

**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

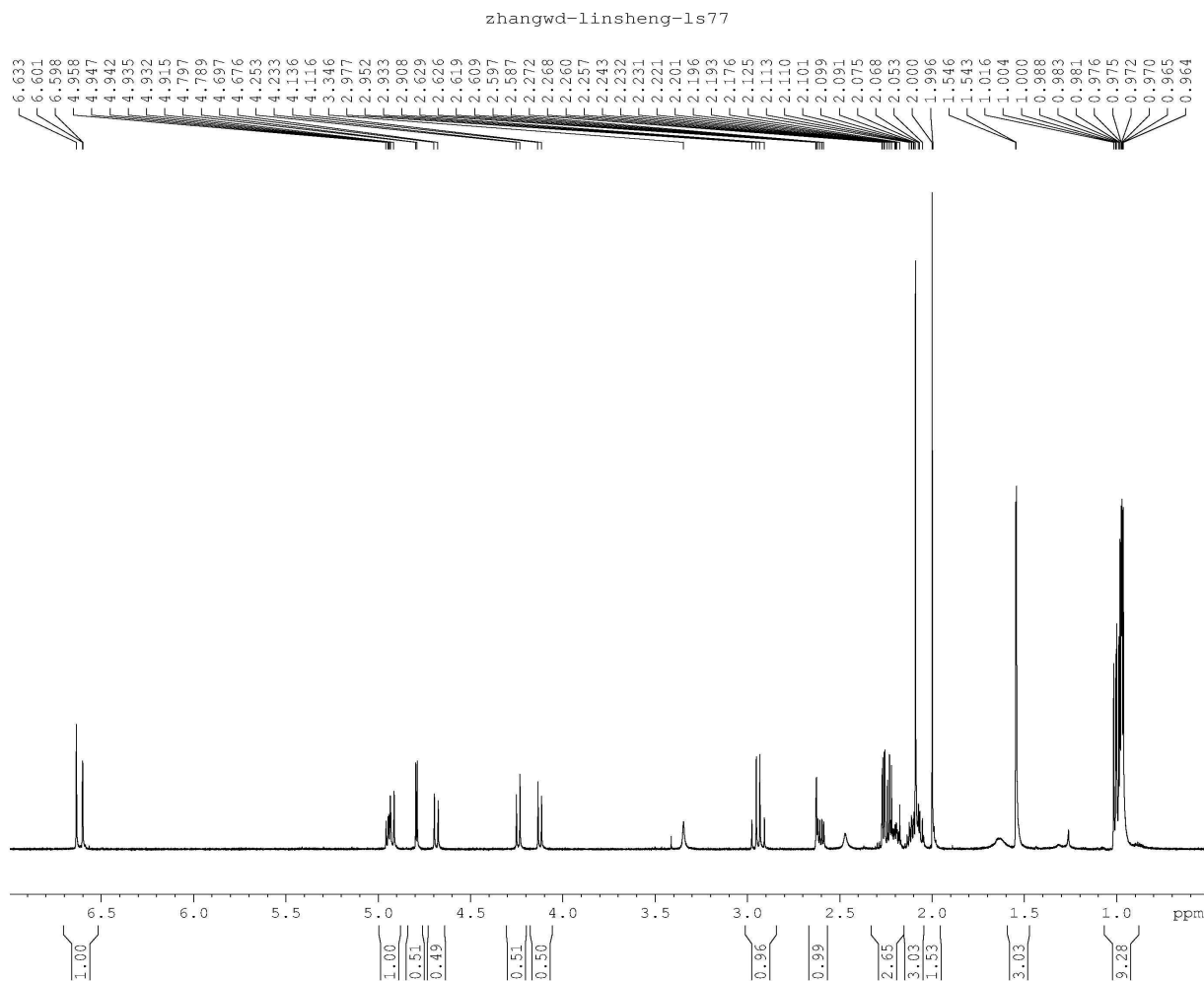
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wdzhangY@hotmail.com

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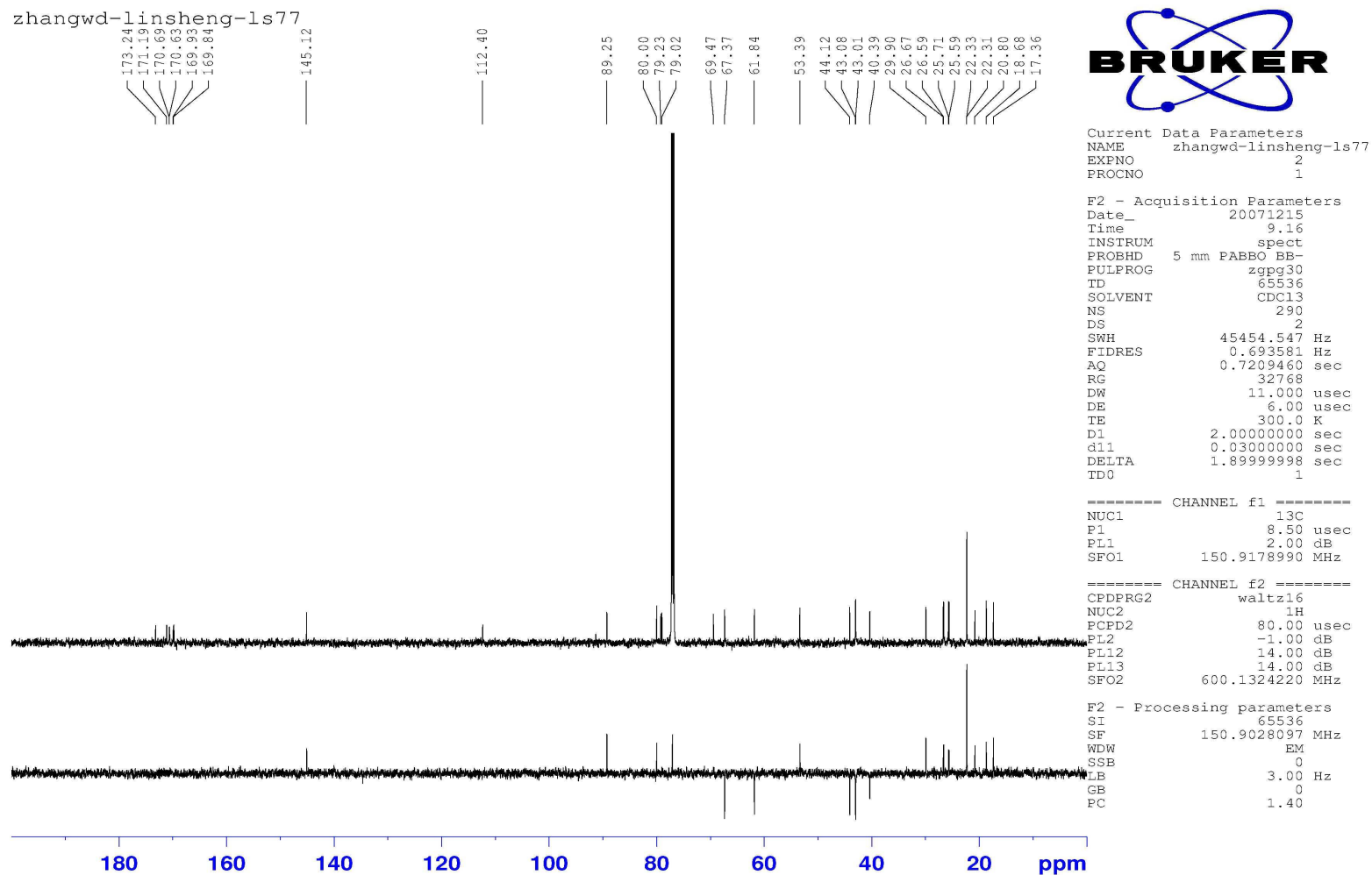
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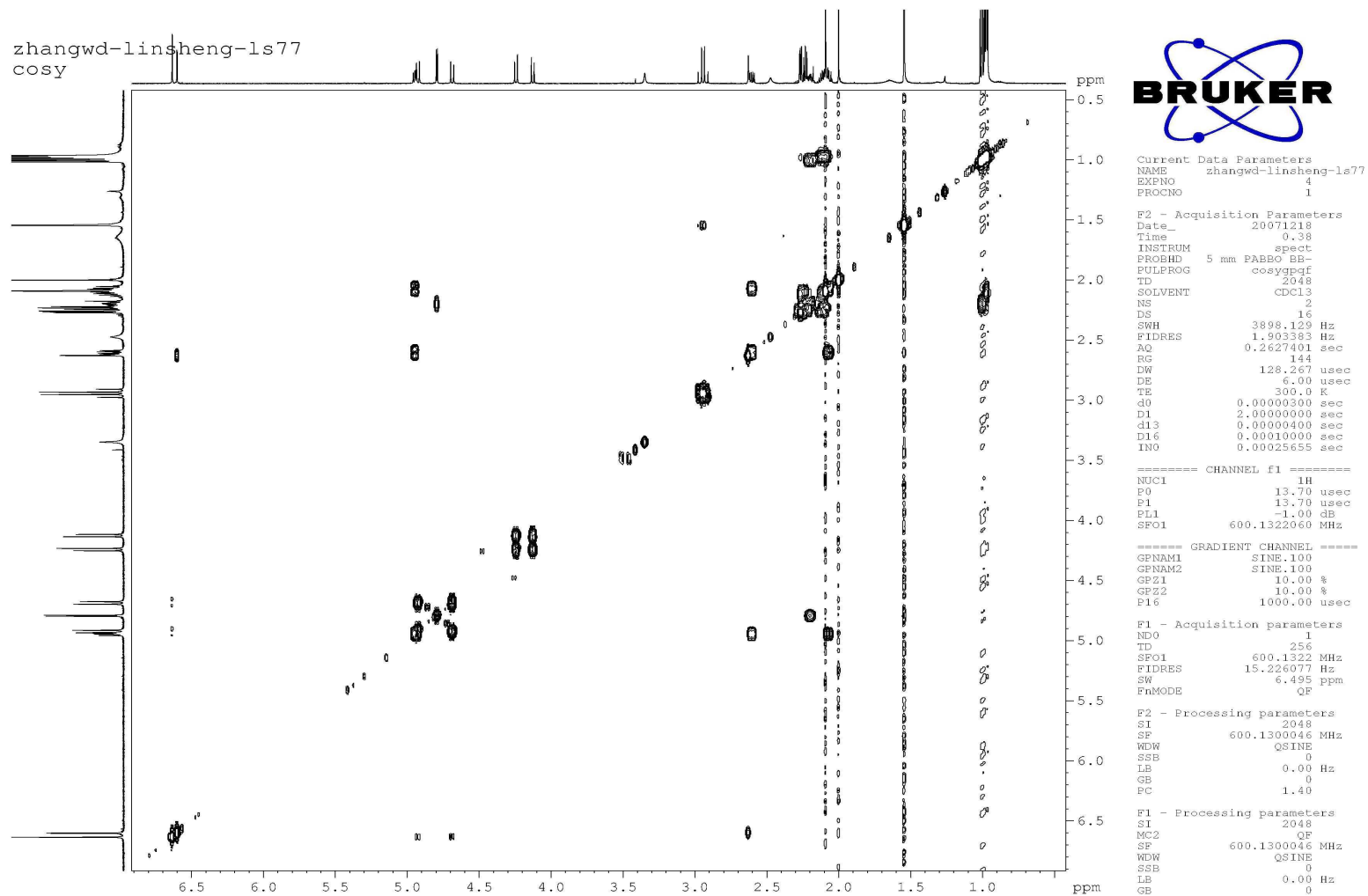
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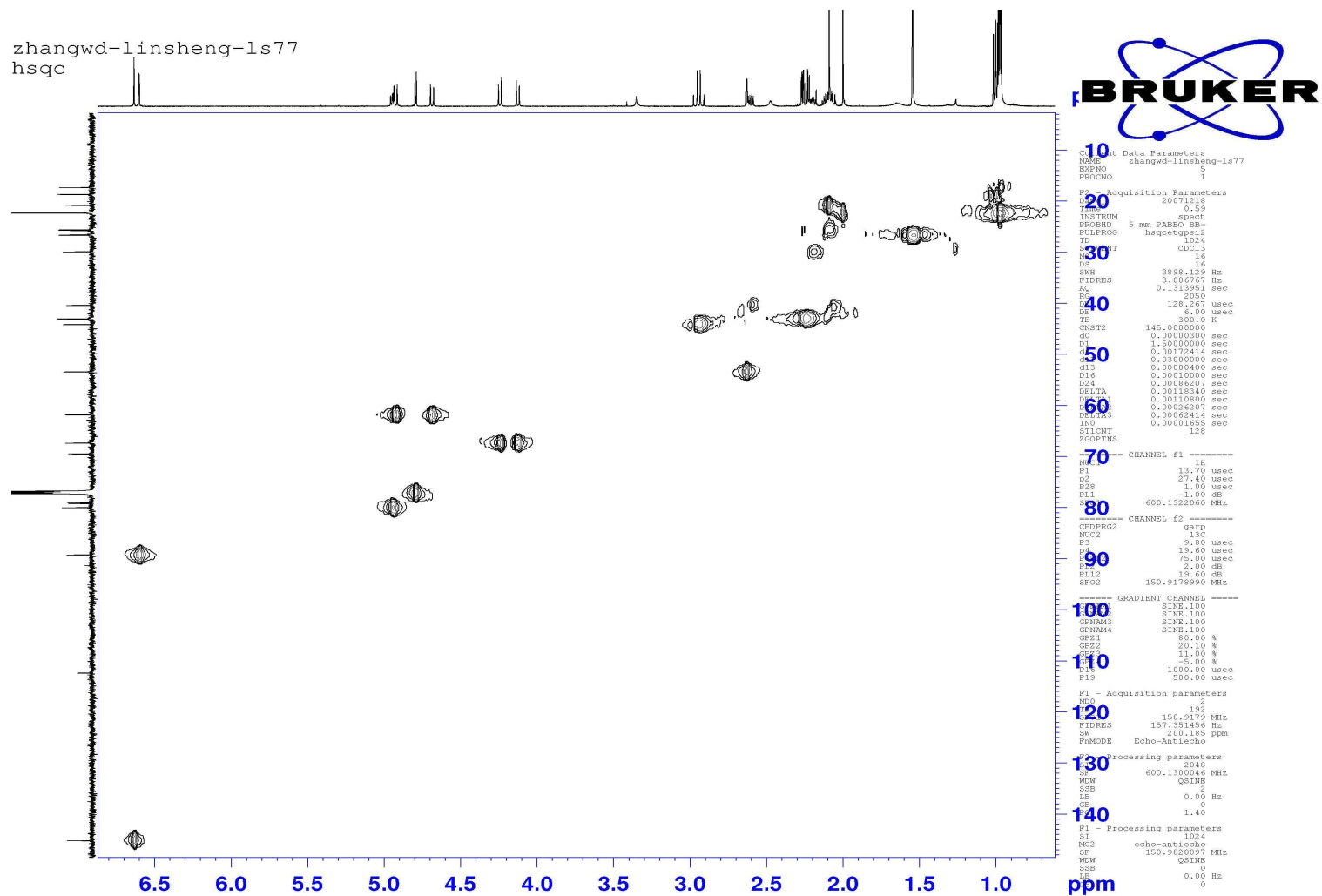
S5. The ^1H NMR Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate A (1)



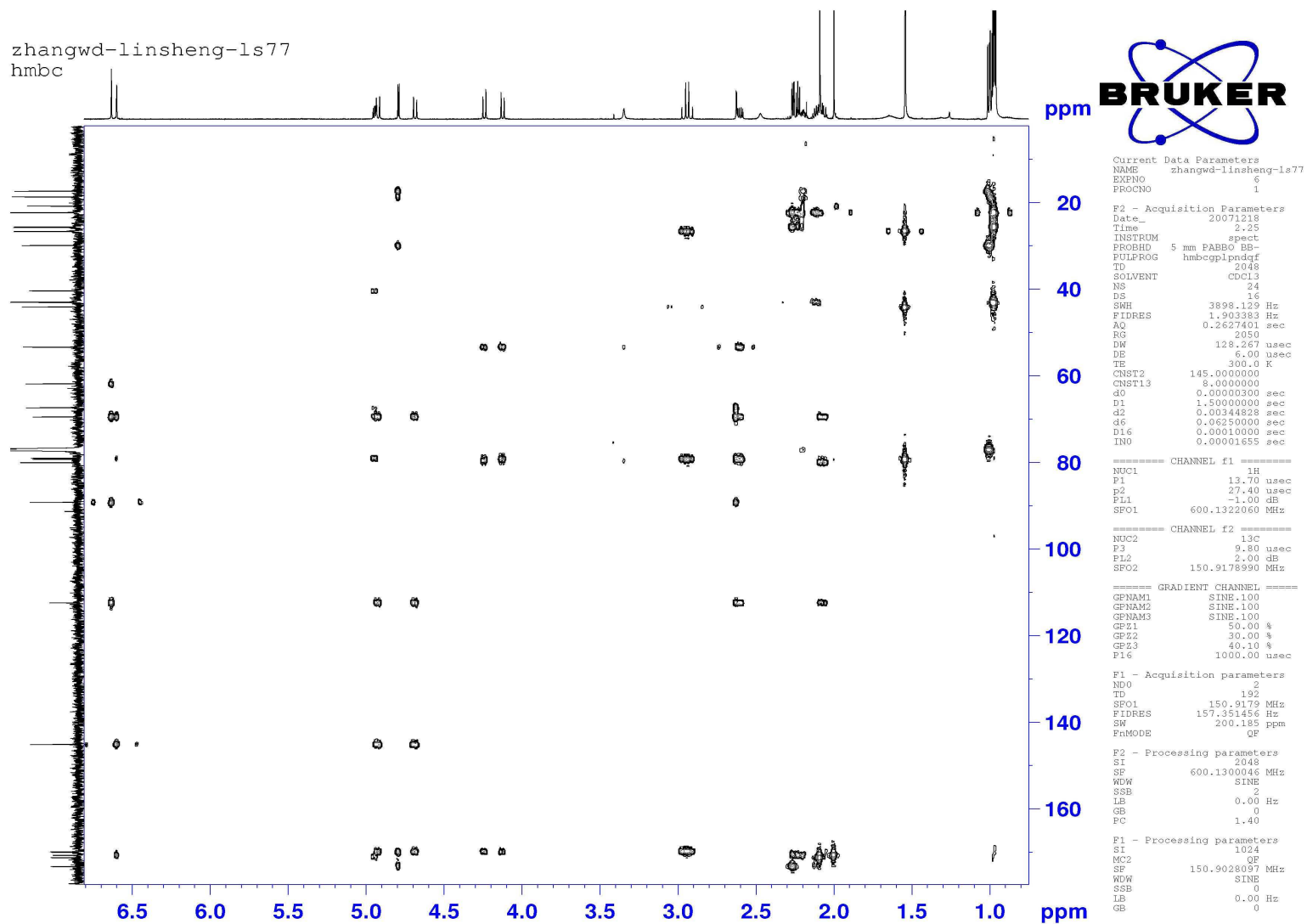
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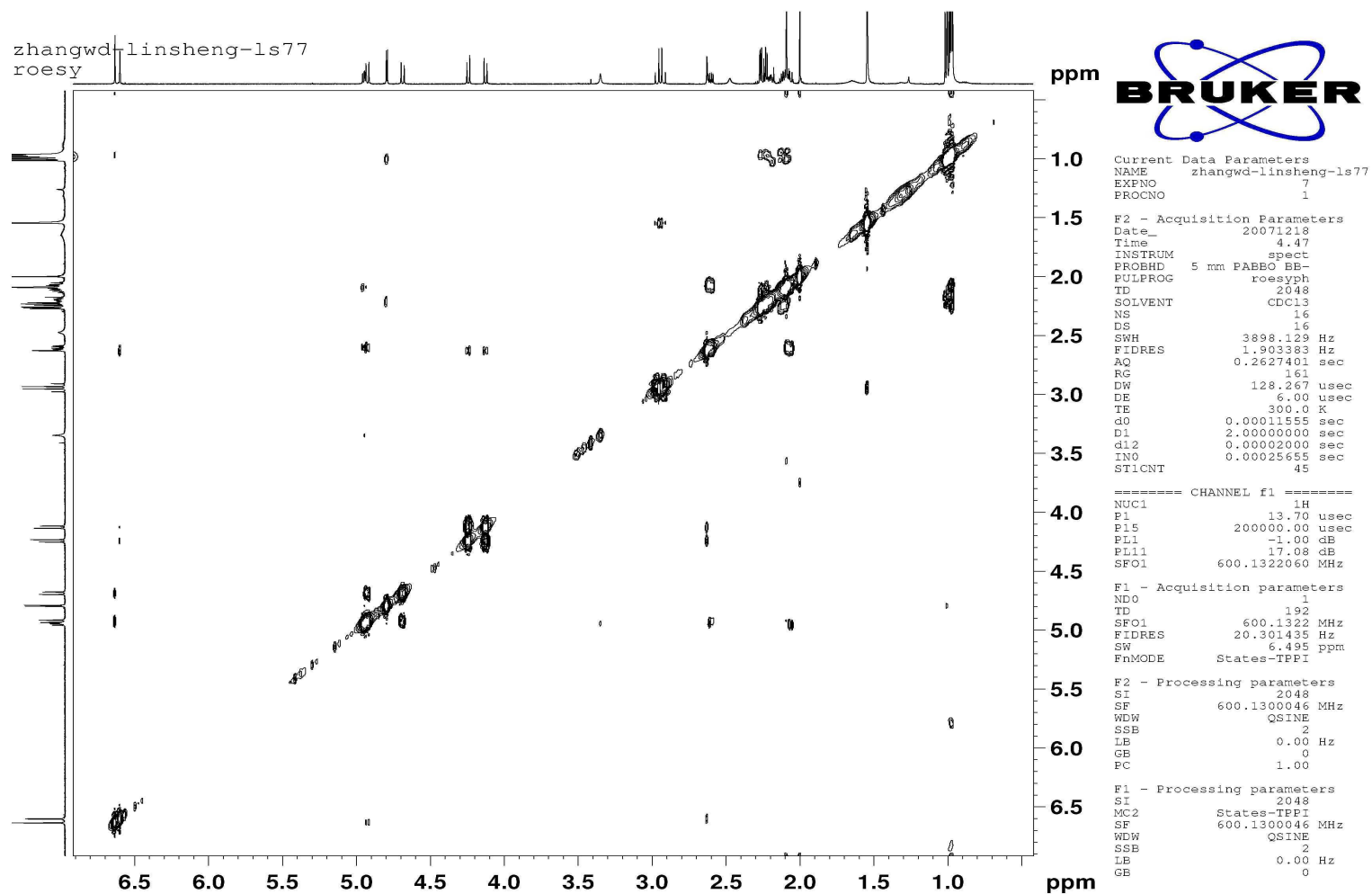
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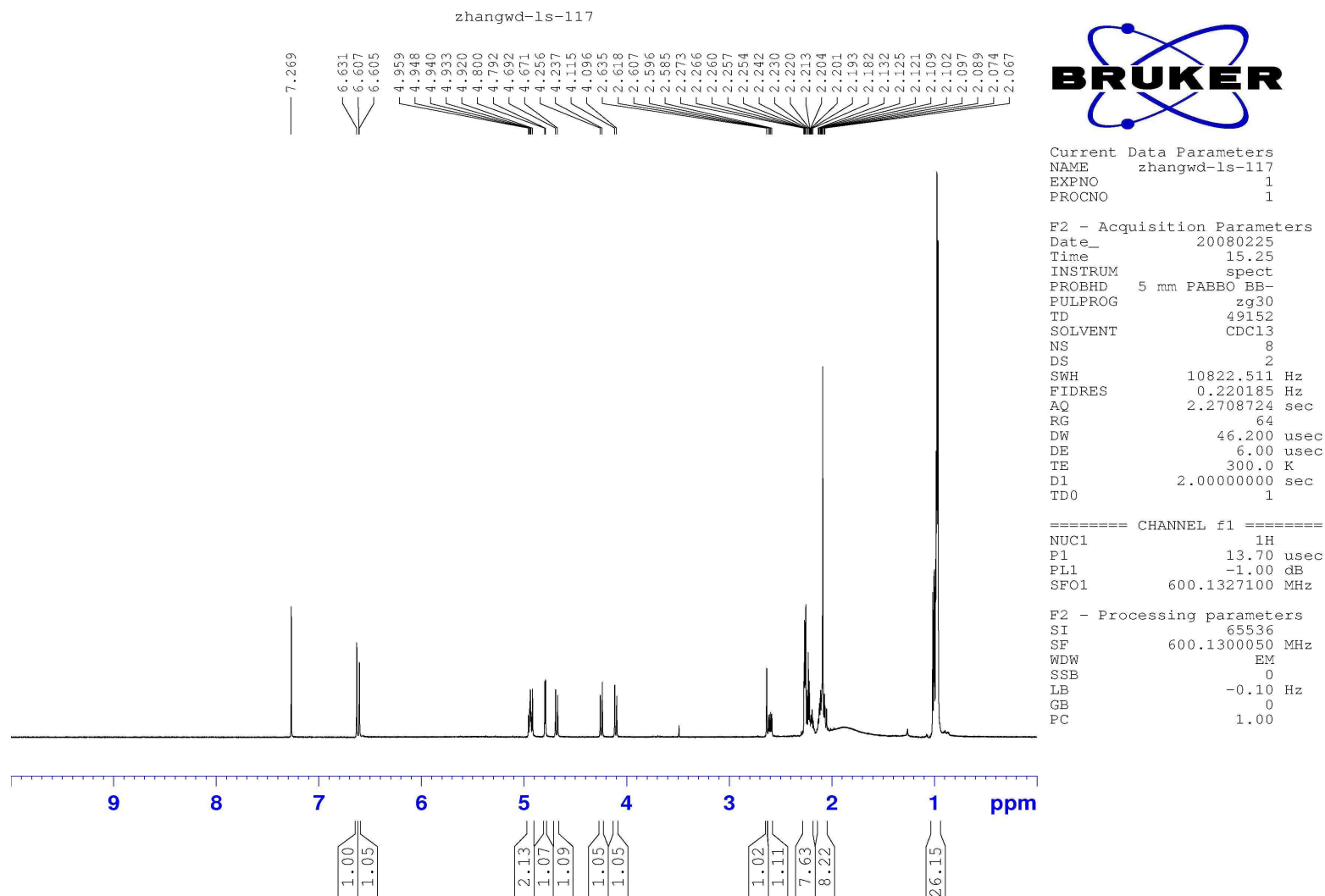
S8. The HSQC Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate A (1)



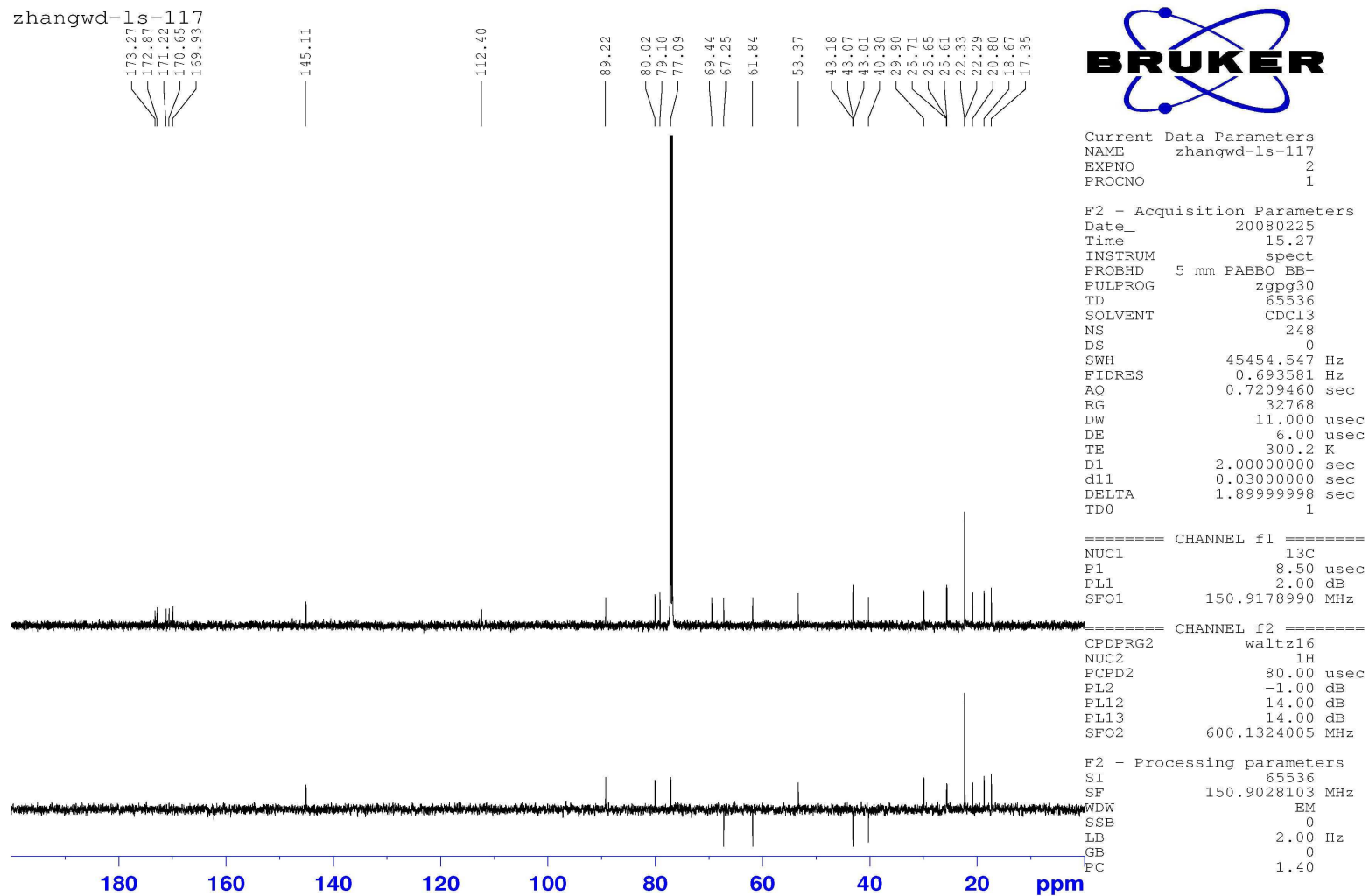
S9. The HMBC Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate A (1)



