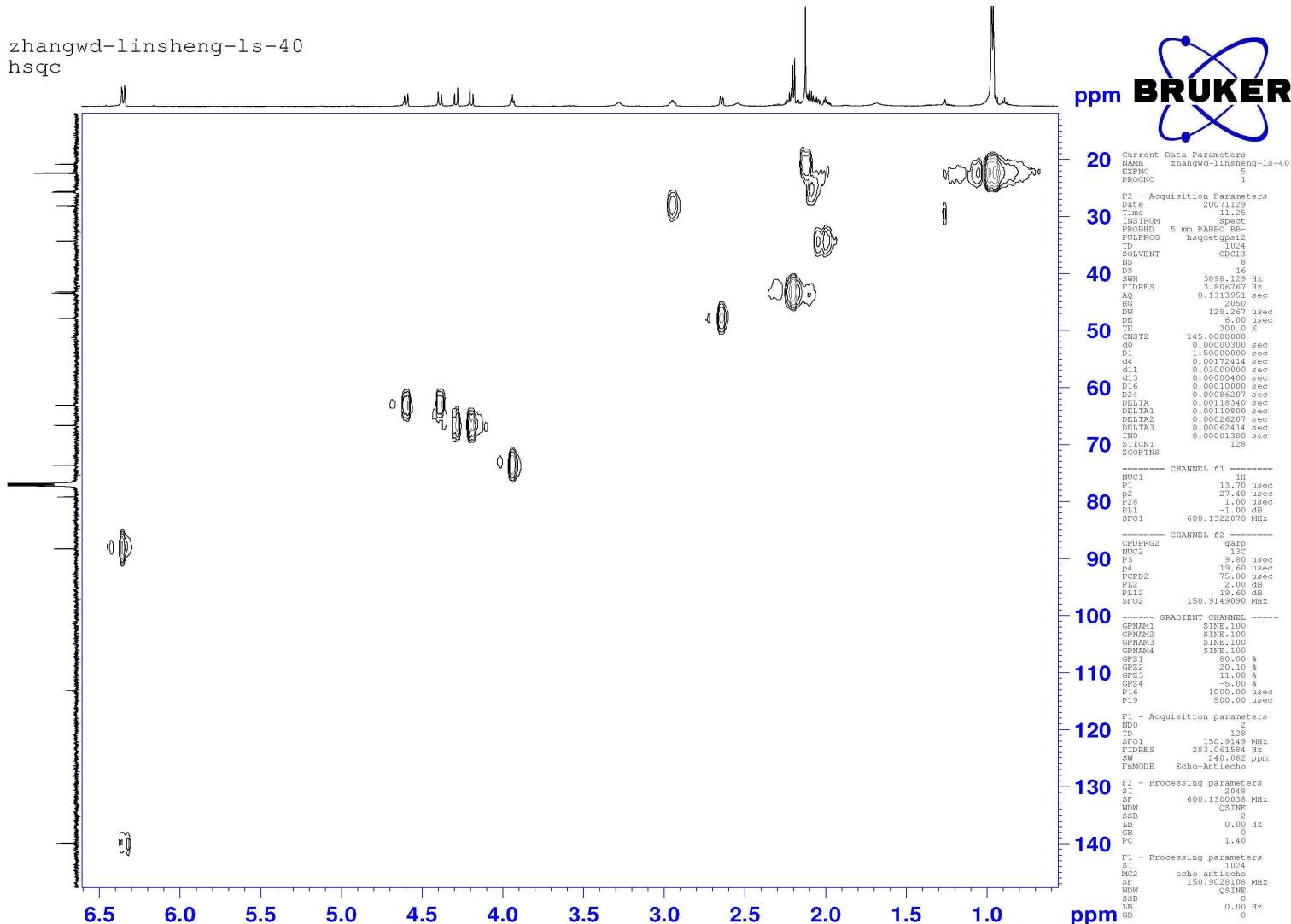
F2 - Processing parameters  
SI 65536  
SF 150.9028108 MHz  
WDW EM  
SSB 0  
LB 3.00 Hz  
GB 0  
PC 1.40

S42. The <sup>13</sup>C NMR and DEPT Spectra (150 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate G (7)

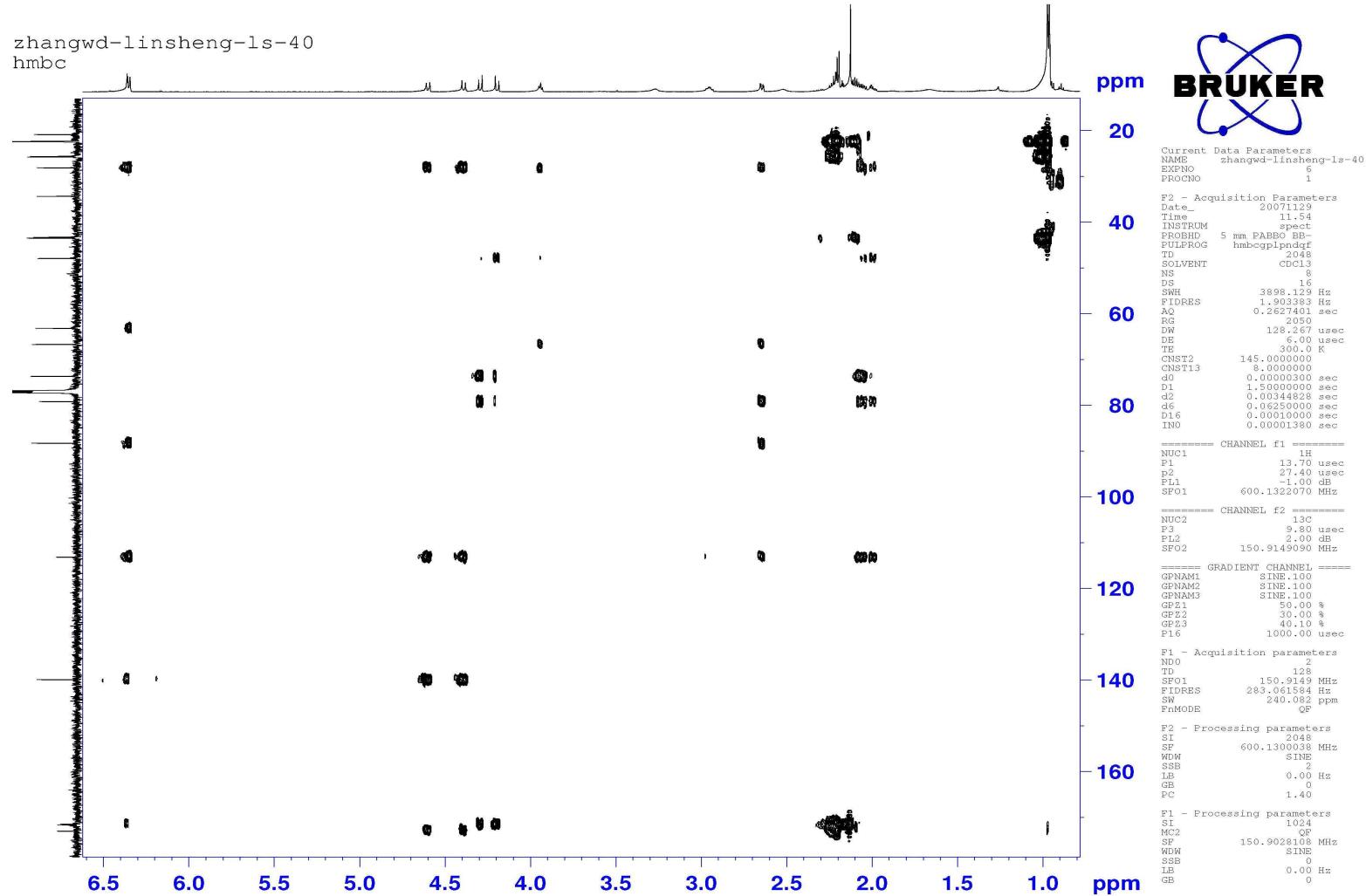


**S43.** The  $^1\text{H}$ - $^1\text{H}$ COSY Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate G (7)

zhangwd-linsheng-ls-40  
hsqc

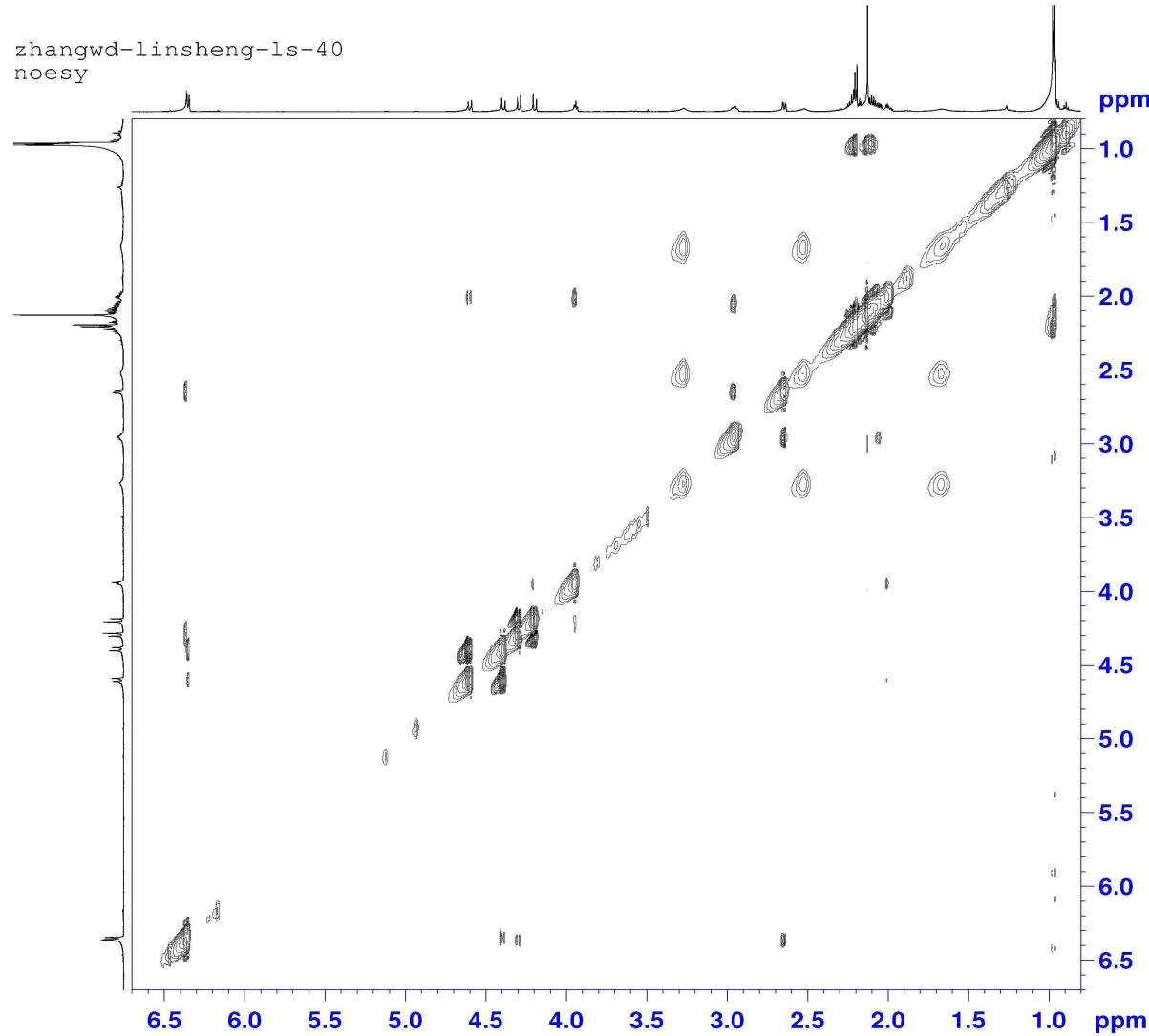


S44. The HSQC Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate G (7)



**S45.** The HMBC Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate G (7)

zhangwd-linsheng-ls-40  
noesy



Current Data Parameters  
NAME zhangwd-linsheng-ls-40  
EXPNO 7  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20071129  
Time\_ 12.27  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG noesypnh  
TD 2048  
SOLVENT CDCl3  
NS 8  
DS 16  
SWH 3898.129 Hz  
FIDRES 1.903383 Hz  
AQ 0.2627401 sec  
RG 16  
DW 128.267 usec  
DE 6.00 usec  
TE 300.0 K  
d0 0.00011083 sec  
D1 2.00000000 sec  
D2 0.80000001 sec  
IN0 0.00025655 sec  
STLCNT 128

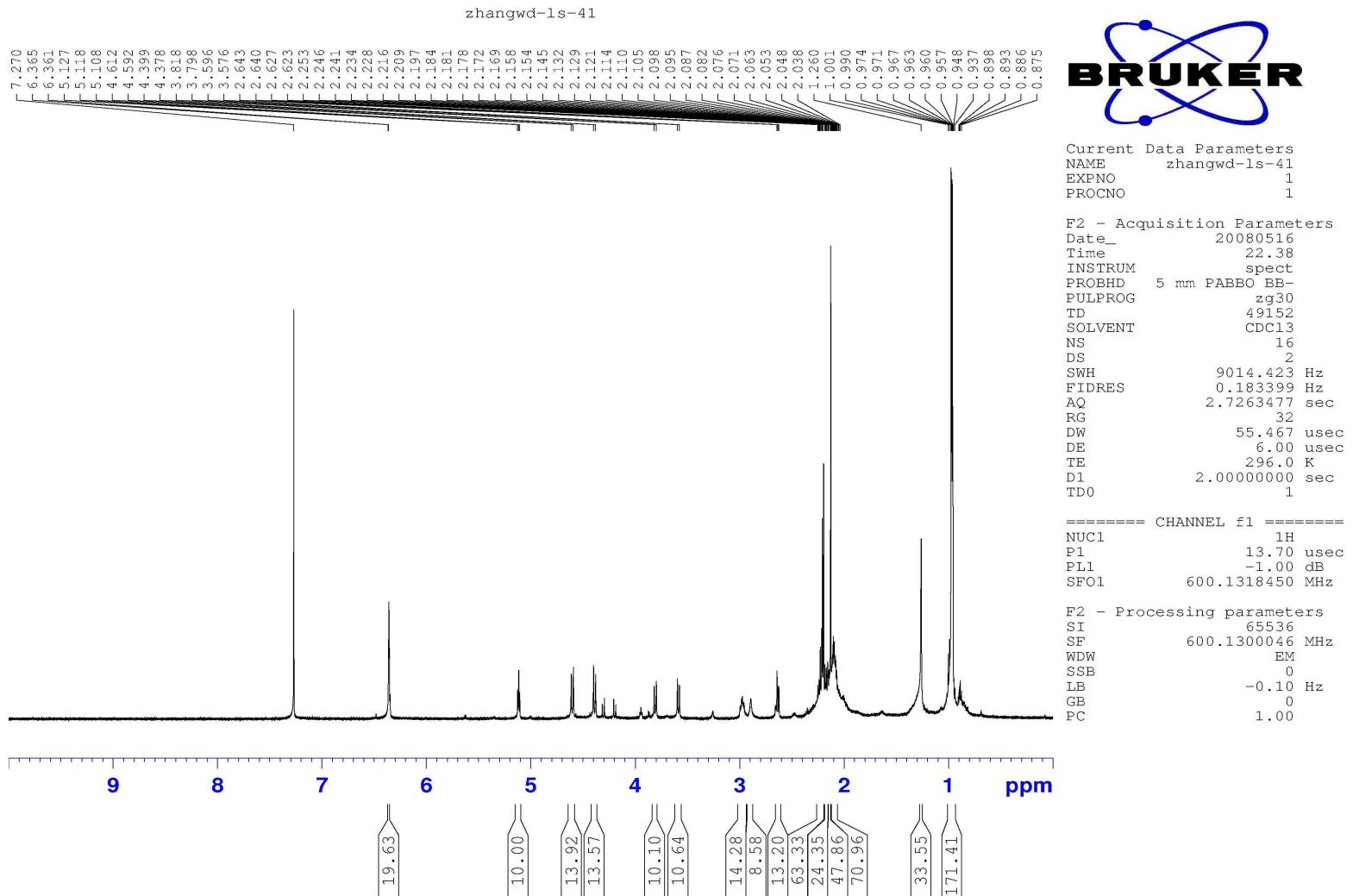
===== CHANNEL f1 =====  
NUC1 1H  
P1 13.70 usec  
PL1 -1.00 dB  
SF01 600.1322070 MHz

F1 - Acquisition parameters  
ND0 1  
TD 128  
SF01 600.1322 MHz  
FIDRES 30.452154 Hz  
SW 6.495 ppm  
FnMODE States-TPPI

F2 - Processing parameters  
SI 2048  
SF 600.1300038 MHz  
WDW QSINE  
SSB 2  
LB 0.00 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 2048  
MC2 States-TPPI  
SF 600.1300038 MHz  
WDW QSINE  
SSB 2  
LB 0.00 Hz  
GB 0

S46. The NOESY Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate G (7)



**S47. The  $^1\text{H}$  NMR Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate H (8)**

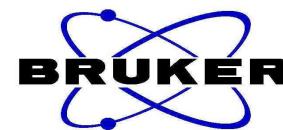
zhangwd-ls-41

112.44  
111.28  
110.76

140.17

113.03

88.22  
80.31  
79.21  
76.14  
73.64  
66.65  
64.56  
63.13  
47.84  
47.48  
43.43  
43.39  
43.21  
34.30  
32.60  
29.69  
28.07  
27.95  
25.71  
25.59  
22.39  
22.32  
22.30  
21.15  
20.83



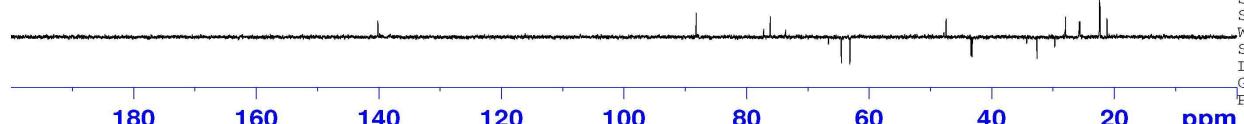
Current Data Parameters  
NAME zhangwd-ls-41  
EXPNO 2  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080517  
Time 2.06  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 4096  
DS 0  
SWH 45454.547 Hz  
FIDRES 0.693581 Hz  
AQ 0.7209460 sec  
RG 32768  
DW 11.000 usec  
DE 6.00 usec  
TE 298.7 K  
D1 2.0000000 sec  
d11 0.0300000 sec  
DELTA 1.8999998 sec  
TD0 1

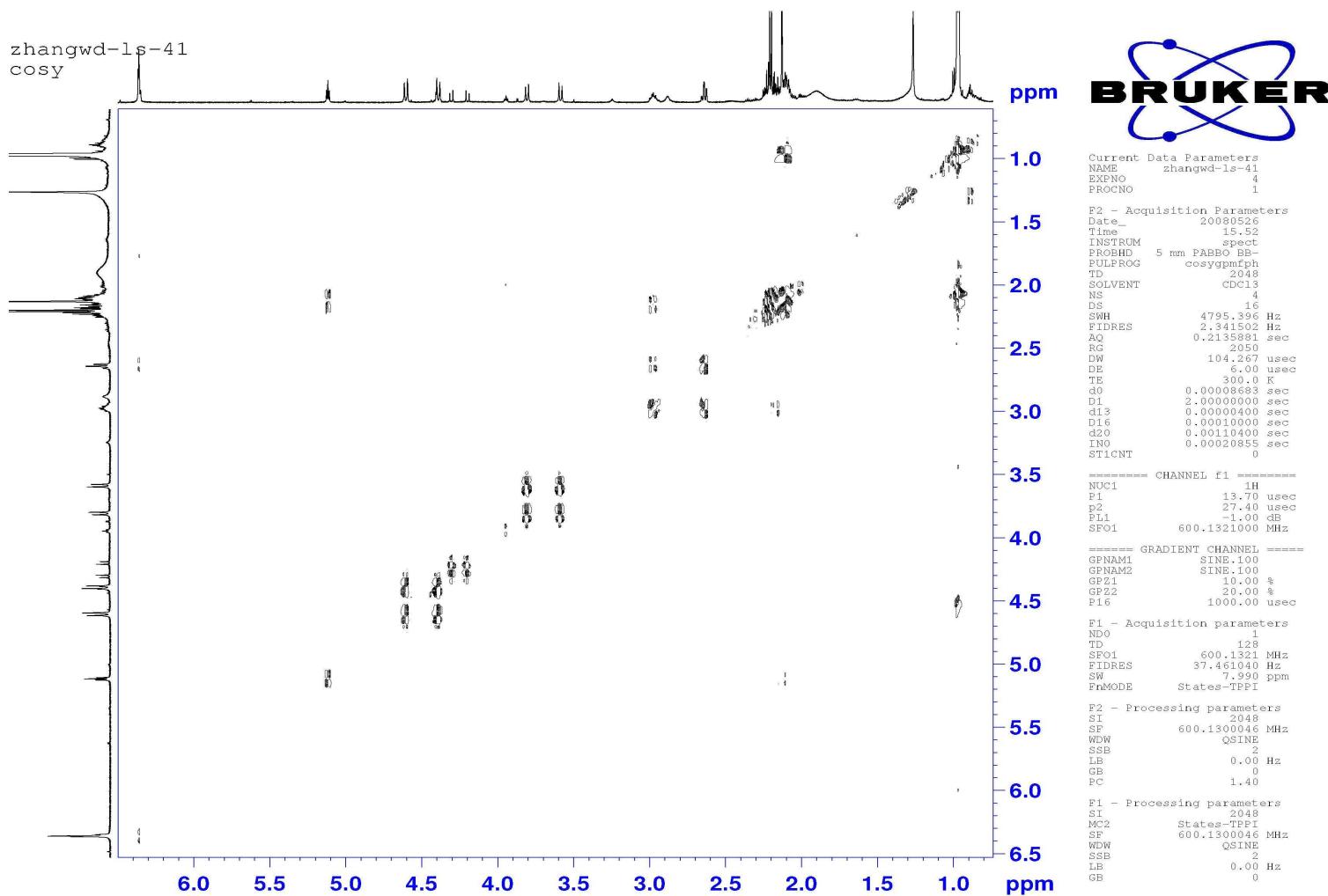
===== CHANNEL f1 =====  
NUC1 13C  
P1 8.50 usec  
PL1 2.00 dB  
SFO1 150.9178990 MHz

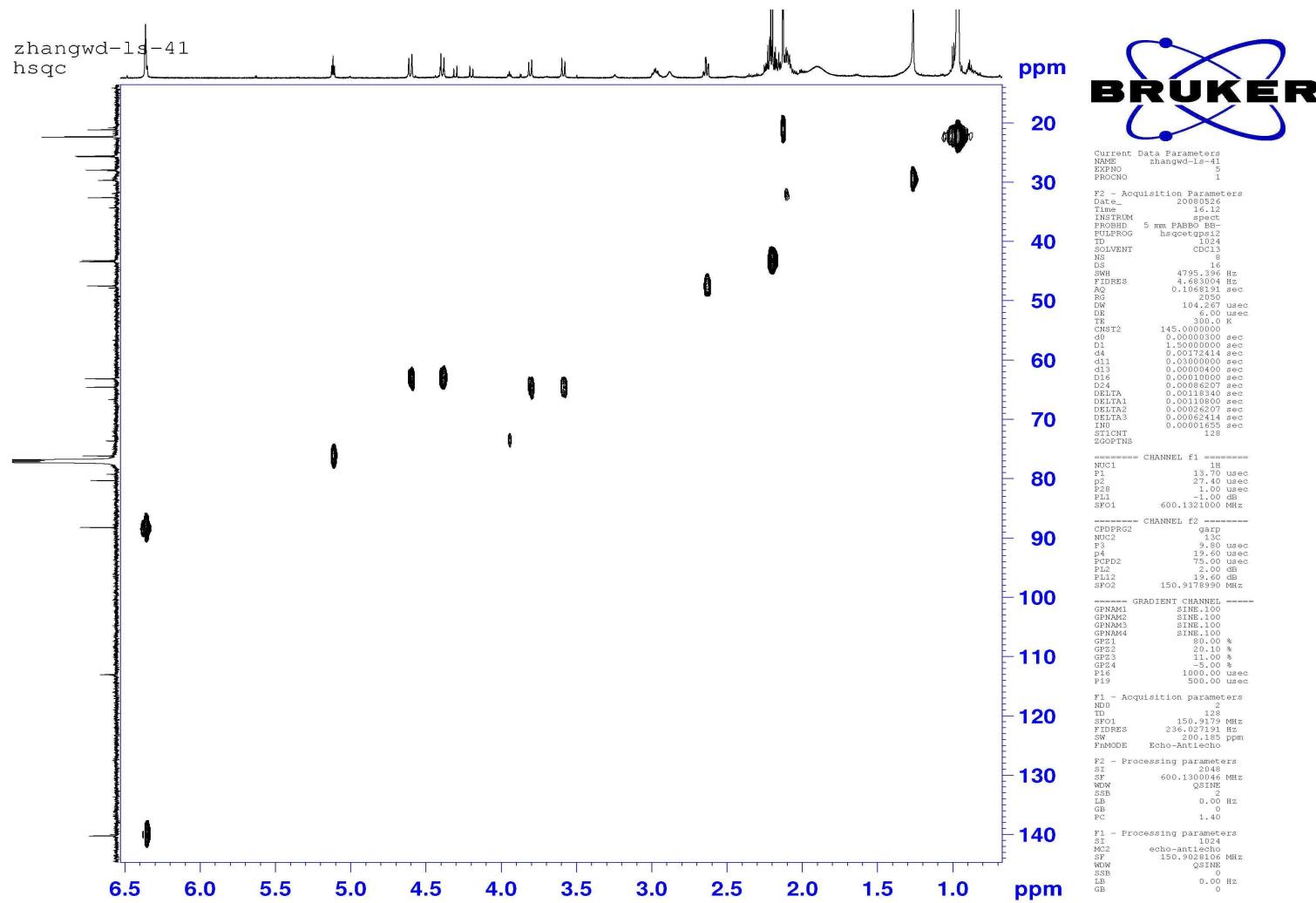
===== CHANNEL f2 =====  
CPDPRG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.00 dB  
PL13 14.00 dB  
SFO2 600.1324005 MHz

F2 - Processing parameters  
SI 65536  
SF 150.9028106 MHz  
WDW EM  
SSB 0  
LB 2.00 Hz  
GB 0  
PC 1.40

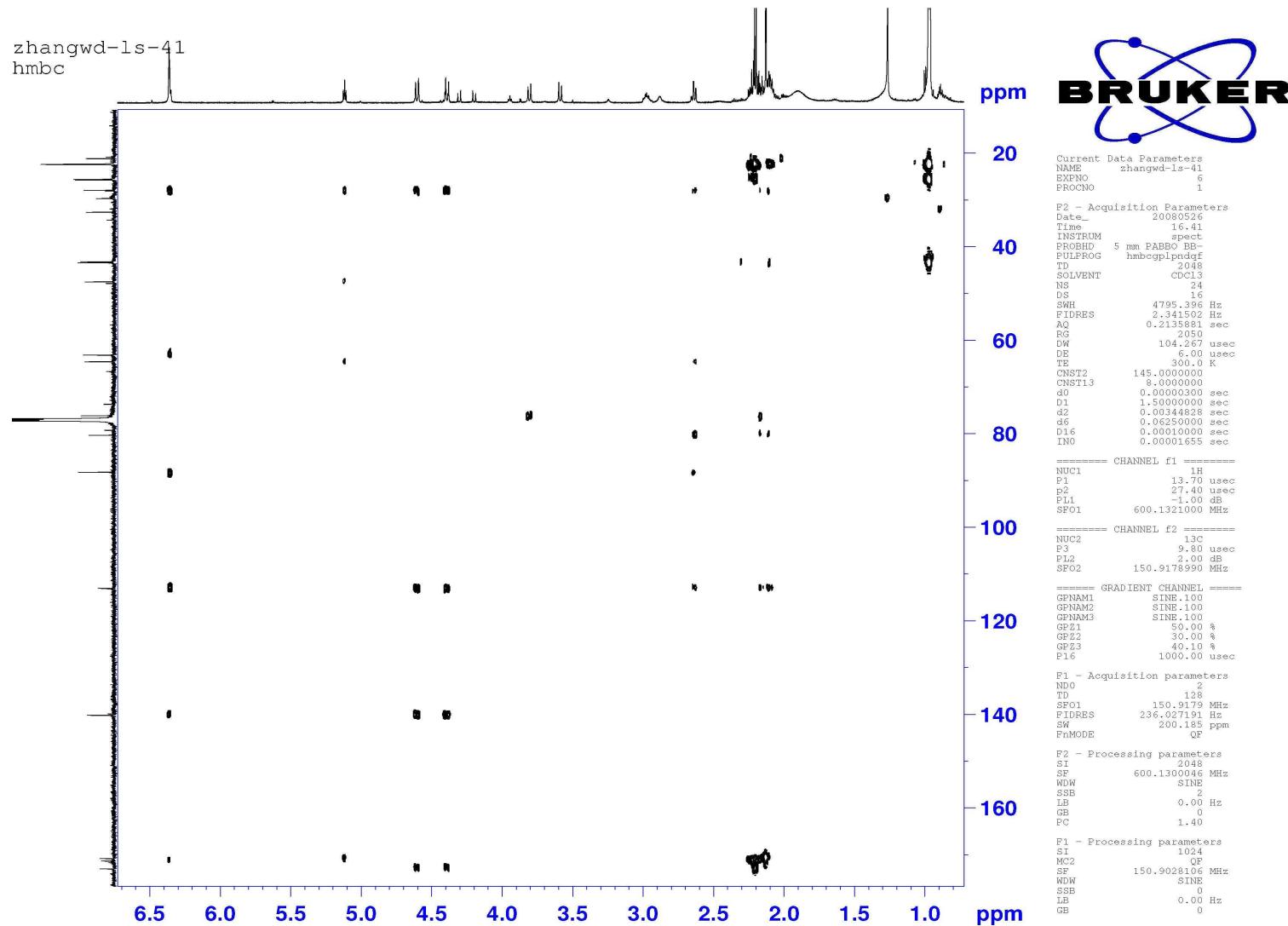


S48. The <sup>13</sup>C NMR and DEPT Spectra (150 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate H (8)

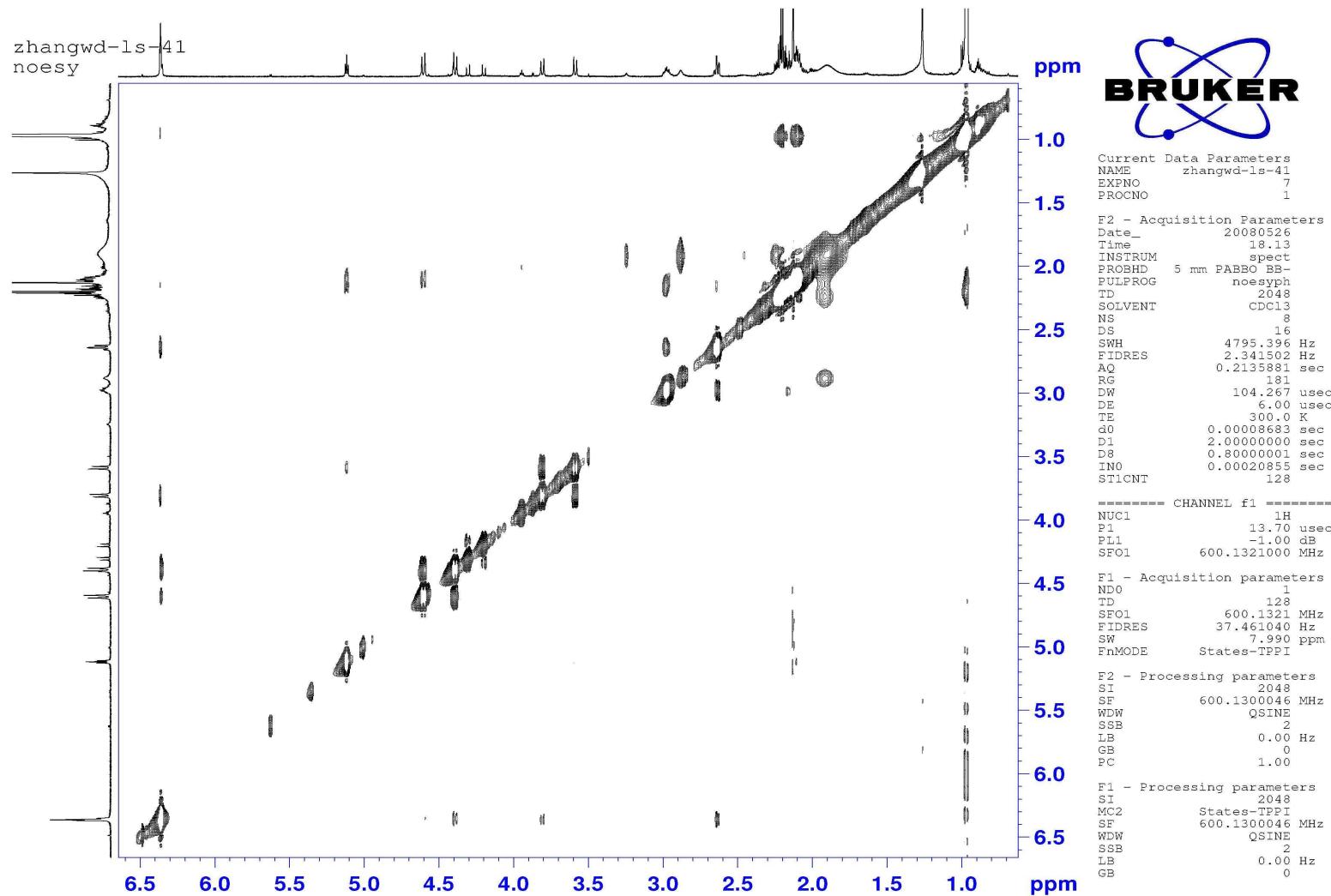




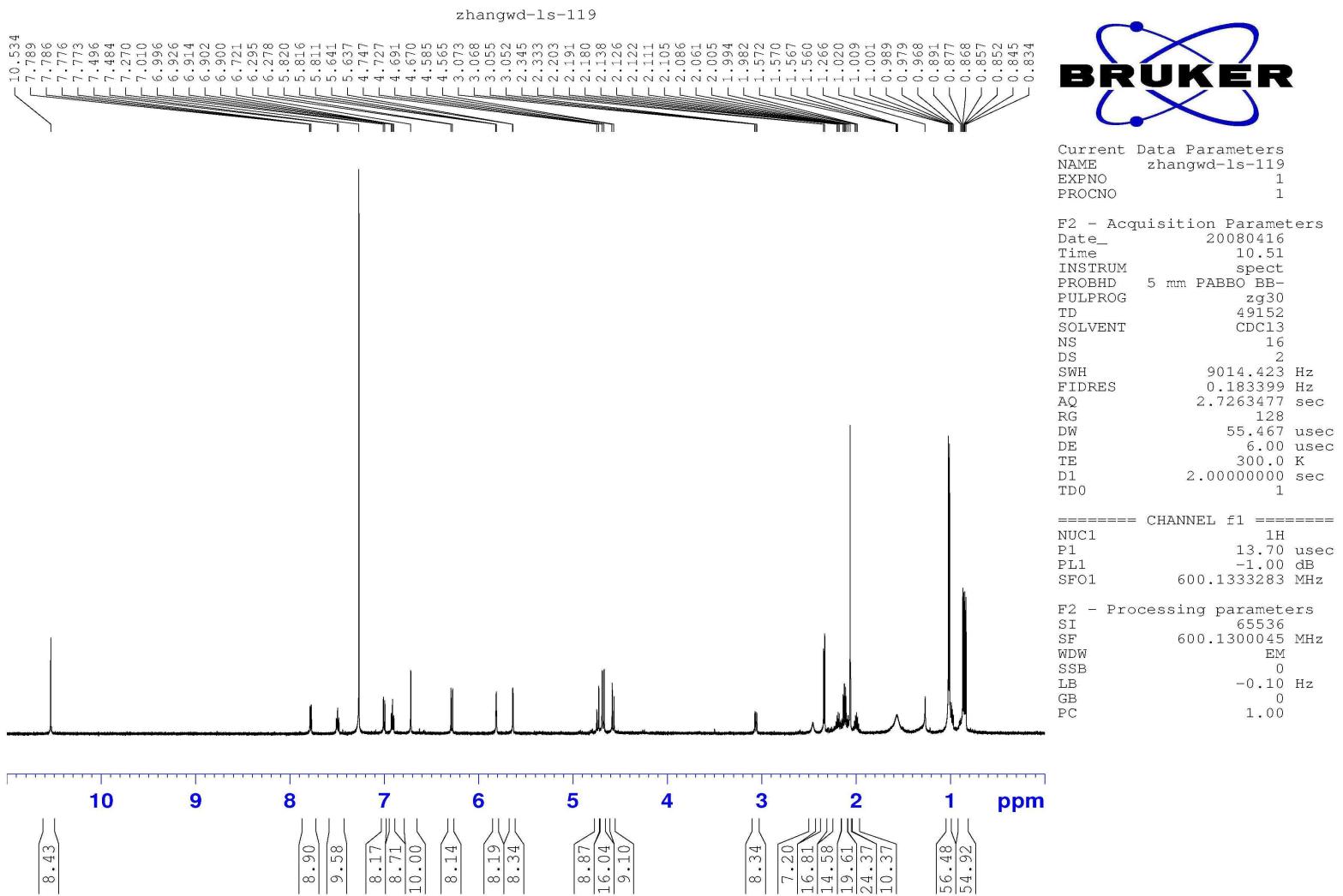
S50. The HSQC Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate H (8)



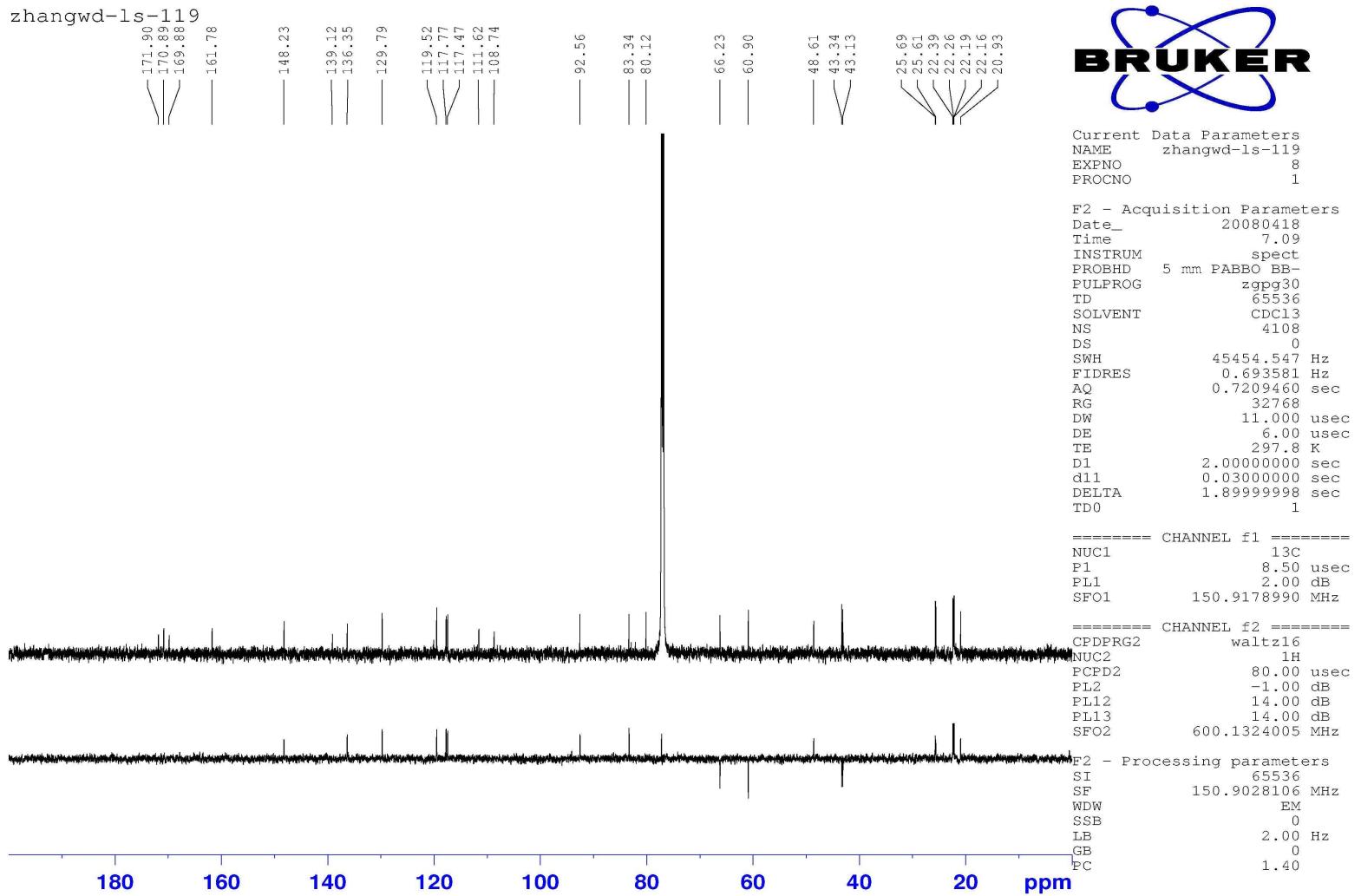
S51. The HMBC Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate H (8)



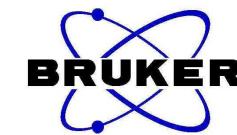
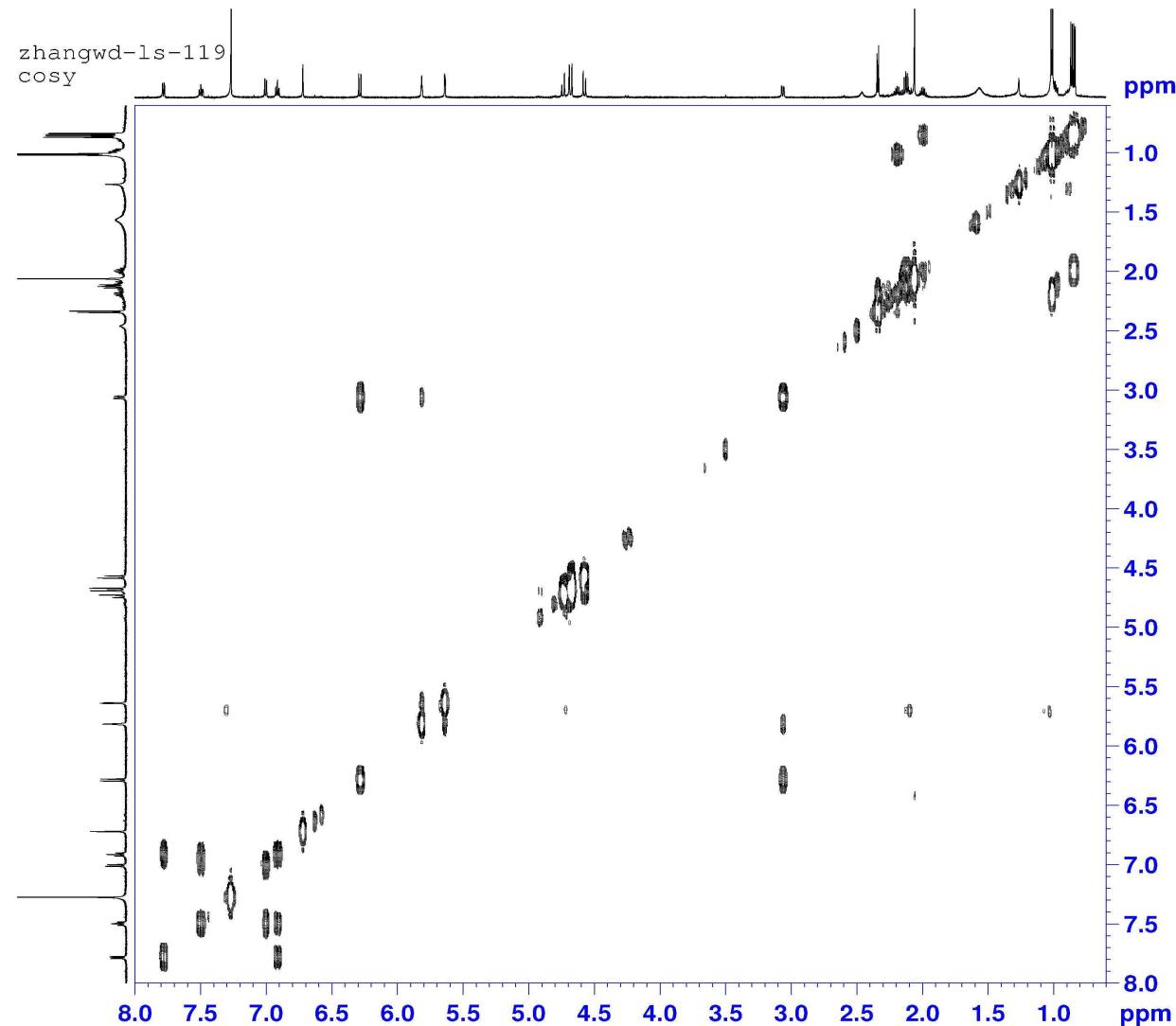
S52. The NOESY Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate H (8)