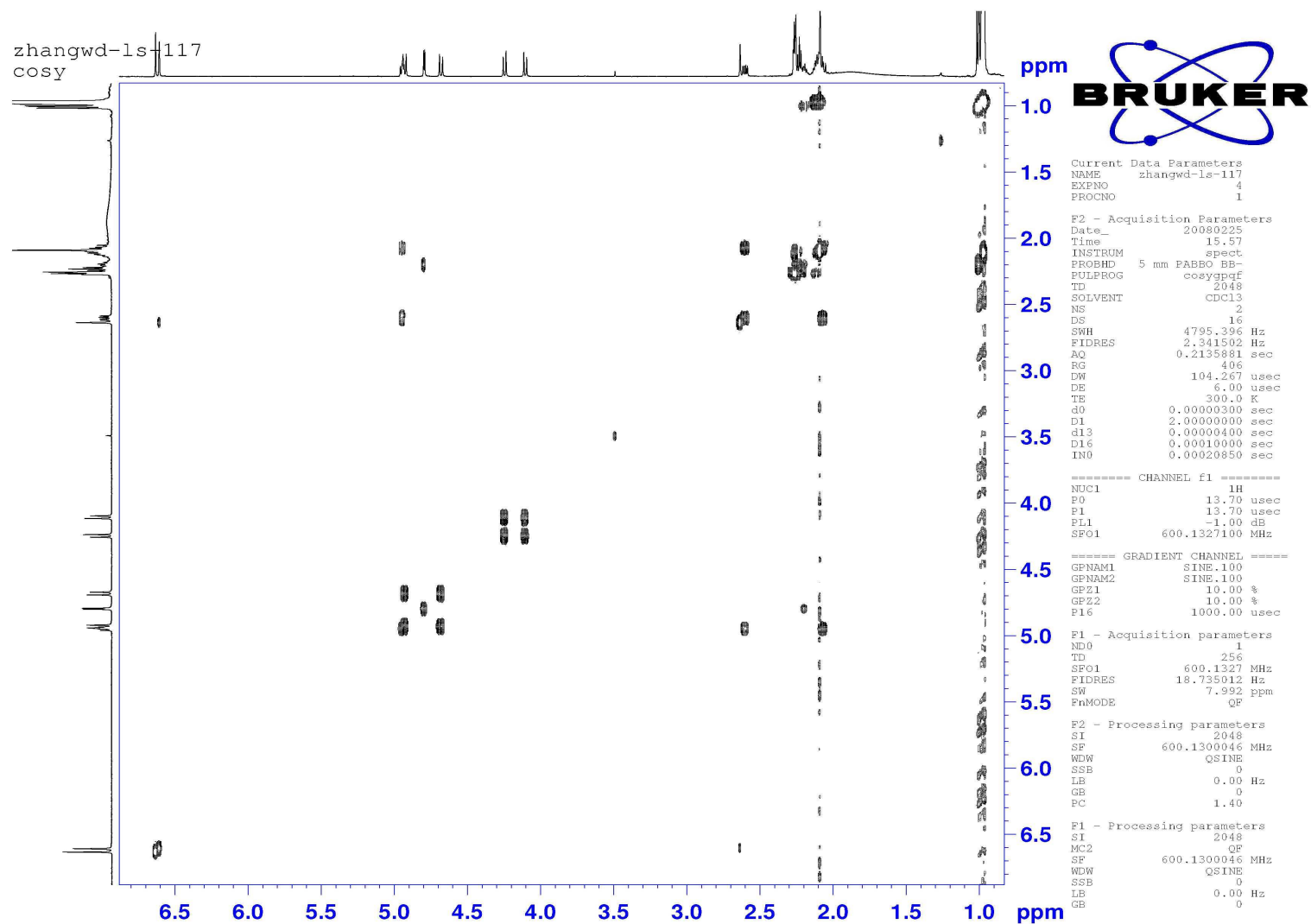
S10. The ROESY Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate A (1)



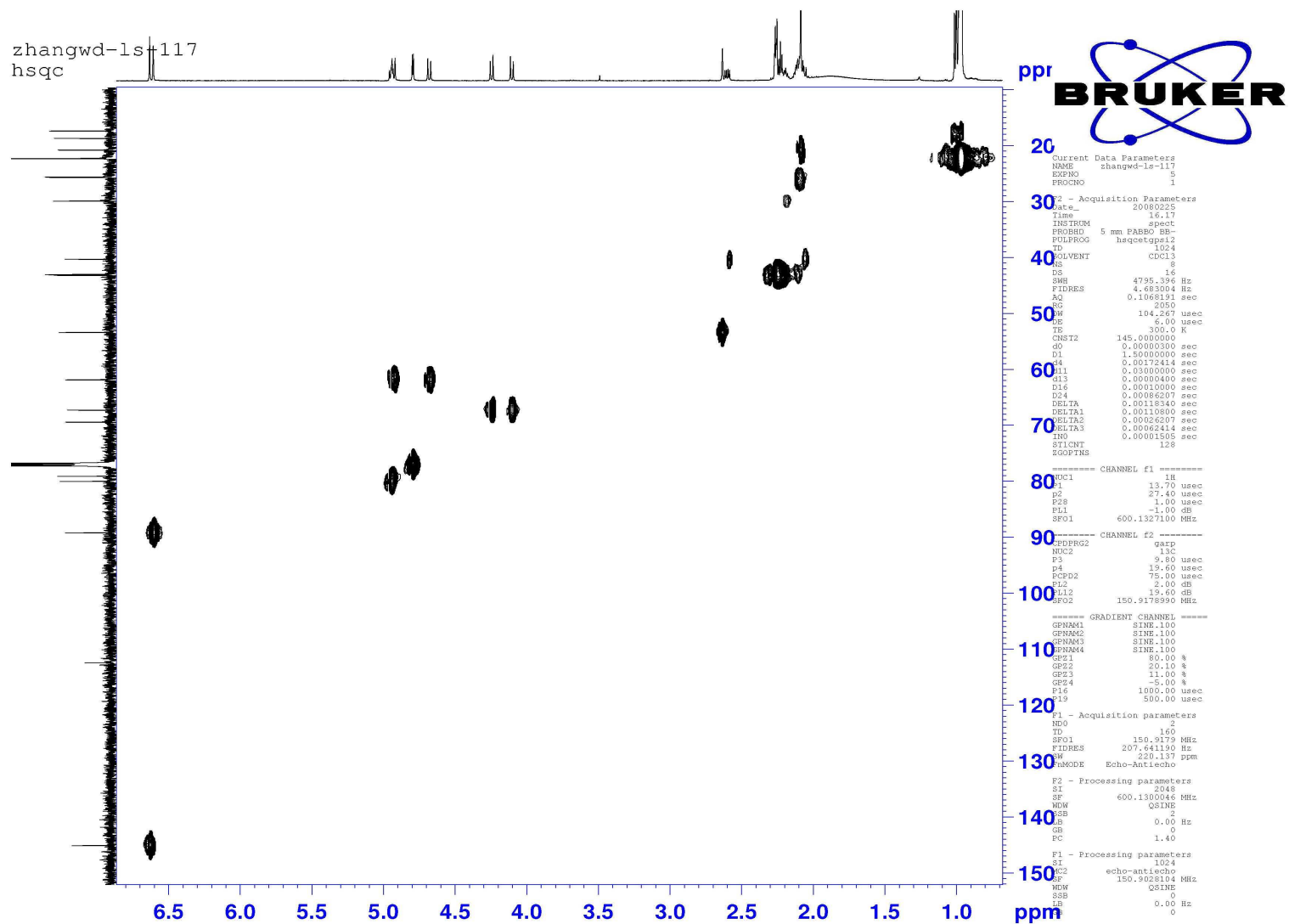
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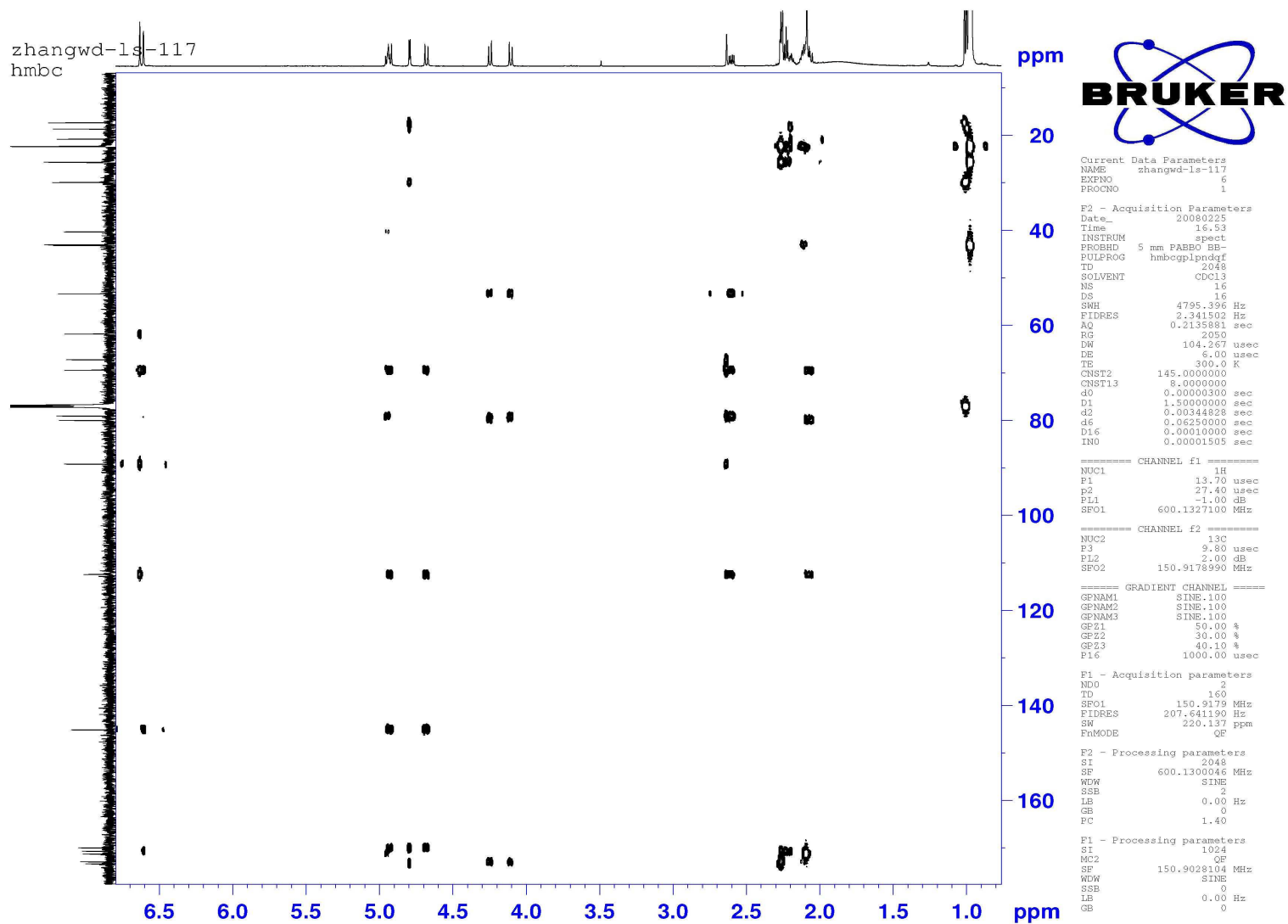
S12. The ^{13}C NMR and DEPT Spectra (150 MHz, CDCl_3) of Jatamanvaltrate B (2)



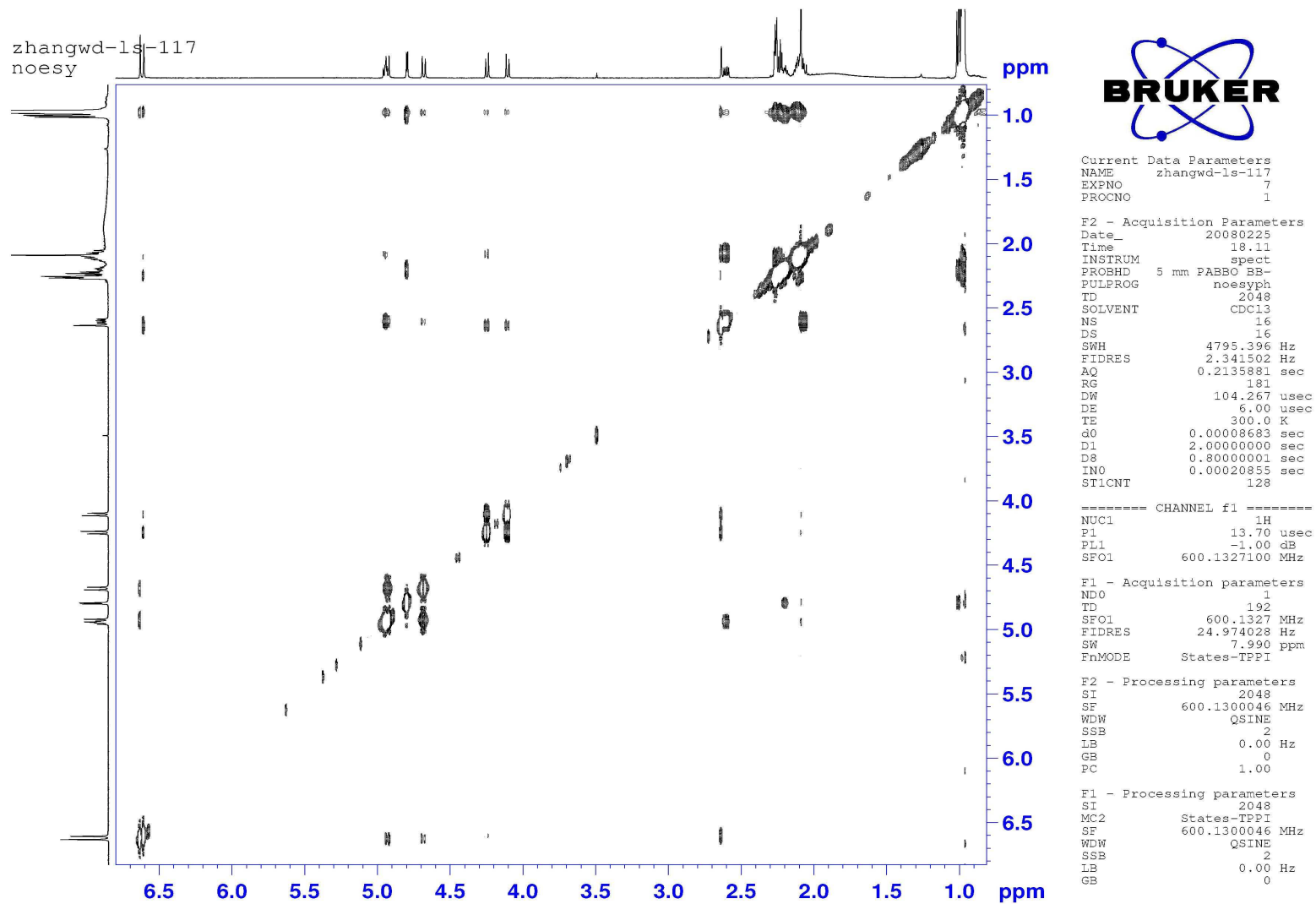
S13. The ^1H - ^1H COSY Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate B (2)



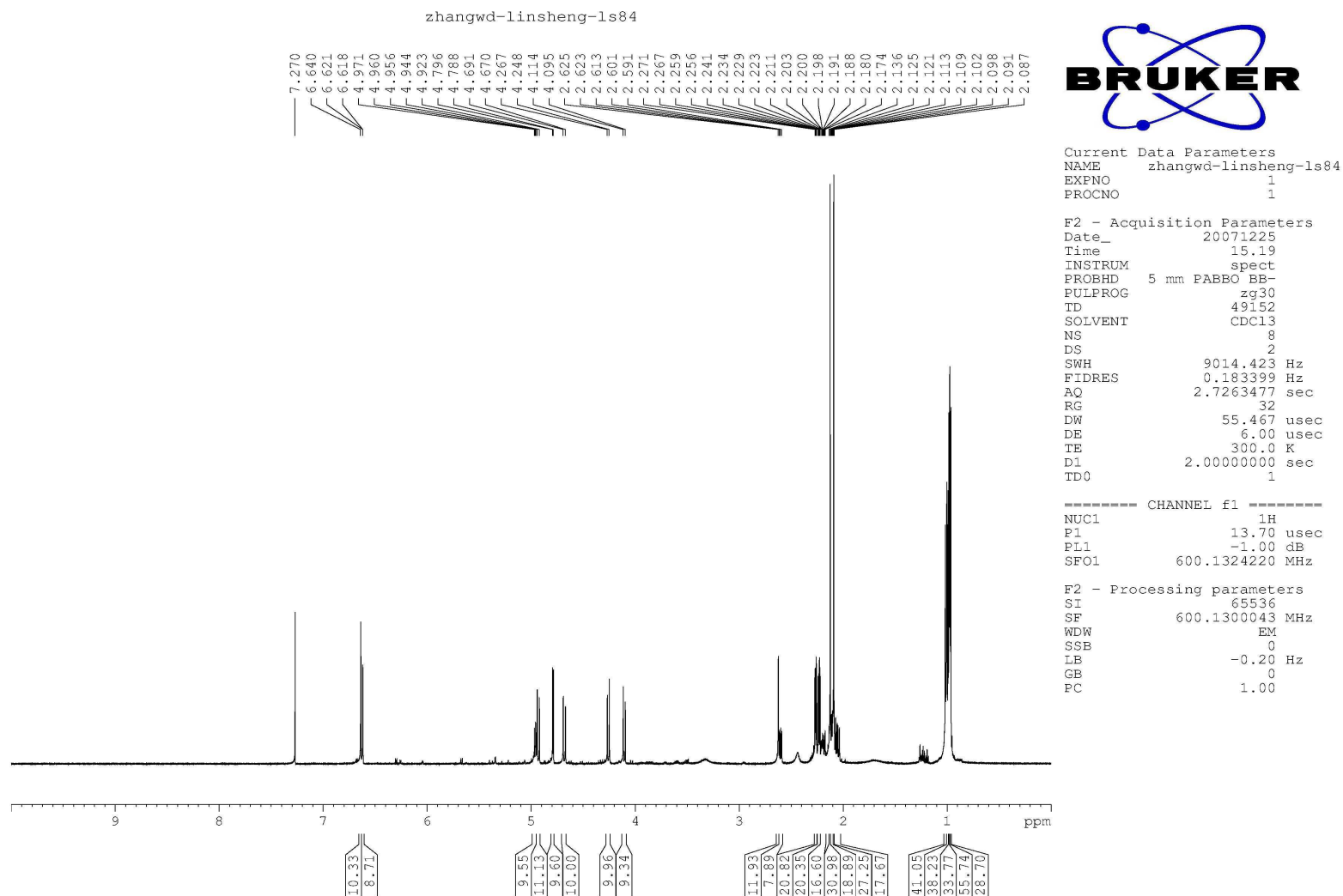
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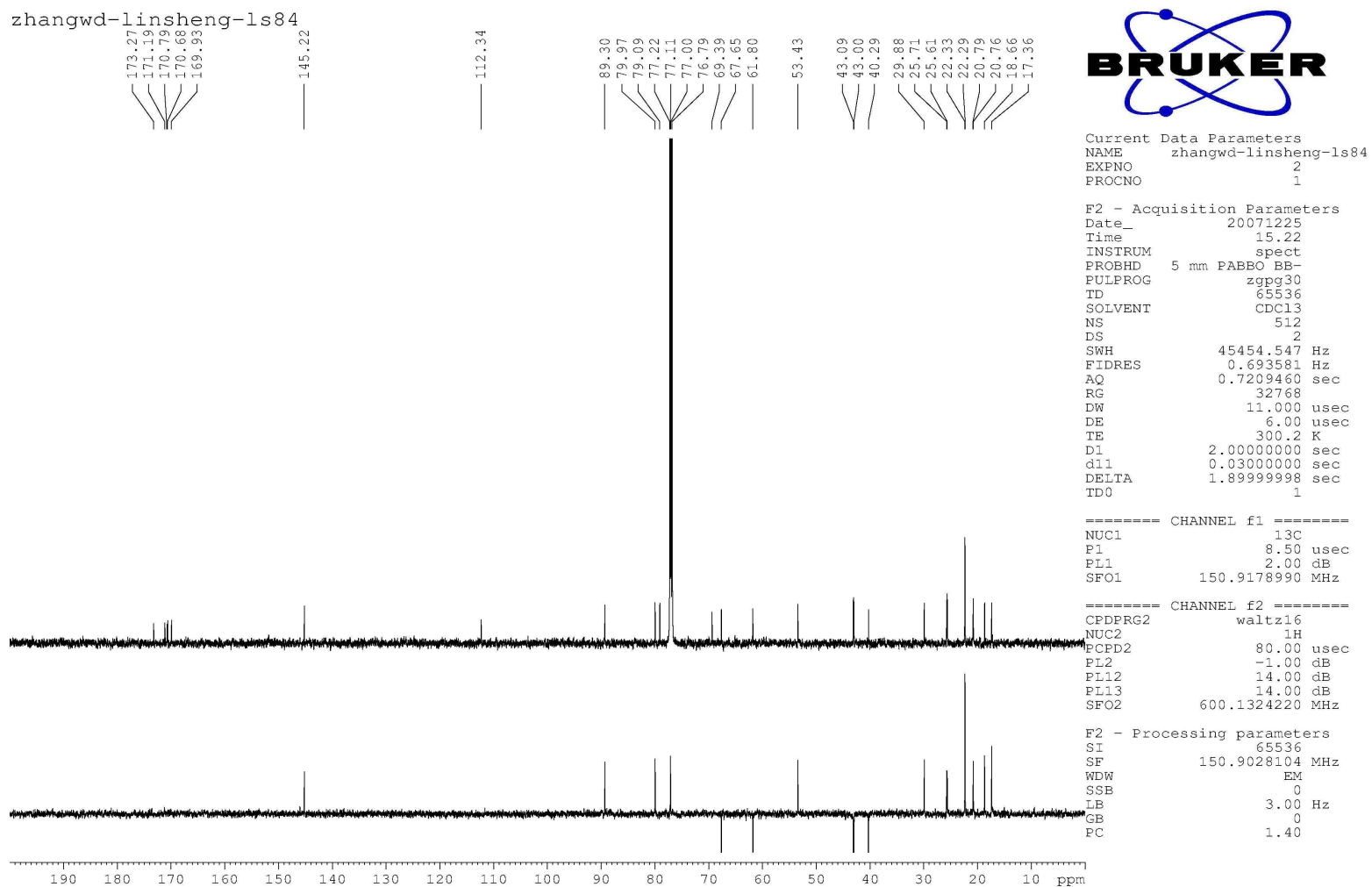
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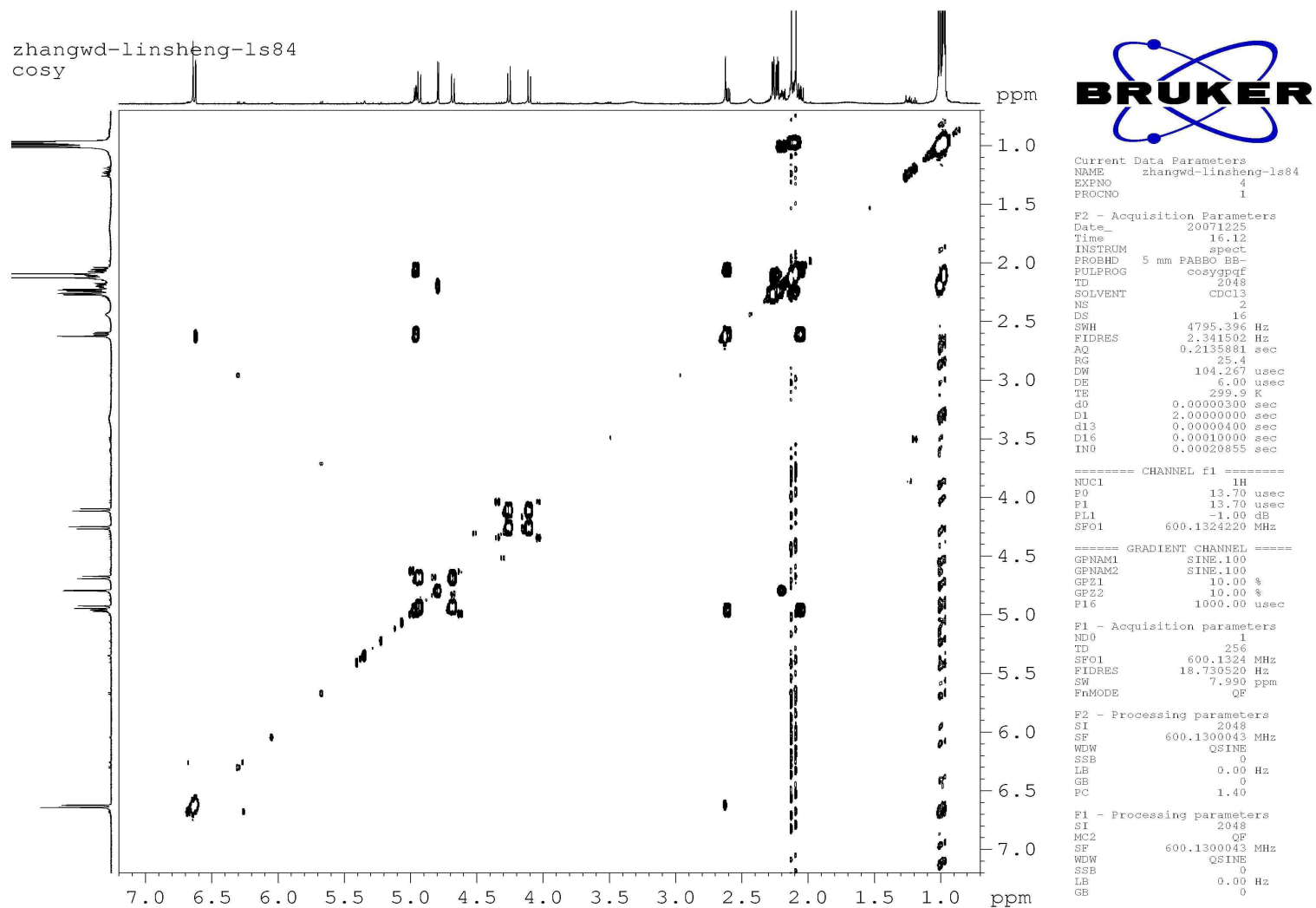
S16. The NOESY Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate B (2)



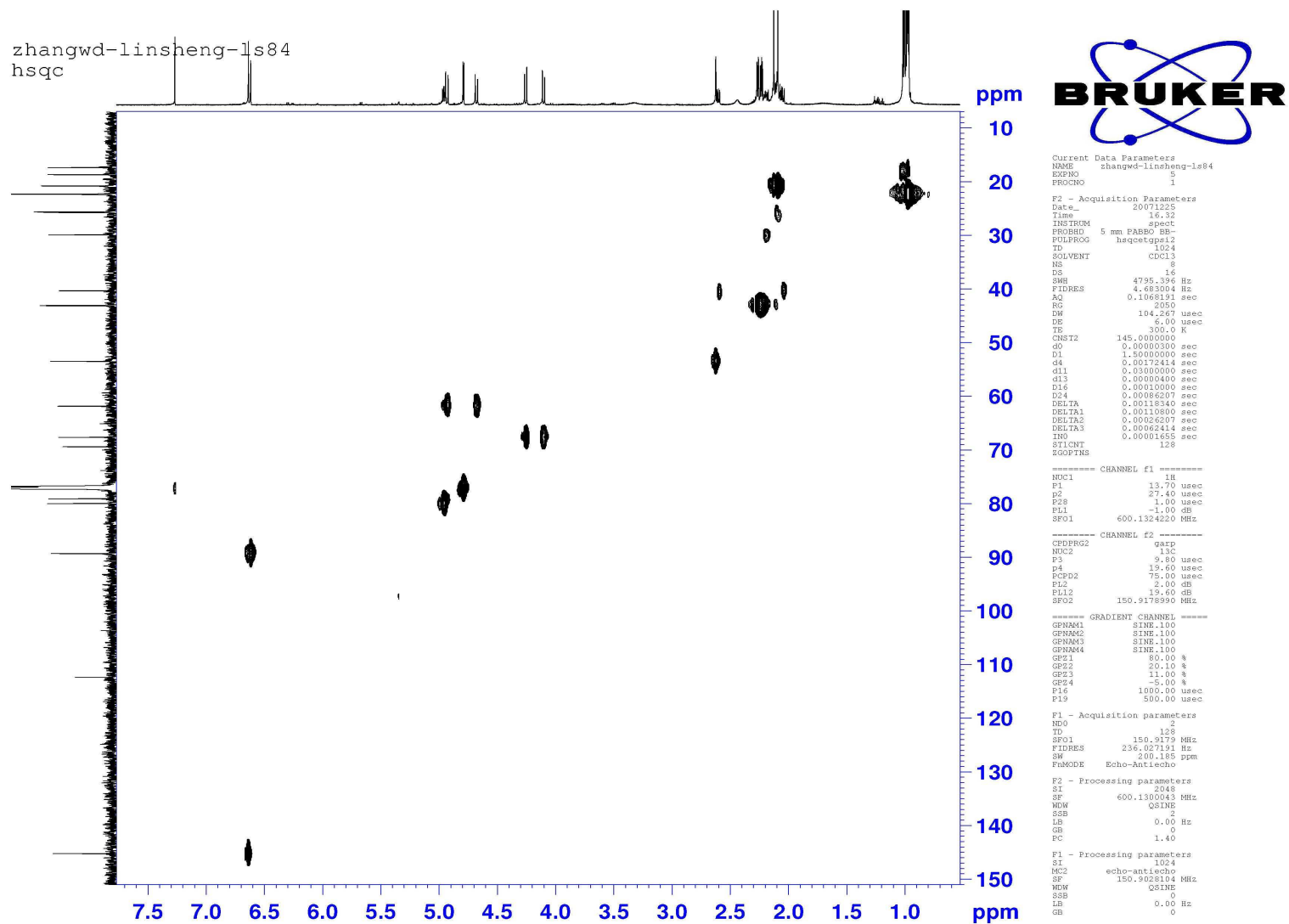
S17. The ^1H NMR Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate C (3)