**S53. The <sup>1</sup>H NMR Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate I (9)**



**S54.** The  $^{13}\text{C}$  NMR and DEPT Spectra (150 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate I (9)



Current Data Parameters  
 NAME zhangwd-ls-119  
 EXPNO 4  
 PROCNO 1

E2 - Acquisition Parameters  
 Date 20080418  
 Time 0.16  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosygpff  
 TD 2048  
 SOLVENT CDCl3  
 NS 1  
 DS 16  
 SWH 6313.4 Hz  
 FIDRES 3.082584 Hz  
 A0 0.1622516 sec  
 RG 1290  
 DW 79.200 usec  
 DE 6.00 usec  
 TE 295.6 K  
 d0 0.00000300 sec  
 D1 2.0000000 sec  
 d13 0.00000400 sec  
 D16 0.00010000 sec  
 IN0 0.00015840 sec

===== CHANNEL f1 ======

NUC1 1H  
 F0 13.70 usec  
 F1 13.70 usec  
 PL1 -1.00 dB  
 SFO1 600.1334260 MHz

===== GRADIENT CHANNEL =====

GPNAME1 SINE,100  
 GPNAME2 SINE,100  
 GPZ1 10.00 %  
 GPZ2 10.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters

ND0 1  
 TD 160  
 SFO1 600.1334 MHz  
 FIDRES 39.457069 Hz  
 SW 10.520 ppm  
 FmMODE QF

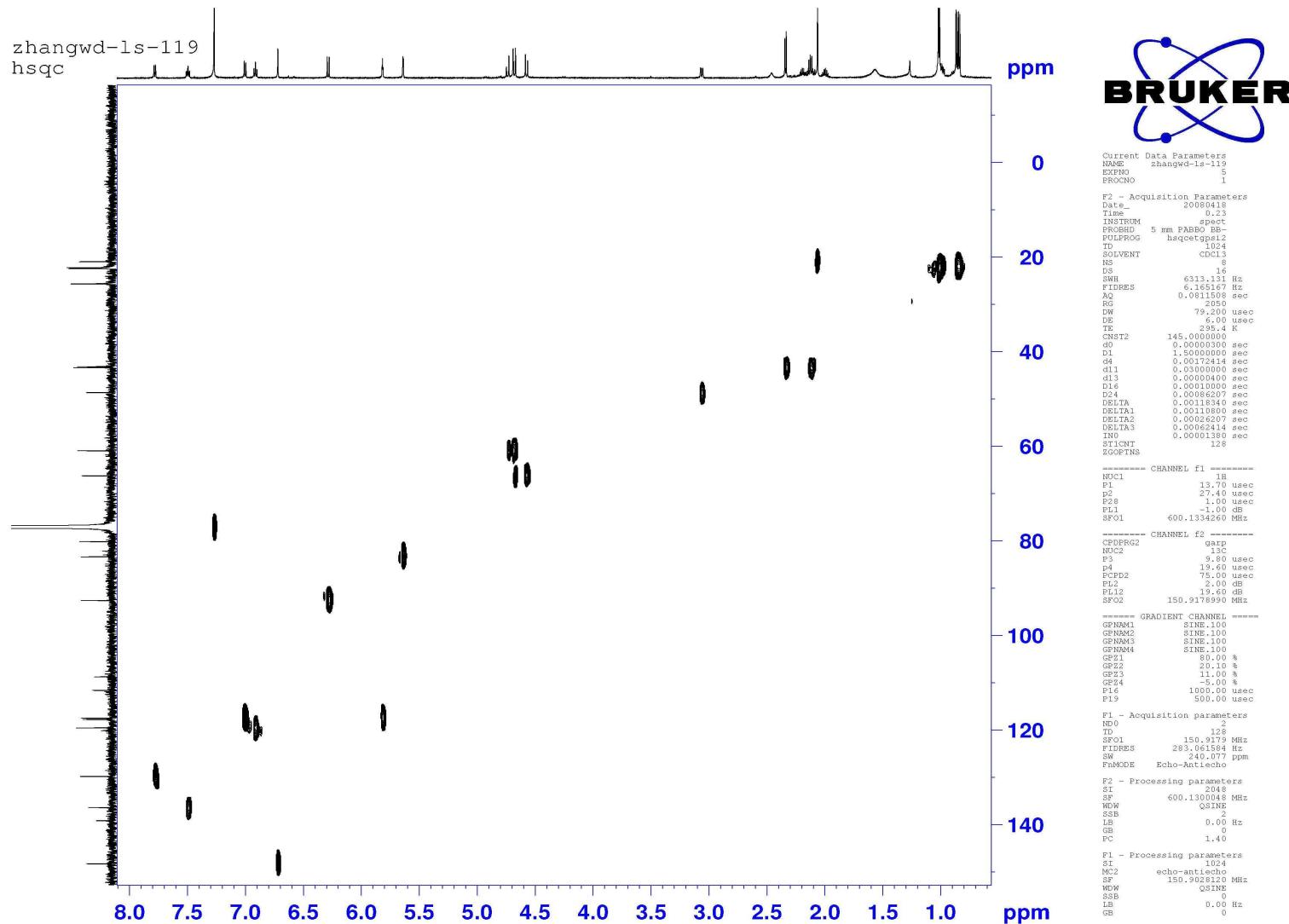
P2 - Processing parameters

SI 2048  
 SF 600.1300048 MHz  
 WDW QSINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.40

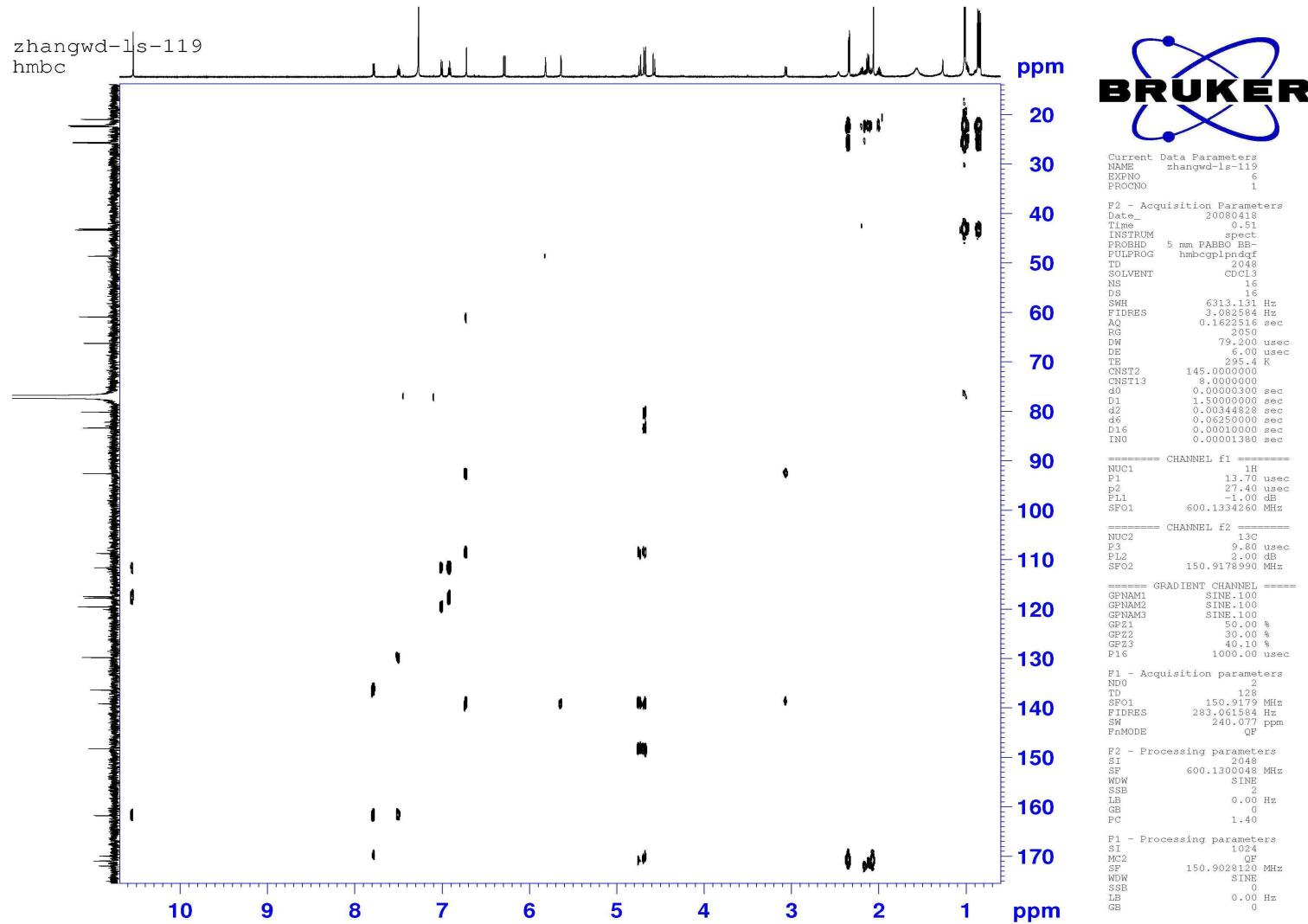
P1 - Processing parameters

SI 2048  
 MC2 QF  
 SF 600.1300048 MHz  
 WDW QSINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

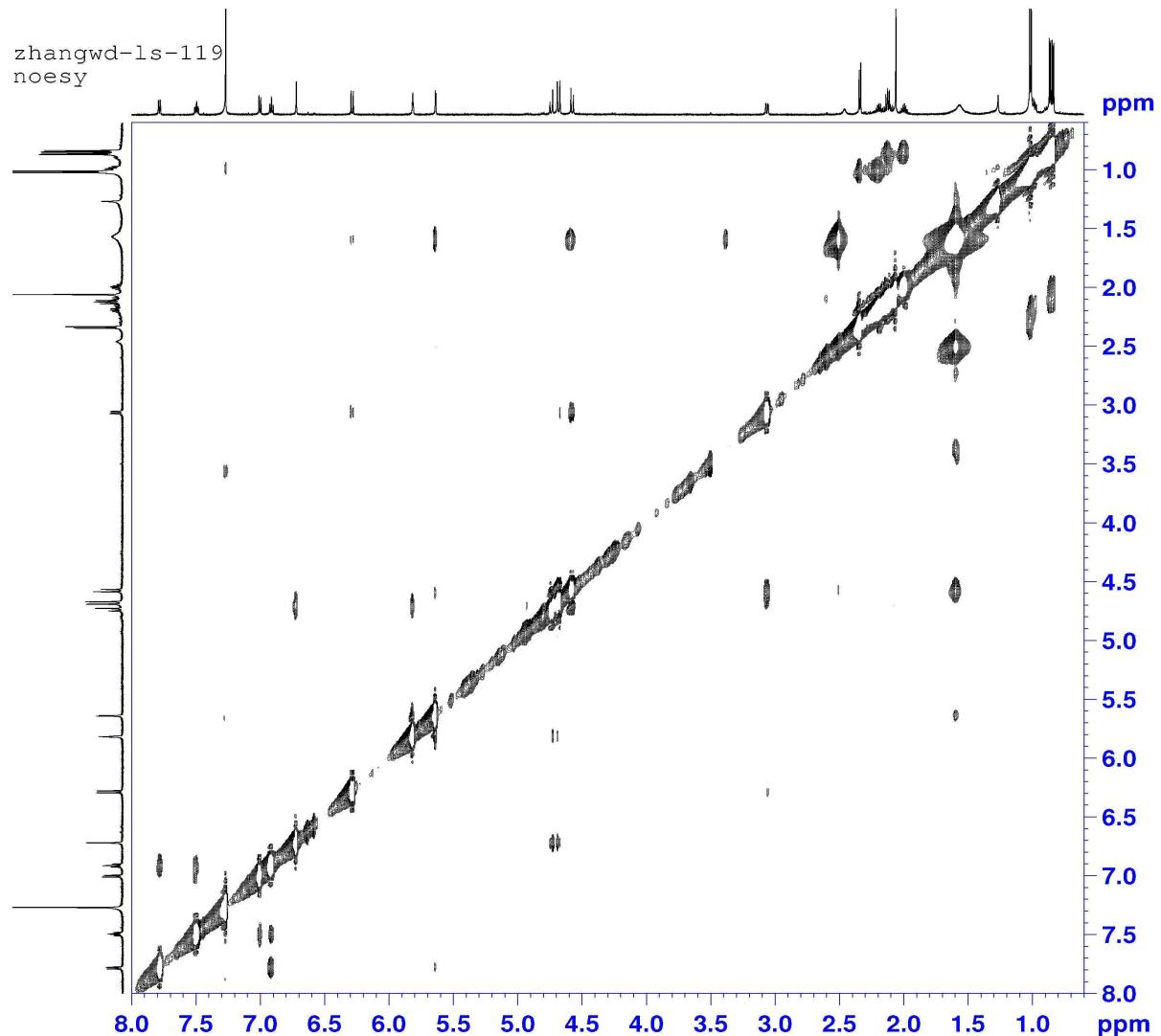
S55. The  $^1\text{H}$ - $^1\text{H}$ COSY Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate I (9)



S56. The HSQC Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate I (9)



S57. The HMBC Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate I (9)



Current Data Parameters  
NAME zhangwd-ls-119  
EXPNO 7  
PROCNO 1

F2 - Acquisition Parameters  
Date\_ 20080418  
Time 1.52  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG noesypb  
TD 2048  
SOLVENT CDCl3  
NS 16  
DS 16  
SWH 6313.131 Hz  
FIDRES 3.082584 Hz  
AQ 0.1622516 sec  
RG 406  
DW 79.200 usec  
DE 6.00 usec  
TE 295.2 K  
d0 0.00006176 sec  
D1 2.0000000 sec  
D8 0.80000001 sec  
INO 0.00015840 sec  
ST1CNT 128

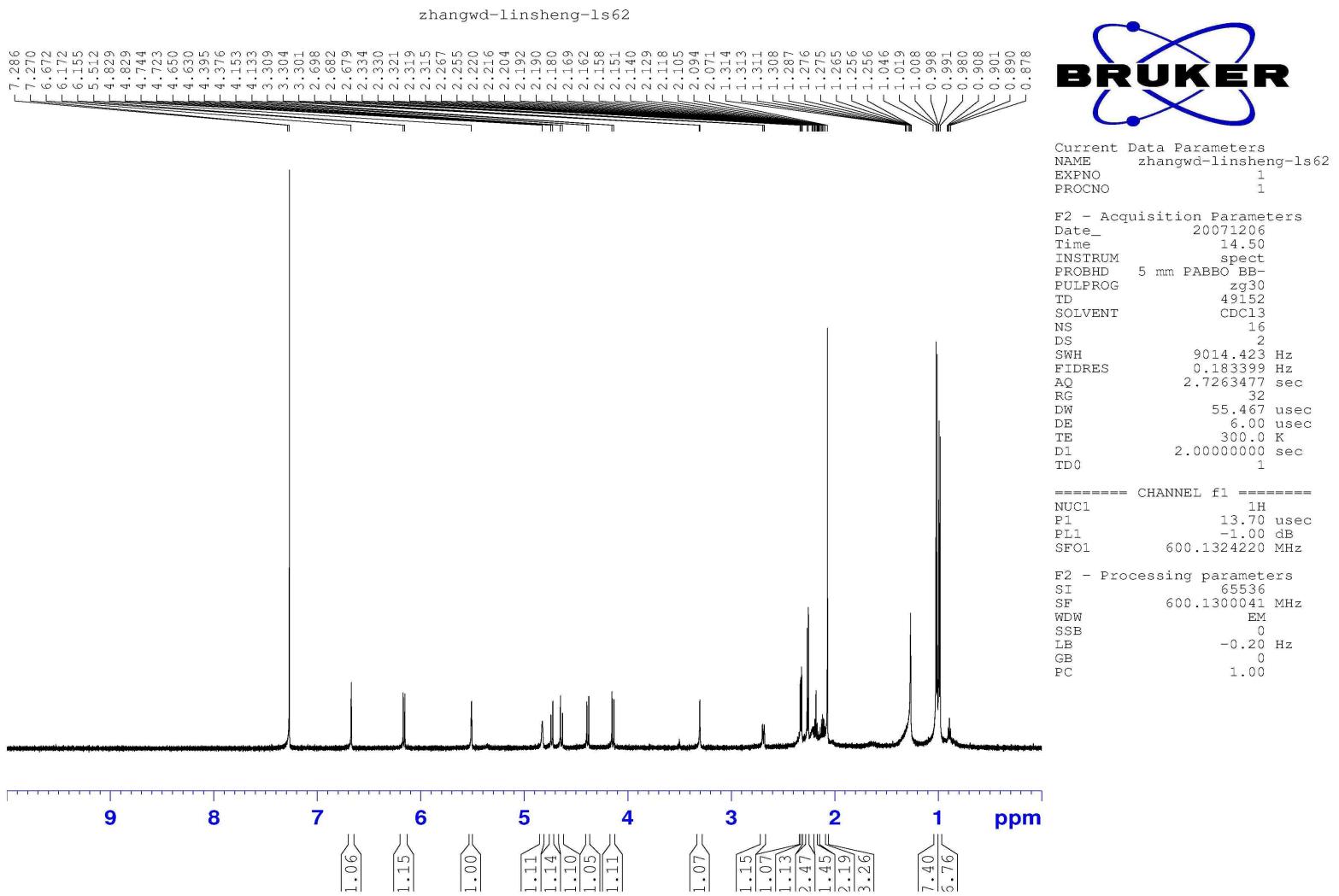
===== CHANNEL f1 =====  
NUC1 1H  
P1 13.70 usec  
PL1 -1.00 dB  
SFO1 600.1334260 MHz

F1 - Acquisition parameters  
ND0 1  
TD 160  
SFO1 600.1334 MHz  
FIDRES 39.457069 Hz  
SW 10.520 ppm  
FnMODE States-TPPPI

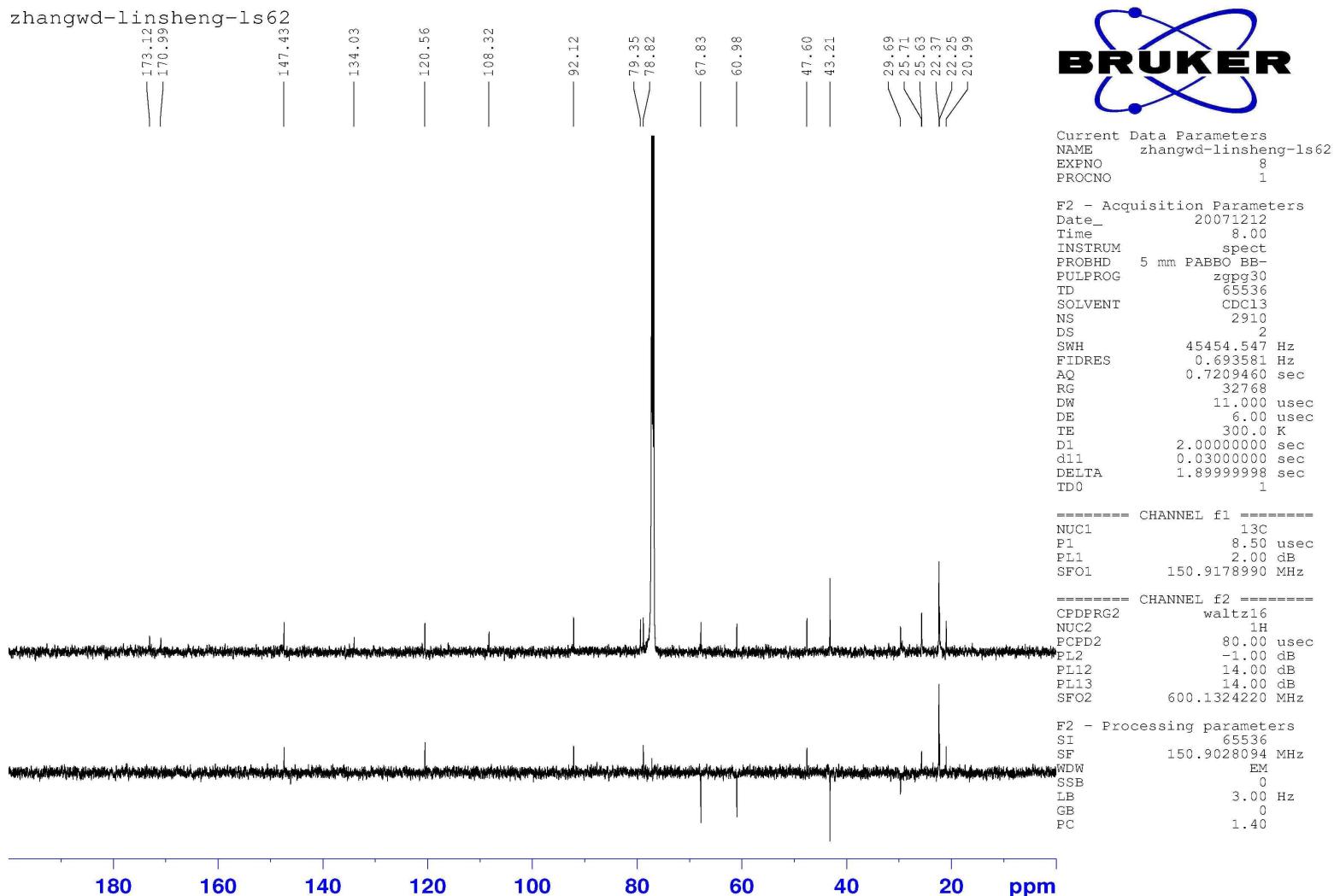
F2 - Processing parameters  
SI 2048  
SF 600.1300048 MHz  
WDW QSINE  
SSB 2  
LB 0.00 Hz  
GB 0  
PC 1.00

F1 - Processing parameters  
SI 2048  
MC2 States-TPPPI  
SF 600.1300048 MHz  
WDW QSINE  
SSB 2  
LB 0.00 Hz  
GB 0