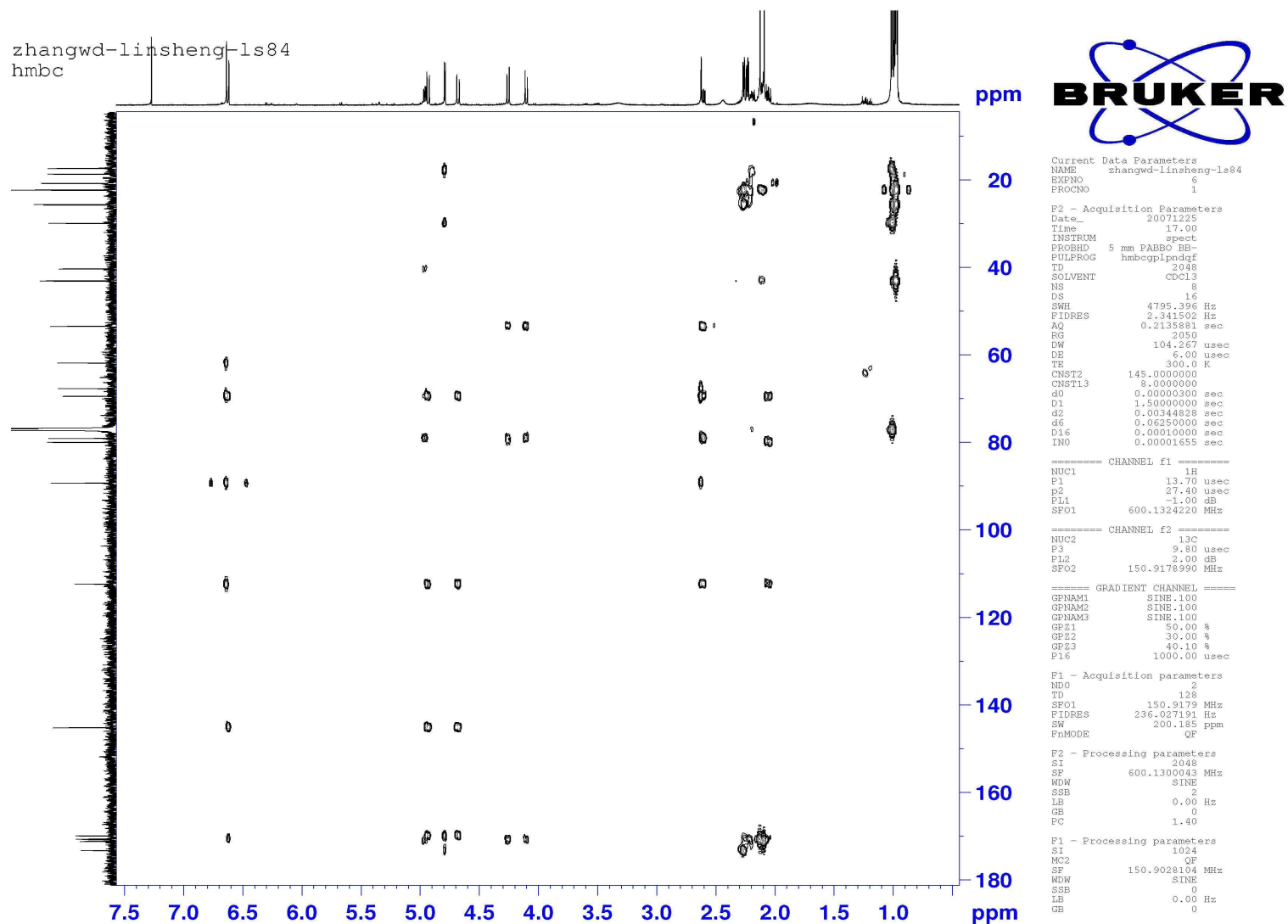
S18. The ^{13}C NMR and DEPT Spectra (150 MHz, CDCl_3) of Jatamanvaltrate C (3)



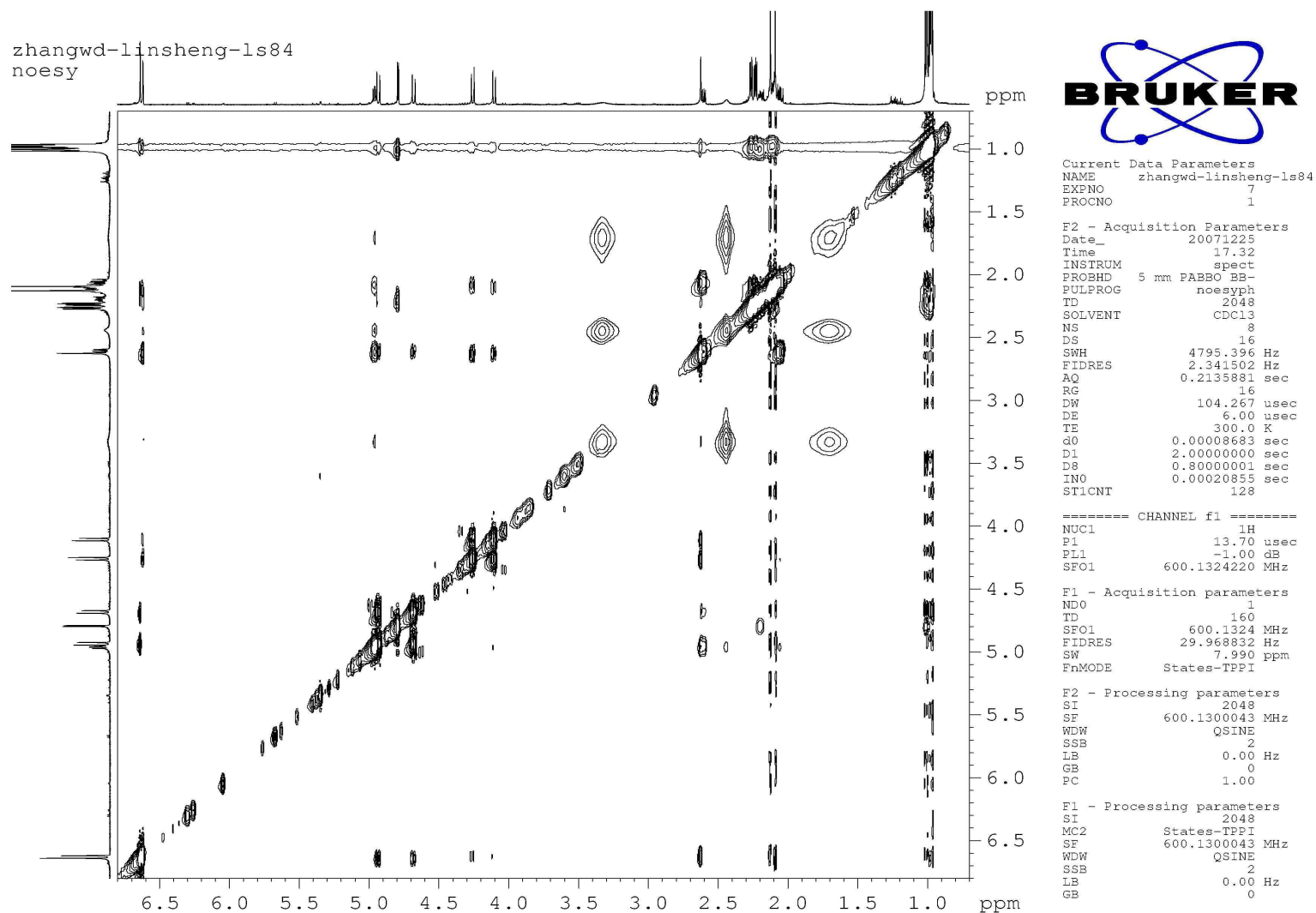
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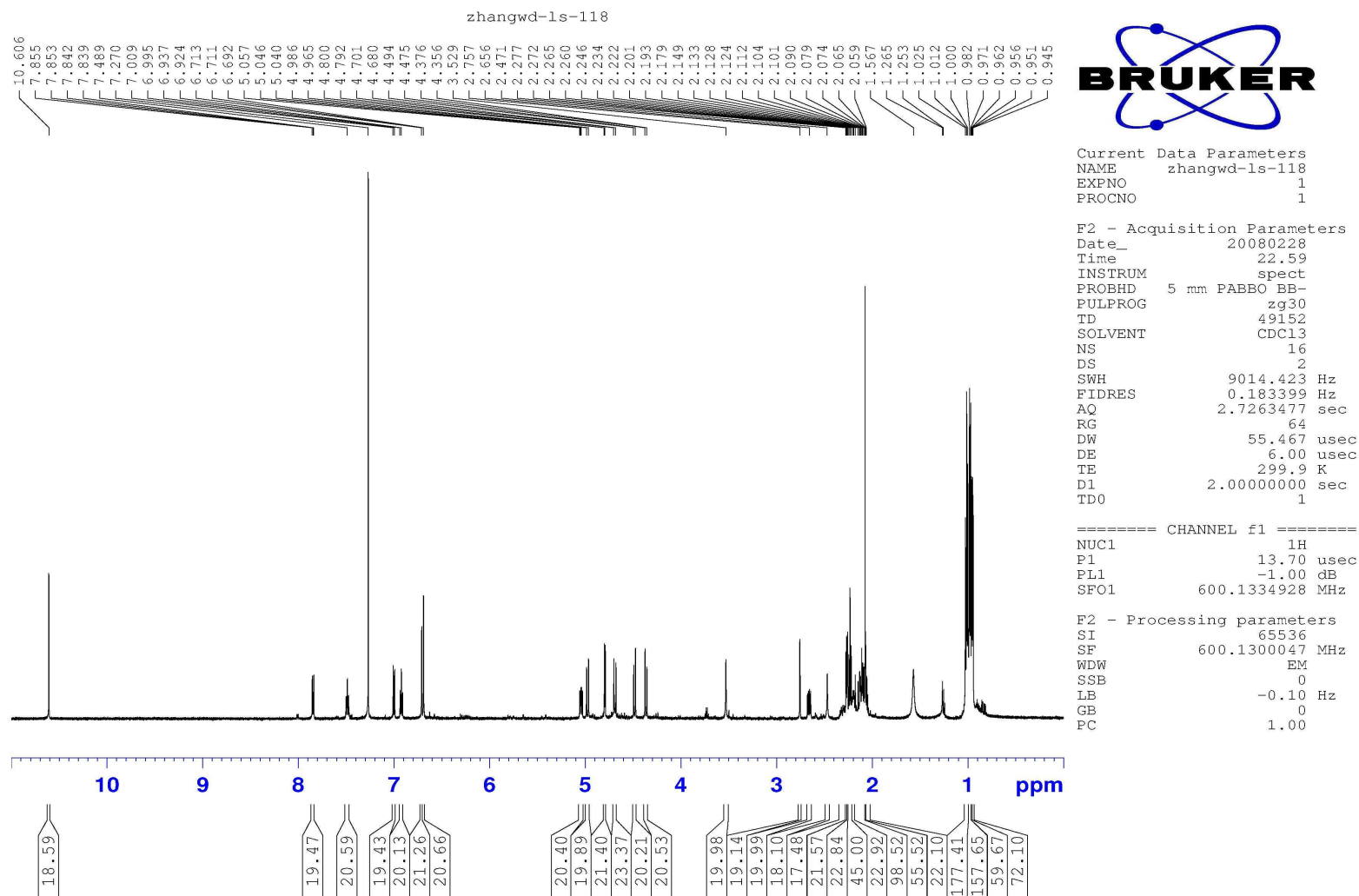
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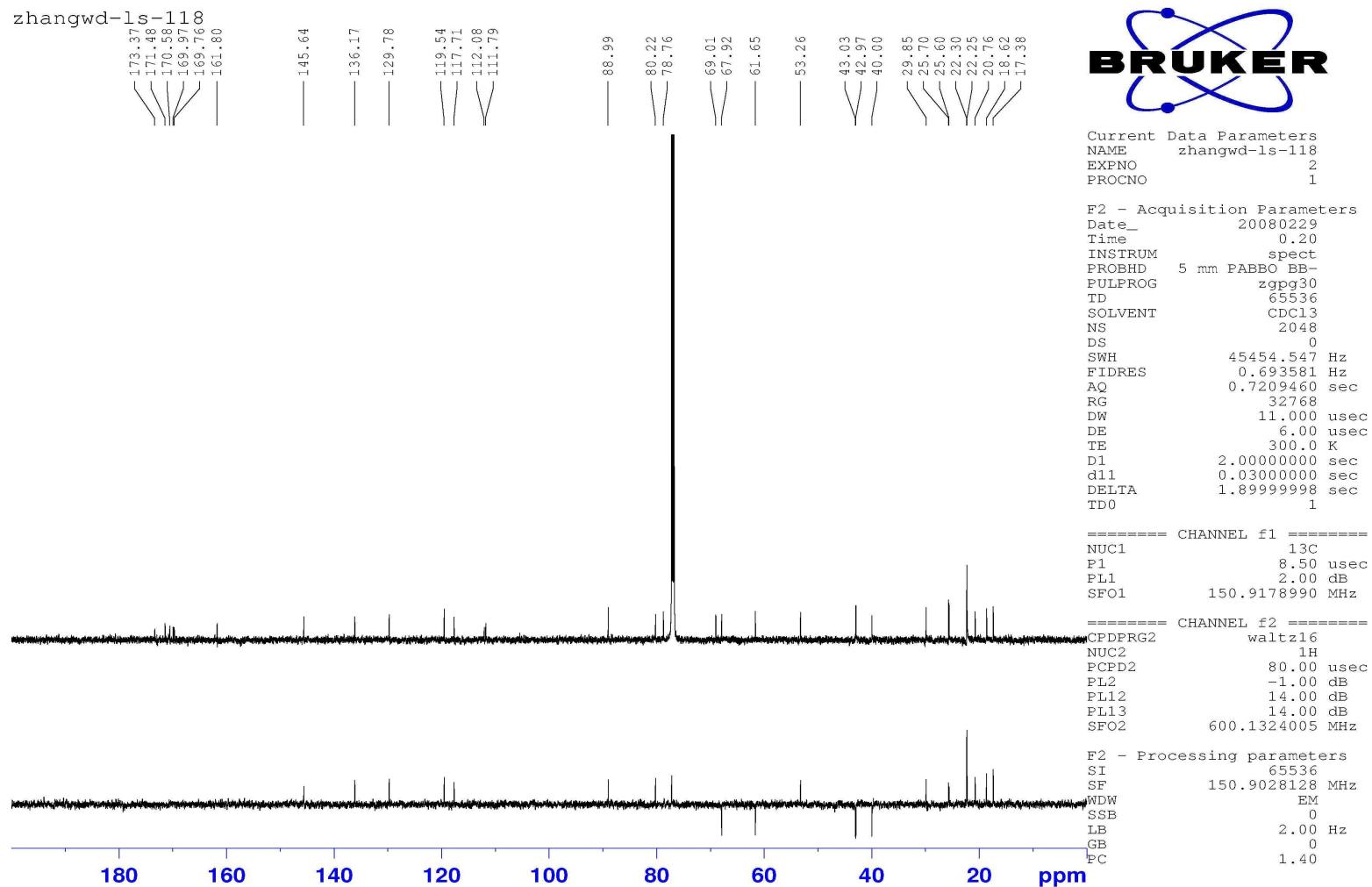
S21. The HMBC Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate C (3)



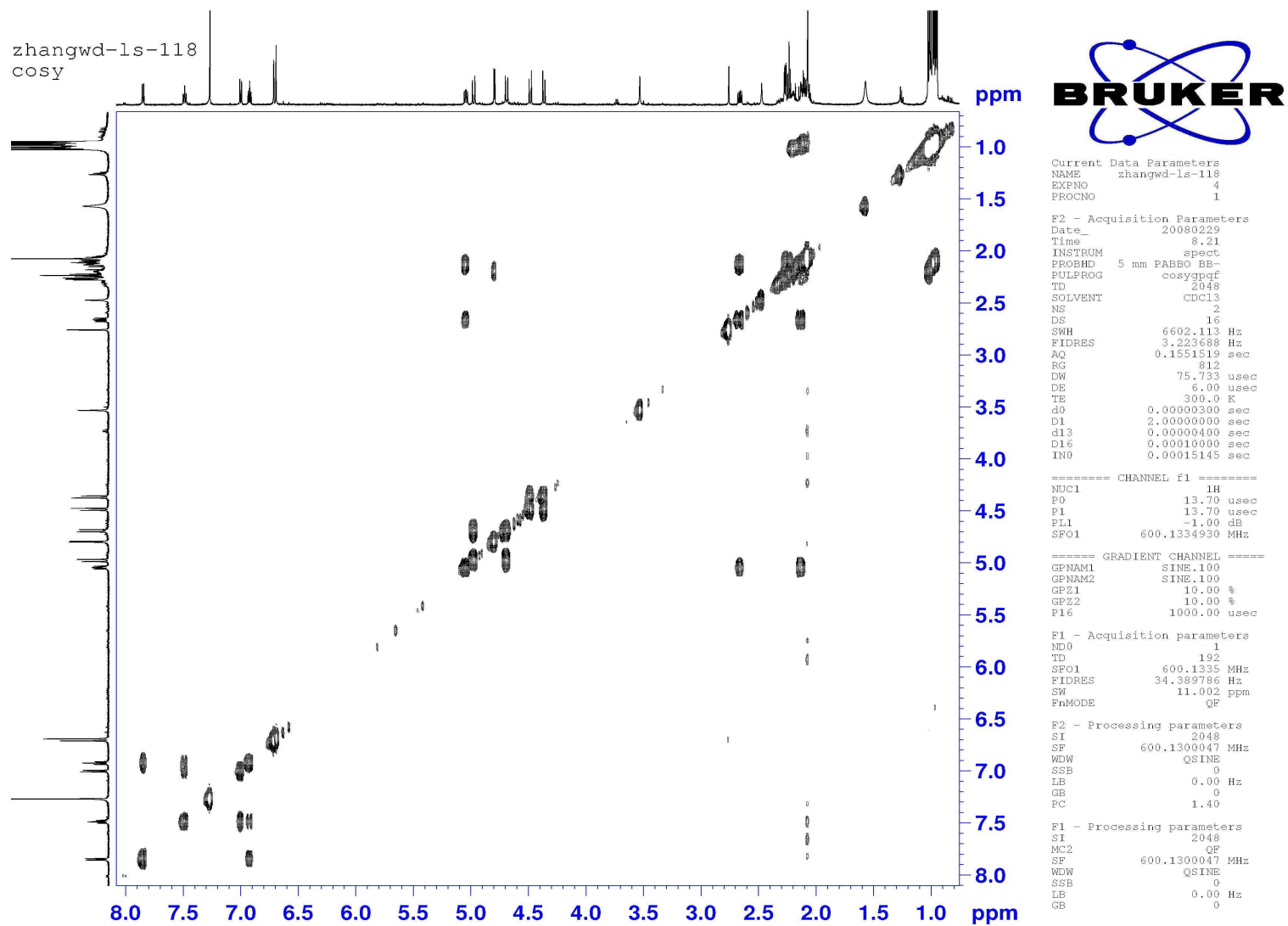
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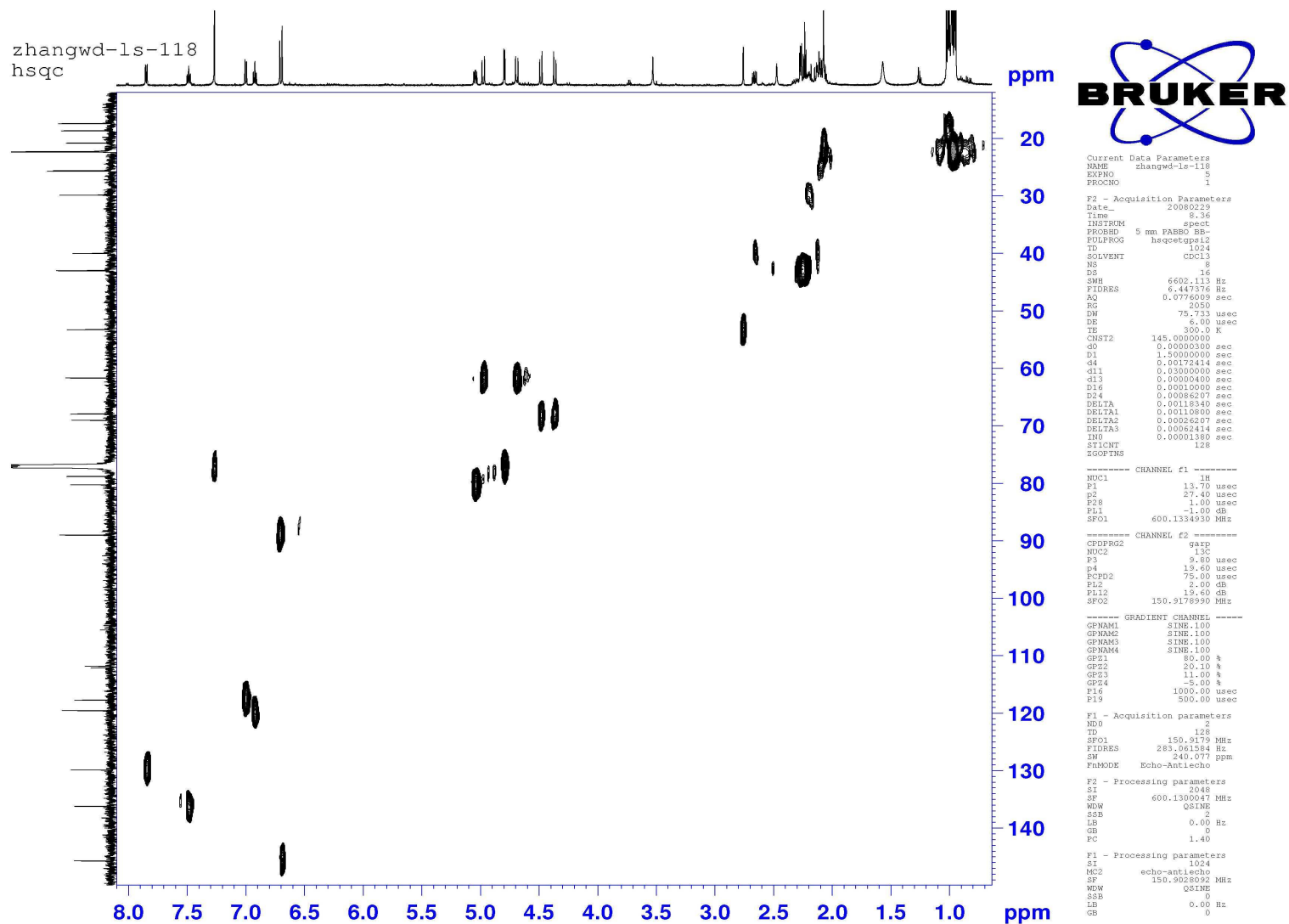
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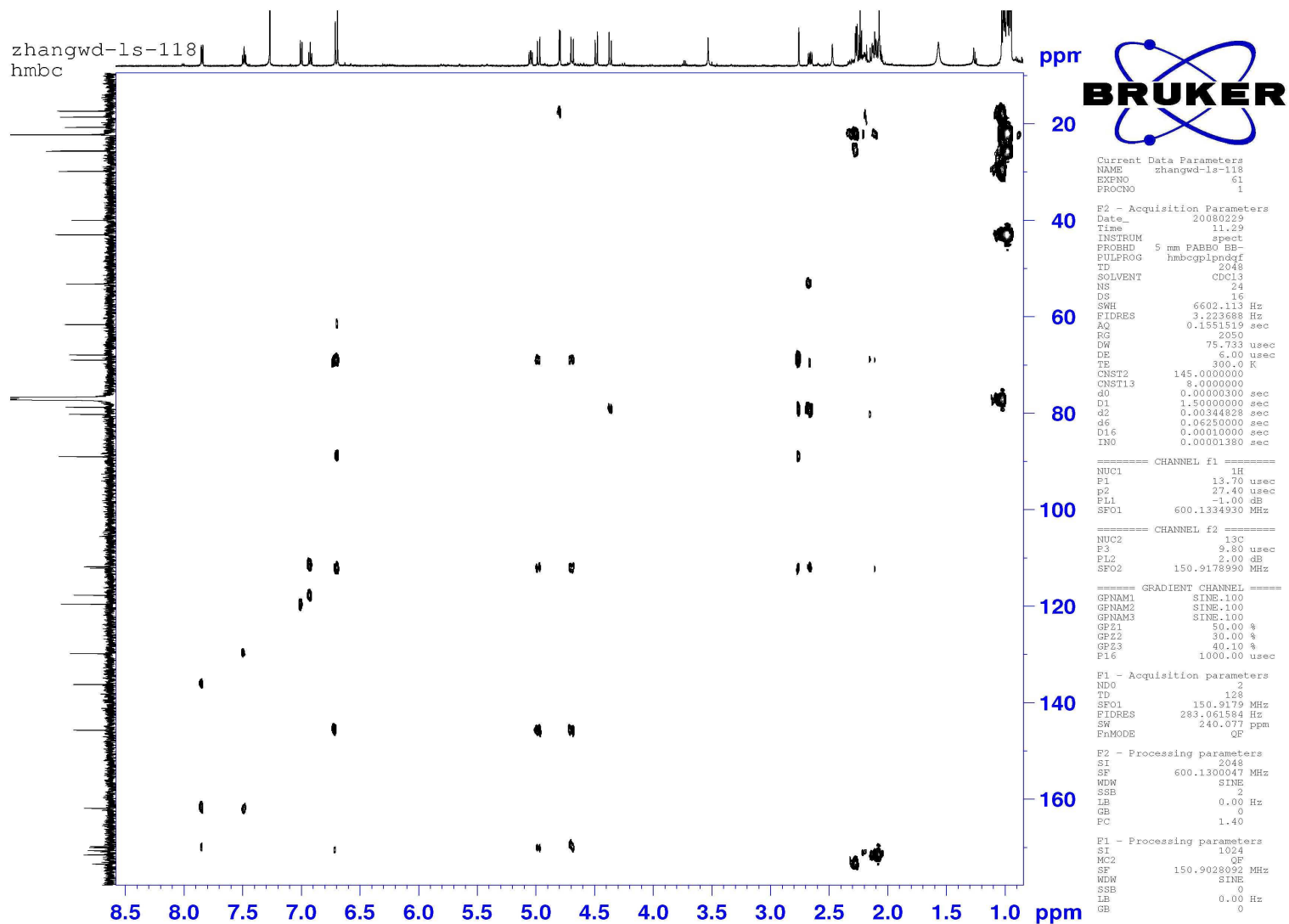
S24. The ^{13}C NMR and DEPT Spectra (150 MHz, CDCl_3) of Jatamanvaltrate D (4)



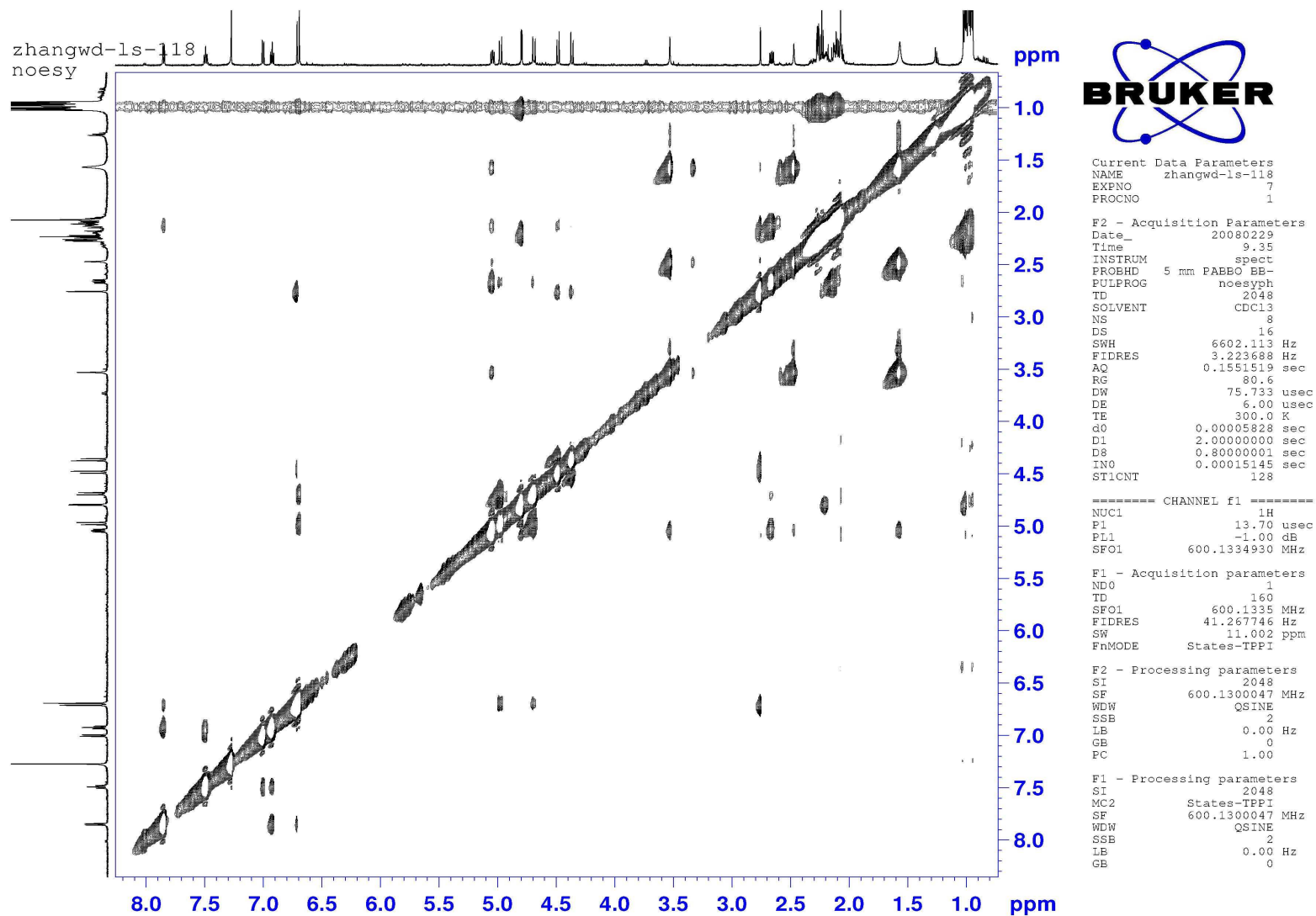
S25. The ^1H - ^1H COSY Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate D (4)



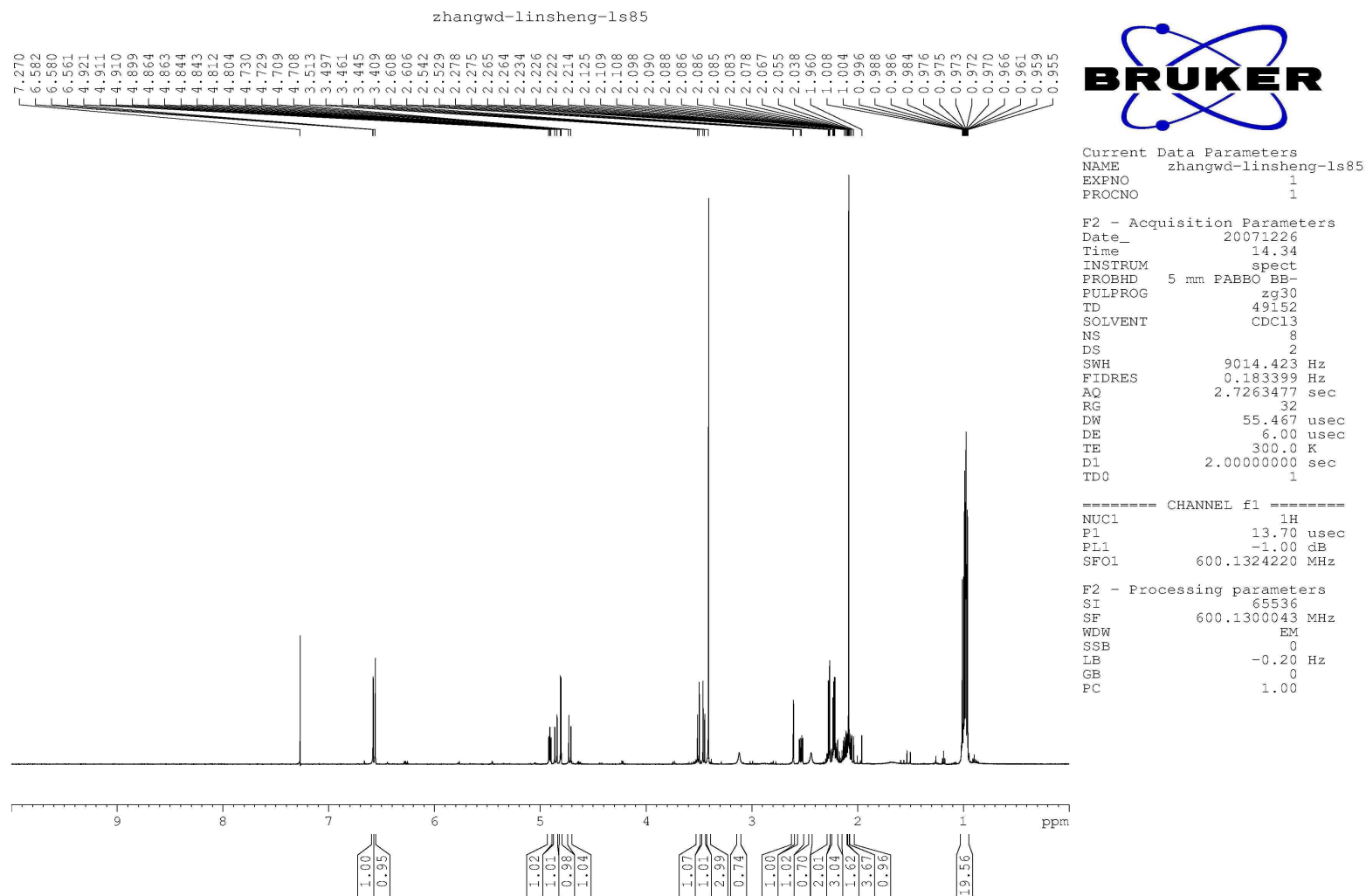
S26. The HSQC Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate D (4)



S27. The HMBC Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate D (4)

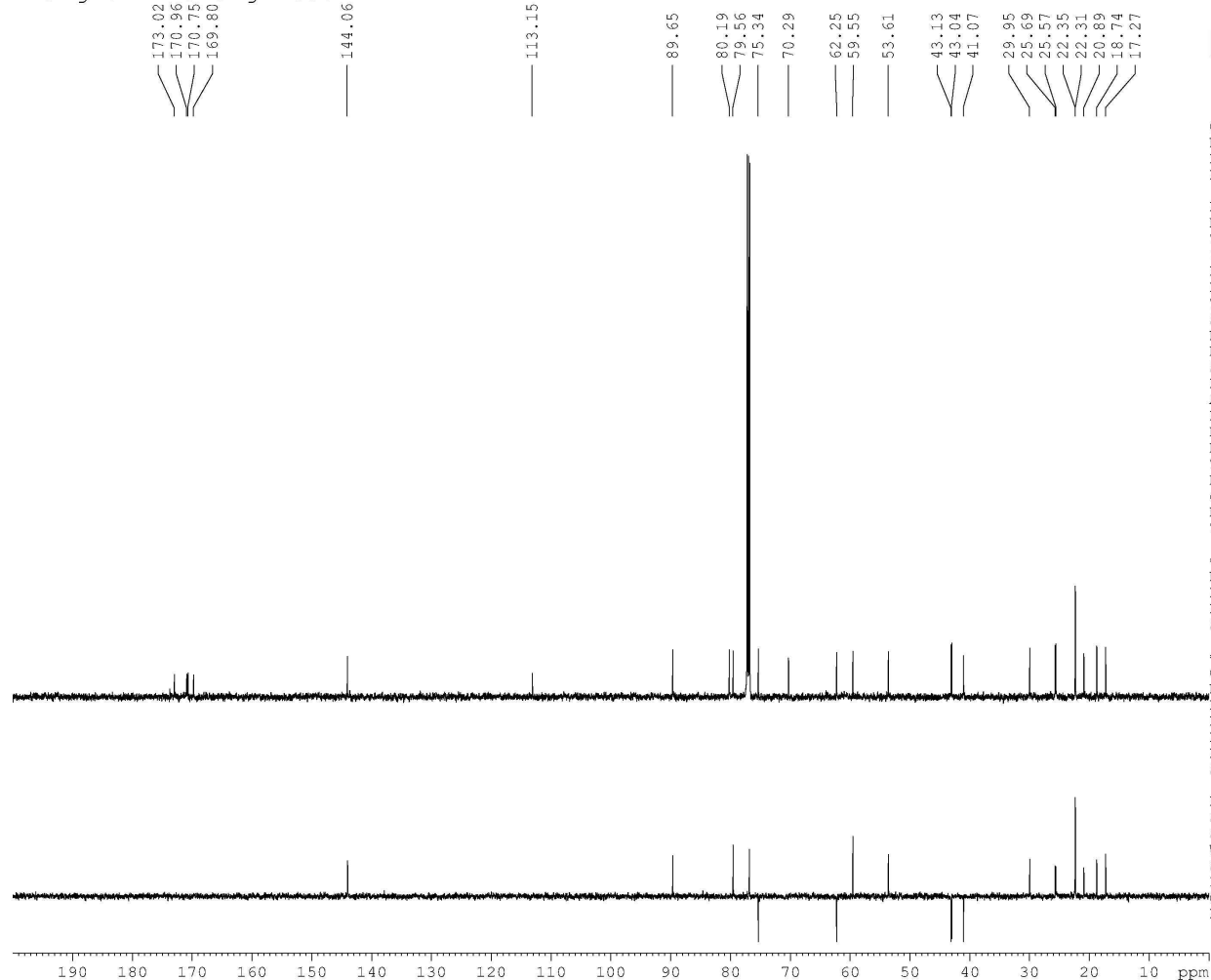


S28. The NOESY Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate D (4)



S29. The ^1H NMR Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate E (5)

zhangwd-linsheng-ls85



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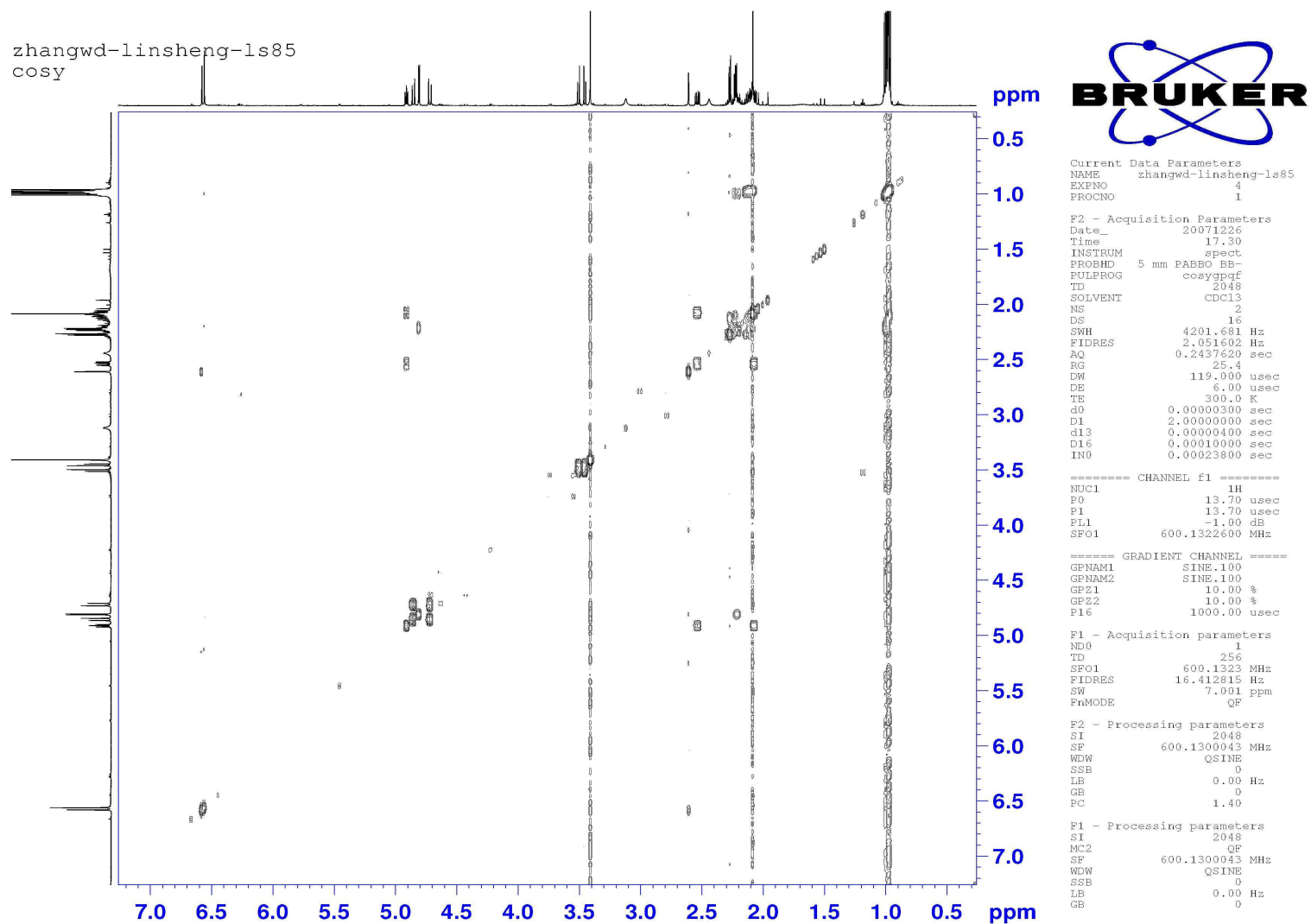
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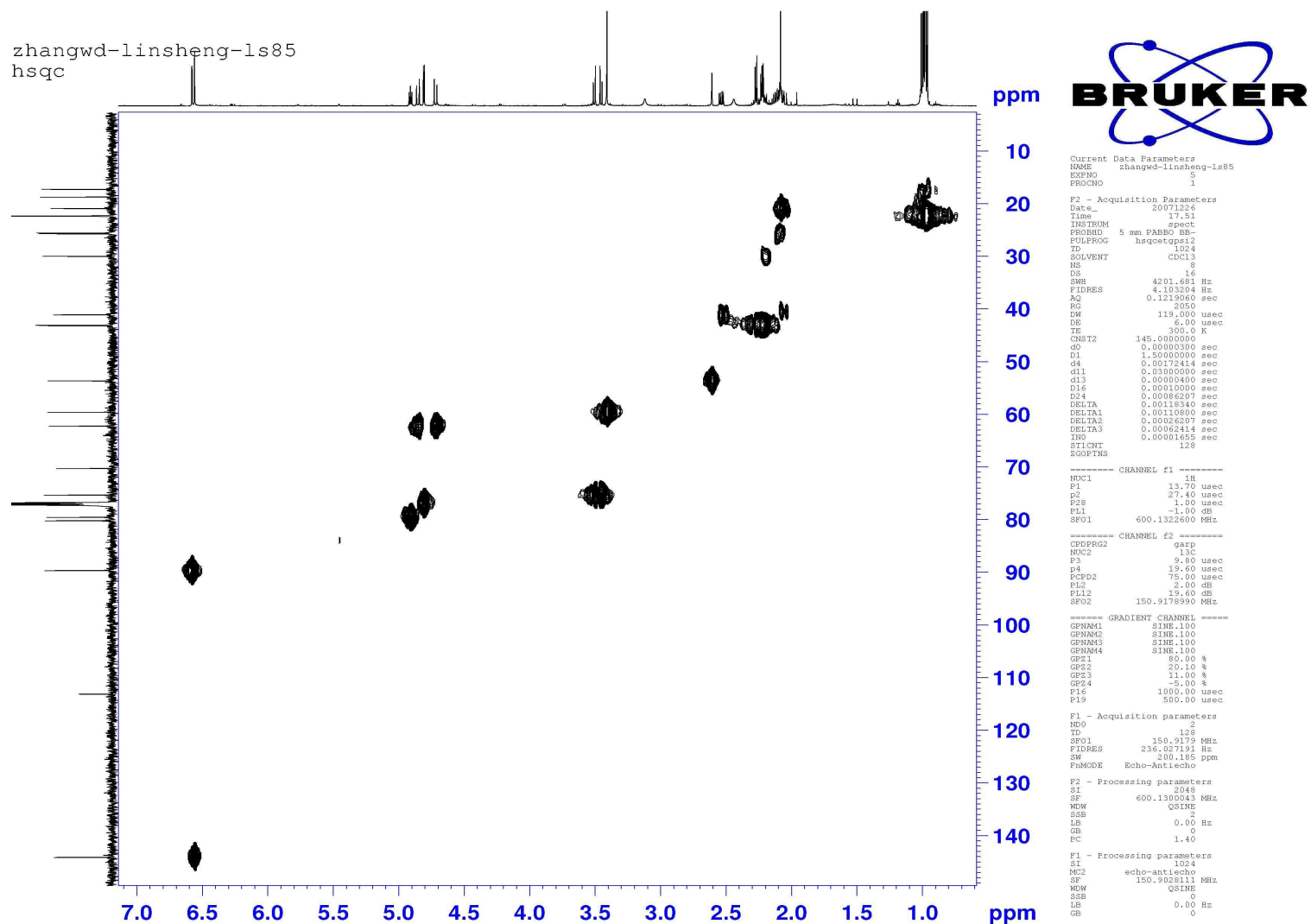
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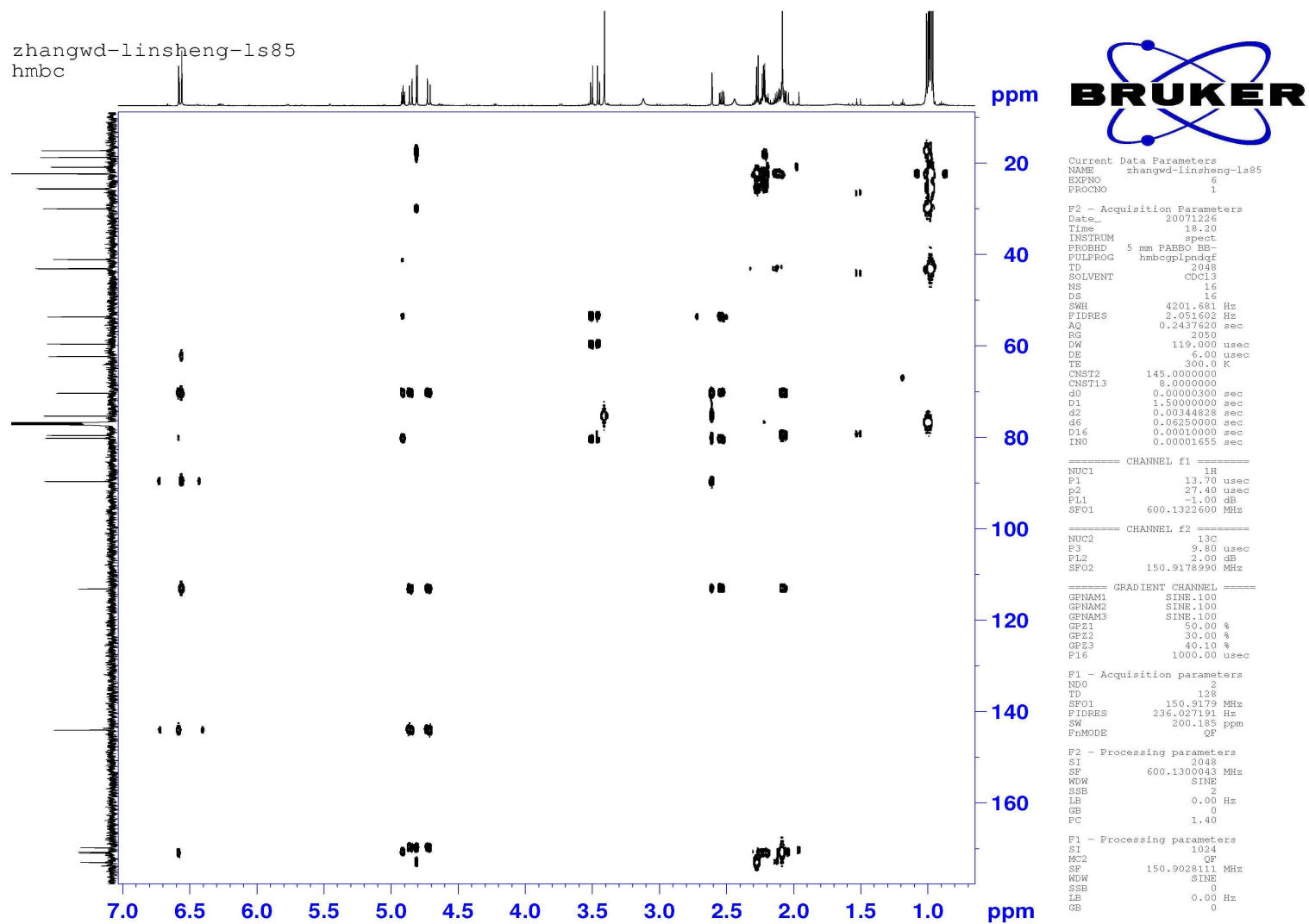
S30. The ^{13}C NMR and DEPT Spectra (150 MHz, CDCl_3) of Jatamanvaltrate E (5)



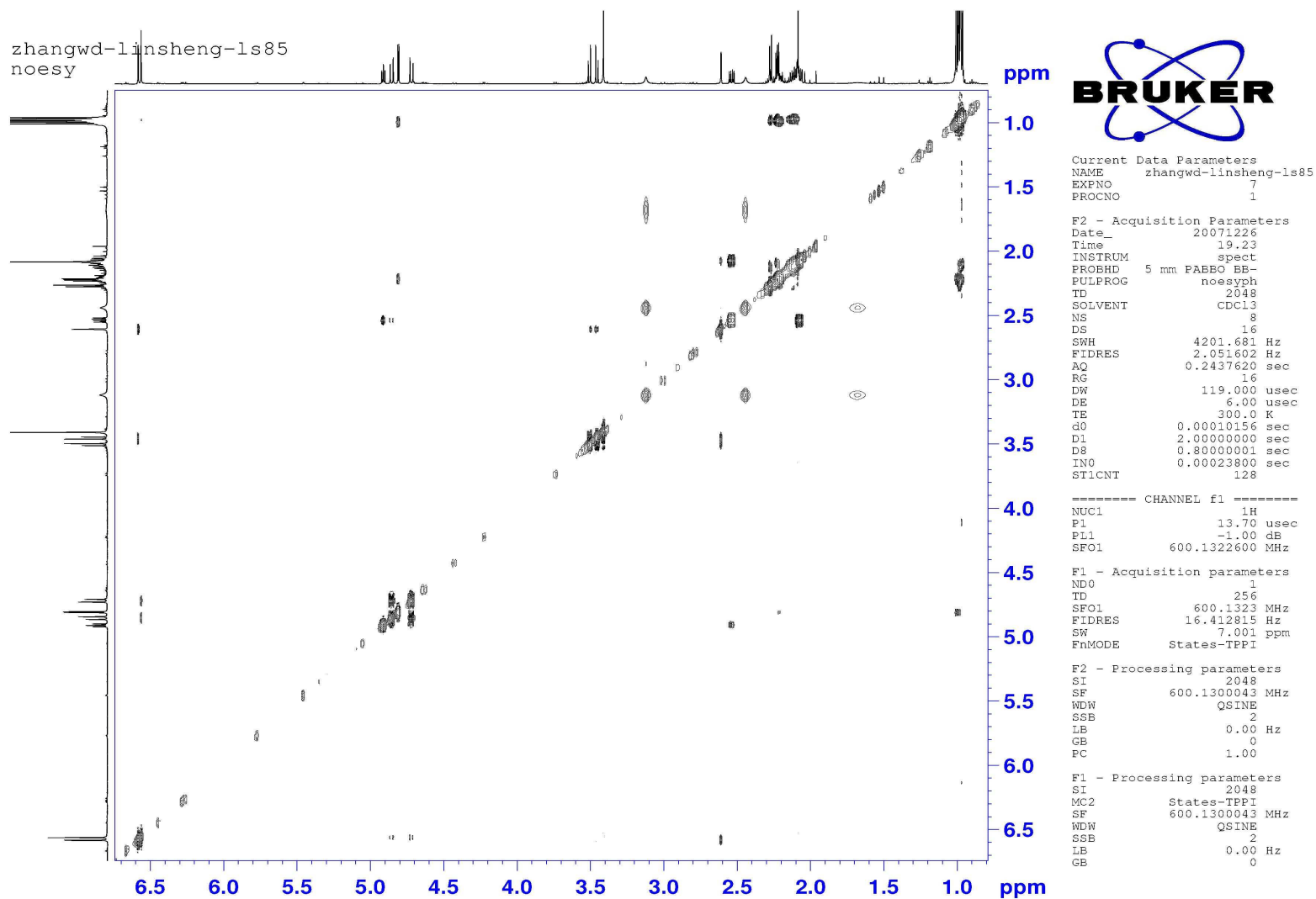
S31. The ^1H - ^1H COSY Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate E (5)



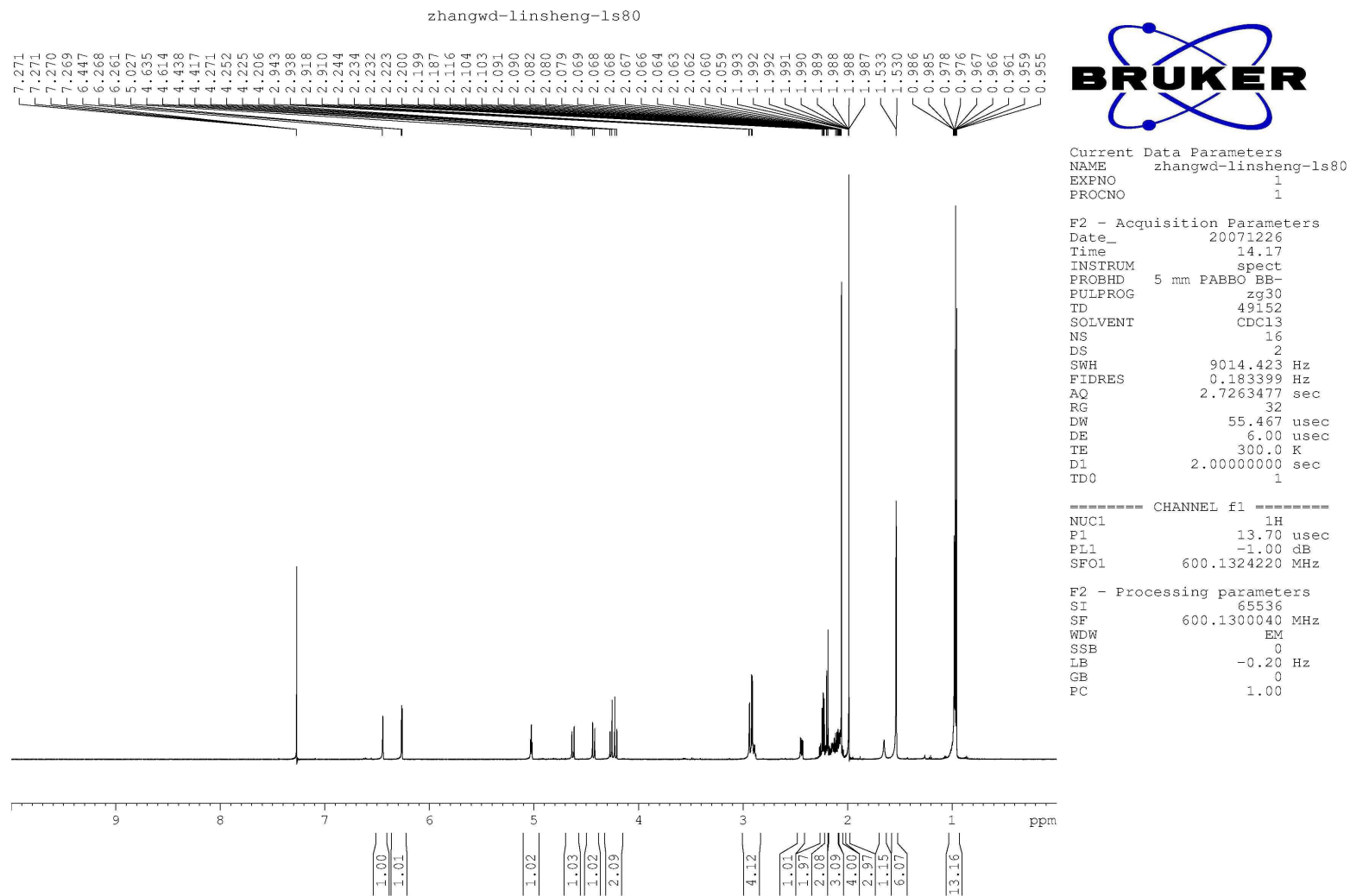
S32. The HSQC Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate E (5)



S33. The HMBNMR Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate E (5)