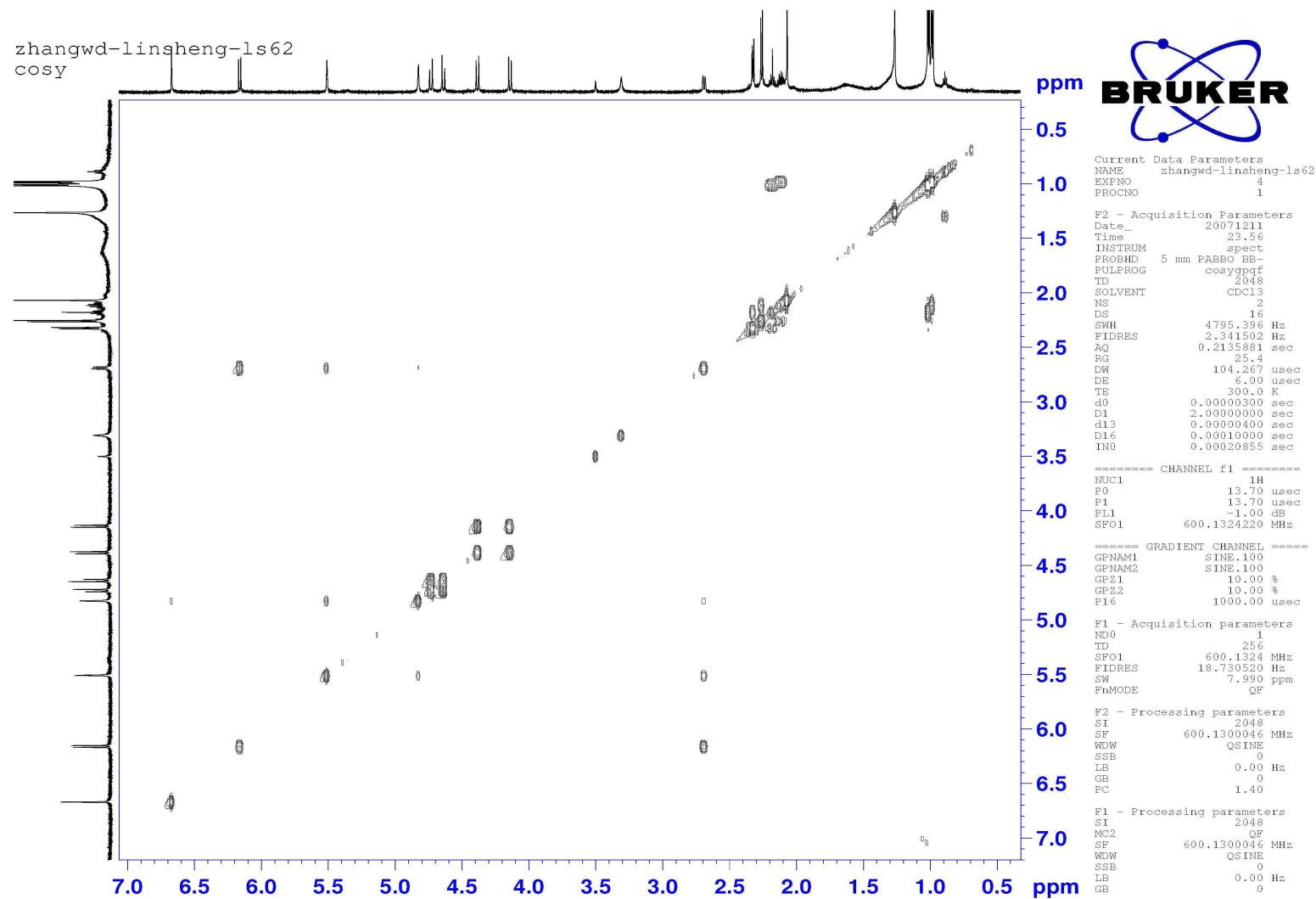
S58. The NOESY Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate I (9)



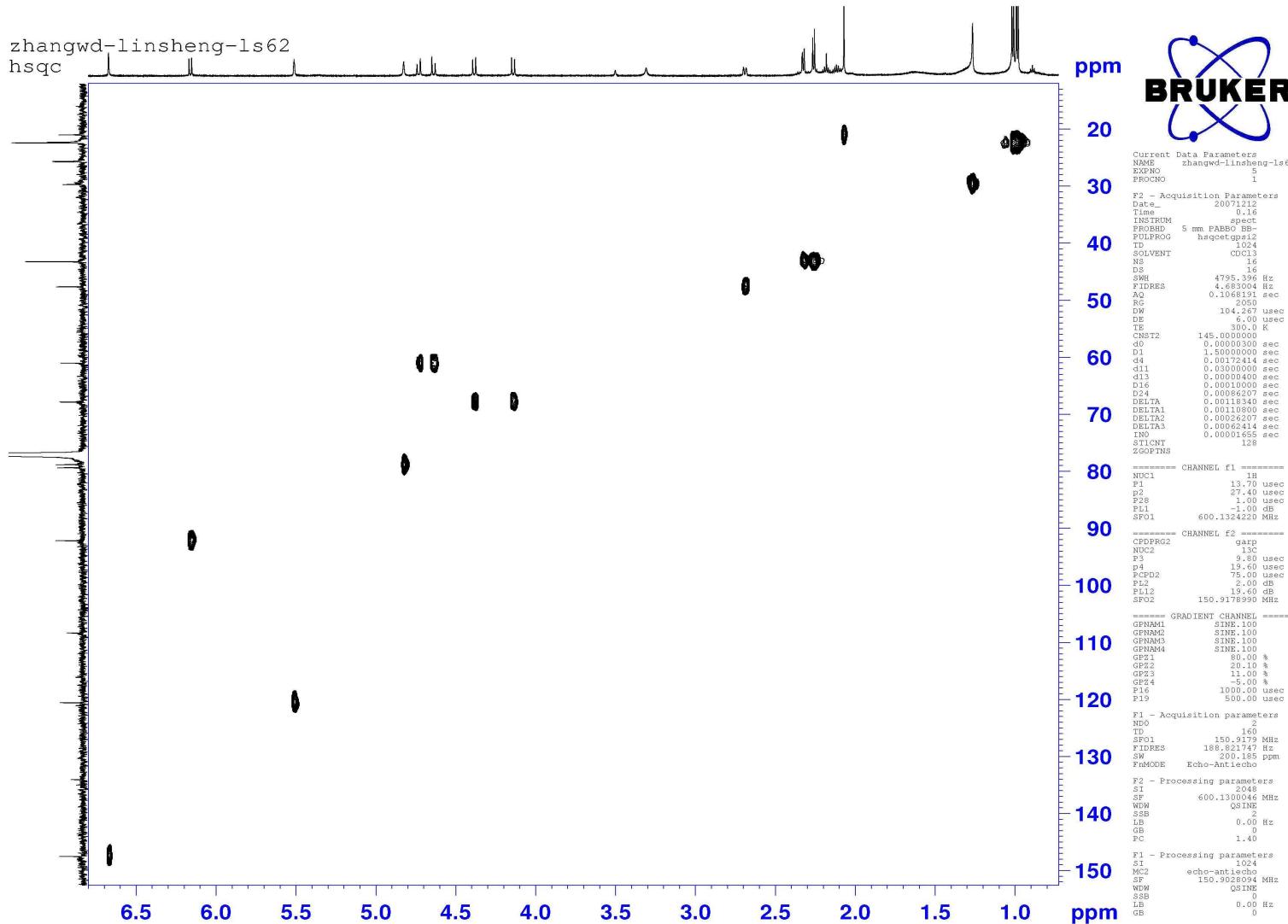
**S59.** The  $^1\text{H}$  NMR Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate J (10)



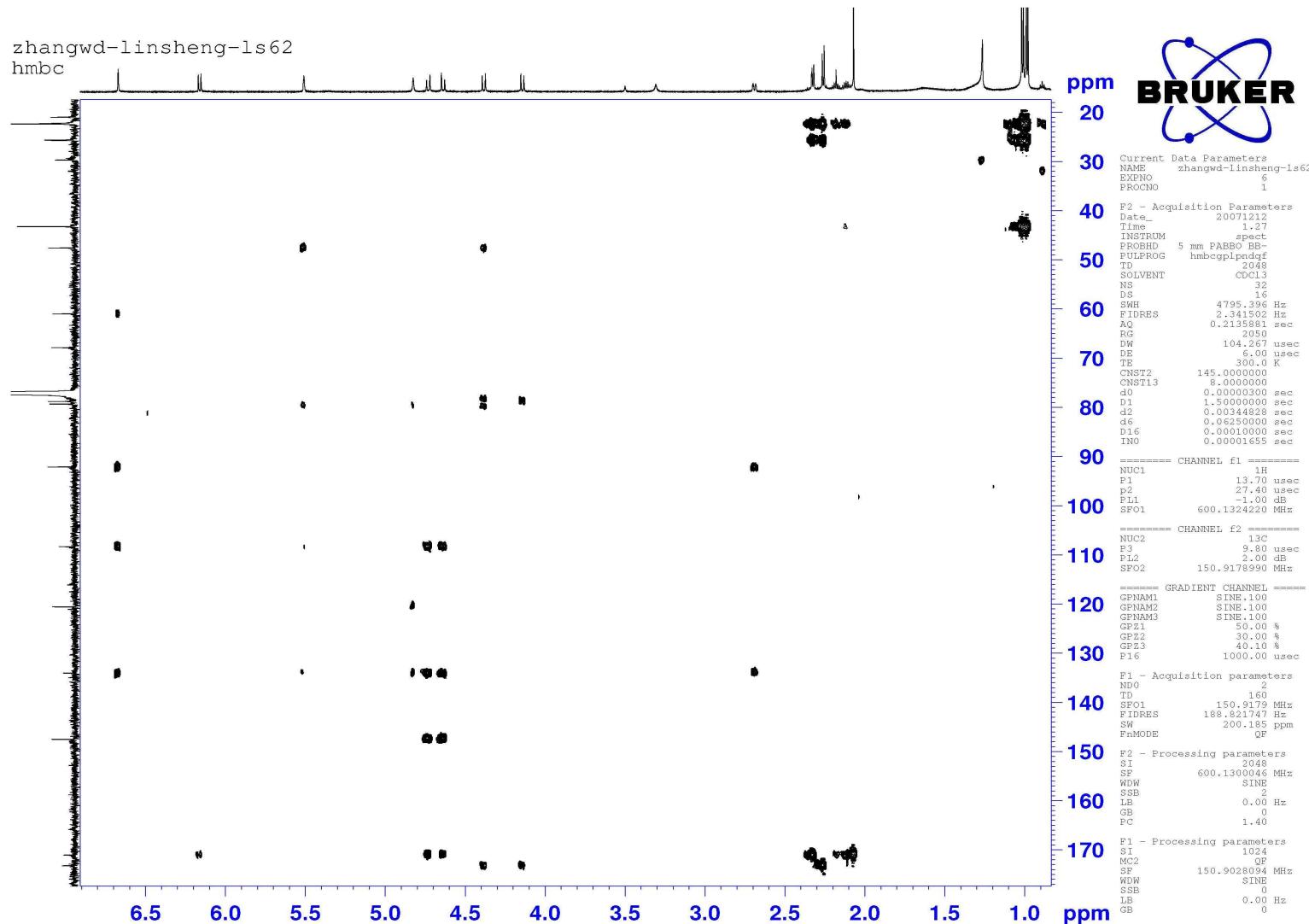
S60. The  $^{13}\text{C}$  NMR and DEPT Spectra (150 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate J (10)



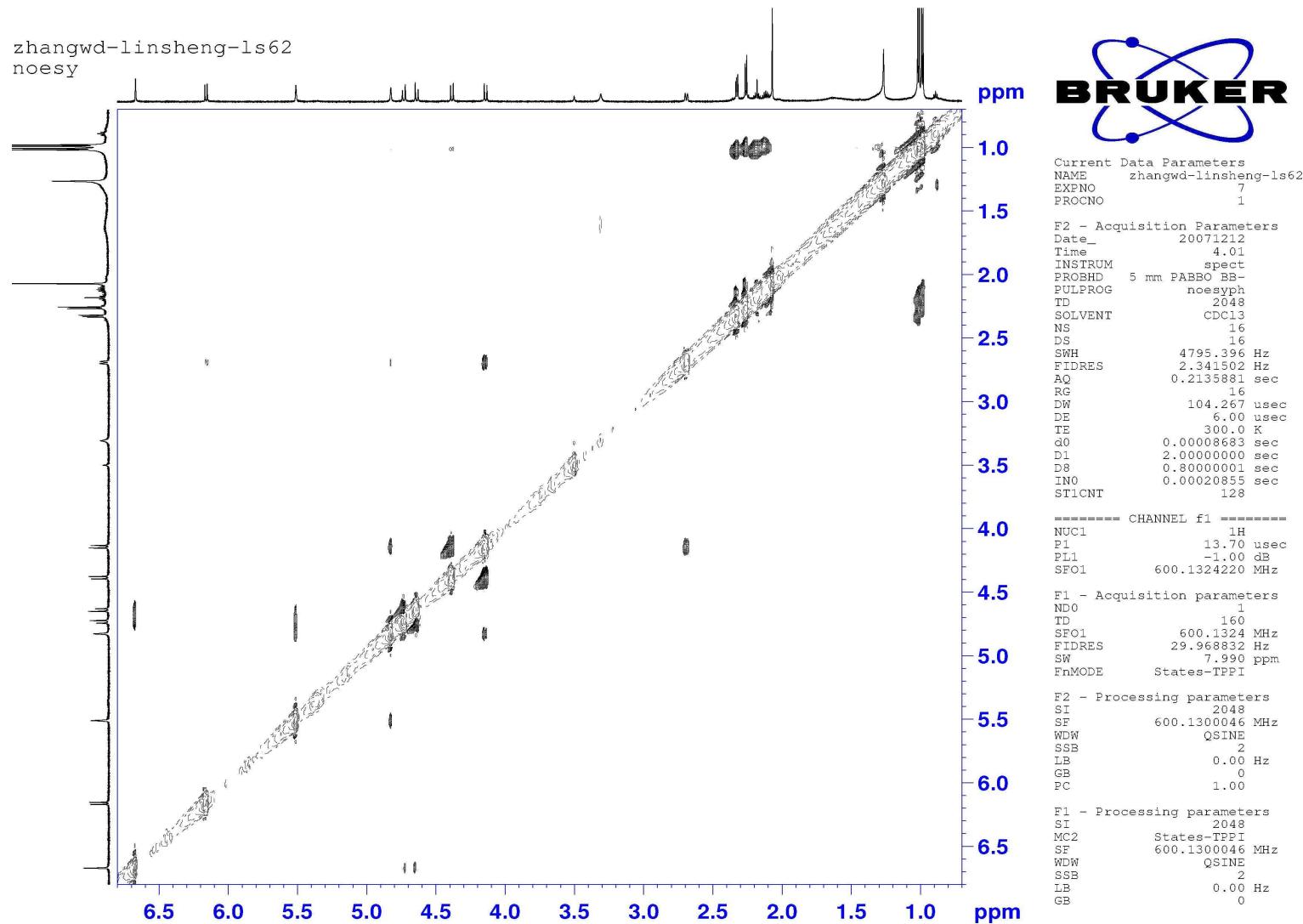
**S61. The <sup>1</sup>H-<sup>1</sup>HCOSY Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate J (10)**



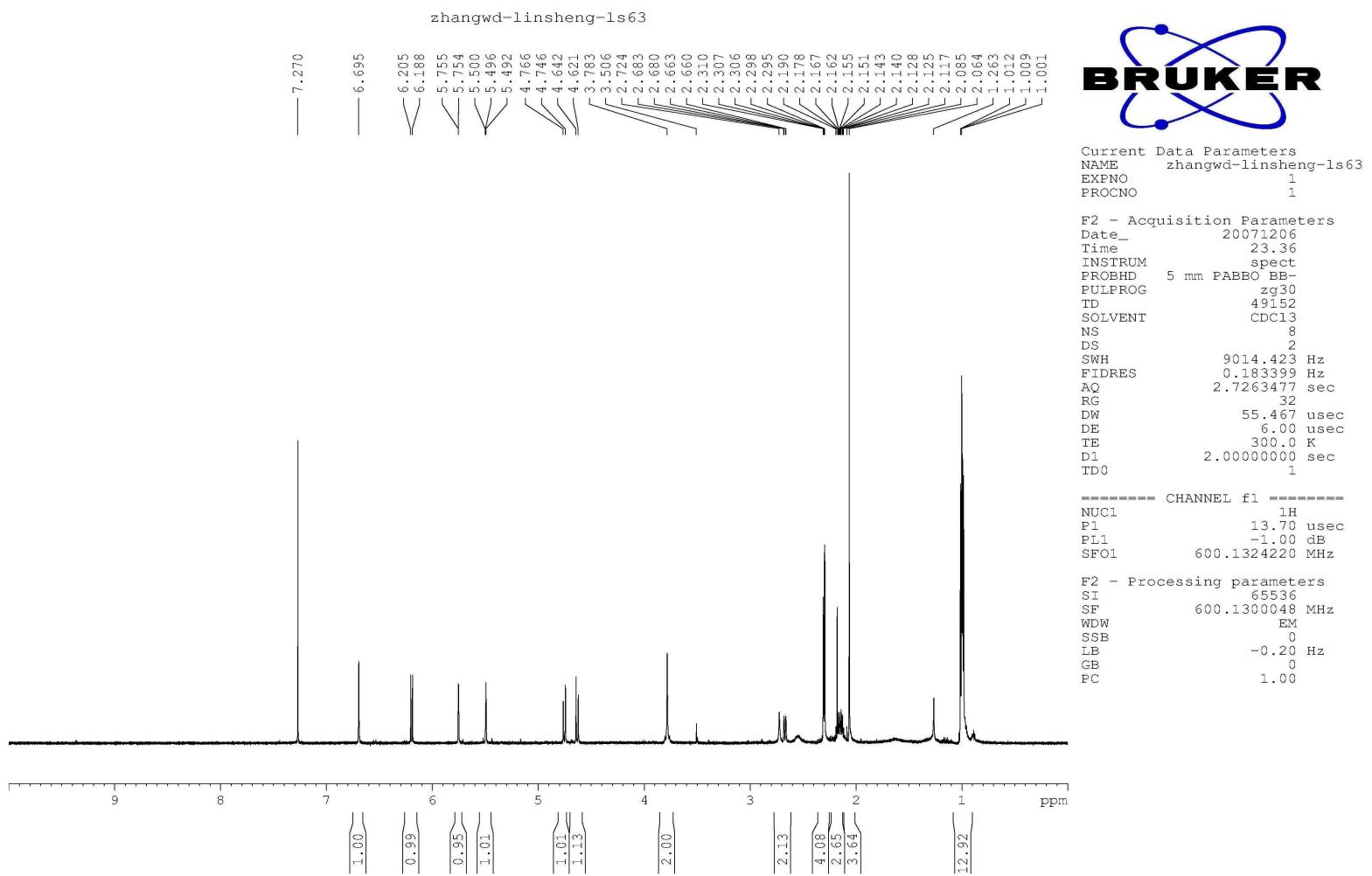
S62. The HSQC Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate J (10)



S63. The HMBC Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate J (10)

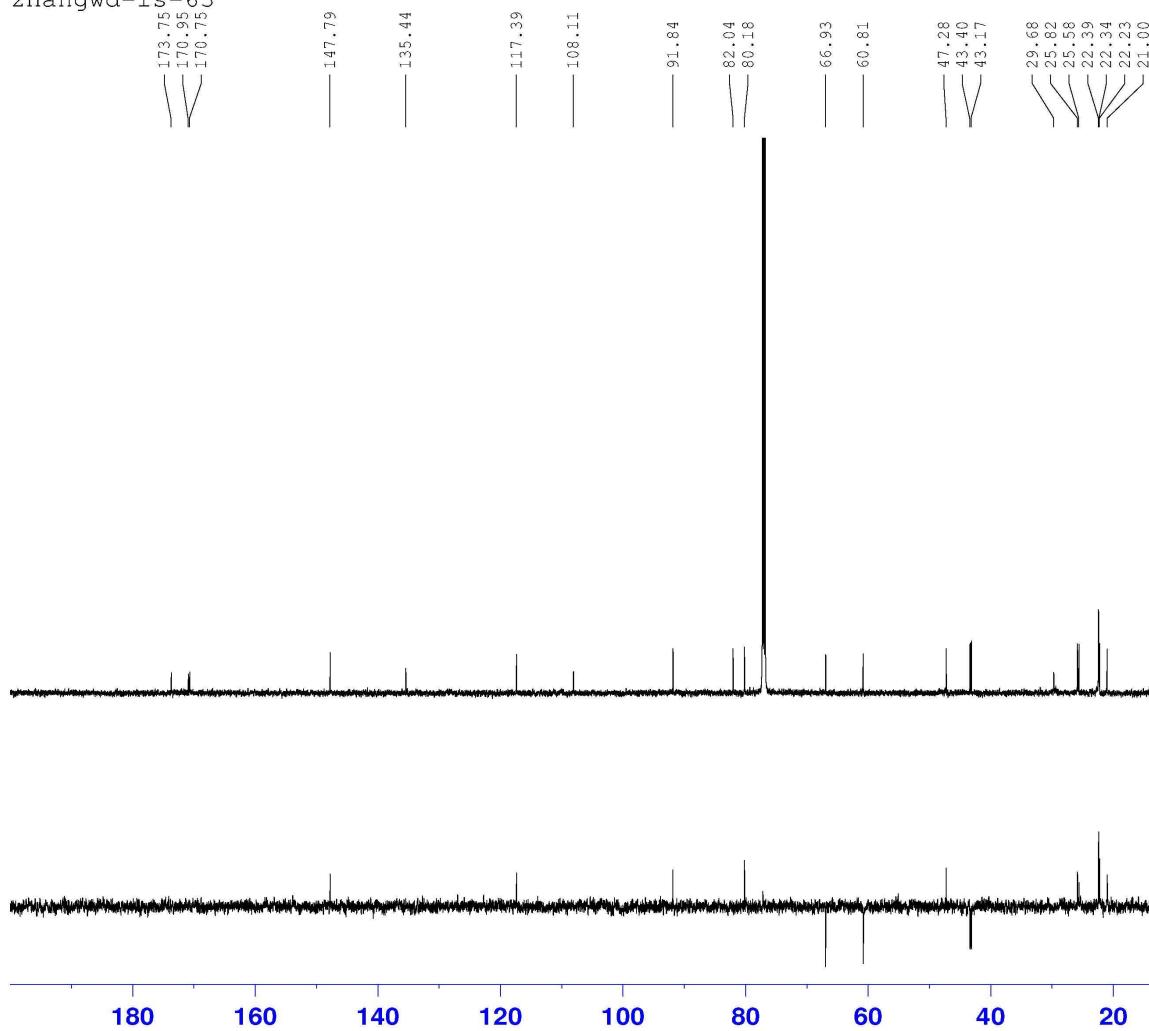


**S64. The NOESY Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate J (10)**



**S65. The  $^1\text{H}$  NMR Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate K (11)**

zhangwd-ls-63



Current Data Parameters  
NAME zhangwd-ls-63  
EXPNO 3  
PROCNO 1

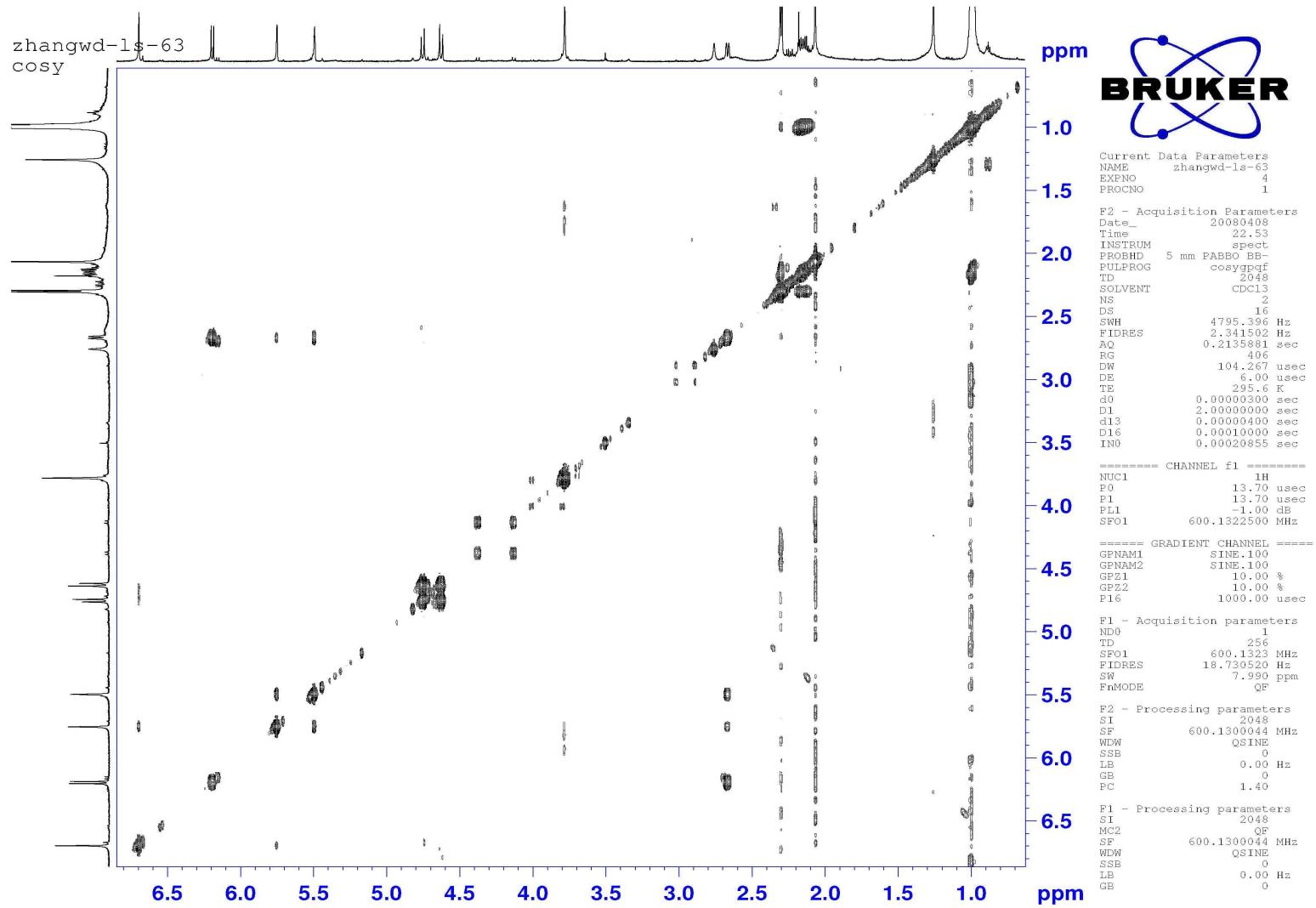
F2 - Acquisition Parameters  
Date\_ 20080408  
Time 22.52  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG zgpg30  
TD 65536  
SOLVENT CDCl3  
NS 1024  
DS 0  
SWH 45454.547 Hz  
FIDRES 0.693581 Hz  
AQ 0.7209460 sec  
RG 32768  
DW 11.000 usec  
DE 6.00 usec  
TE 296.9 K  
D1 2.0000000 sec  
d11 0.03000000 sec  
DELTA 1.8999998 sec  
TD0 1