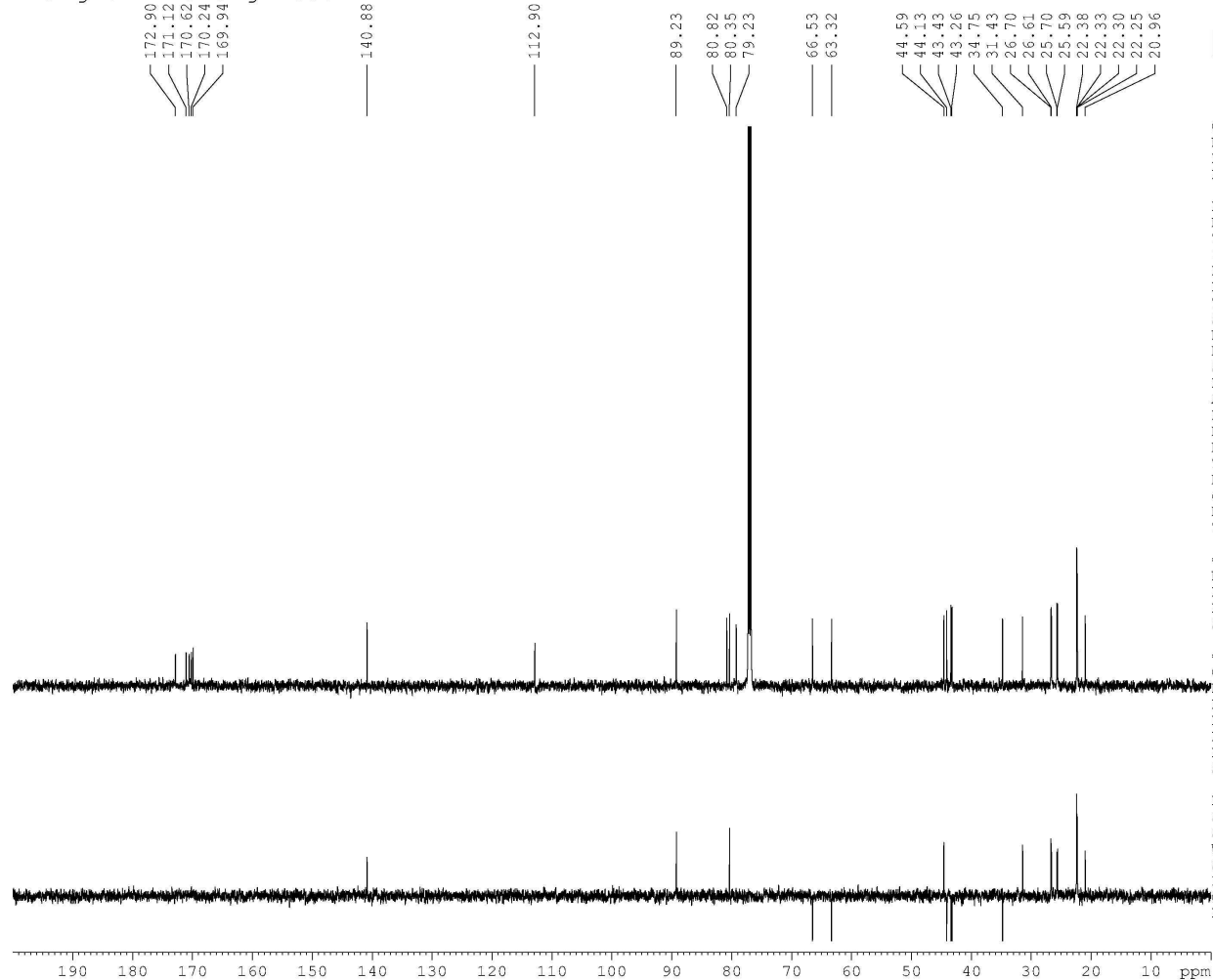


S34. The NOESY Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate E (5)



S35. The ^1H NMR Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate F (6)

zhangwd-linsheng-ls80



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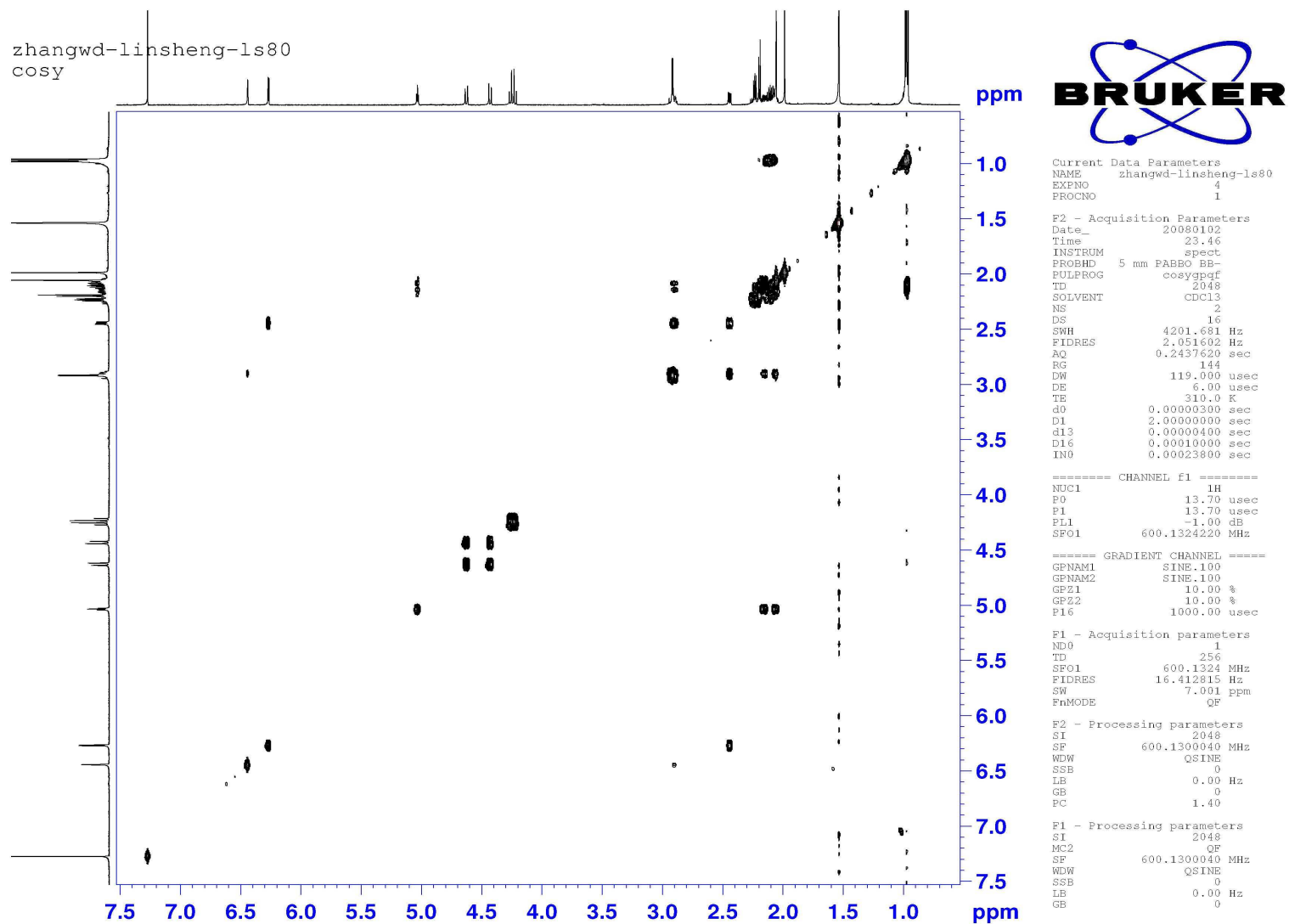
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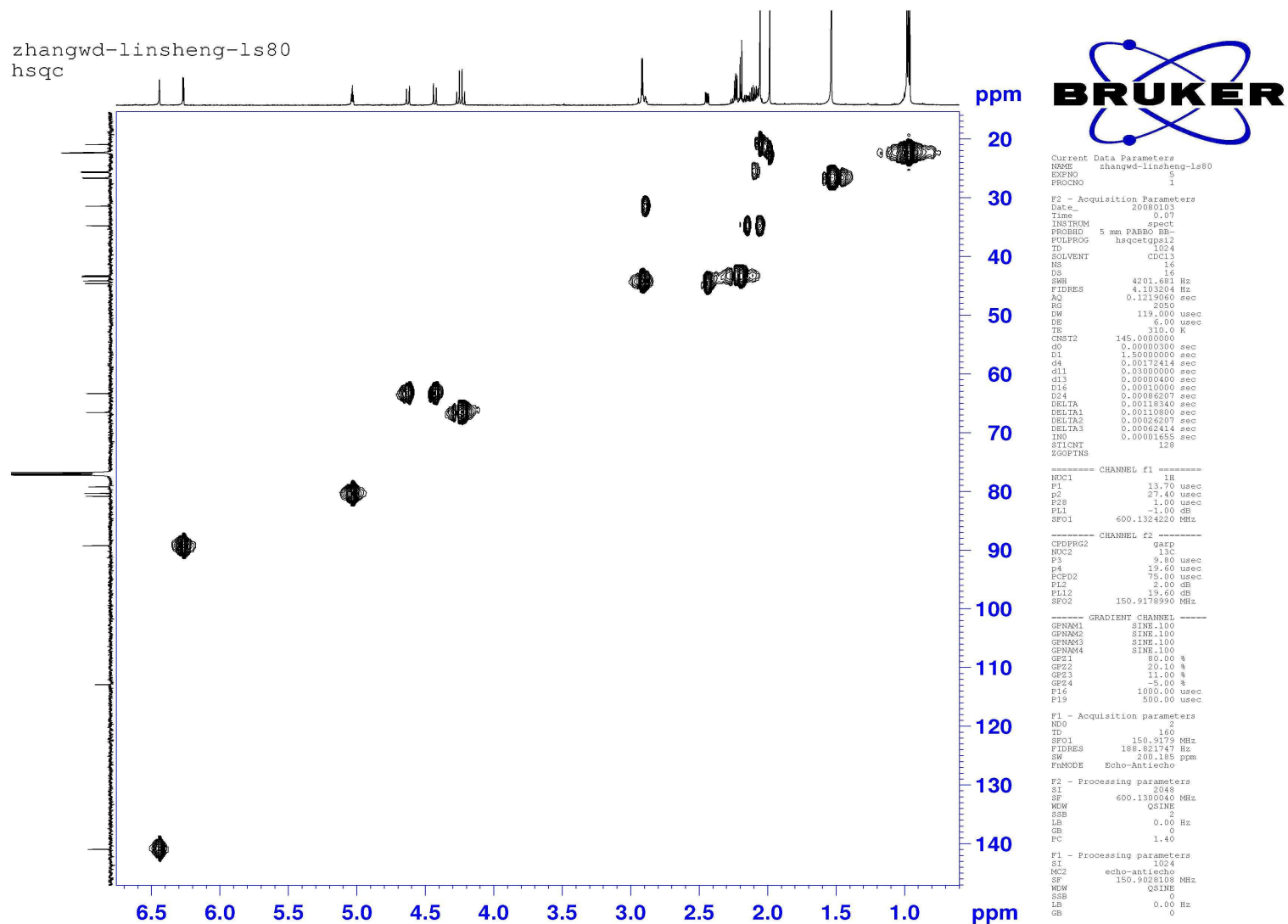
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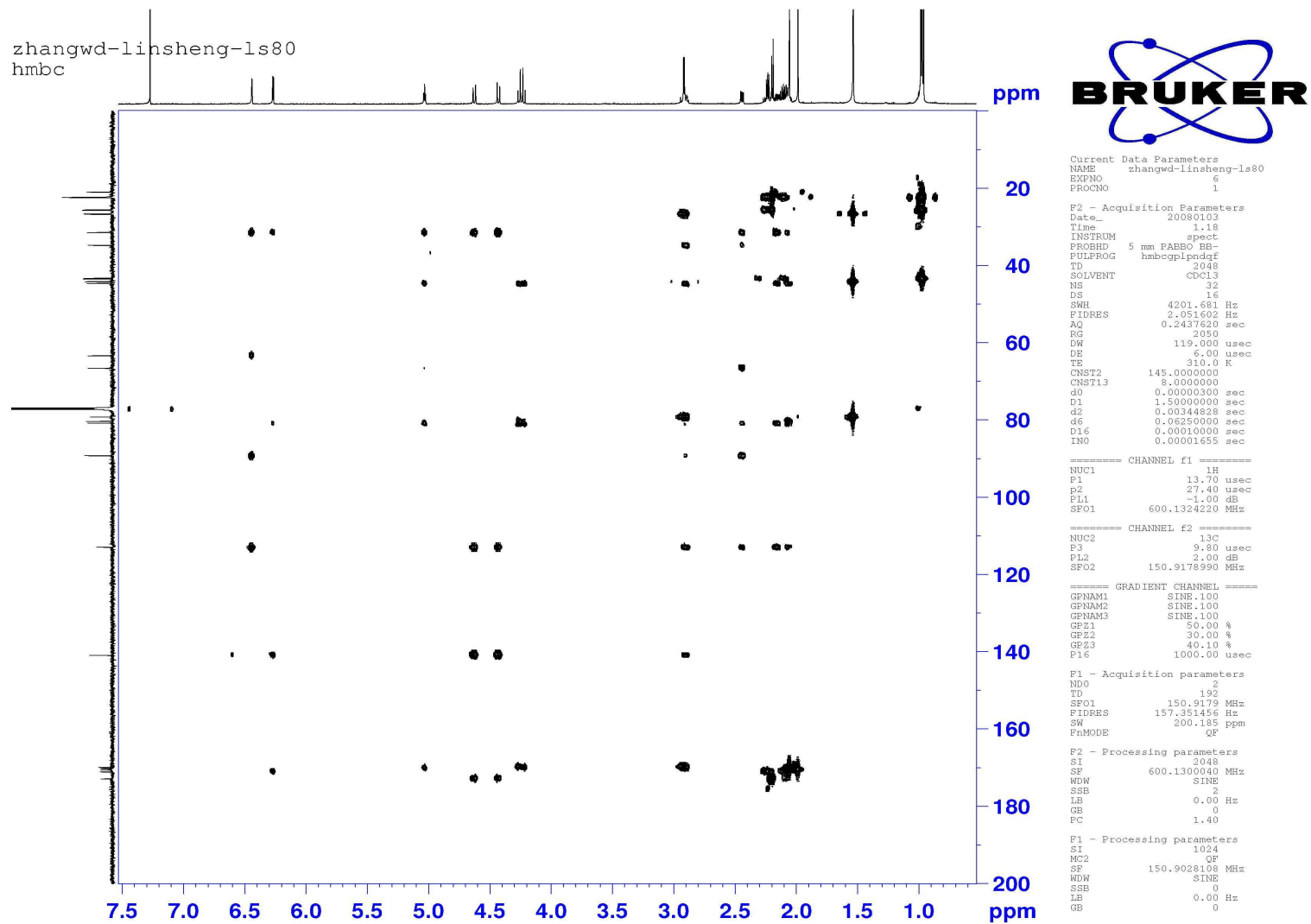
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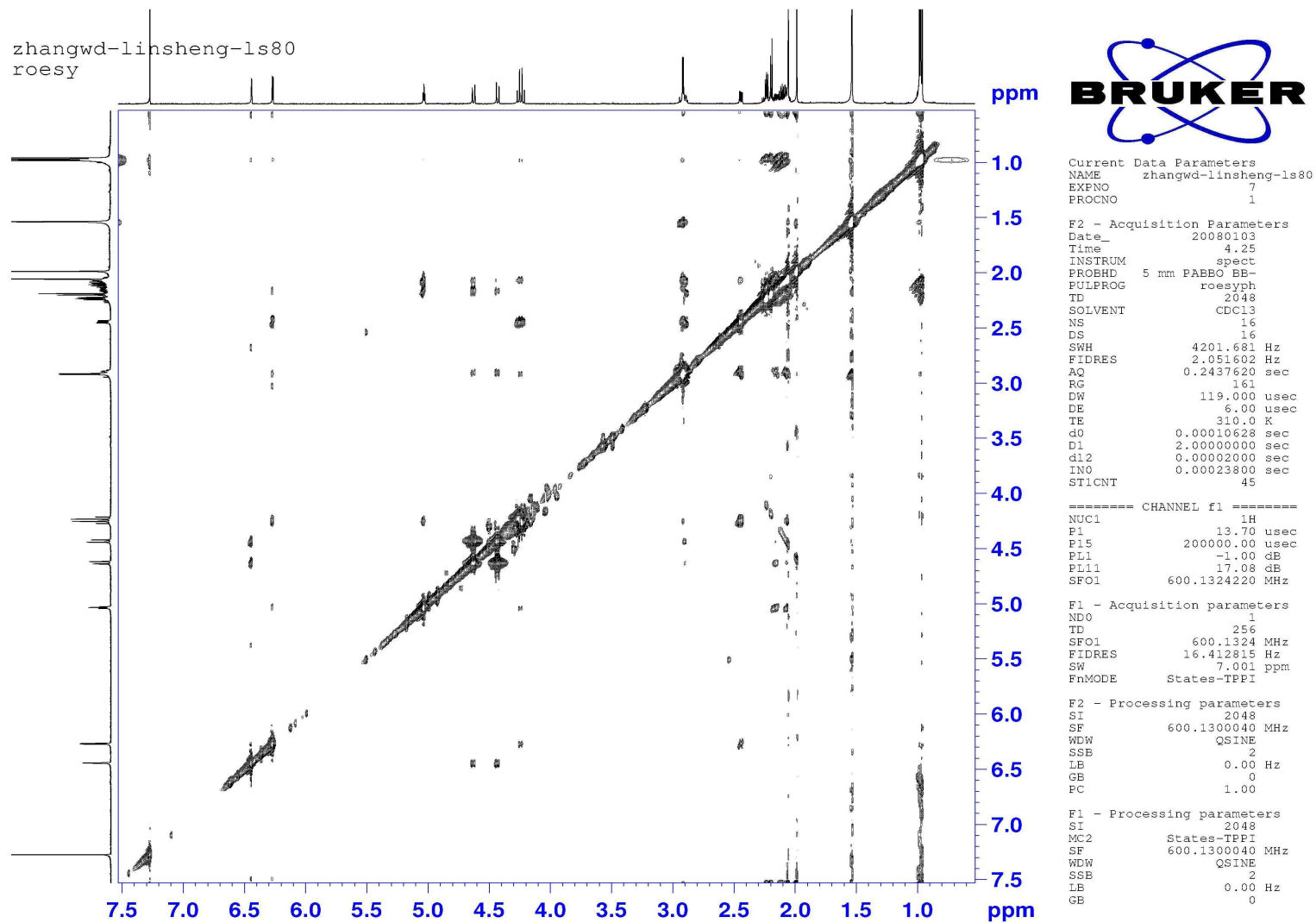
S37. The ^1H - ^1H COSY Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate F (6)



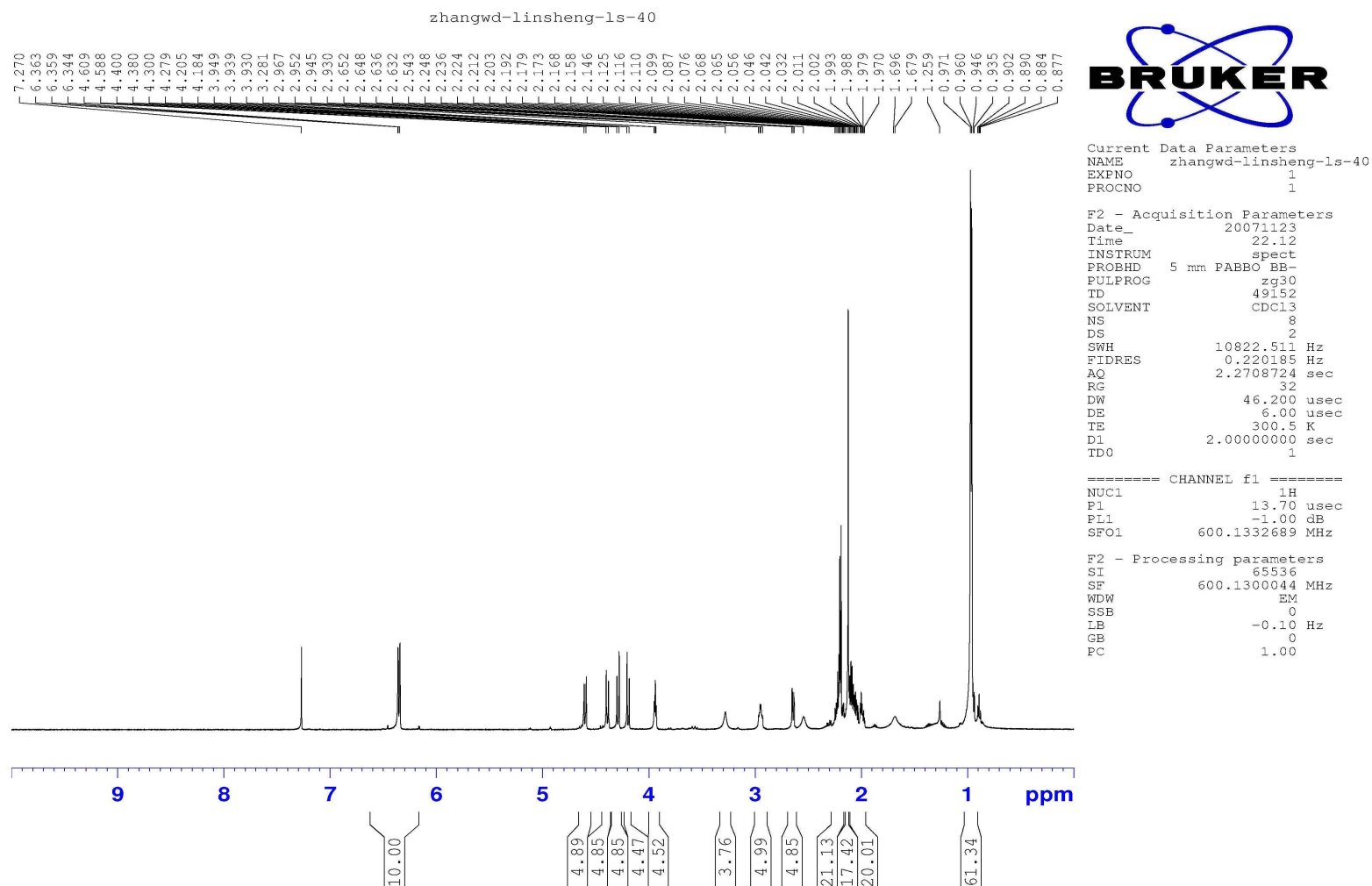
S38. The HSQC Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate F (6)



S39. The HMBC Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate F (6)

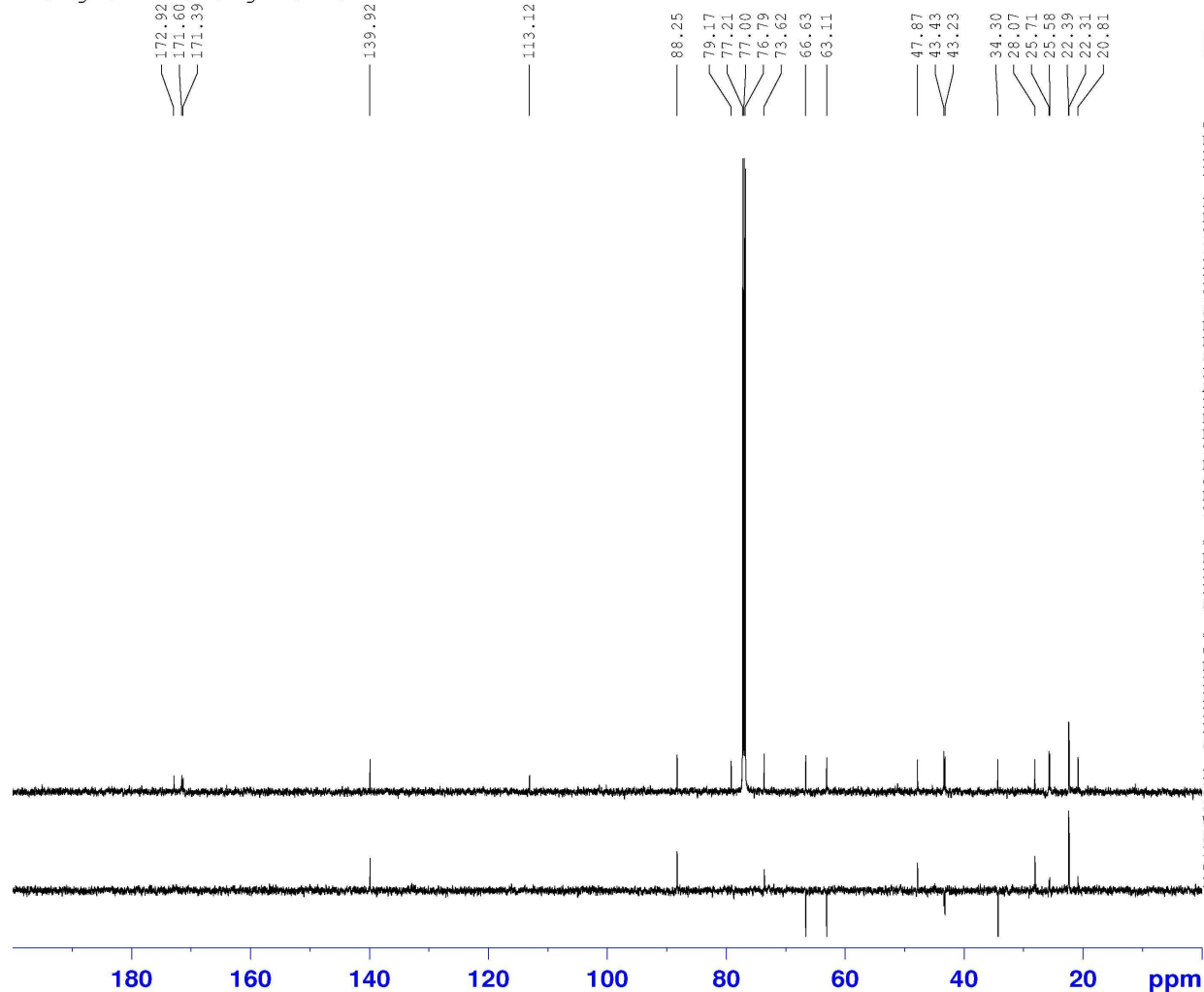


S40. The ROESY Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate F (6)



S41. The ^1H NMR Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate G (7)

zhangwd-linsheng-ls-40



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EXPNO 2
PROCNO 1

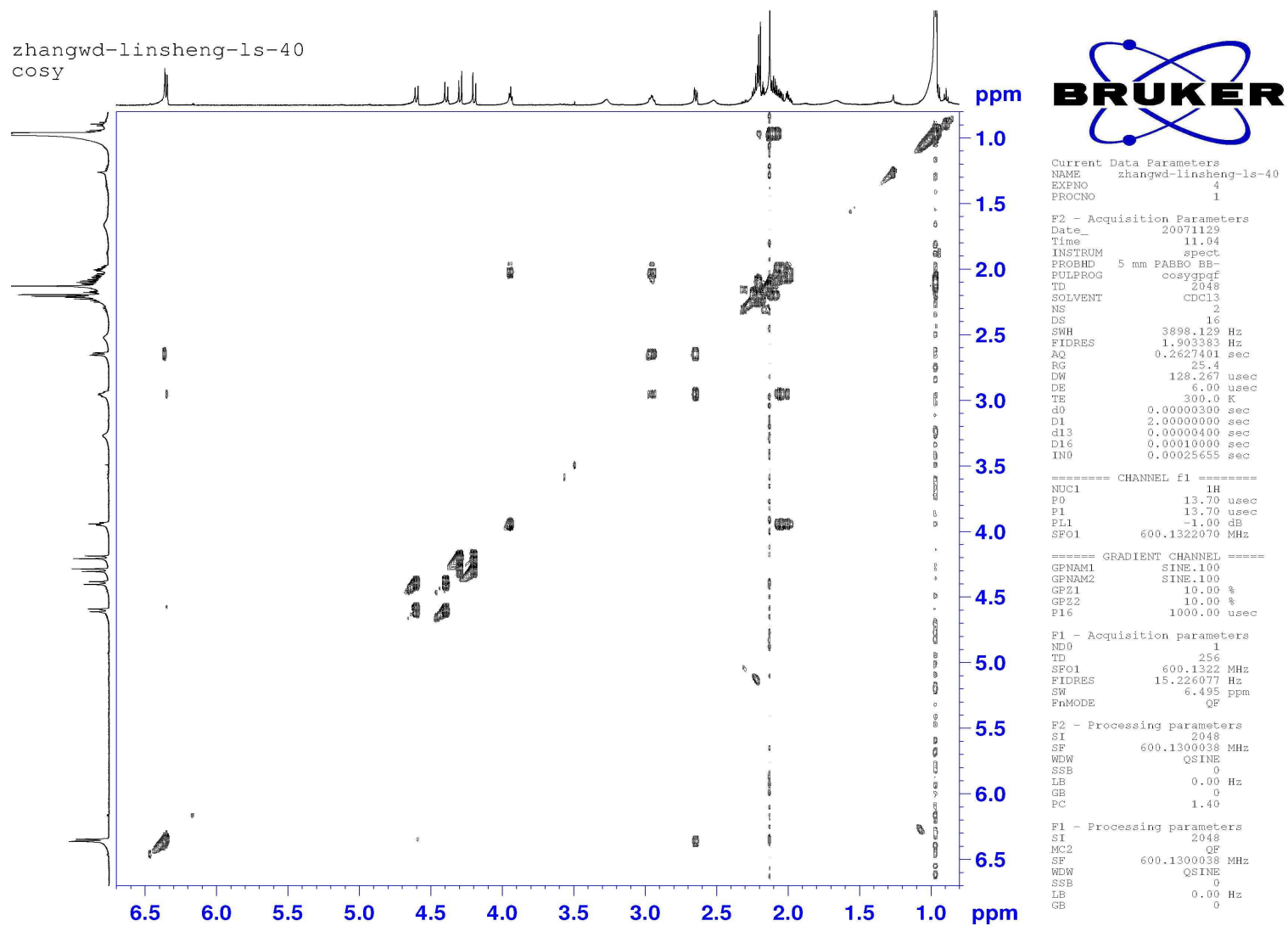
F2 - Acquisition Parameters
Date_ 20071123
Time 22.25
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 278
DS 2
SWH 45454.547 Hz
FIDRES 0.693581 Hz
AQ 0.7209460 sec
RG 32768
DW 11.000 usec
DE 6.00 usec
TE 300.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 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