===== CHANNEL f1 ======  
NUC1 13C  
P1 8.50 usec  
PL1 2.00 dB  
SFO1 150.9178990 MHz

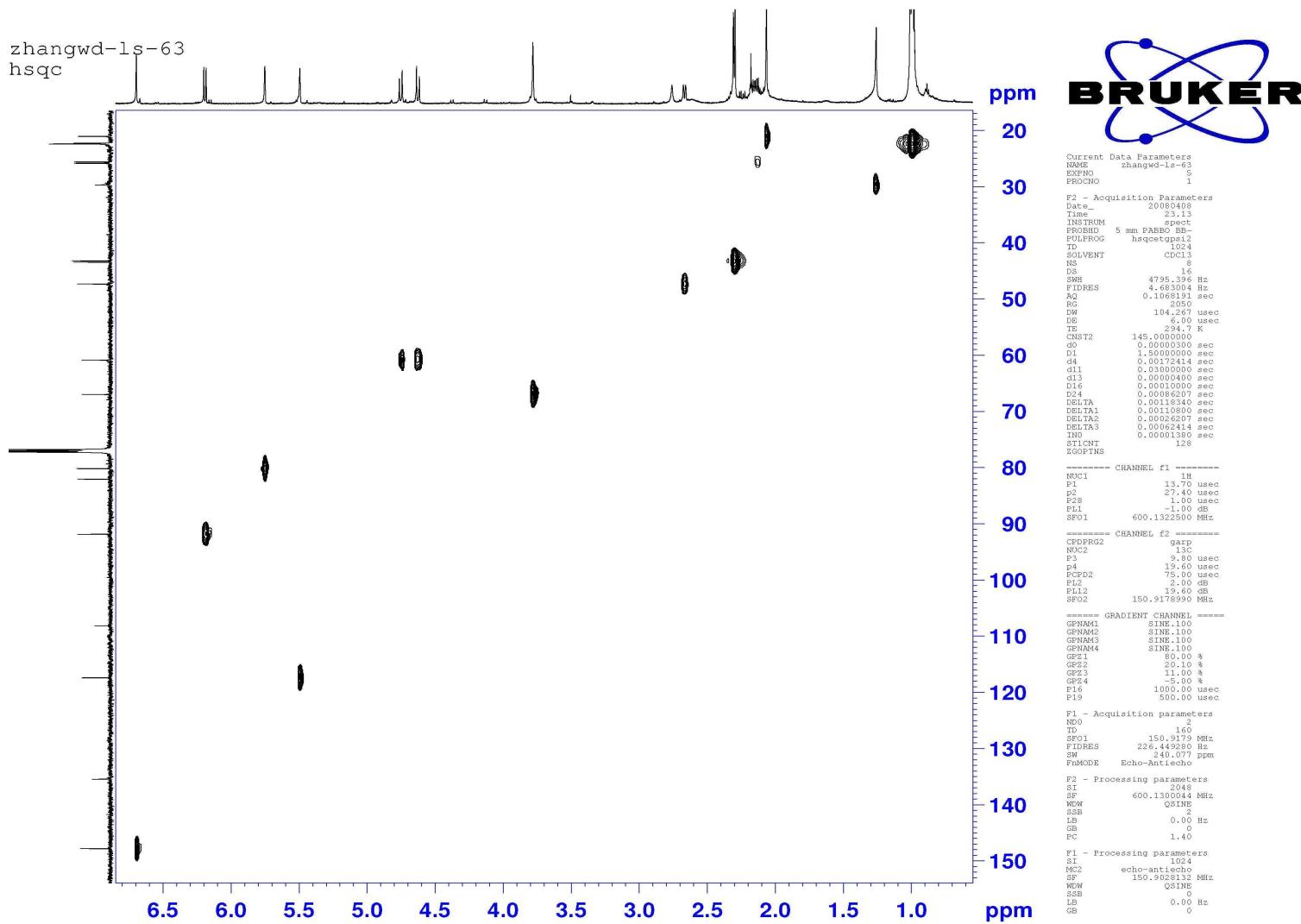
===== CHANNEL f2 ======  
CPDPG2 waltz16  
NUC2 1H  
PCPD2 80.00 usec  
PL2 -1.00 dB  
PL12 14.00 dB  
PL13 14.00 dB  
SFO2 600.1324005 MHz

F2 - Processing parameters  
SI 65536  
SF 150.9028120 MHz  
WDW EM  
SSB 0  
LB 2.00 Hz  
GB 0  
PC 1.40

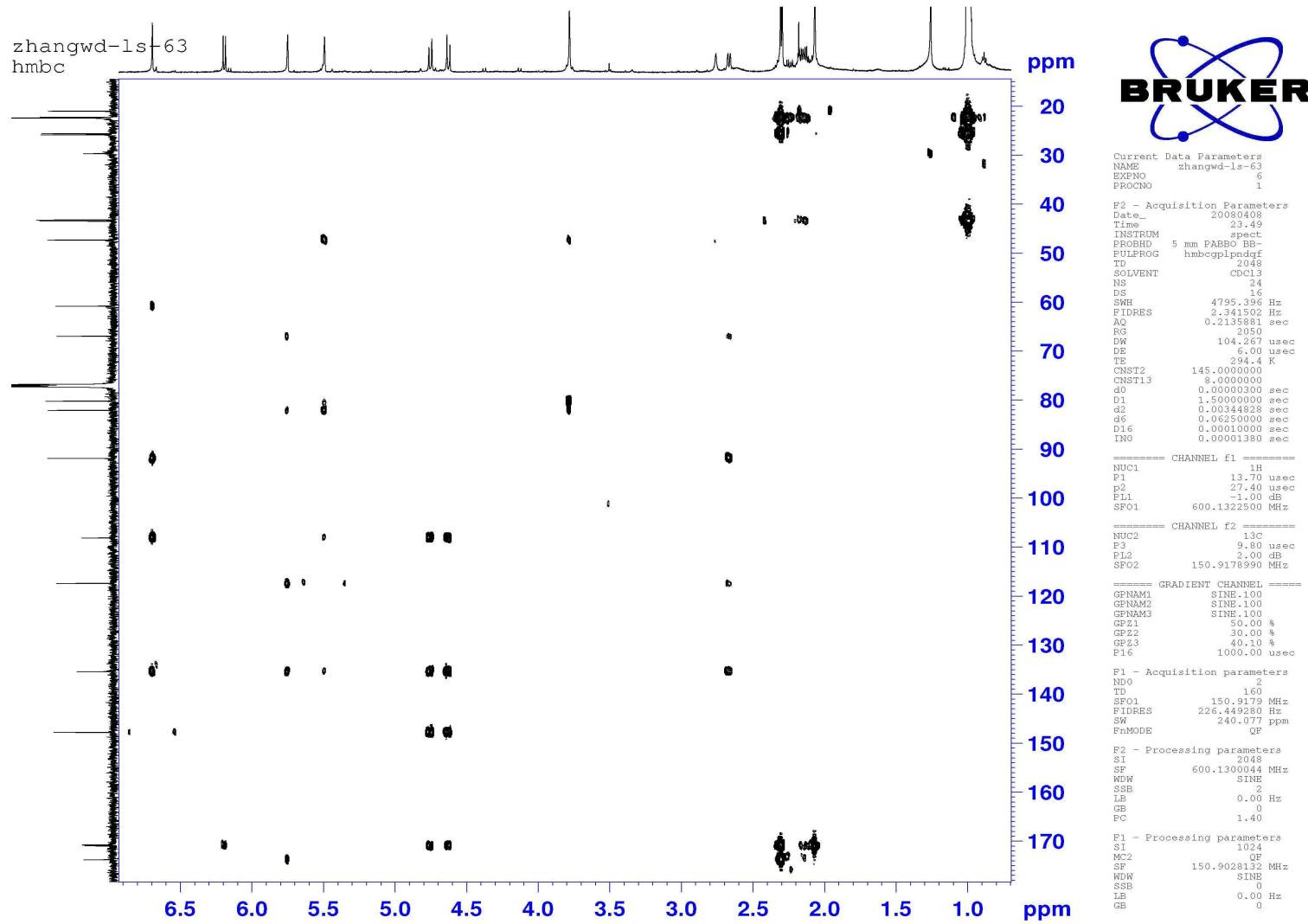
S66. The <sup>13</sup>C NMR and DEPT Spectra (150 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate K (11)



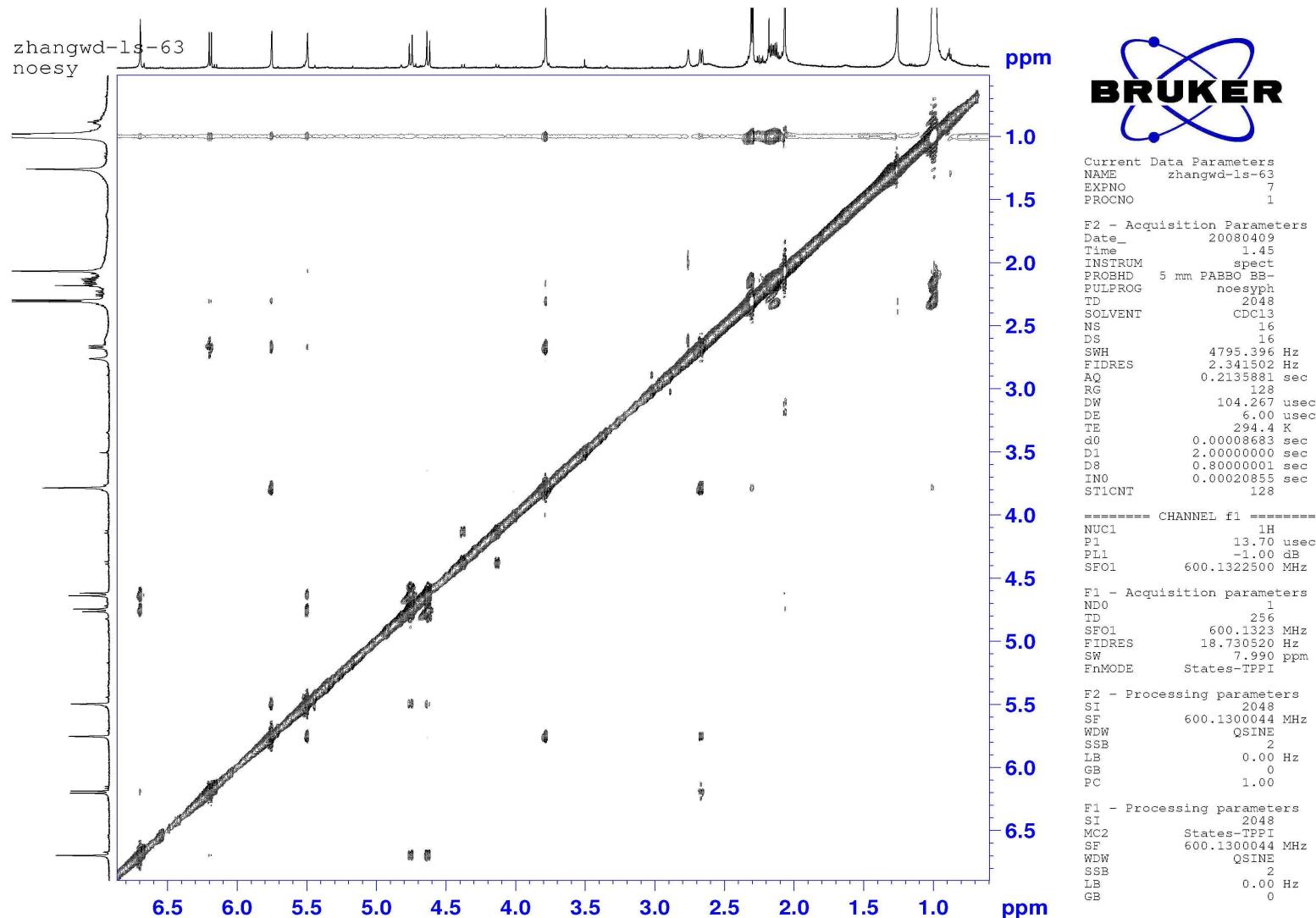
**S67. The  $^1\text{H}$ - $^1\text{H}$ COSY Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate K (11)**



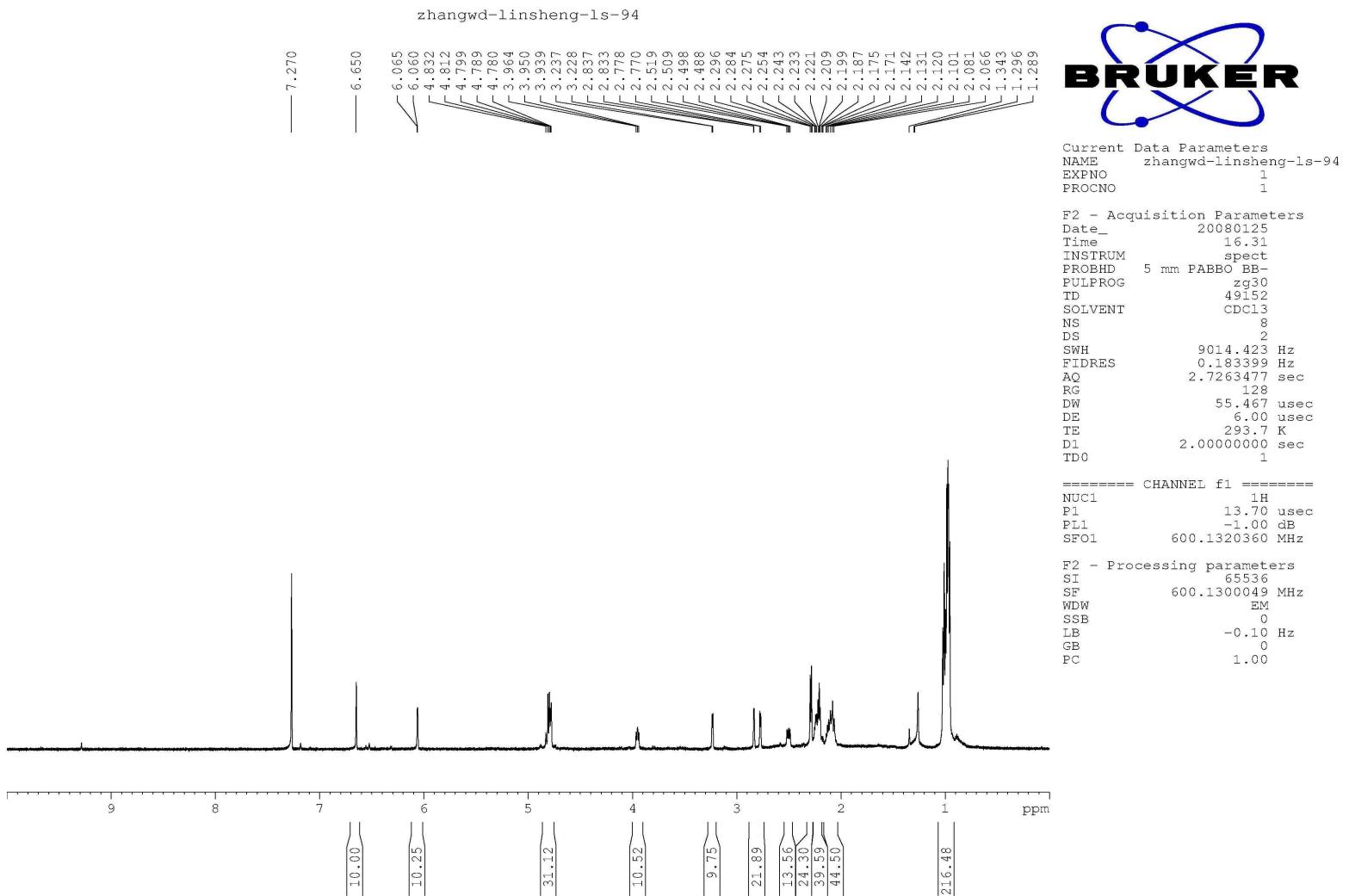
**S68. The HSQC Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate K (11)**



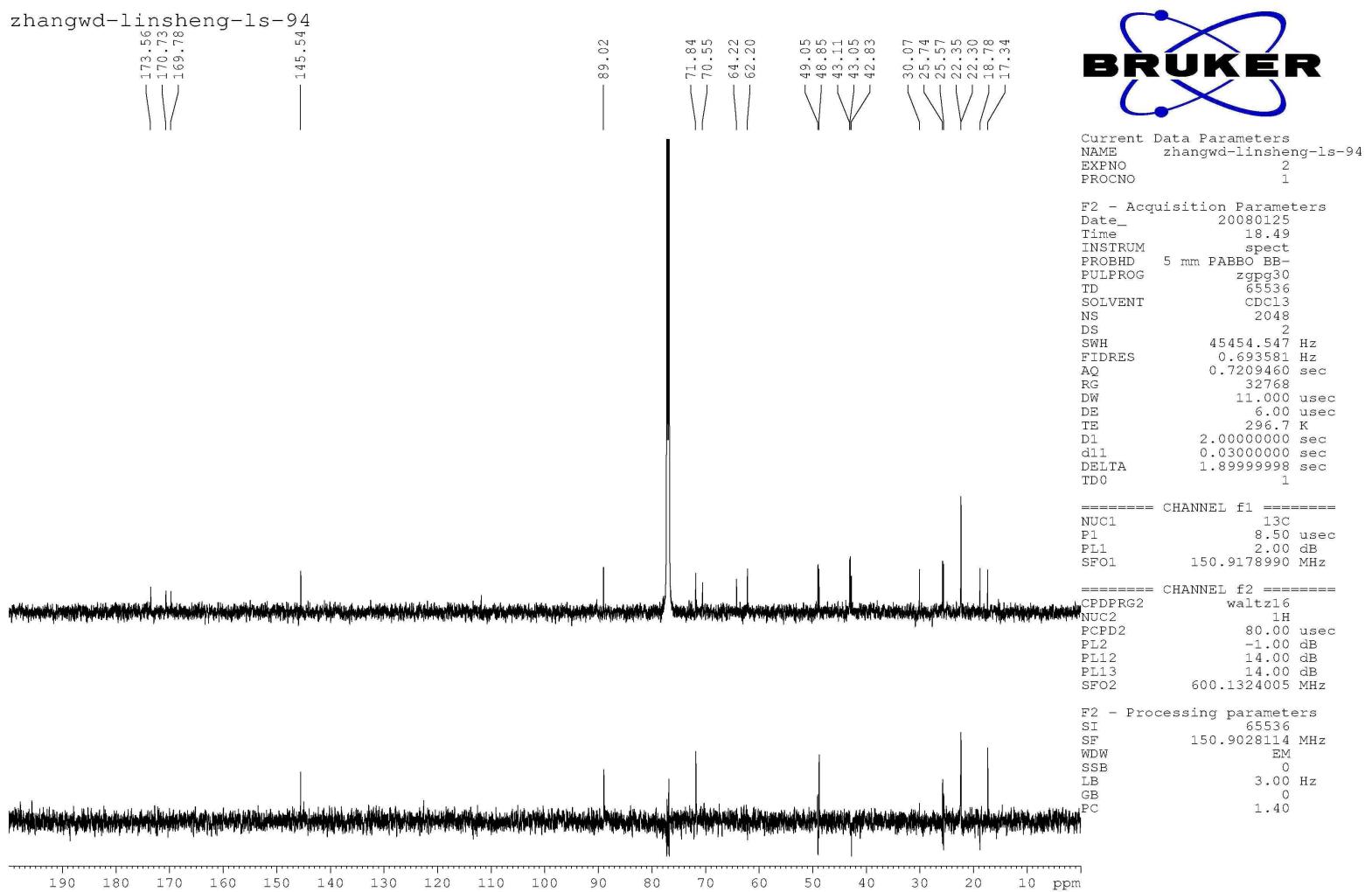
S69. The HMBC Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate K (11)