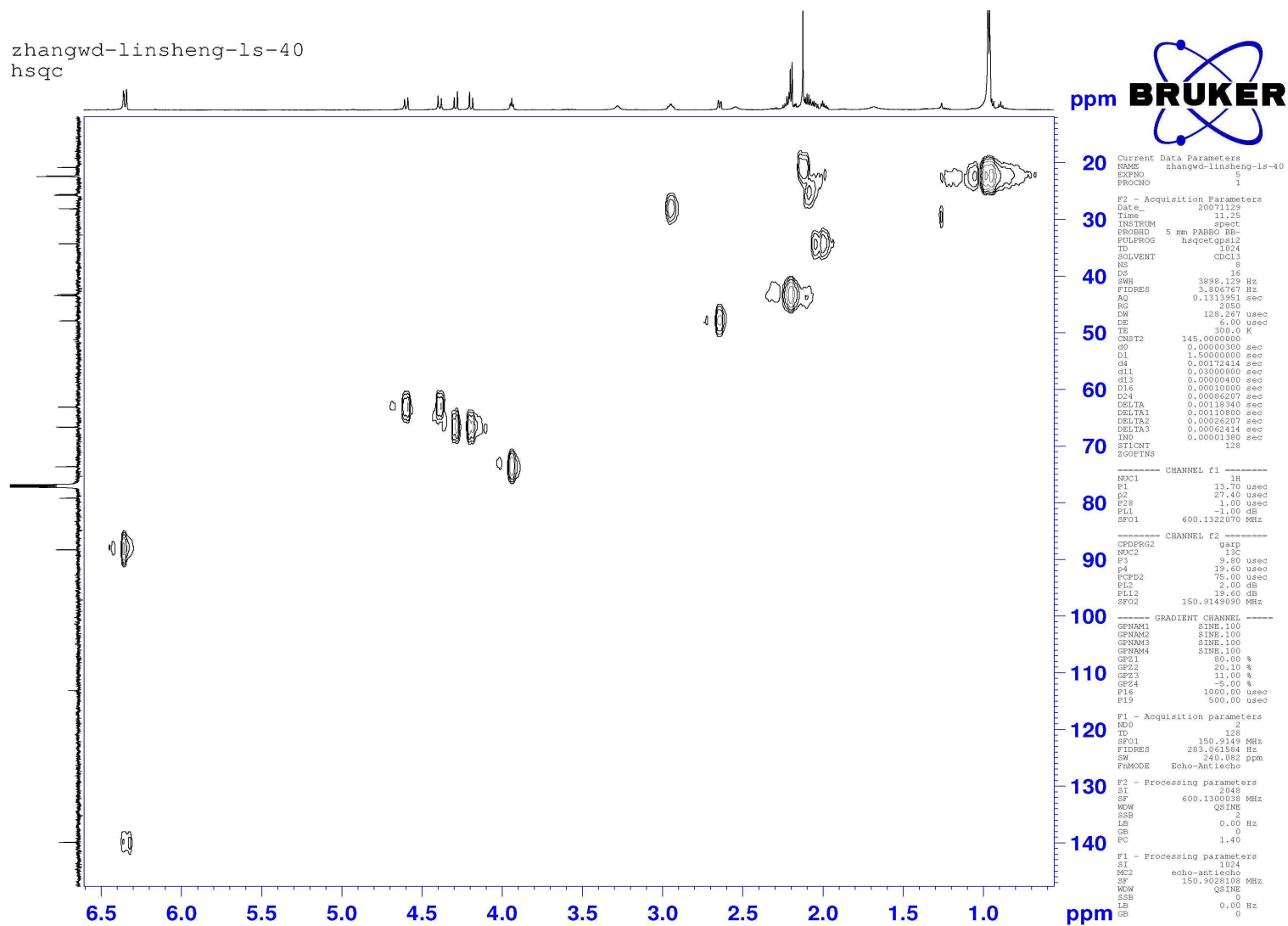
F2 - Processing parameters
SI 65536
SF 150.9028108 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

S42. The ^{13}C NMR and DEPT Spectra (150 MHz, CDCl_3) of Jatamanvaltrate G (7)

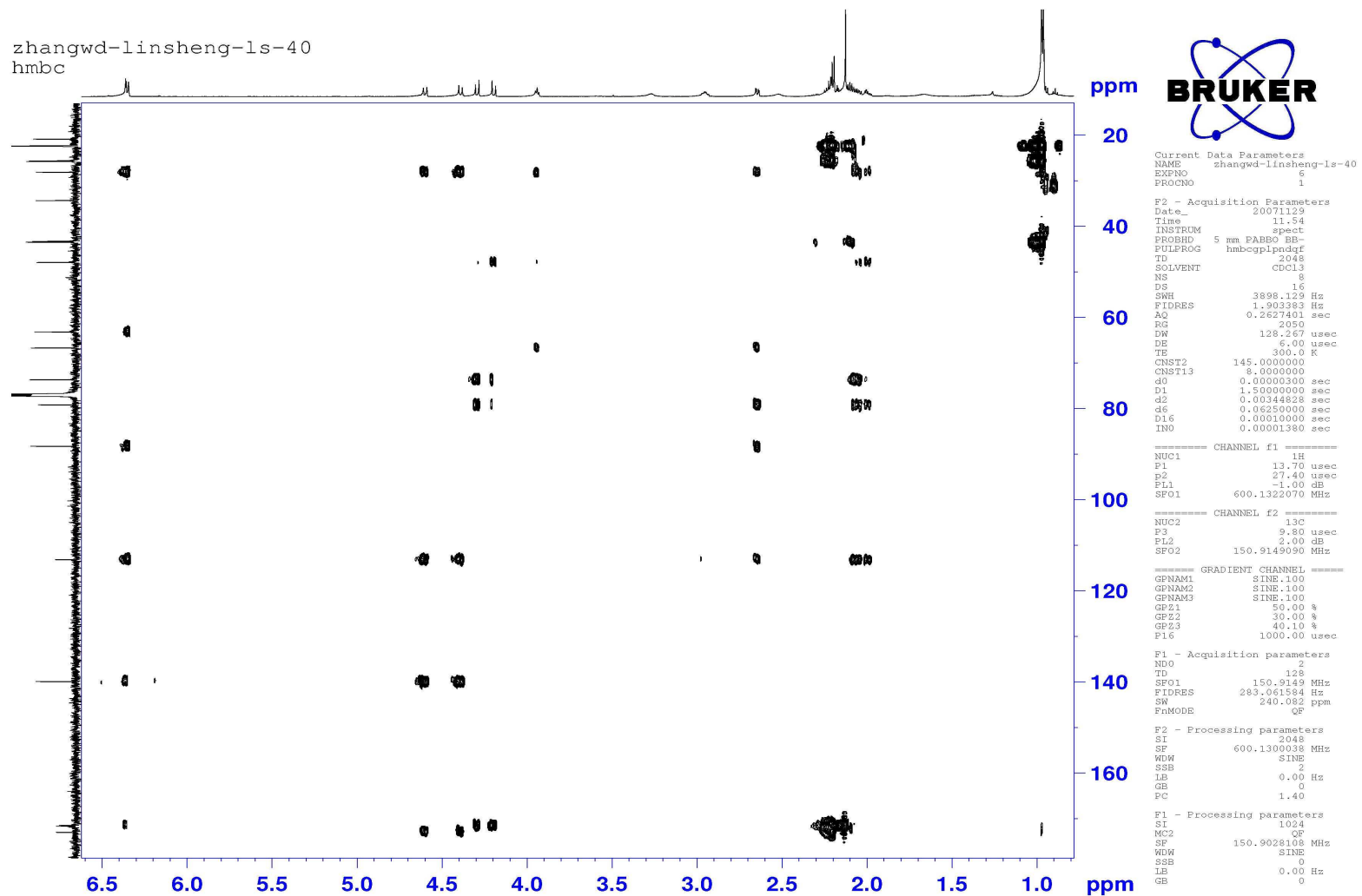


S43. The ^1H - ^1H COSY Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate G (7)

zhangwd-linsheng-ls-40
hsqc

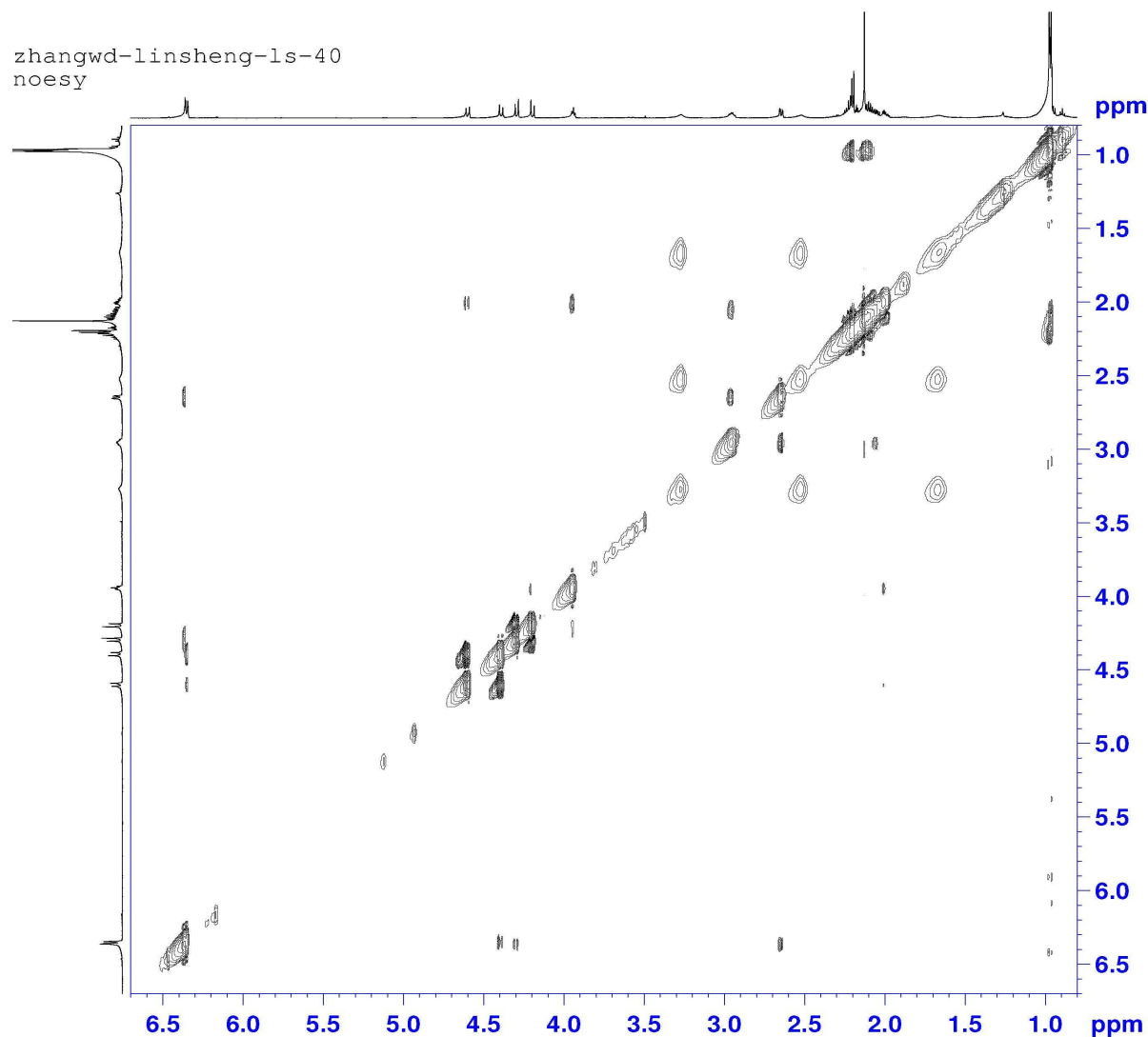


S44. The HSQC Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate G (7)



S45. The HMBC Spectrum (600 MHz, CDCl_3) 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 noesyph
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
D8 0.80000001 sec
IN0 0.00025655 sec
STICNT 128

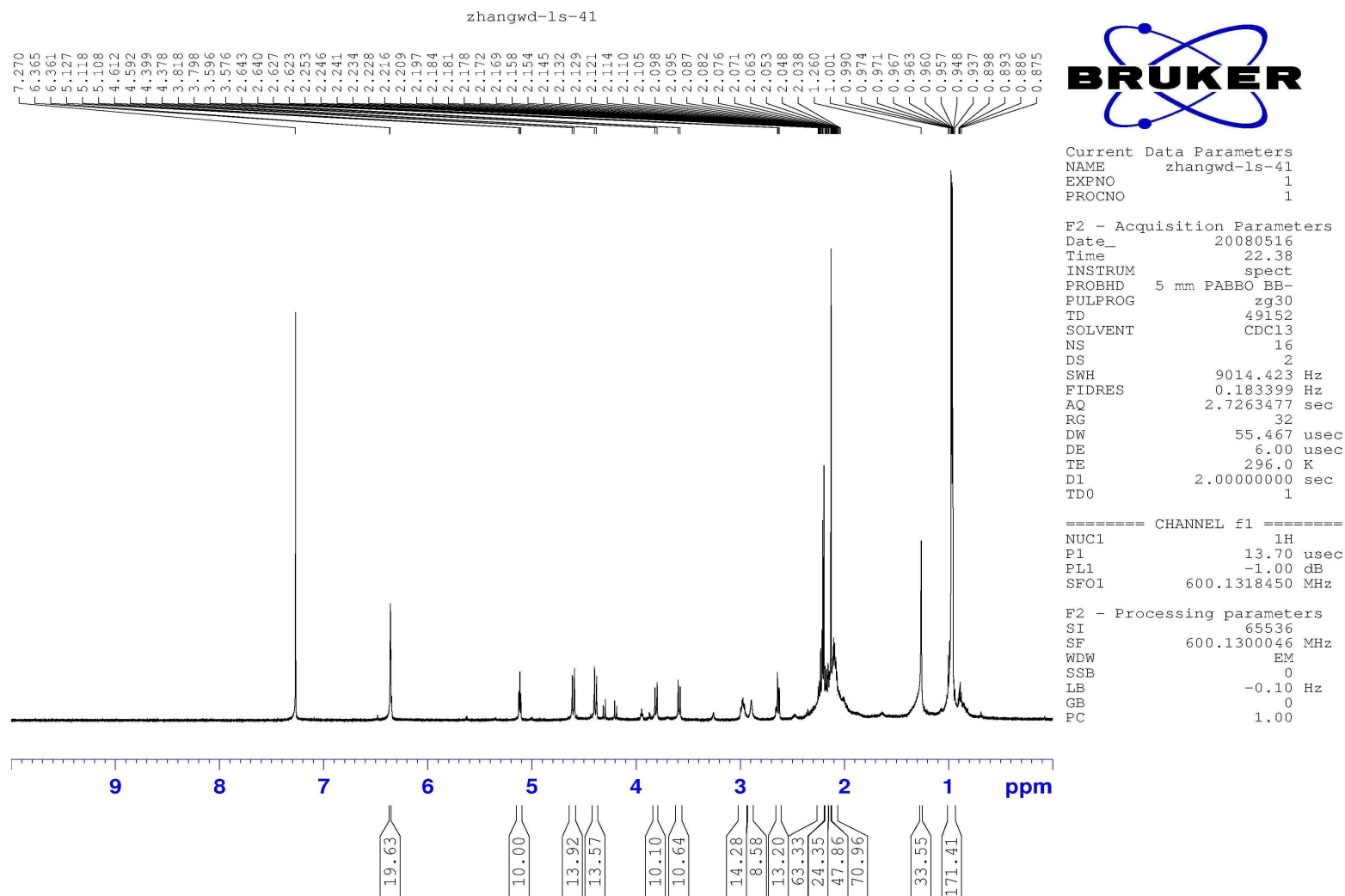
----- CHANNEL f1 -----
NUC1 1H
P1 13.70 usec
PL1 -1.00 dB
SFO1 600.1322070 MHz

F1 - Acquisition parameters
ND0 1
TD 128
SFO1 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

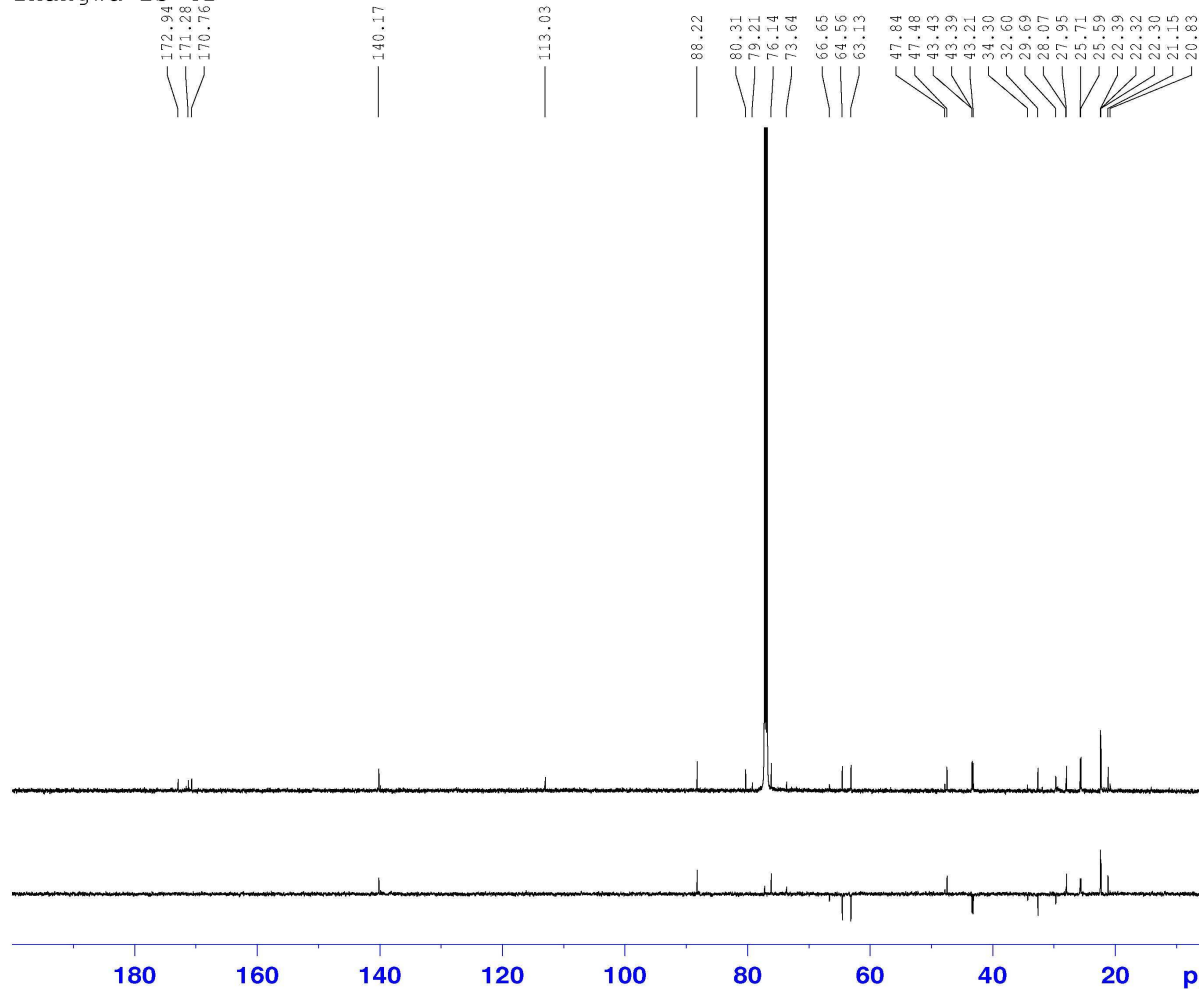
F1 - Processing parameters
SI 2048
MC2 States-TPPI
SF 600.1300038 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

S46. The NOESY Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate G (7)



S47. The ^1H NMR Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate H (8)

zhangwd-ls-41



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

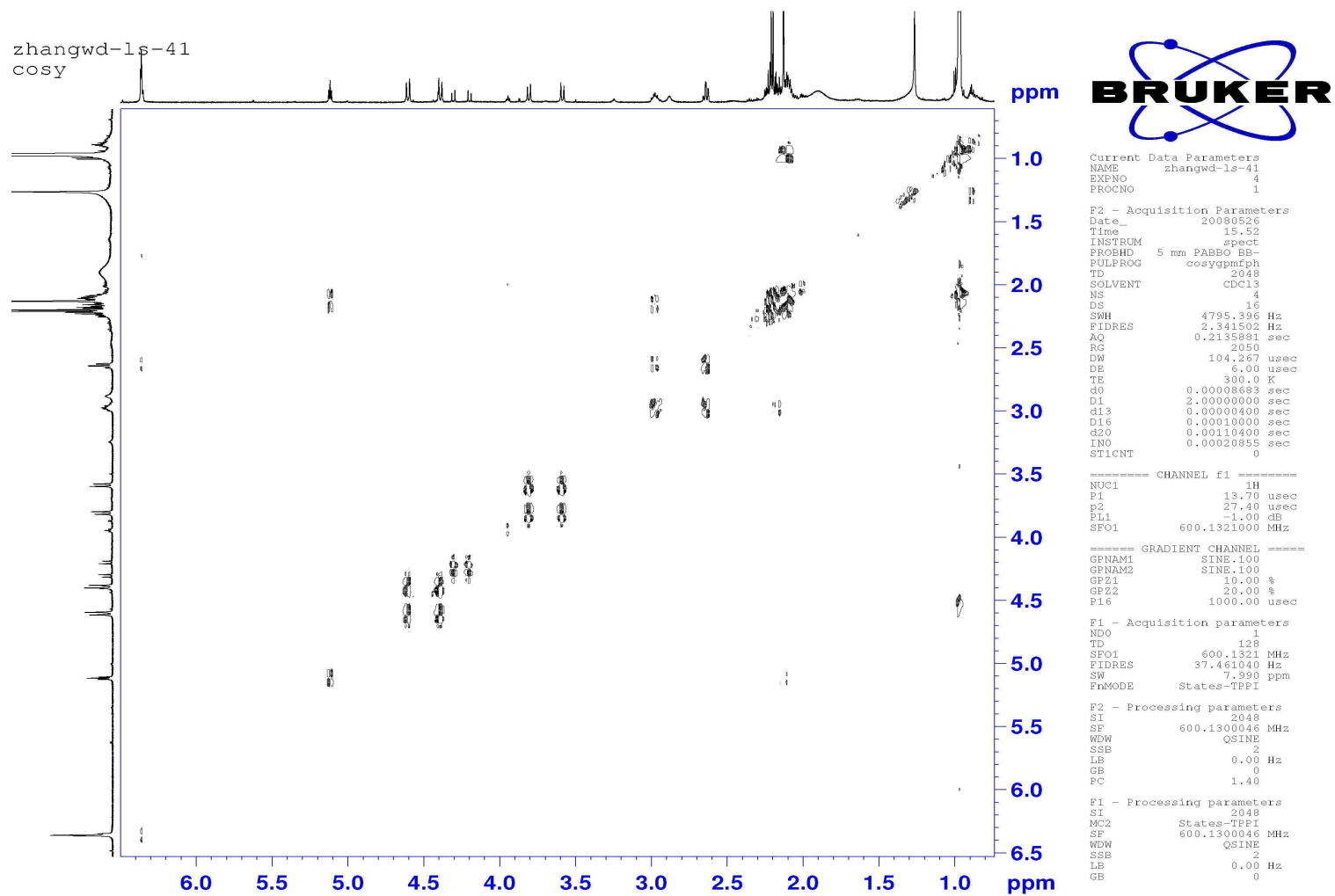
F2 - Acquisition Parameters
 Date_ 20080517
 Time 2.06
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 4096
 DS 0
 SWH 45454.547 Hz
 FIDRES 0.693581 Hz
 AQ 0.7209460 sec
 RG 32768
 DW 11.000 usec
 DE 6.00 usec
 TE 298.7 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.899999998 sec
 TD0 1

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

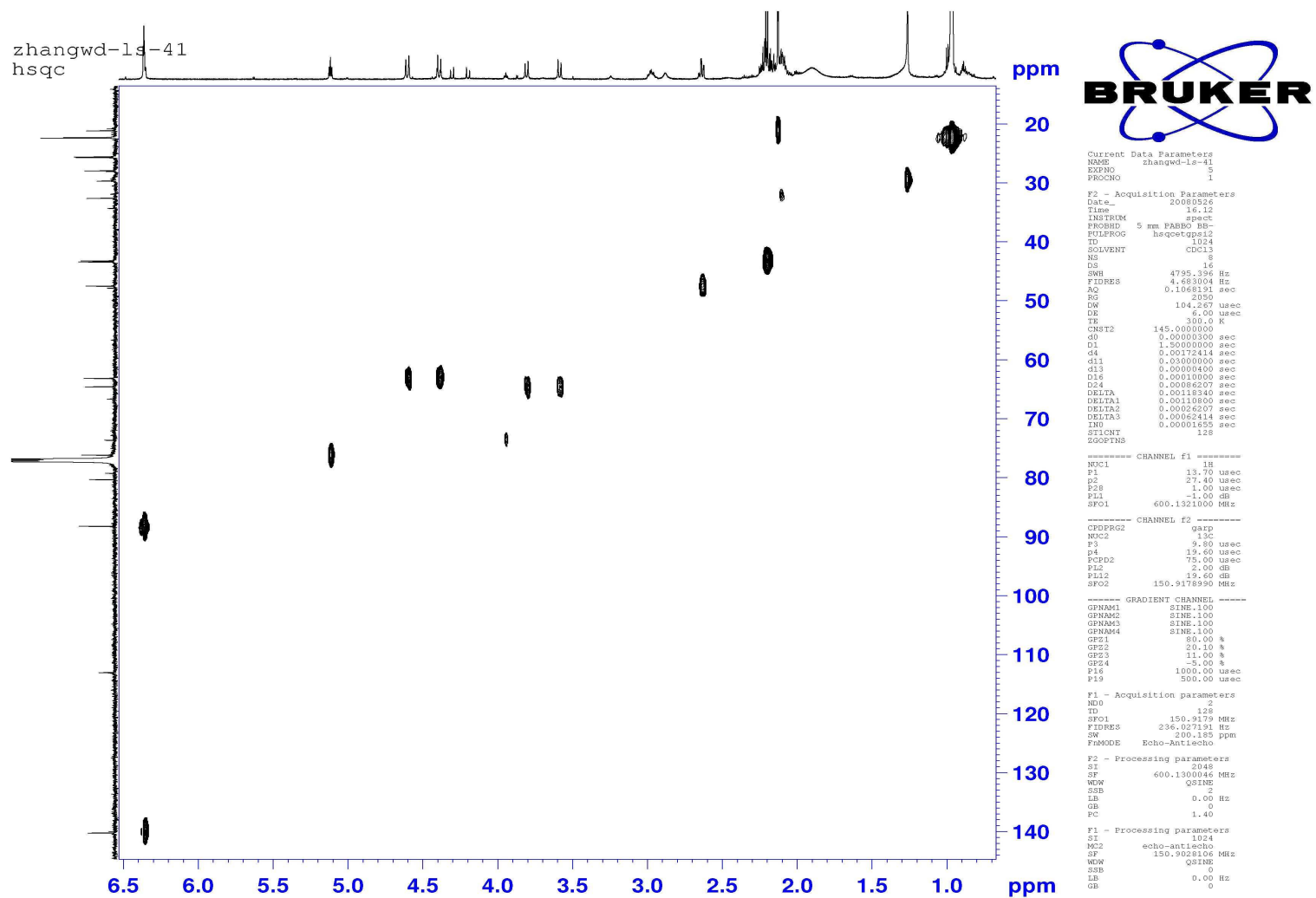
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 14.00 dB
 PL13 14.00 dB
 SFO2 600.1324005 MHz

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

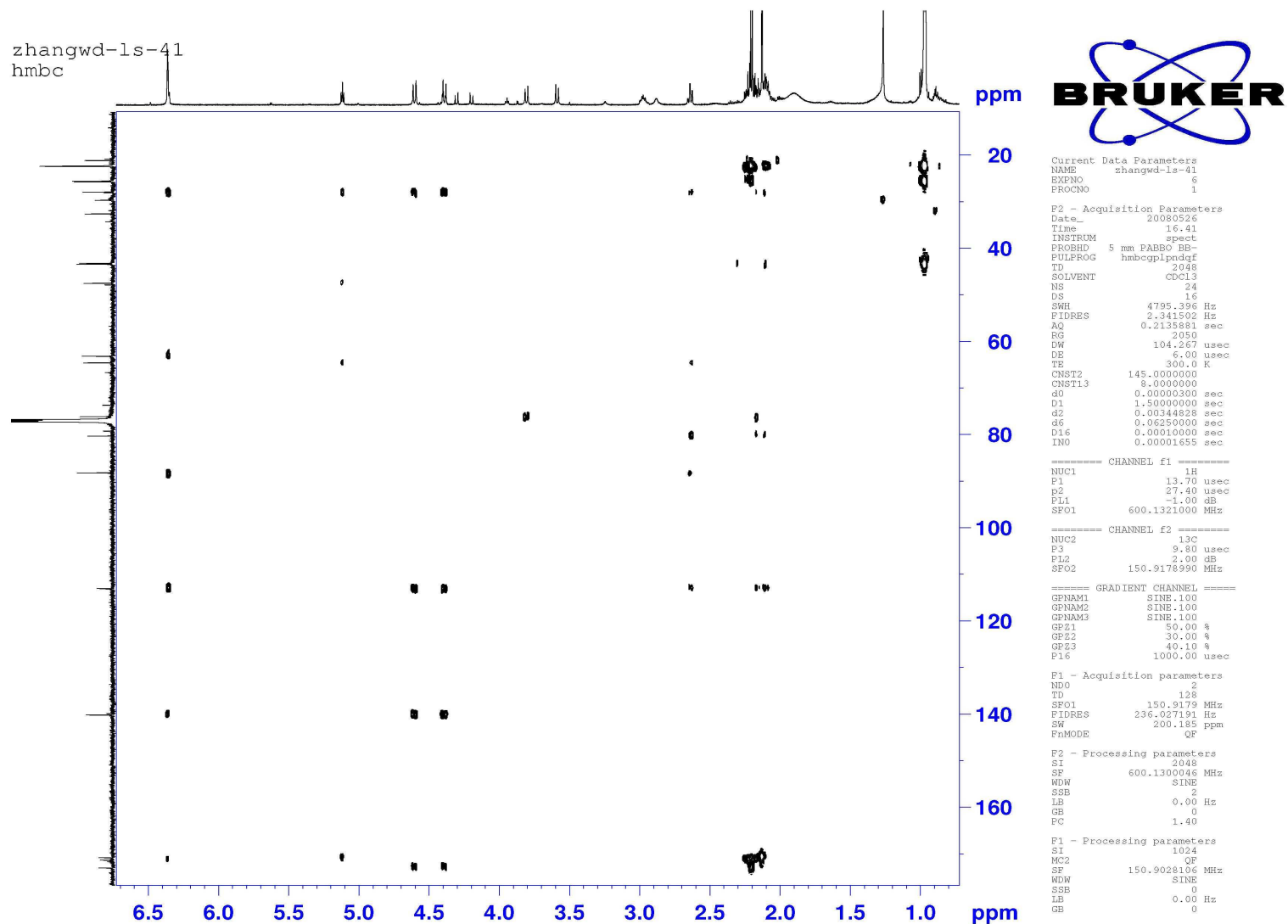
S48. The ^{13}C NMR and DEPT Spectra (150 MHz, CDCl_3) of Jatamanvaltrate H (8)



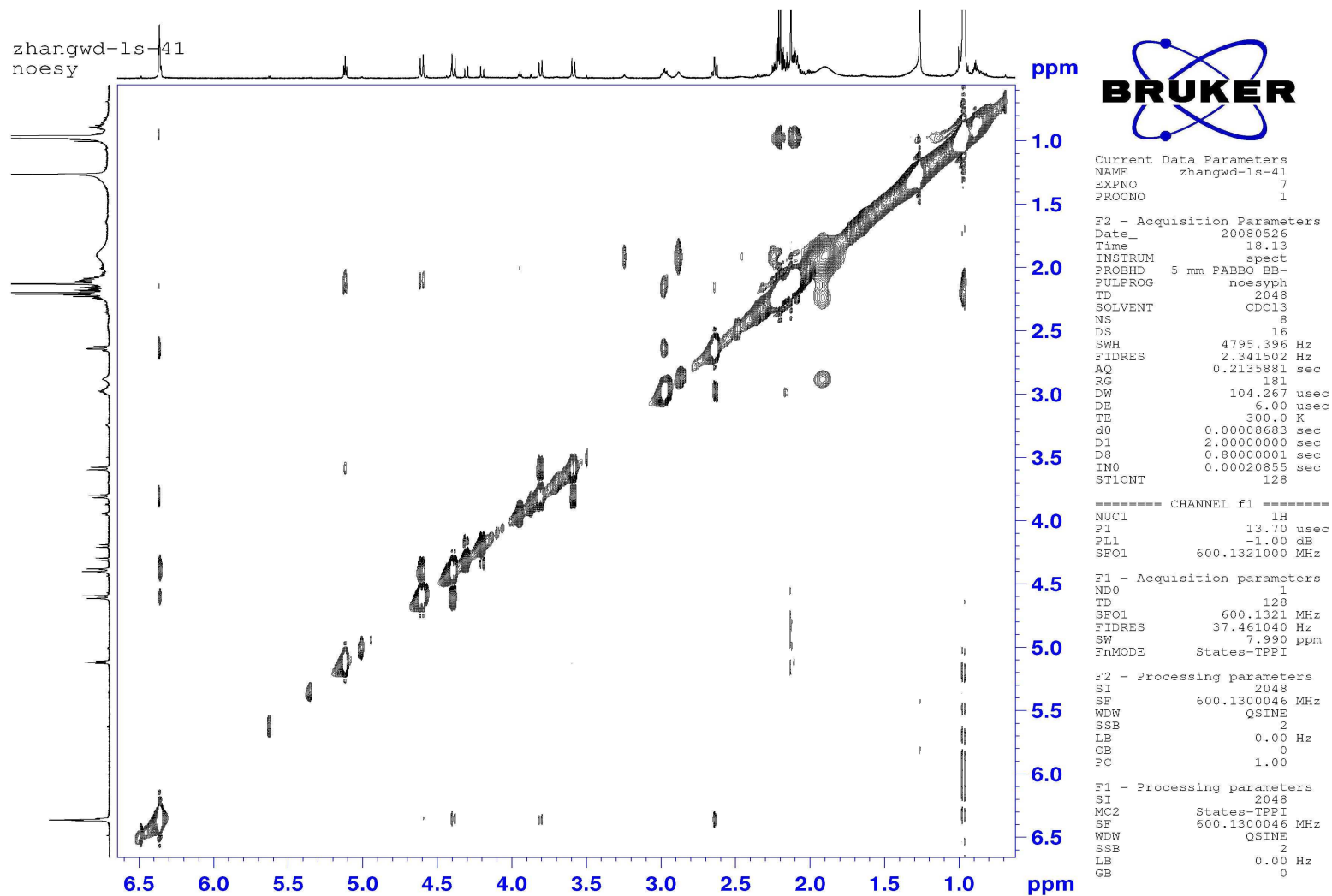
S49. The ^1H - ^1H COSY Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate H (8)



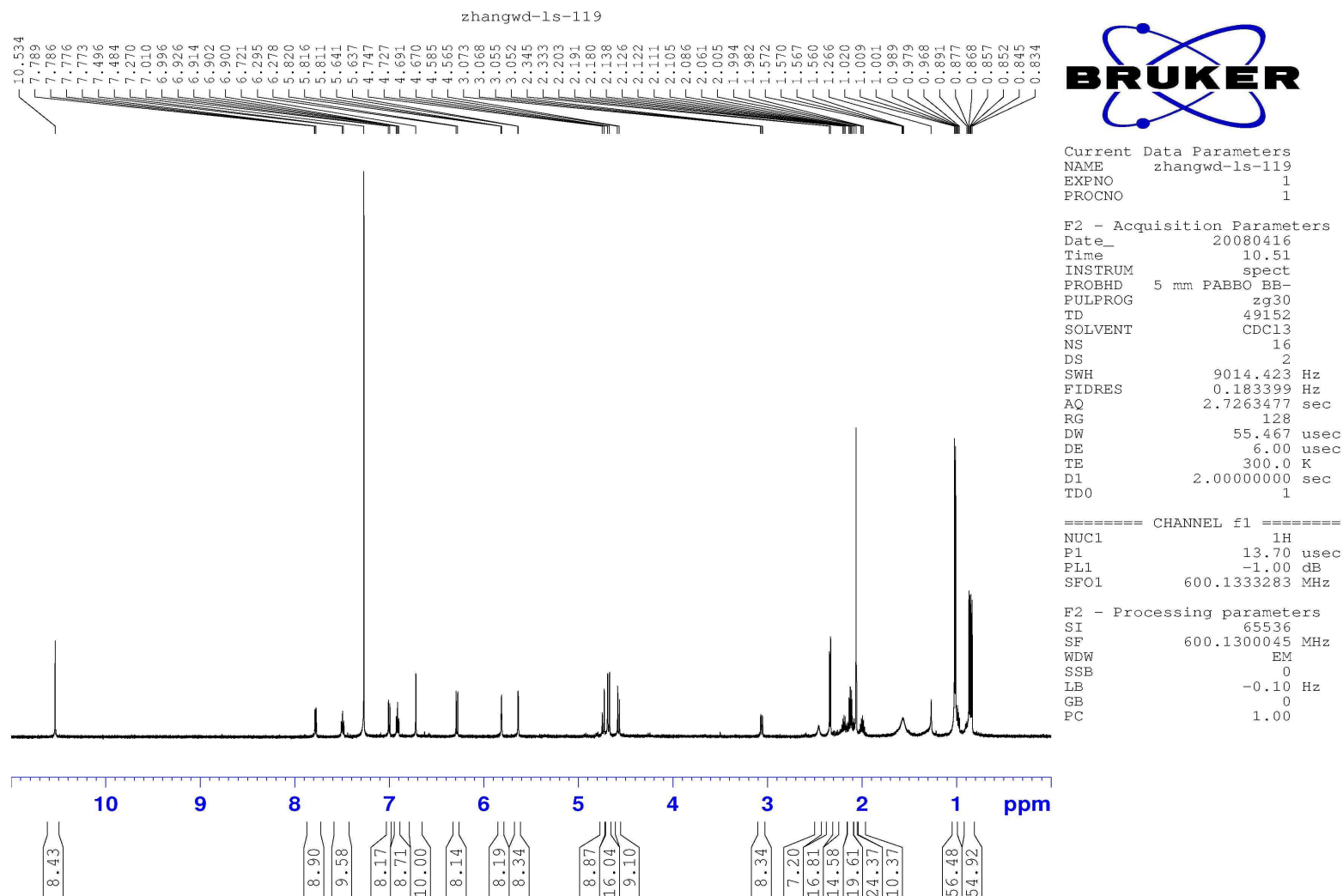
S50. The HSQC Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate H (8)



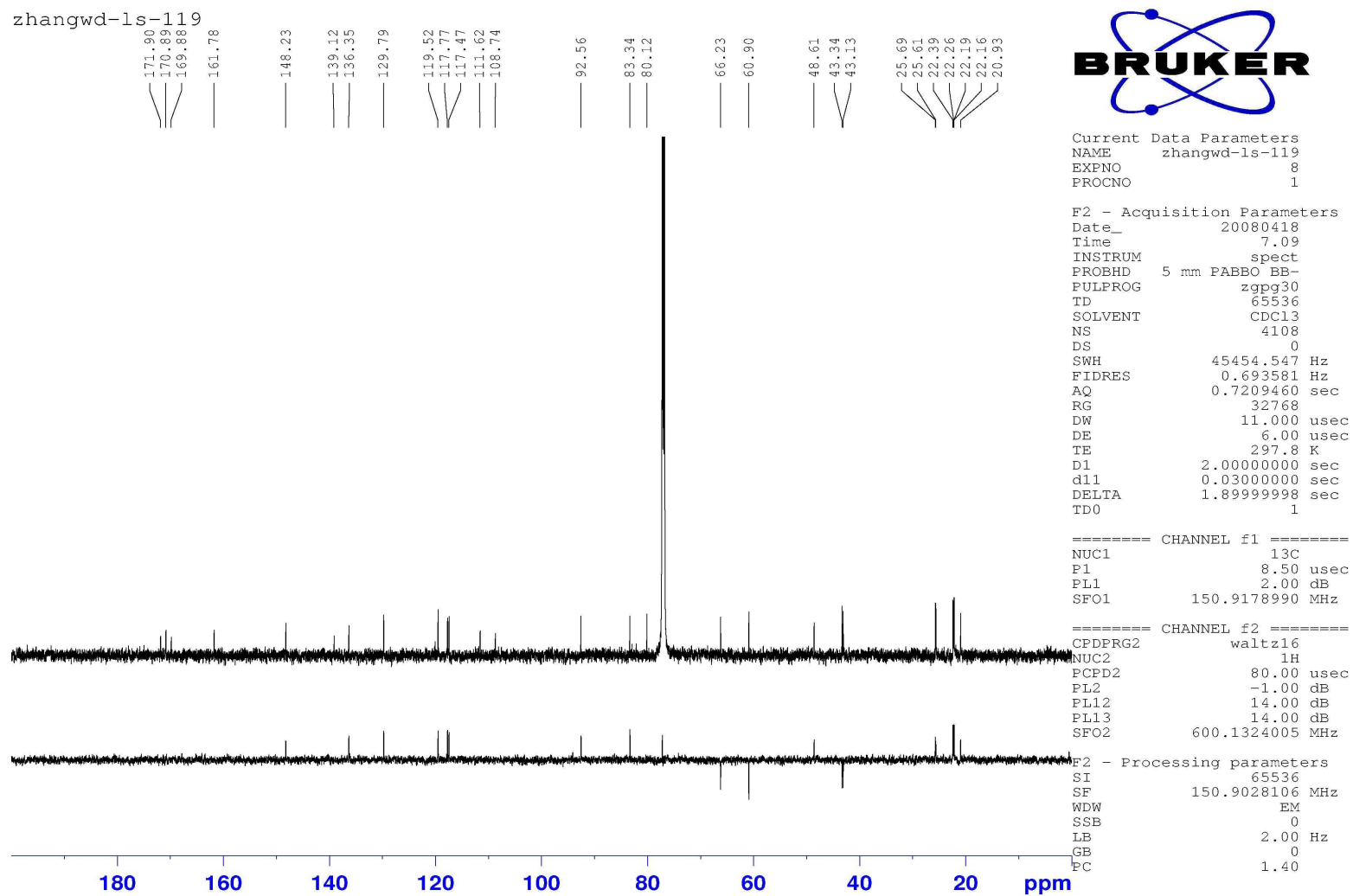
S51. The HMBC Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate H (8)



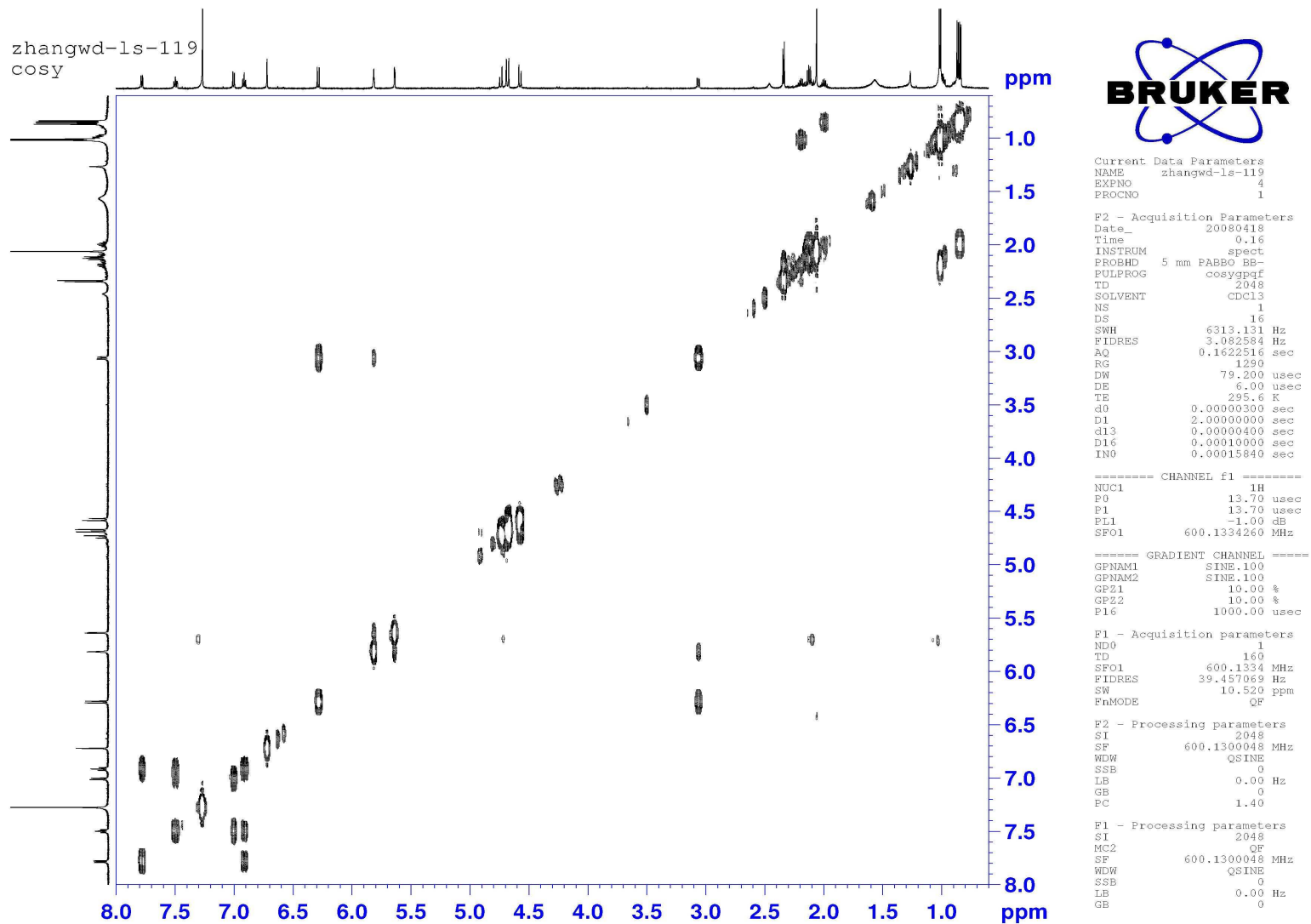
S52. The NOESY Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate H (8)



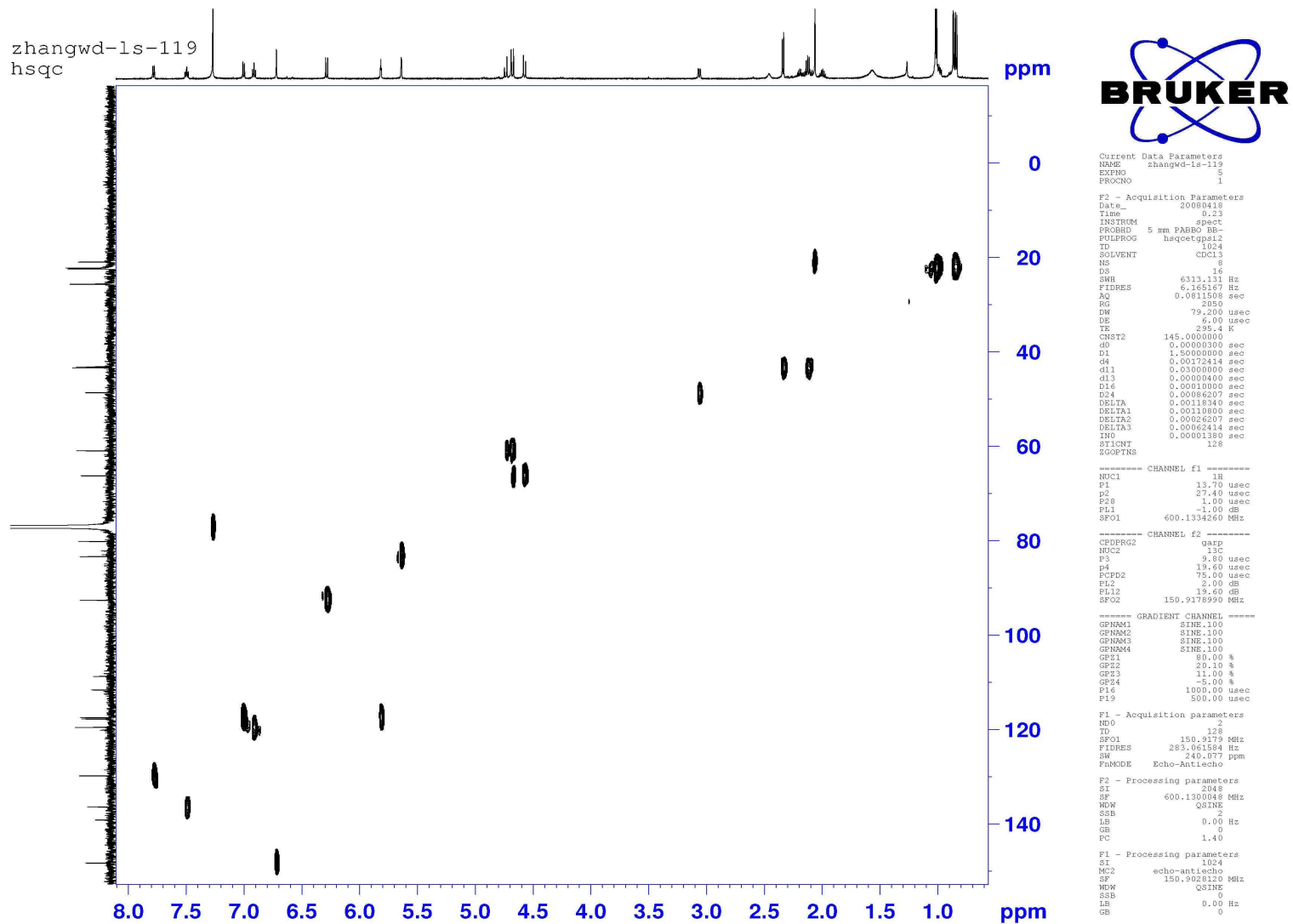
S53. The ^1H NMR Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate I (9)



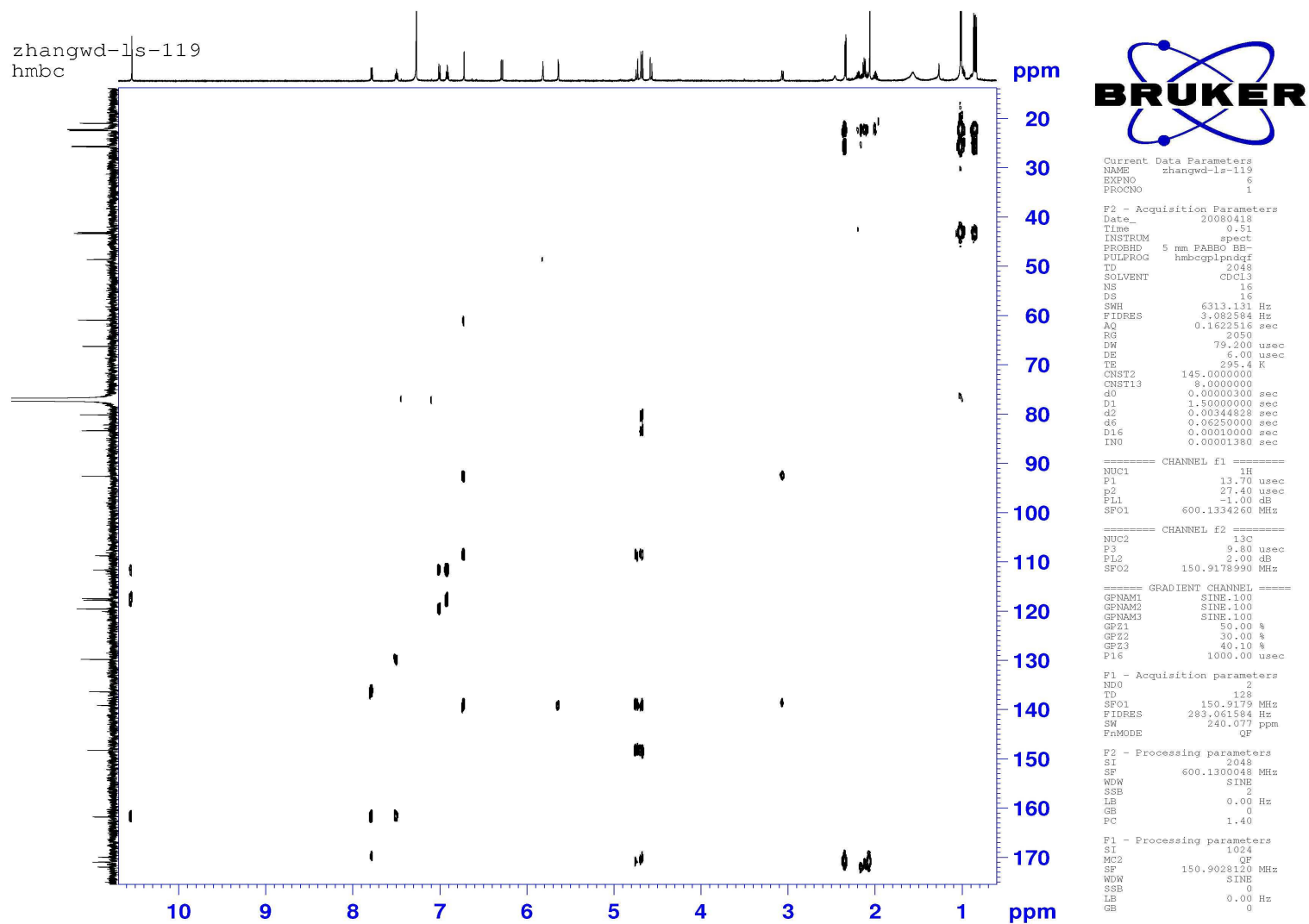
S54. The ^{13}C NMR and DEPT Spectra (150 MHz, CDCl_3) of Jatamanvaltrate I (9)



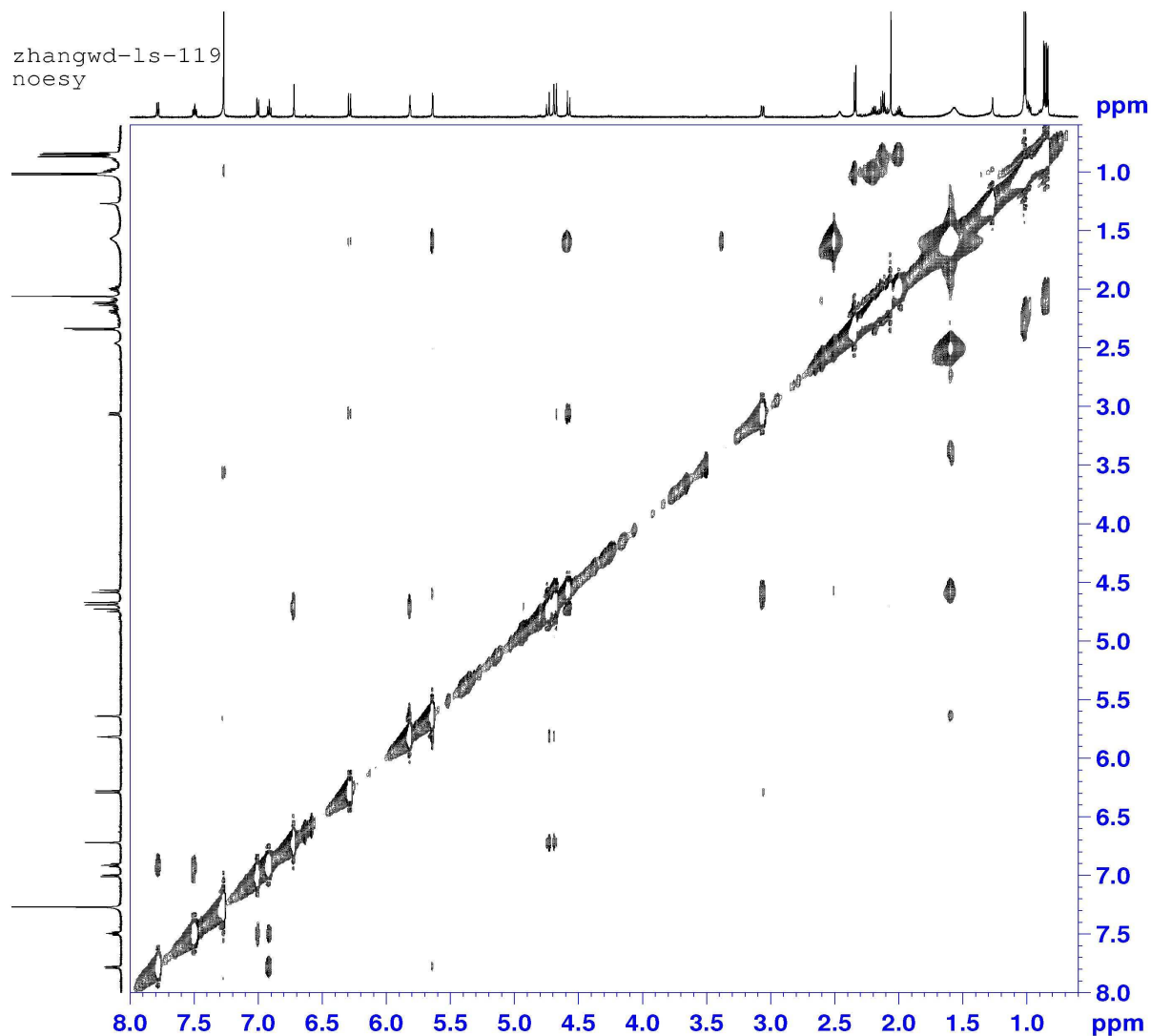
S55. The ^1H - ^1H COSY Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate I (9)



S56. The HSQC Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate I (9)



S57. The HMBNMR Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate I (9)



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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   noesyph
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         2.00000000 sec
D8         0.80000001 sec
IN0        0.00015840 sec
ST1CNT     128