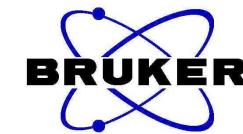
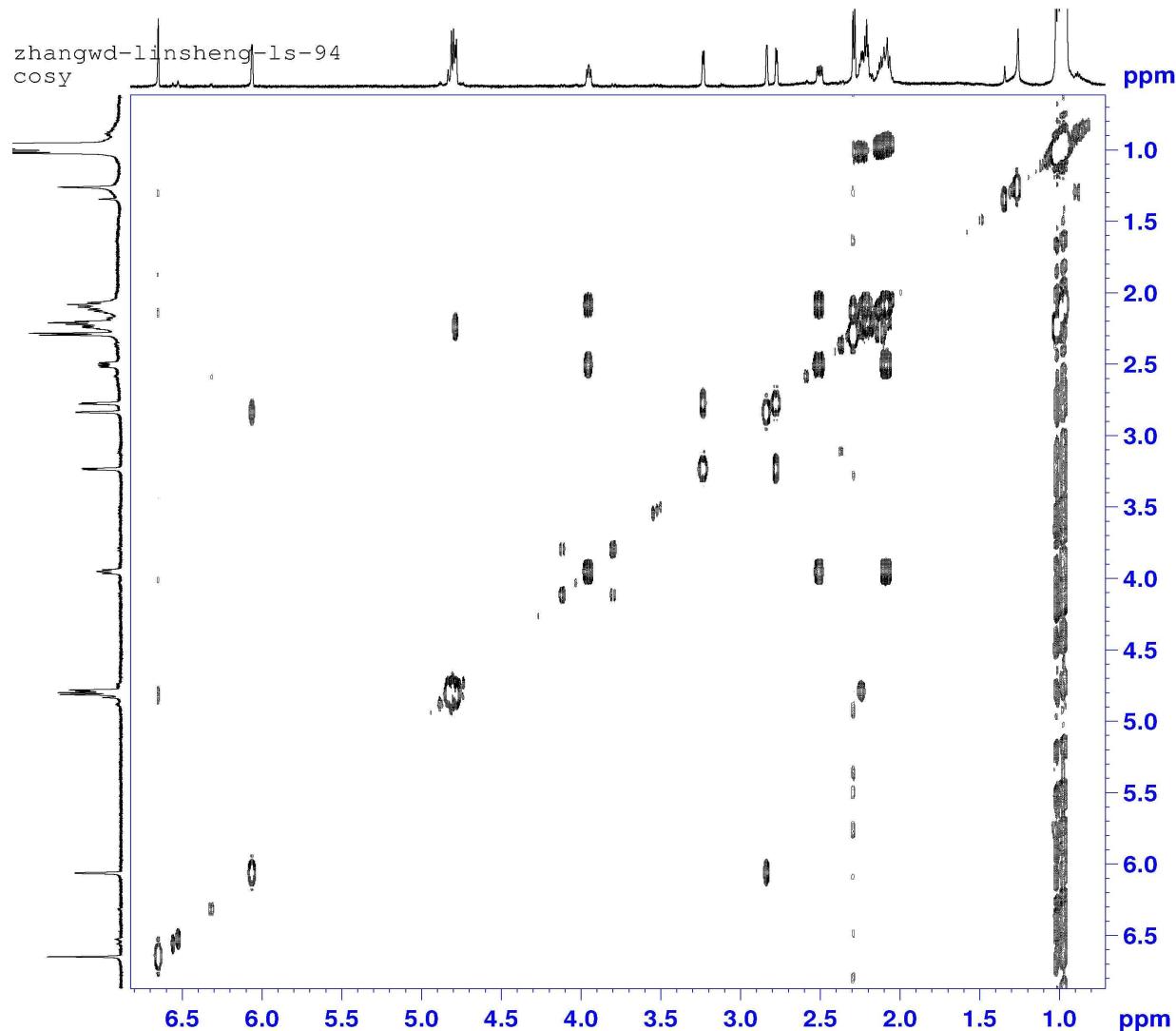
**S70. The NOESY Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate K (11)**



**S71. The <sup>1</sup>H NMR Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate L (12)**



**S72. The  $^{13}\text{C}$  NMR and DEPT Spectra (150 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate L (12)**



Current Data Parameters  
NAME zhangwd-linsheng-ls-94  
EXPNO 4  
PROCNO 1

F2 - Acquisition Parameters  
Date 20080125  
Time 19.14  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG cosyppgf  
TD 2048  
SOLVENT CDCl3  
NS 2  
DS 18  
SWH 4795.38 Hz  
FIDRES 2.341504 Hz  
ACQTIME 0.2135881 sec  
RG 645  
DW 104.867 usec  
DE 6.00 usec  
TE 294.7 K  
d0 0.00000300 sec  
D1 2.0000000 sec  
d13 0.00000400 sec  
D16 0.00010000 sec  
IN0 0.00020855 sec

===== CHANNEL f1 =====  
NUC1 1H  
P0 13.70 usec  
P1 13.70 usec  
PL1 -1.00 dB  
SF01 600.1320360 MHz

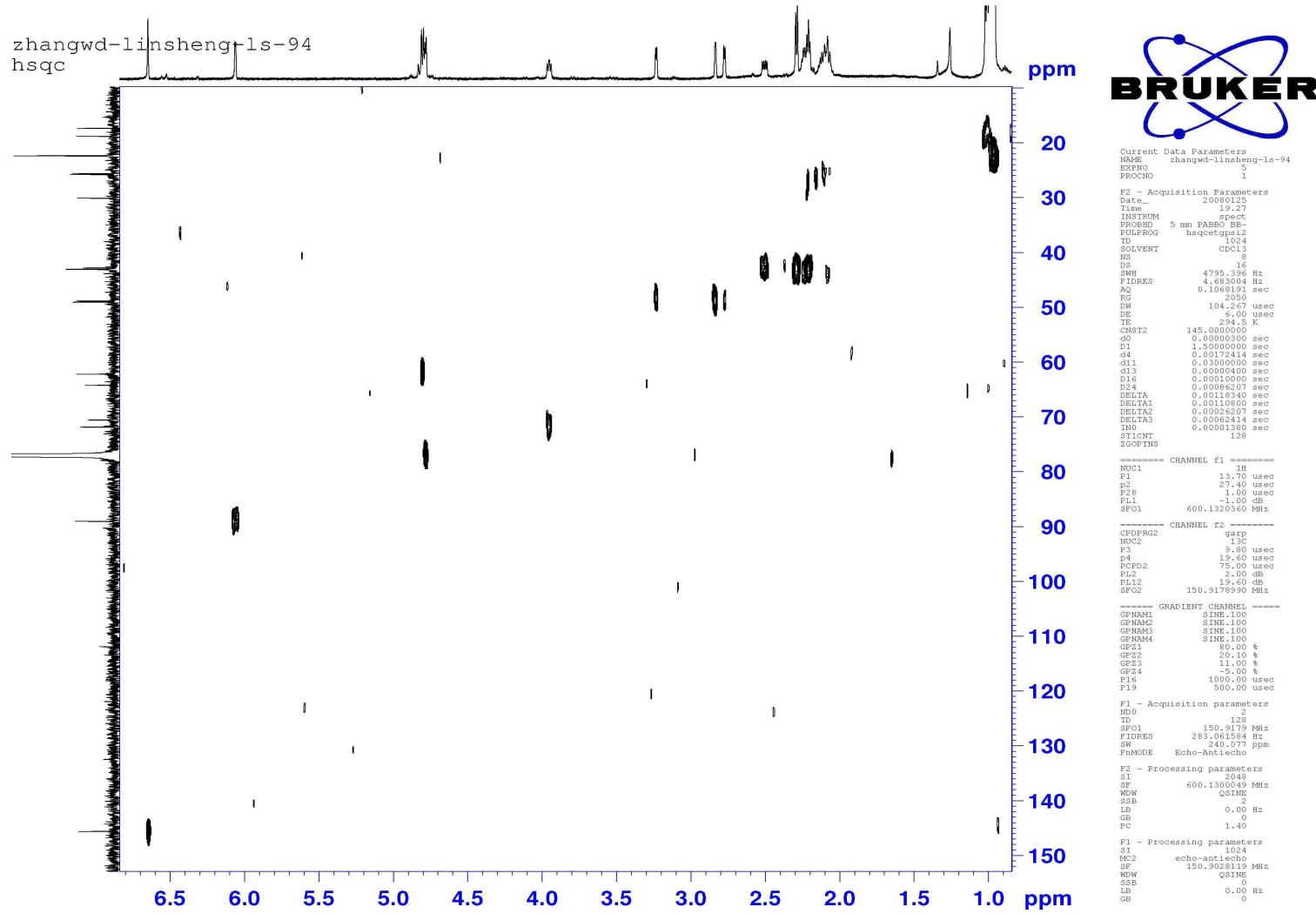
===== GRADIENT CHANNEL =====  
GRNM1 SINE,100  
GRNM2 SINE,100  
GPZ1 10.00 %  
GPZ2 10.00 %  
PL6 1000.00 usec

F1 - Acquisition parameters  
ND0 1  
TD 160  
SF01 600.132 MHz  
FIDRES 29.968832 Hz  
SW 7.990 ppm  
FMODE QF

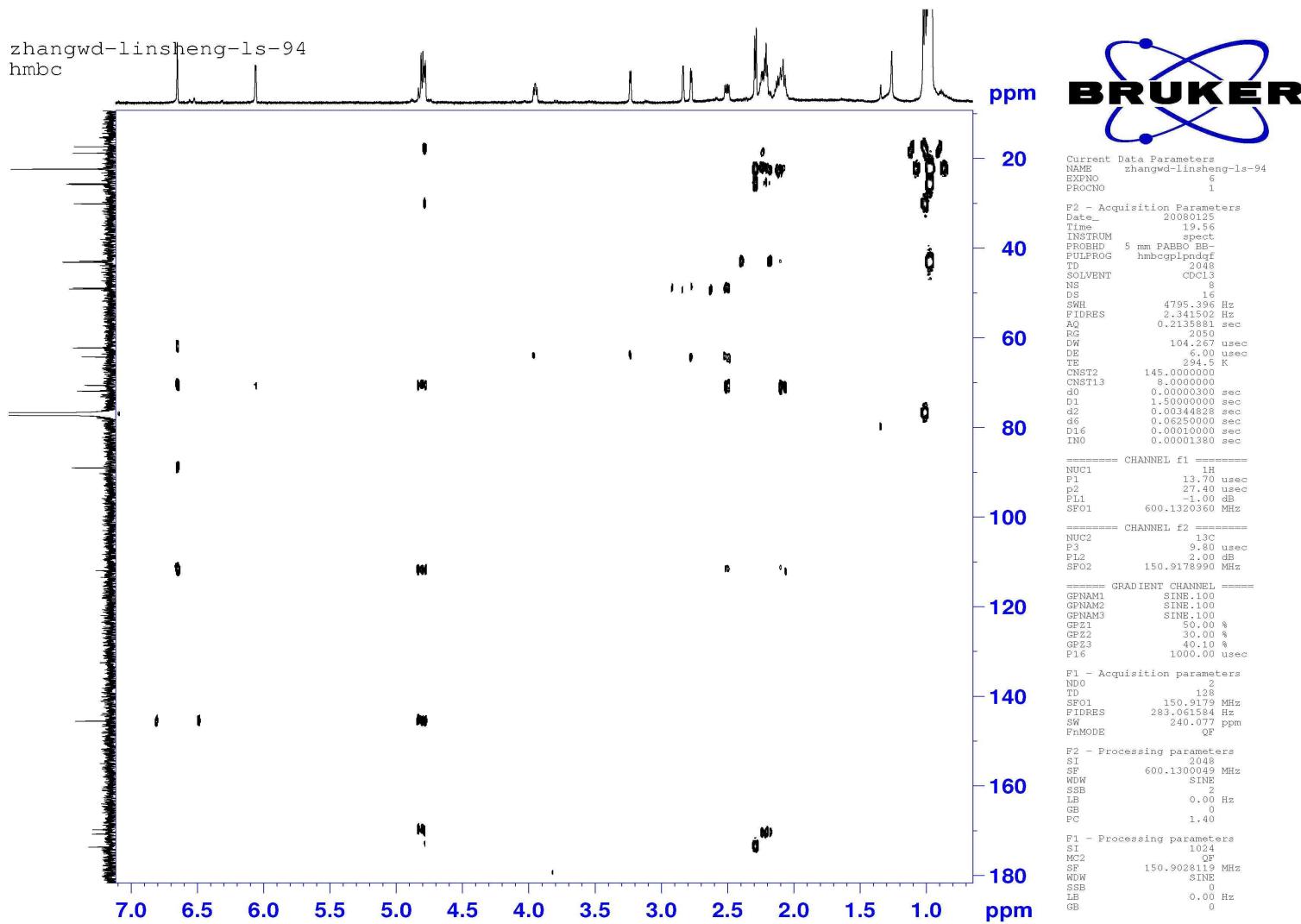
F2 - Processing parameters  
SI 2048  
SF 600.1300049 MHz  
WDW QSIMD  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 2048  
MC2 QF  
SF 600.1300049 MHz  
WDW QSINE  
SSB 0  
LB 0.00 Hz  
GB 0

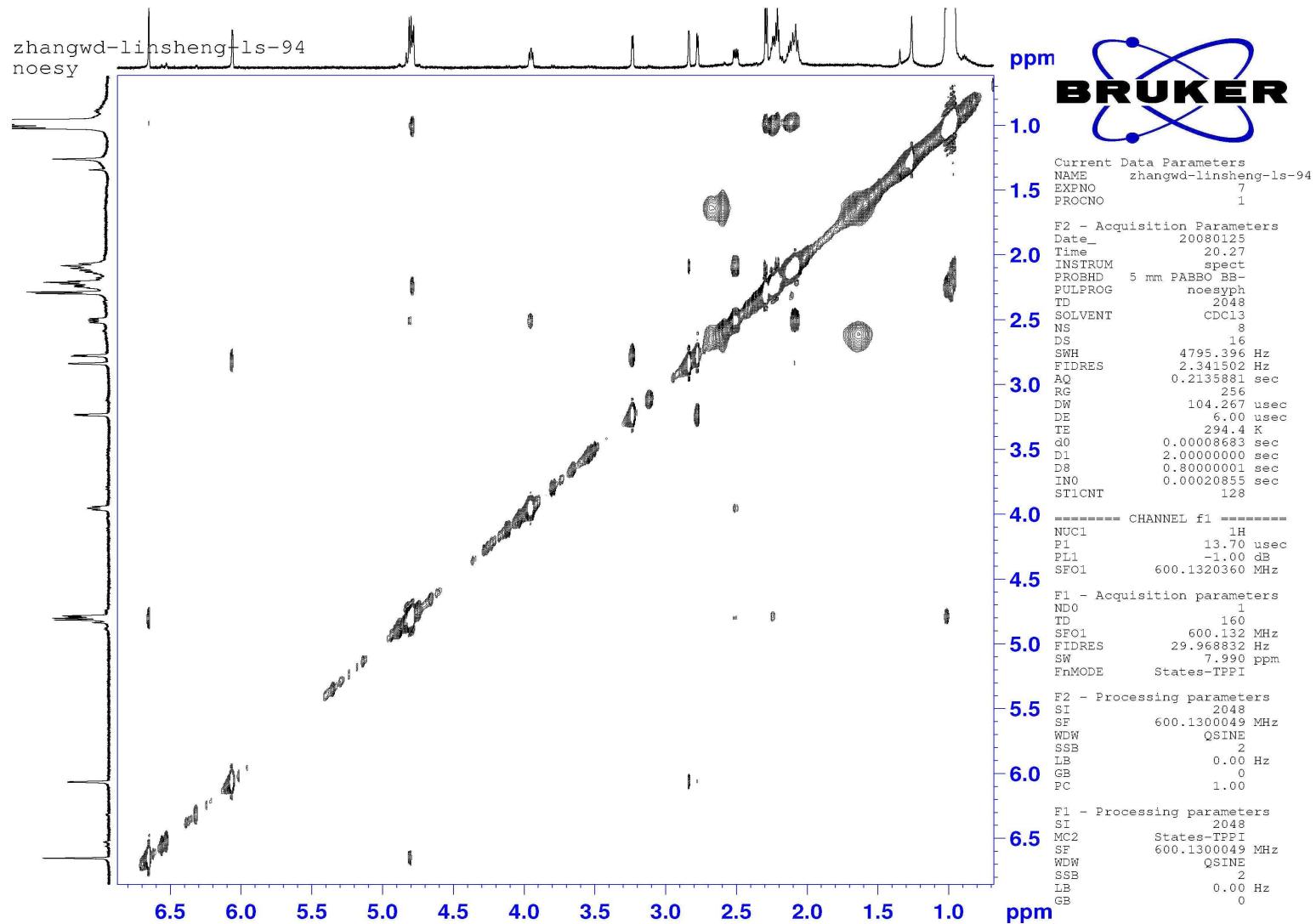
S73. The  $^1\text{H}$ - $^1\text{H}$ COSY Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate L (12)



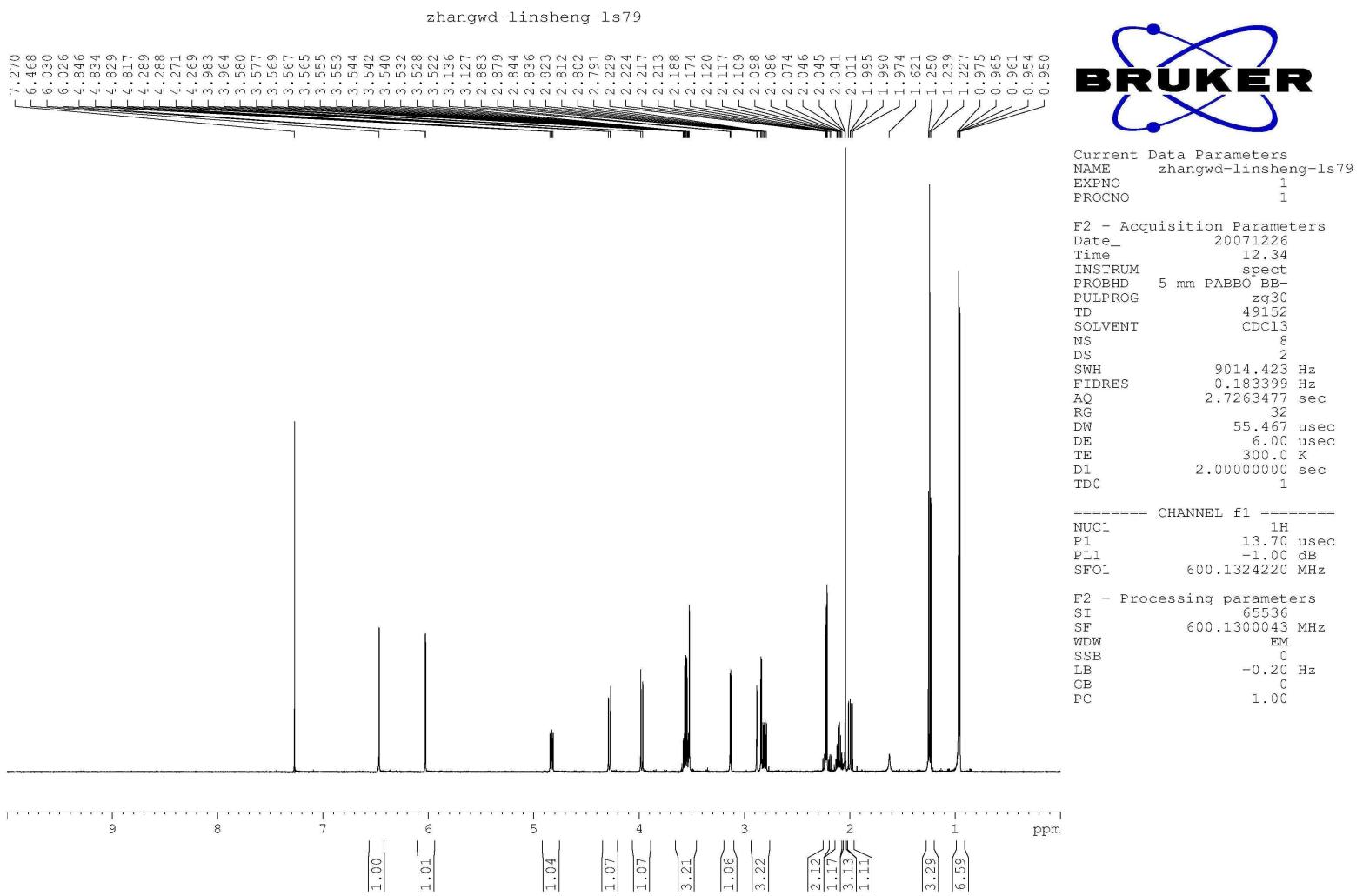
S74. The HSQC Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate L (12)



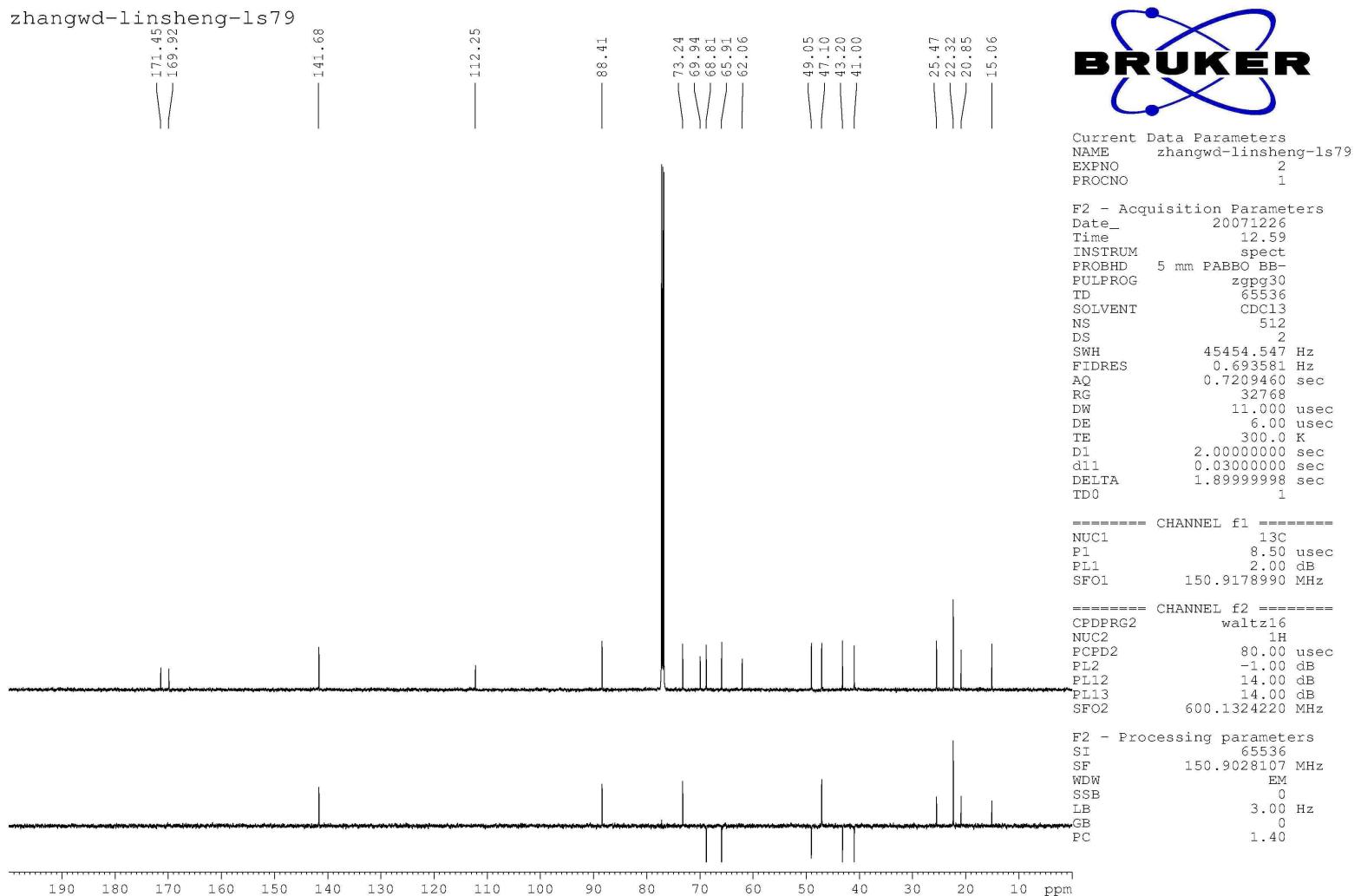
**S75. The HMBC Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate L (12)**



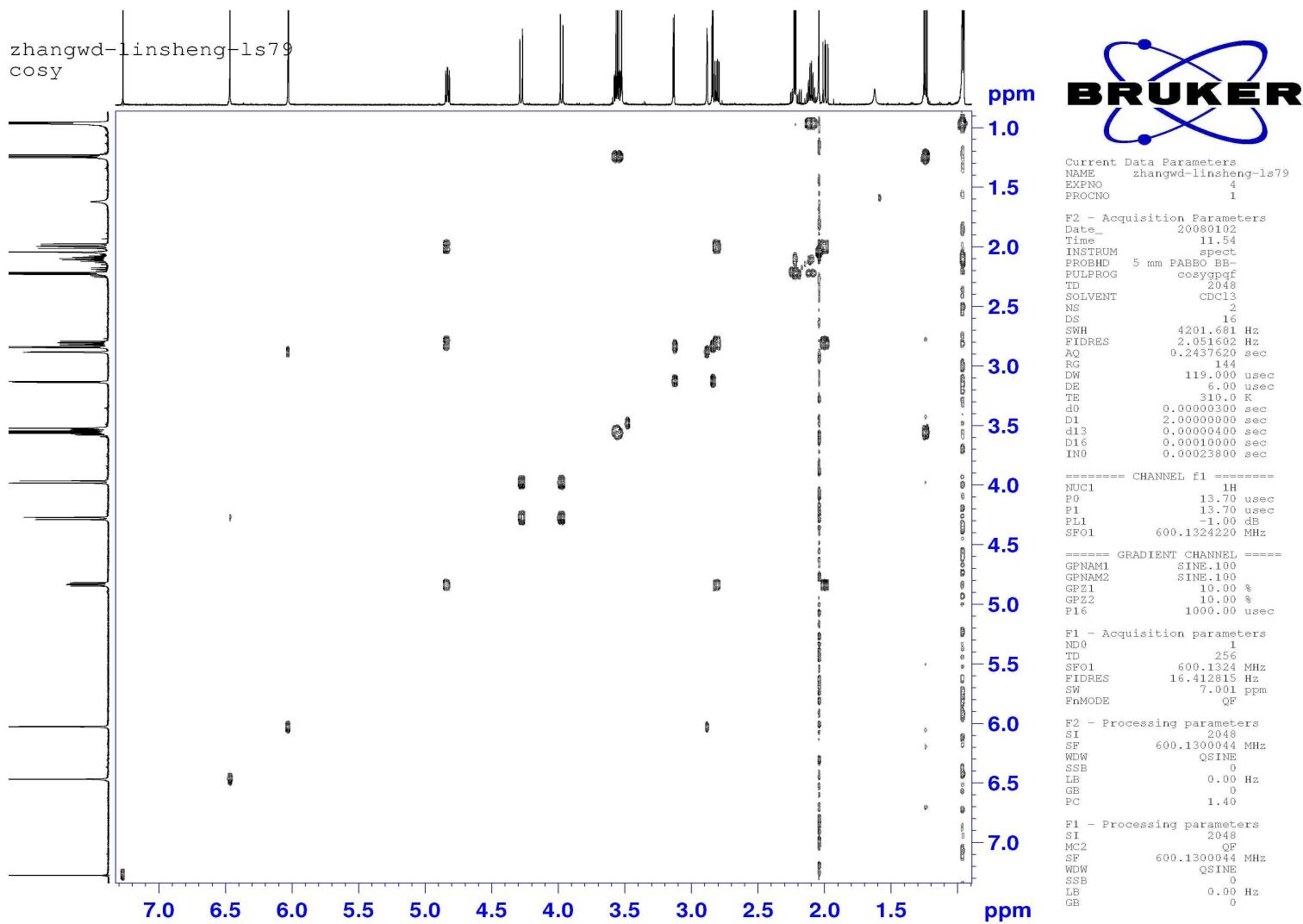
S76. The NOESY Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate L (12)



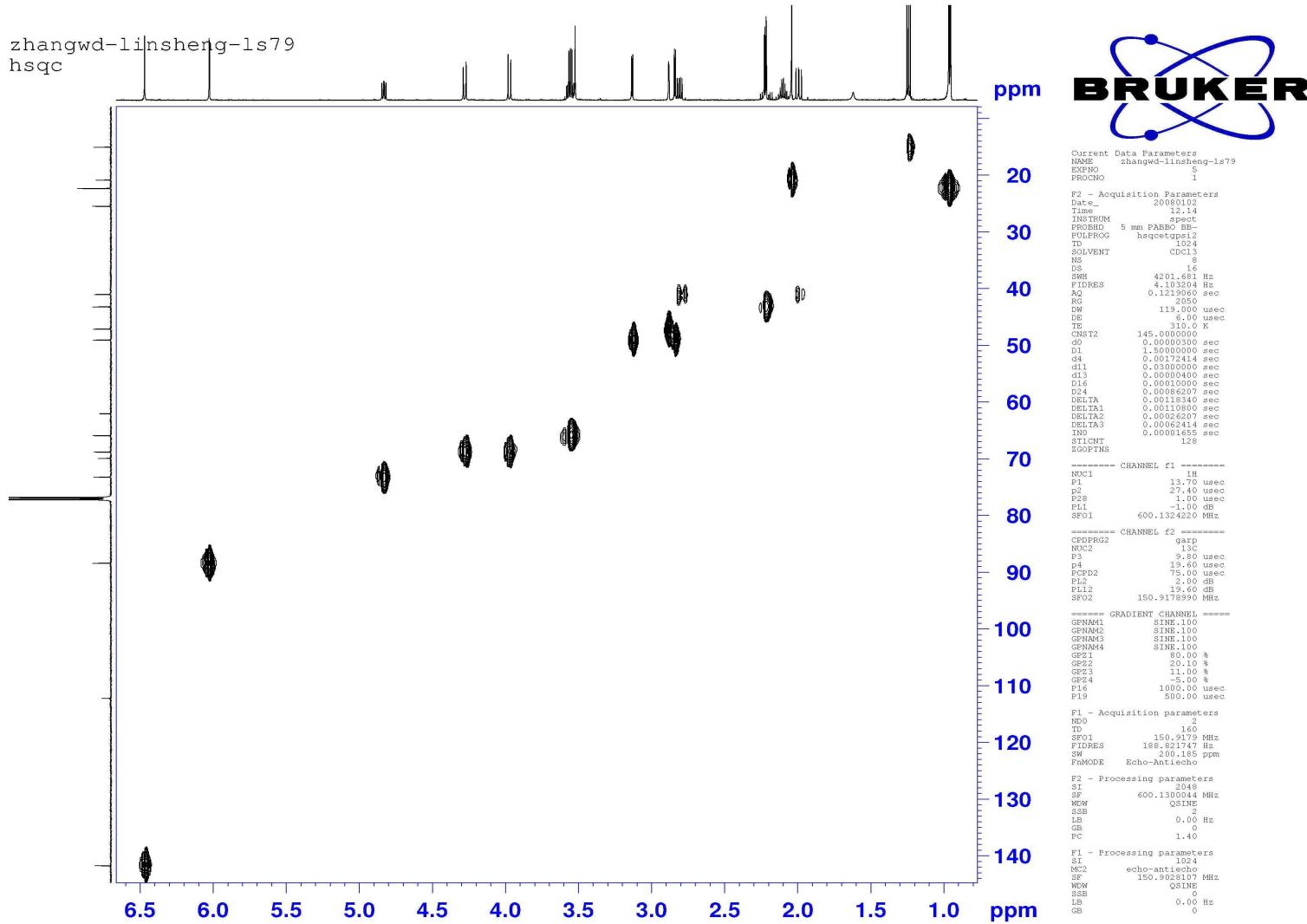
**S77. The  $^1\text{H}$  NMR Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate M (13)**



**S78.** The  $^{13}\text{C}$  NMR and DEPT Spectra (150 MHz,  $\text{CDCl}_3$ ) of jatamanvaltrate M (13)

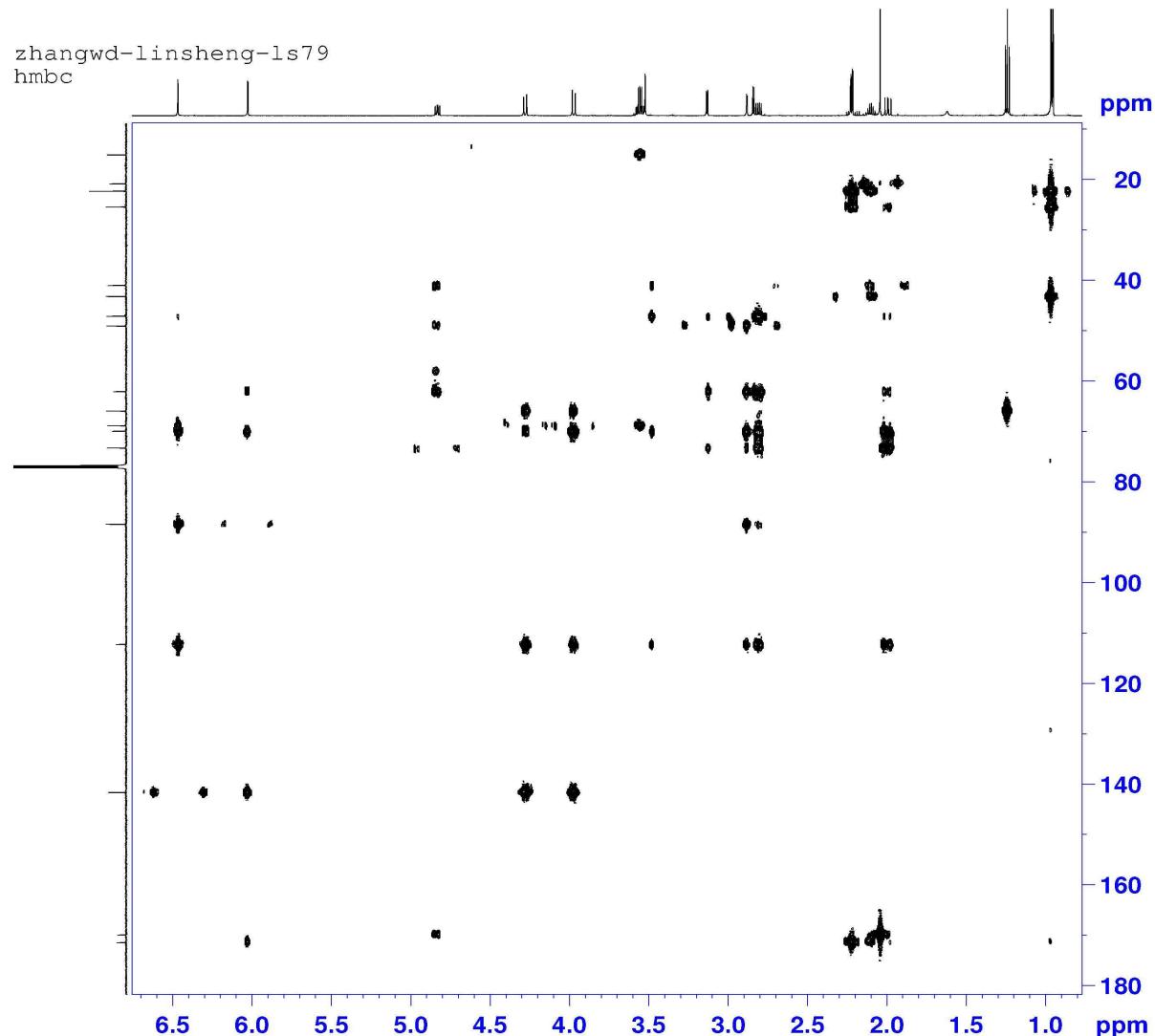


**S79. The  $^1\text{H}$ - $^1\text{H}$ COSY Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Jatamanvaltrate M (13)**



**S80. The HSQC Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate M (13)**

zhangwd-linsheng-ls79  
hmhc



Current Data Parameters  
NAME zhangwd-linsheng-ls79  
EXPNO 6  
PROCNO 1

P2 - Acquisition Parameters  
Date 20080102  
Time 12.51  
INSTRUM spect  
PROBHD 5 mm PABBO BB-  
PULPROG hmbcgraplpr1f  
TD 2048  
SOLVENT CDCl3  
NS 16  
DS 16  
SWH 4201.40 Hz  
FIDRES 2.051602 Hz  
AQ 0.2437620 sec  
RG 2050  
DW 119.000 usec  
DE 6.00 usec  
TE 310.0 K  
CNST2 145.000000  
CNST13 8.000000  
d0 0.00000300 sec  
D1 1.5000000 sec  
d2 0.0344820 sec  
d6 0.0625000 sec  
D16 0.0001000 sec  
INO 0.00001655 sec

===== CHANNEL f1 =====  
NUC1 1H  
P1 13.70 usec  
p2 27.40 usec  
PL1 -1.00 dB  
SFO1 600.1324220 MHz

===== CHANNEL f2 =====  
NUC2 13C  
P3 9.80 usec  
PL2 2.00 dB  
SFO2 150.9178990 MHz

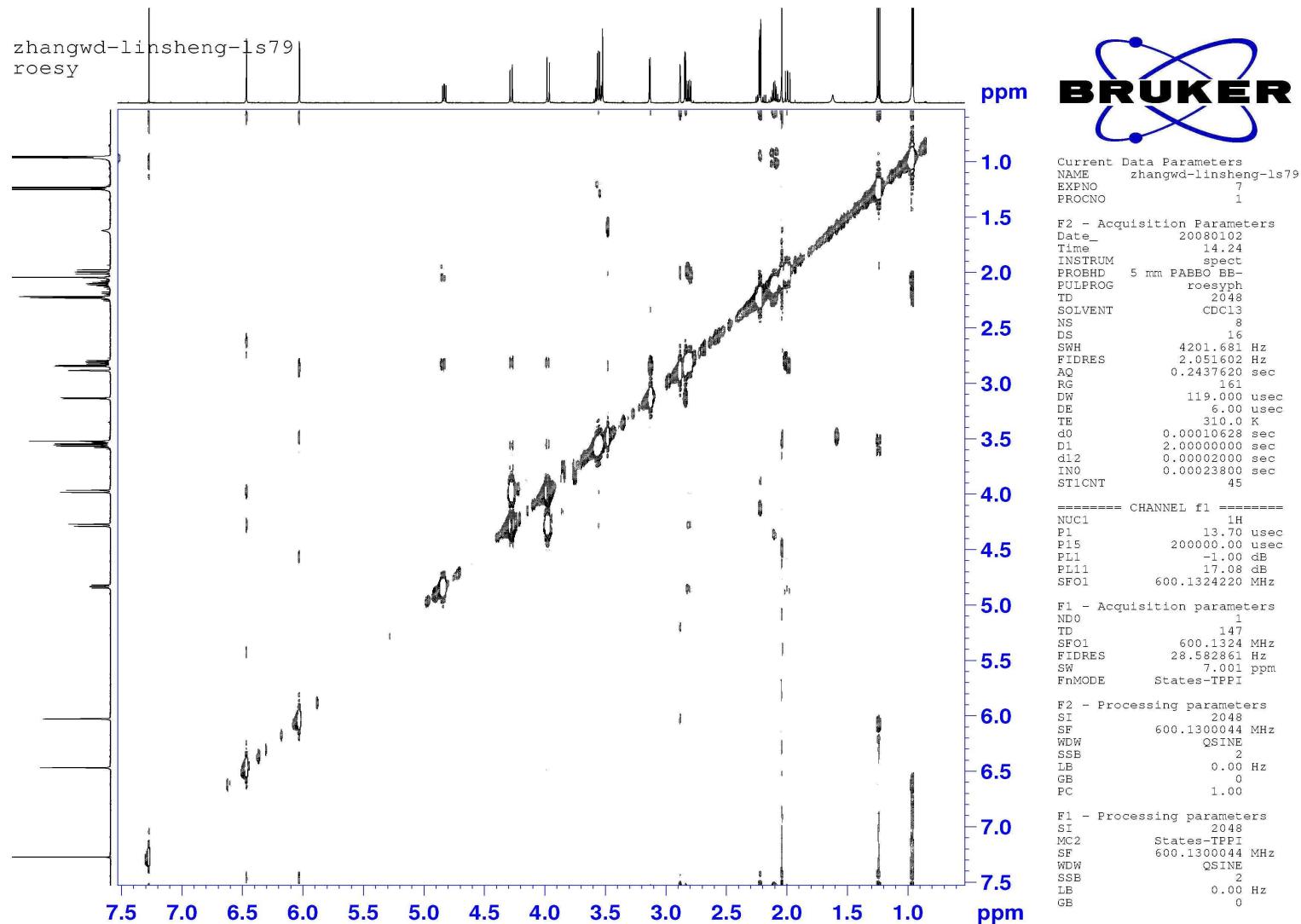
===== GRADIENT CHANNEL =====  
GPNAME1 SINE.100  
GPNAME2 SINE.100  
GPNAME3 SINE.100  
GPZ1 50.00 %  
GPZ2 30.00 %  
GPZ3 40.10 %  
P16 1000.00 usec

P1 - Acquisition parameters  
ND0 2  
TD 192  
SFO1 150.9179 MHz  
FIDRES 157.351456 Hz  
SW 200.185 ppm  
FnMode QF

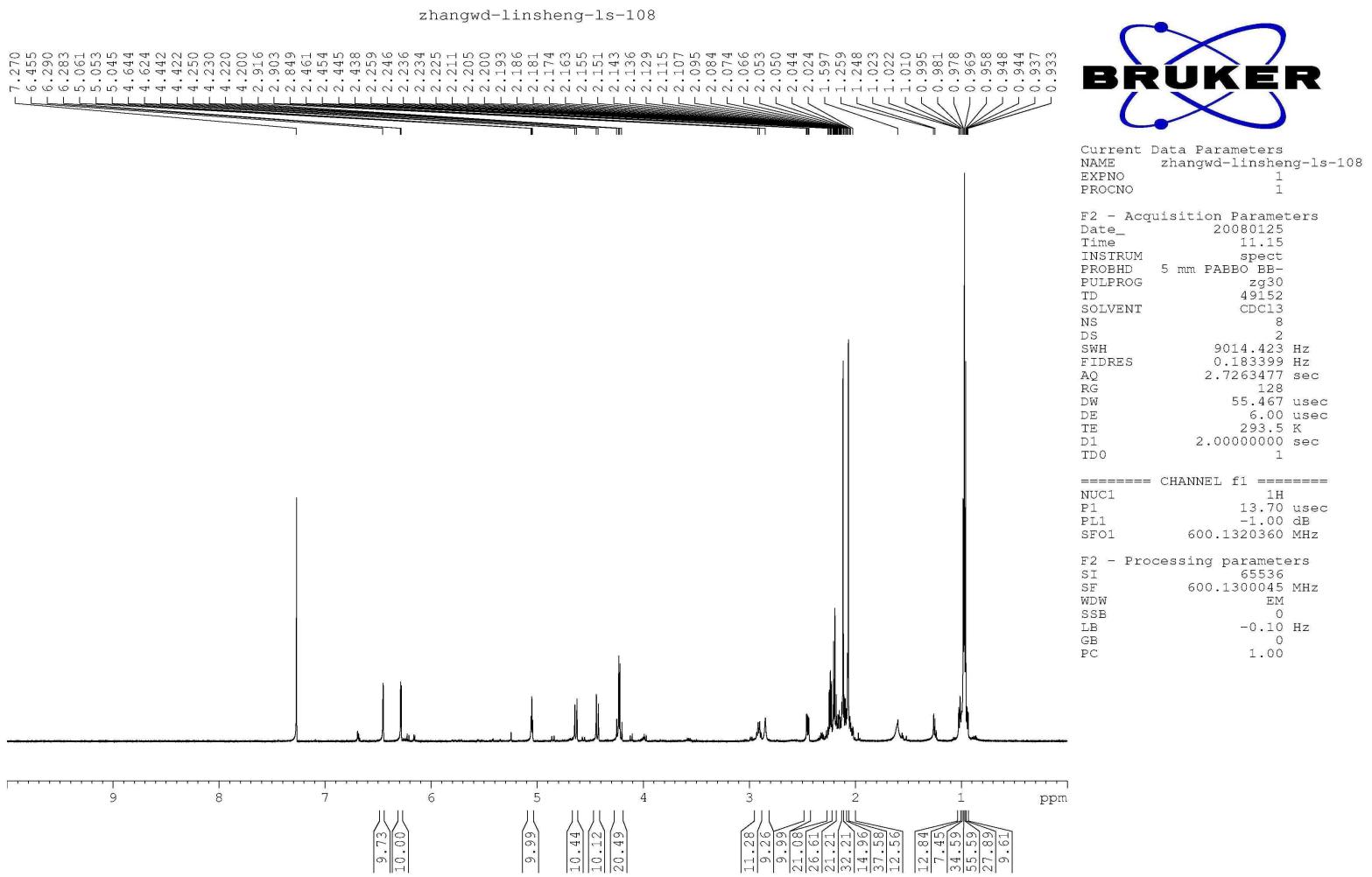
F2 - Processing parameters  
SI 2048  
SF 600.130004 MHz  
SS 1  
SSB 0  
LB 0.00 Hz  
GB 0  
PC 1.40

F1 - Processing parameters  
SI 1024  
MC2 QF  
SF 150.9028107 MHz  
WDW SINE  
SSB 0  
LB 0.00 Hz  
GB 0

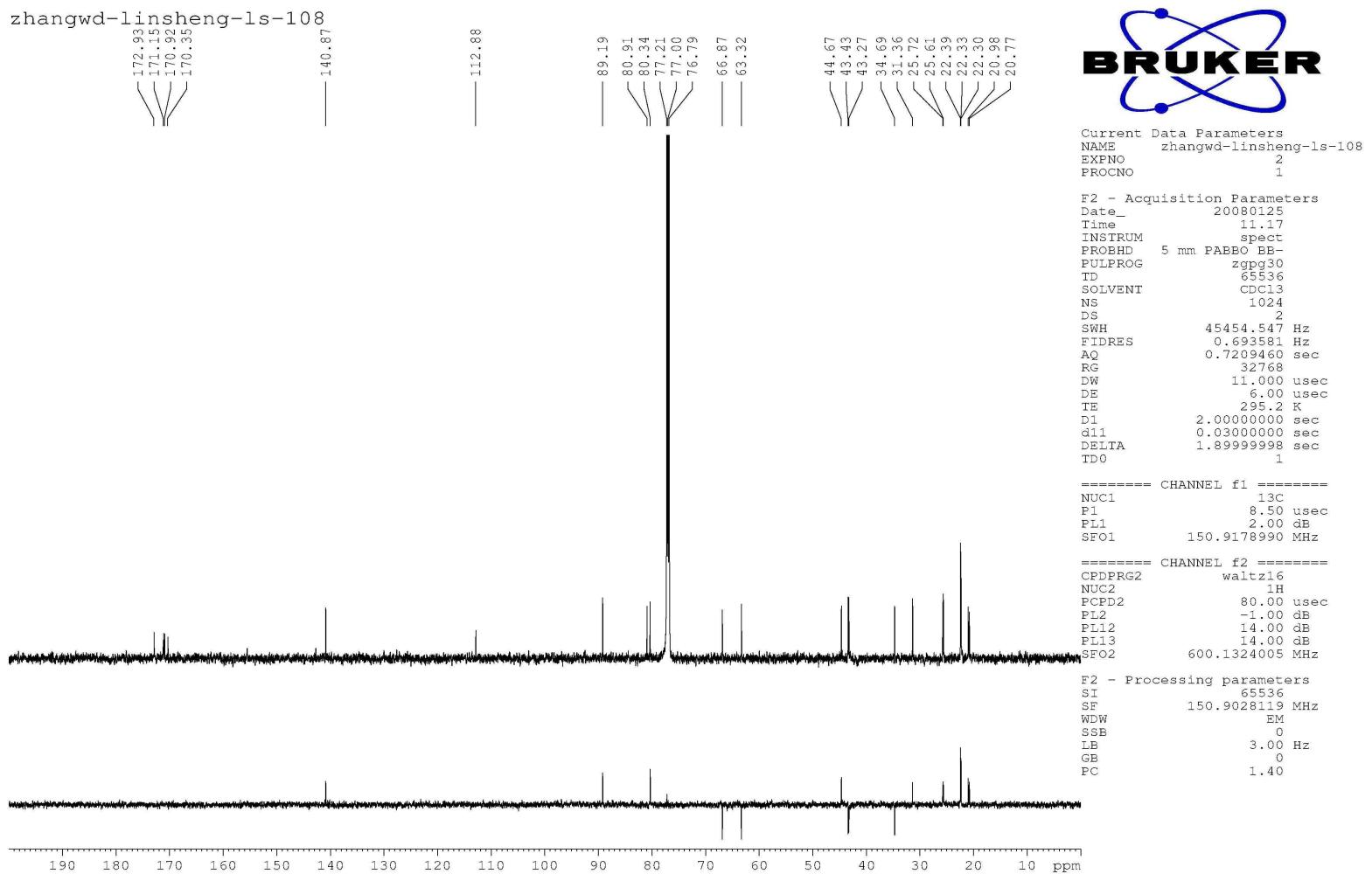
S81. The HMBC Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate M (13)



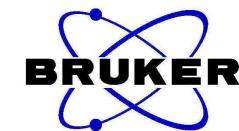
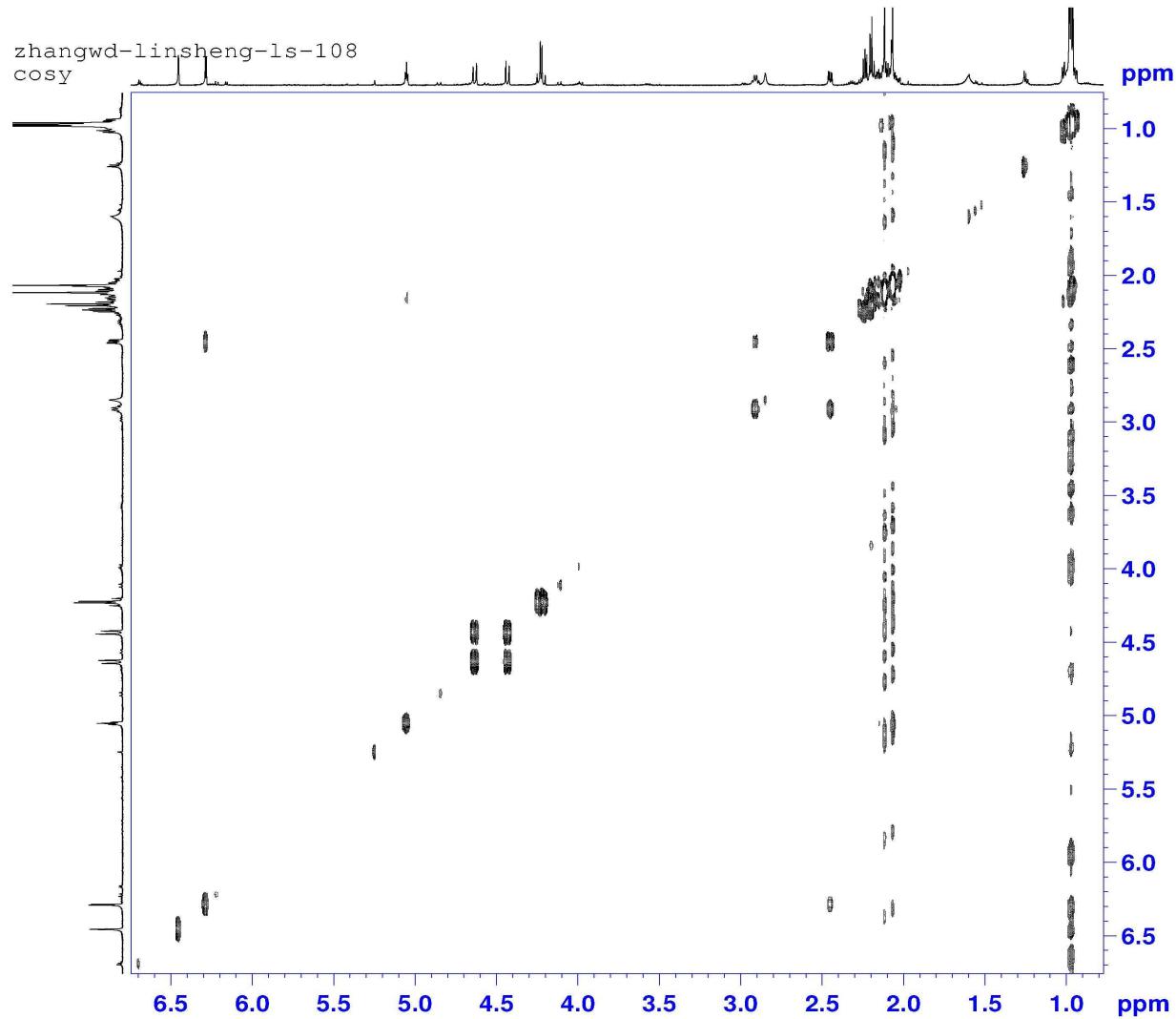
S82. The ROESY Spectrum (600 MHz, CDCl<sub>3</sub>) of Jatamanvaltrate M (13)



**S83. The <sup>1</sup>H NMR Spectrum (600 MHz, CDCl<sub>3</sub>) of Compound (16)**



**S84. The  $^{13}\text{C}$  NMR and DEPT Spectra (150 MHz,  $\text{CDCl}_3$ ) of Compound (16)**



Current Data Parameters  
 NAME zhangwd-linsheng-ls-108  
 EXPNO 4  
 PROCNO 1

F2 - Acquisition Parameters  
 Date\_ 20080125  
 Time 12.21  
 INSTRUM spect  
 PROBHD 5 mm PABBO BB-  
 PULPROG cosyppqf  
 TD 2048  
 SOLVENT CDCl3  
 NS 2  
 DS 16  
 SWH 4795.396 Hz  
 FIDRES 2.341502 Hz  
 AQ 0.2135881 sec  
 RG 322  
 DW 104.267 usec  
 DE 6.00 usec  
 TE 293.9 K  
 CP 0.00000300 sec  
 D1 2.0000000 sec  
 D13 0.00000400 sec  
 D16 0.0001000 sec  
 IN0 0.00020855 sec

===== CHANNEL f1 ======  
 NUC1 1H  
 P0 13.70 usec  
 P1 13.70 usec  
 PL1 -1.00 deg  
 SFO1 600.1320360 MHz

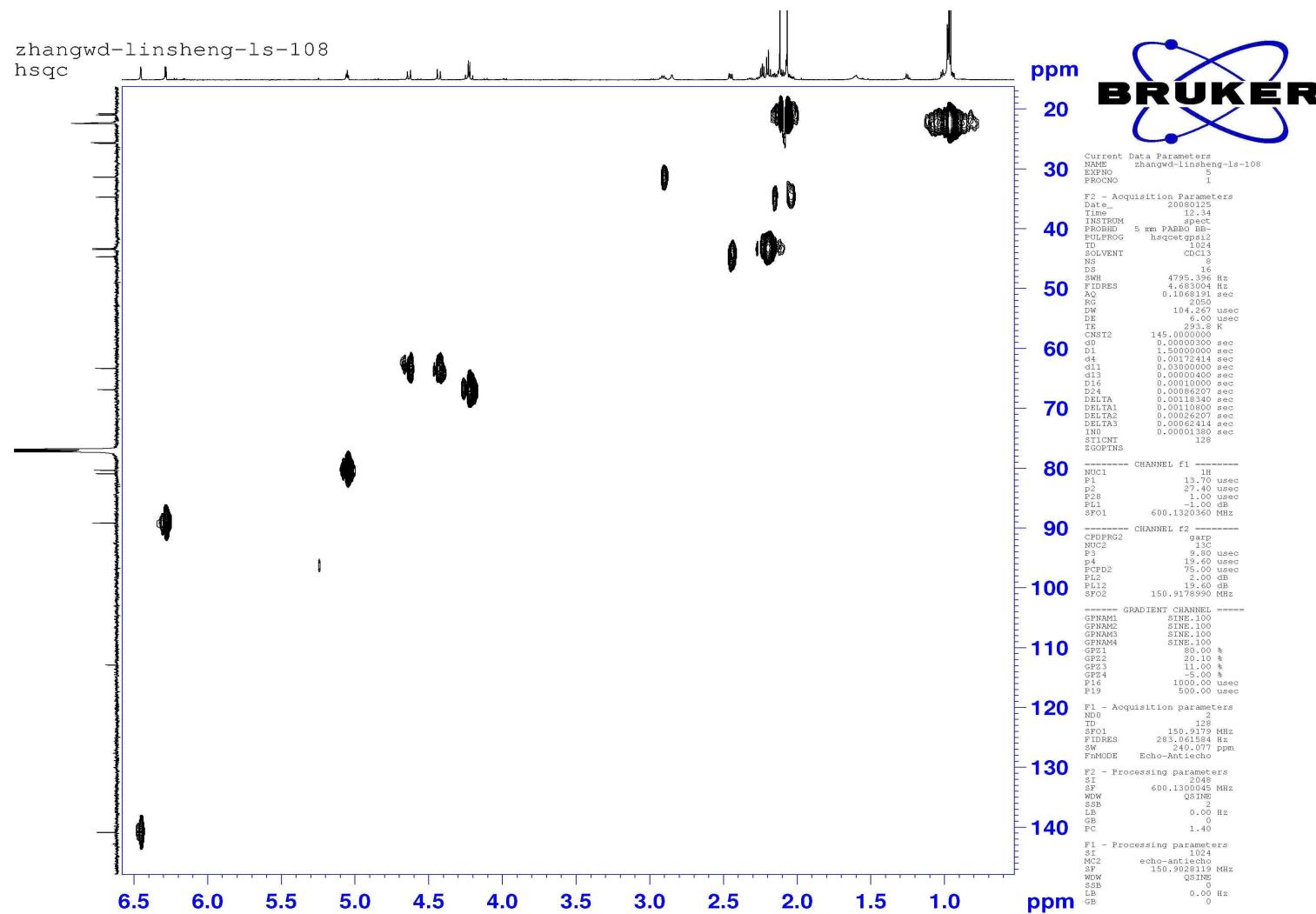
===== GRADIENT CHANNEL =====  
 GPNAME1 SINE.100  
 GPNAME2 SINE.100  
 GPZ1 10.00 %  
 GPZ2 10.00 %  
 P16 1000.00 usec

F1 - Acquisition parameters  
 ND0 1  
 T0 160  
 SFO1 600.132 MHz  
 FIDRES 29.968932 Hz  
 SW 7.990 ppm  
 PRMODE QF

F2 - Processing parameters  
 SI 2048  
 SF 600.1300045 MHz  
 WDW QSINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0  
 PC 1.40

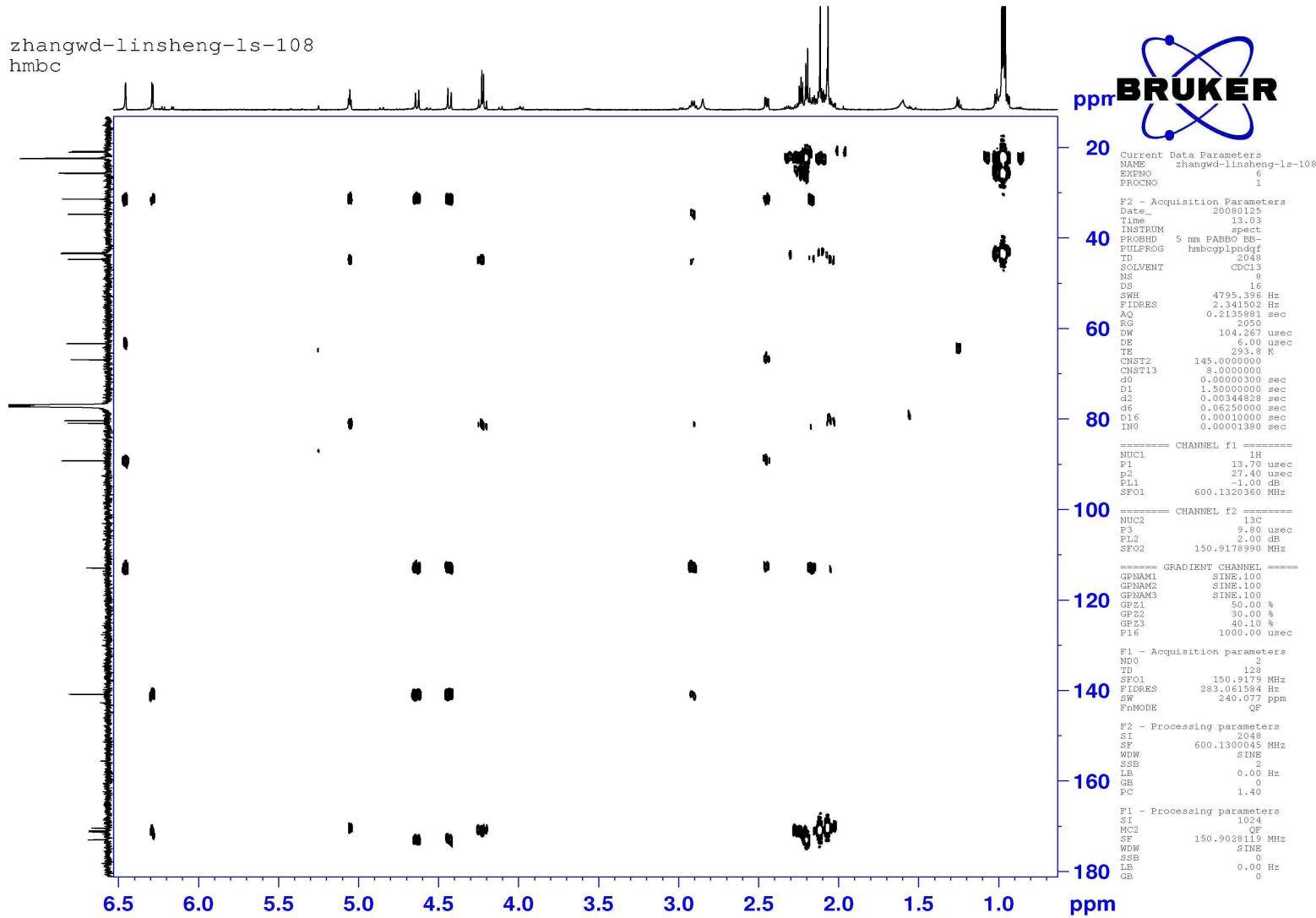
P1 - Processing parameters  
 SI 2048  
 MC2 QF  
 SF 600.1300045 MHz  
 WDW QSINE  
 SSB 0  
 LB 0.00 Hz  
 GB 0

**S85. The  $^1\text{H}$ - $^1\text{H}$ COSY Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Compound (16)**

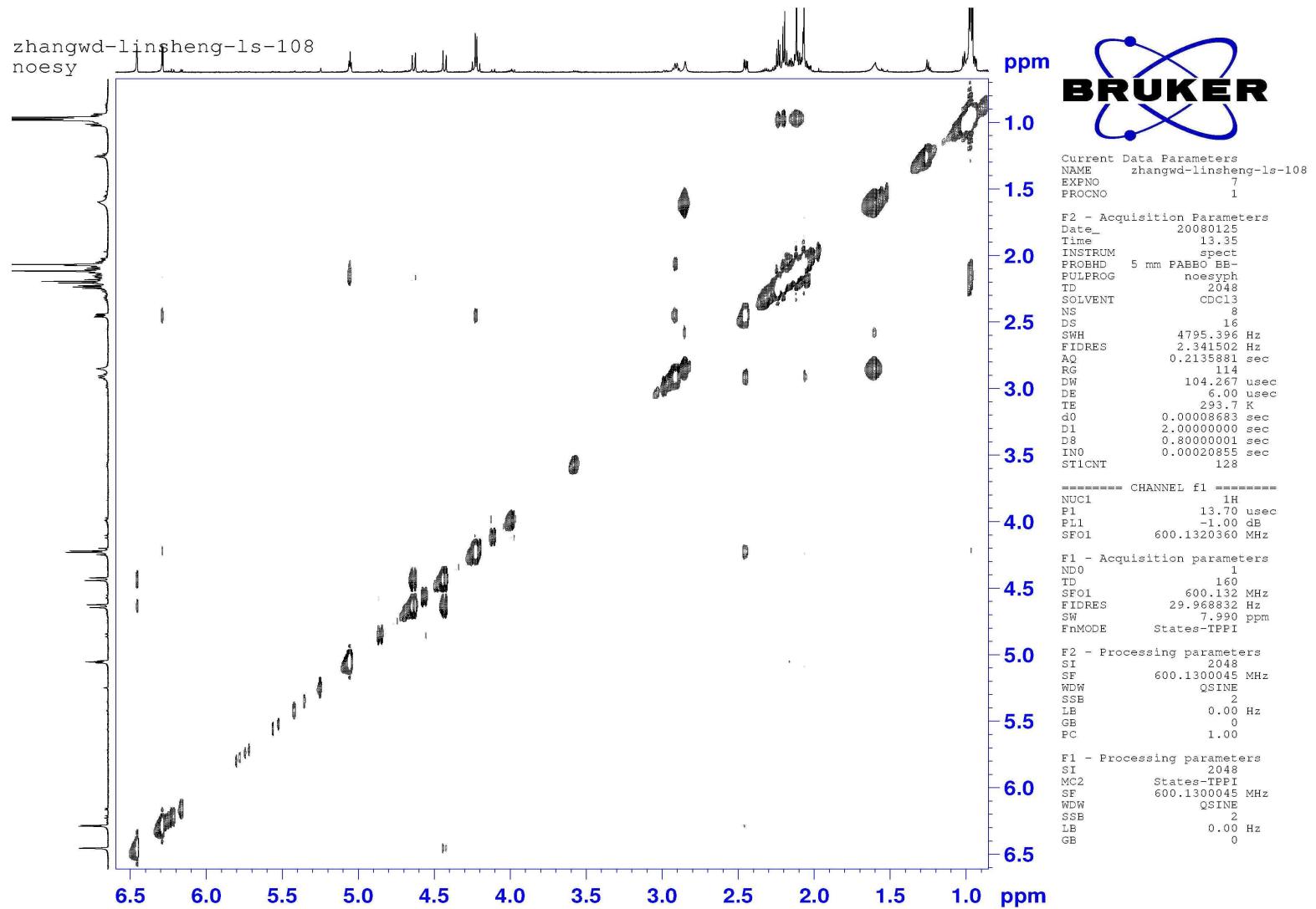


S86. The HSQC Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Compound (16)

zhangwd-linsheng-ls-108  
hmhc



S87. The HMBC Spectrum of Compound (16)



S88. The NOESY Spectrum (600 MHz,  $\text{CDCl}_3$ ) of Compound (16)

**Table S1.** Cytotoxicity of Compounds **1-22** to A549, PC-3M, HCT-8, and Bel7402 Cell Lines

compound	IC <sub>50</sub> ( $\mu$ M)			
	A 549	PC-3M	HCT-8	Bel 7402
<b>1</b>	>10	5.3	>10	>10
<b>2</b>	>10	3.9	6.2	>10
<b>3</b>	>10	>10	>10	>10
<b>4</b>	>10	3.8	4.5	9.7
<b>5</b>	>10	>10	9.7	8.5
<b>6</b>	>10	4.3	>10	8.8
<b>7</b>	>10	5.6	>10	5.9
<b>8</b>	>10	5.2	>10	>10
<b>9</b>	>10	3.9	9.7	>10
<b>10</b>	>10	5.8	>10	>10
<b>11</b>	>10	5.0	>10	7.1
<b>12</b>	>10	3.4	>10	7.6
<b>13</b>	>10	6.3	>10	>10
<b>14</b>	>10	3.1	8.2	9.9
<b>15</b>	>10	3.9	>10	>10
<b>16</b>	3.0	1.6	2.6	4.4
<b>17</b>	8.6	>10	>10	>10
<b>18</b>	7.4	1.9	2.5	4.0
<b>19</b>	7.0	2.2	1.5	2.3
<b>20</b>	>10	3.8	6.6	7.5
<b>21</b>	3.7	1.6	1.8	6.1
<b>22</b>	2.9	1.4	1.0	1.7
paclitaxel <sup>a</sup>	0.0052	0.027	0.037	0.095

<sup>a</sup> paclitaxel was used as a positive control