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

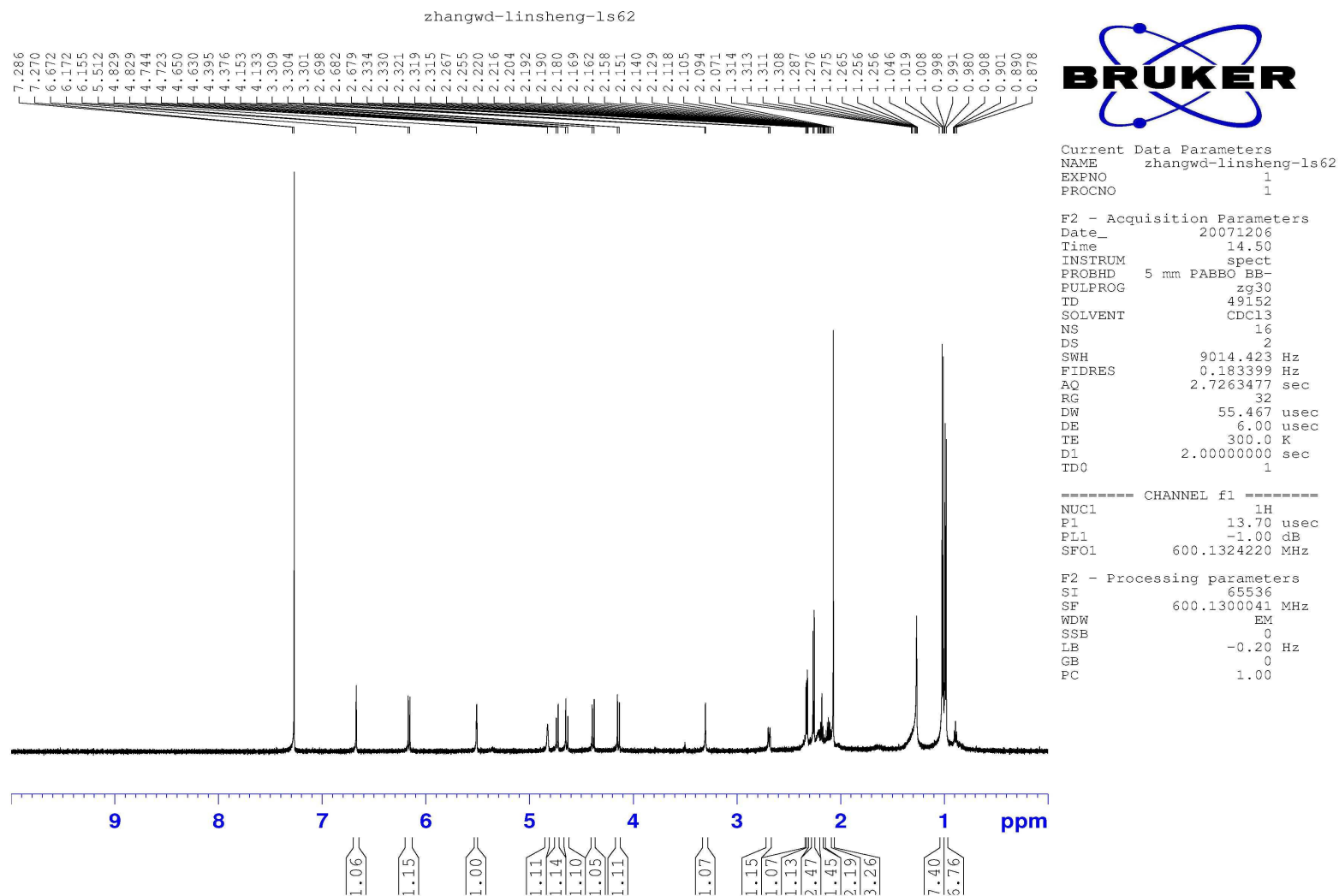
F1 - Acquisition parameters
ND0        1
TD         160
SFO1       600.1334 MHz
FIDRES     39.457069 Hz
SW         10.520 ppm
FnMODE     States-TPPI

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-TPPI
SF         600.1300048 MHz
WDW        QSINE
SSB        2
LB         0.00 Hz
GB         0

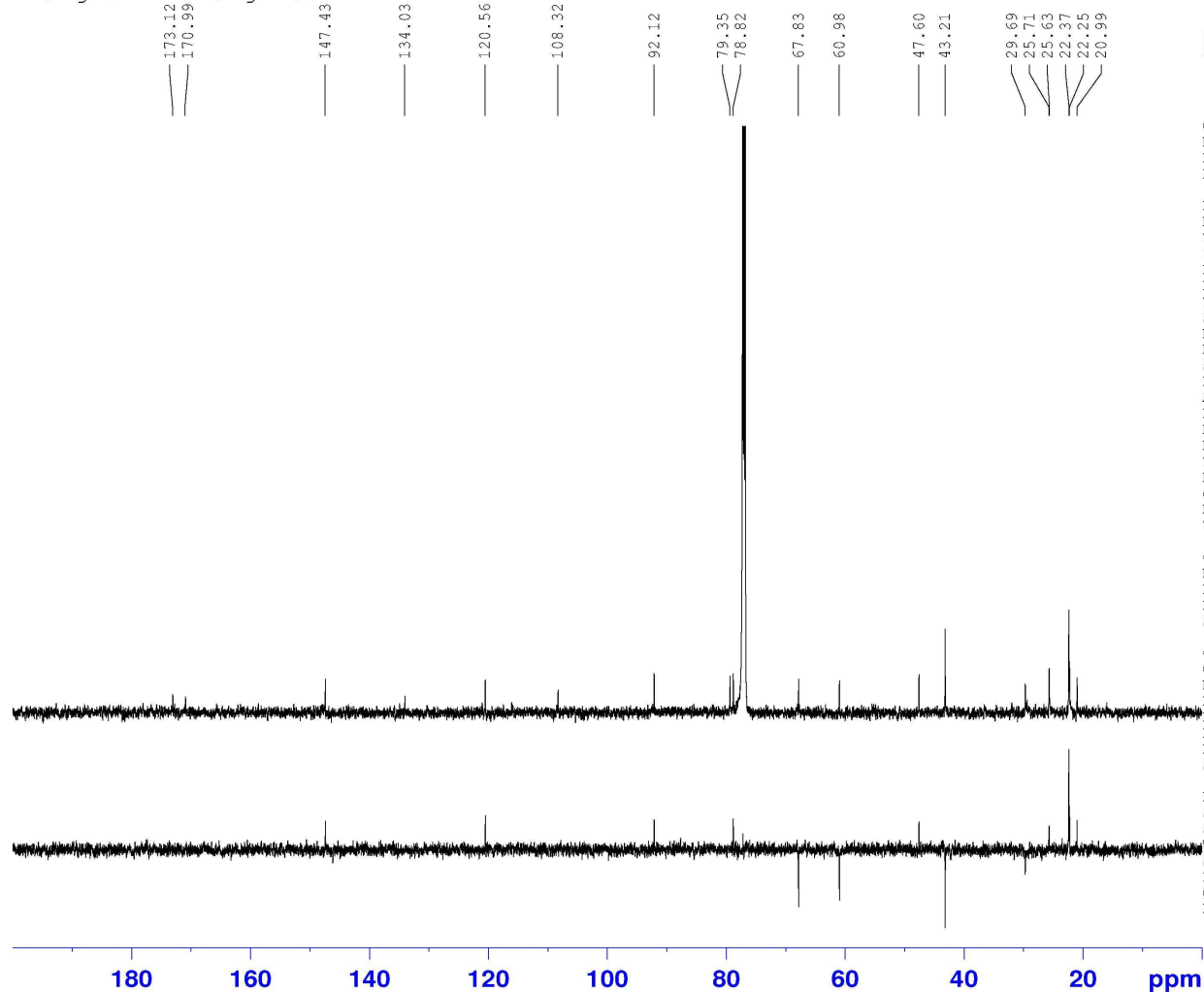
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S58. The NOESY Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate I (9)



S59. The ^1H NMR Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate J (10)

zhangwd-linsheng-ls62



Current Data Parameters
NAME zhangwd-linsheng-ls62
EXPNO 8
PROCNO 1

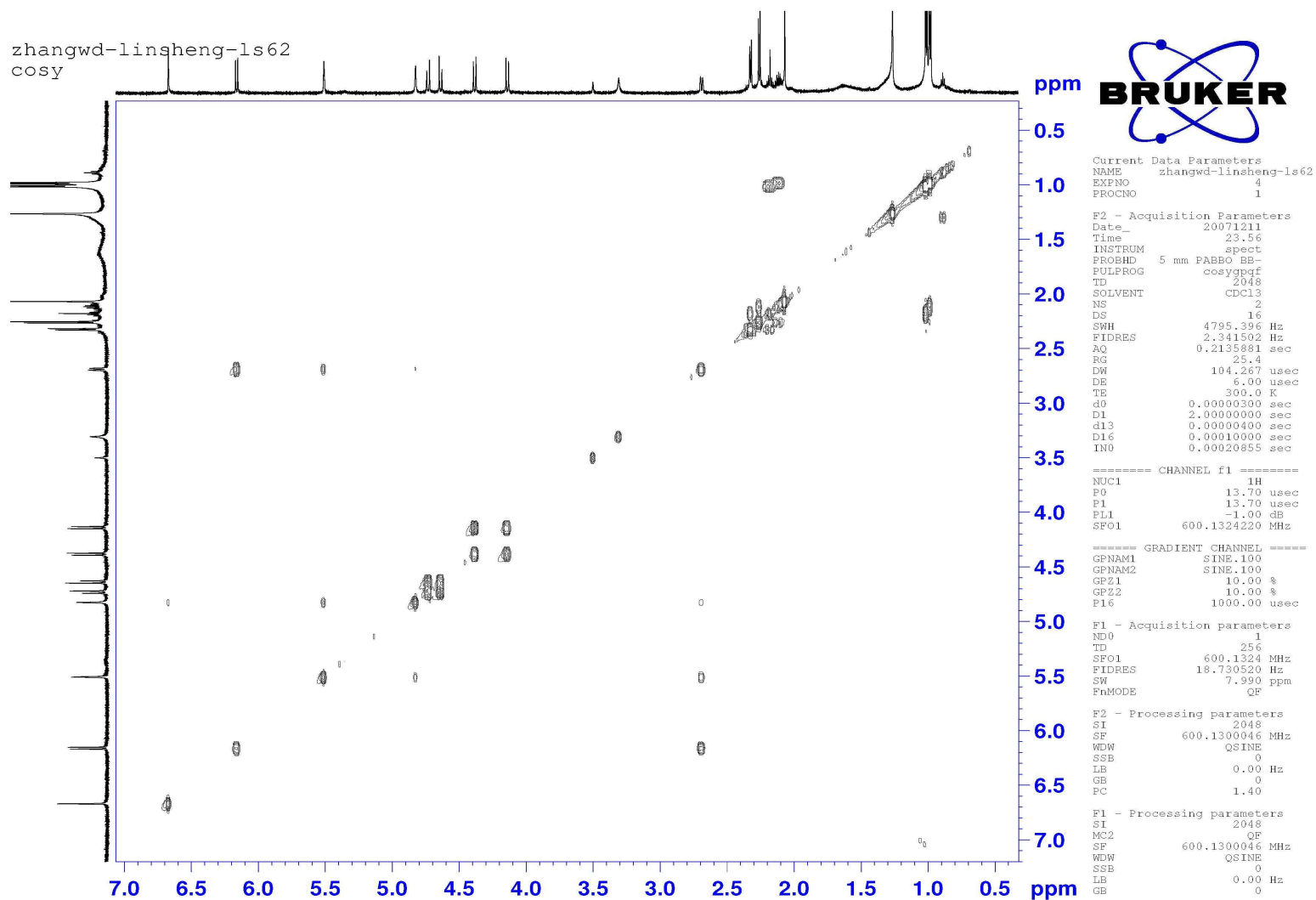
F2 - Acquisition Parameters
Date_ 20071212
Time 8.00
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 2910
DS 2
SWH 45454.547 Hz
FIDRES 0.693581 Hz
AQ 0.7209460 sec
RG 32768
DW 11.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

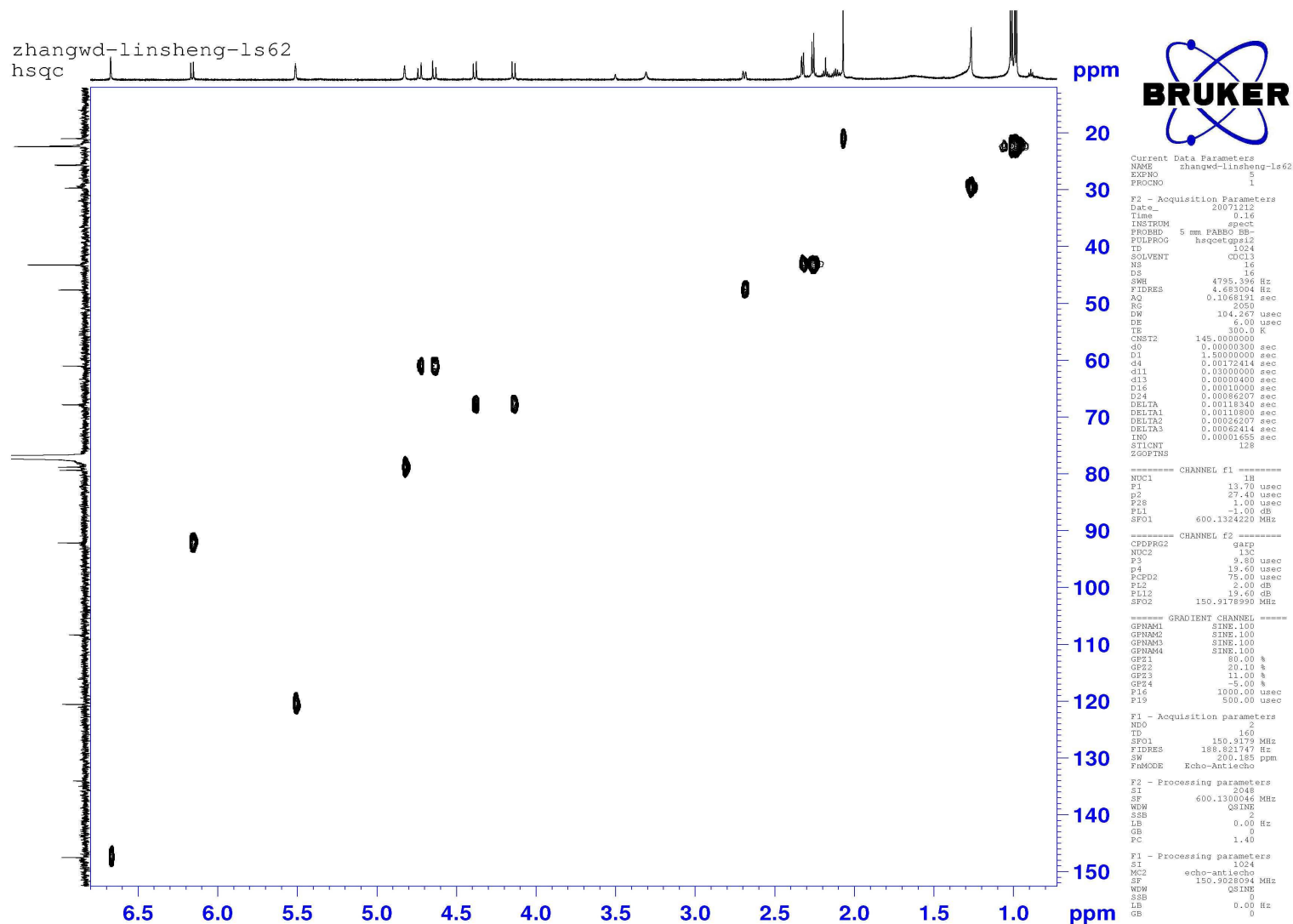
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.00 dB
PL13 14.00 dB
SFO2 600.1324220 MHz

F2 - Processing parameters
SI 65536
SF 150.9028094 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

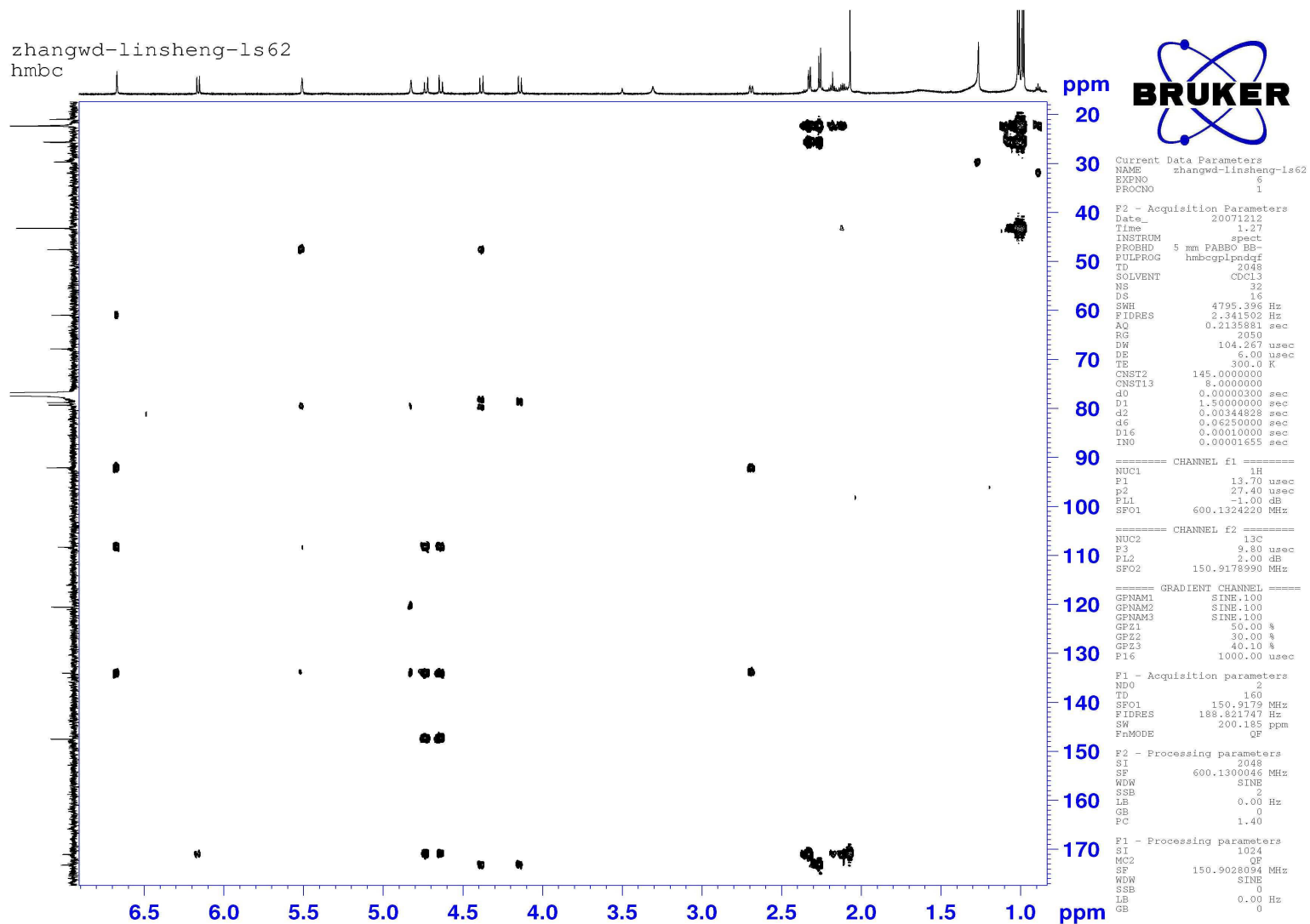
S60. The ^{13}C NMR and DEPT Spectra (150 MHz, CDCl_3) of Jatamanvaltrate J (10)



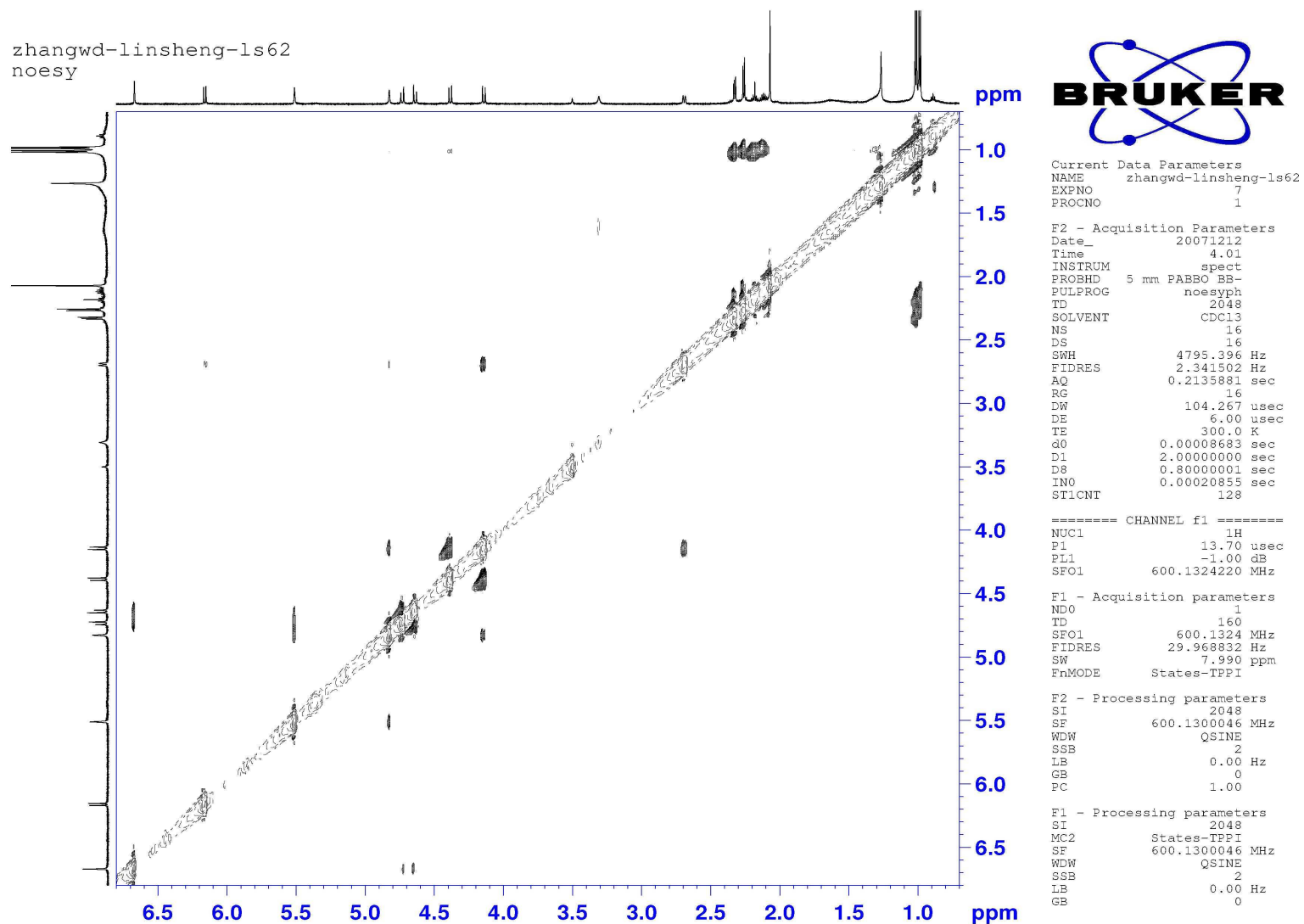
S61. The ^1H - ^1H COSY Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate J (10)



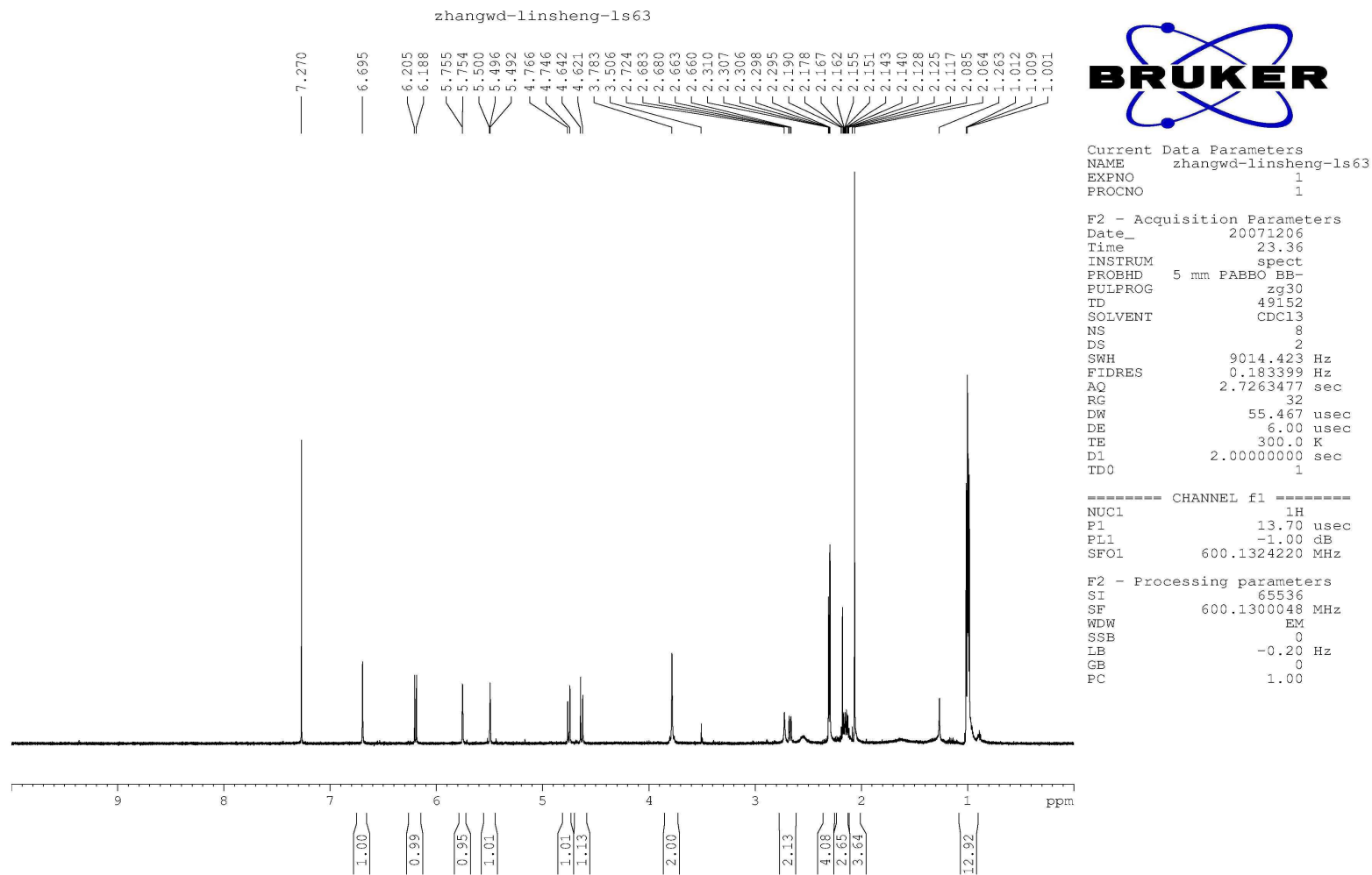
S62. The HSQC Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate J (10)



S63. The HMBC Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate J (10)

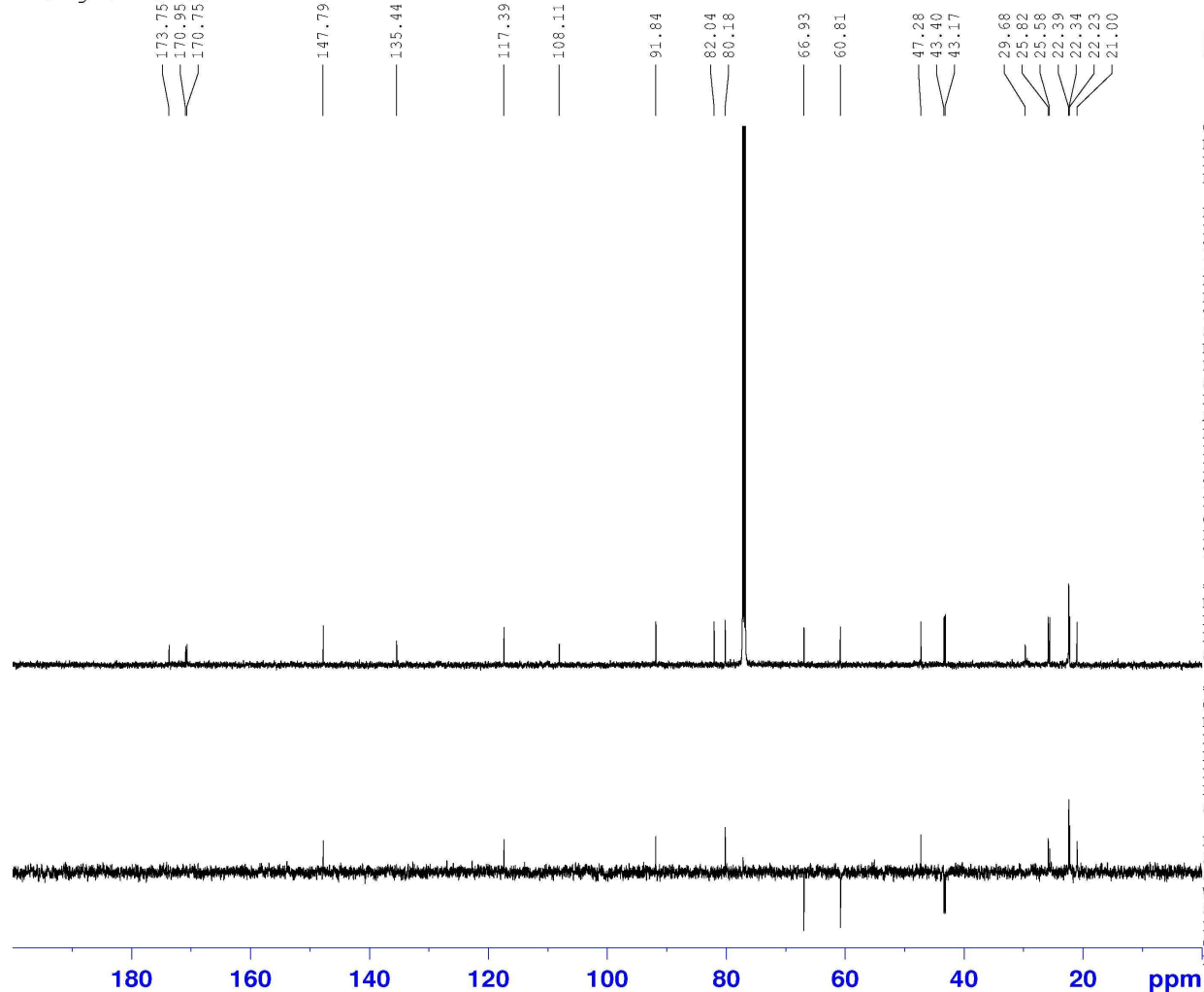


S64. The NOESY Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate J (10)



S65. The ^1H NMR Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate K (11)

zhangwd-ls-63



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

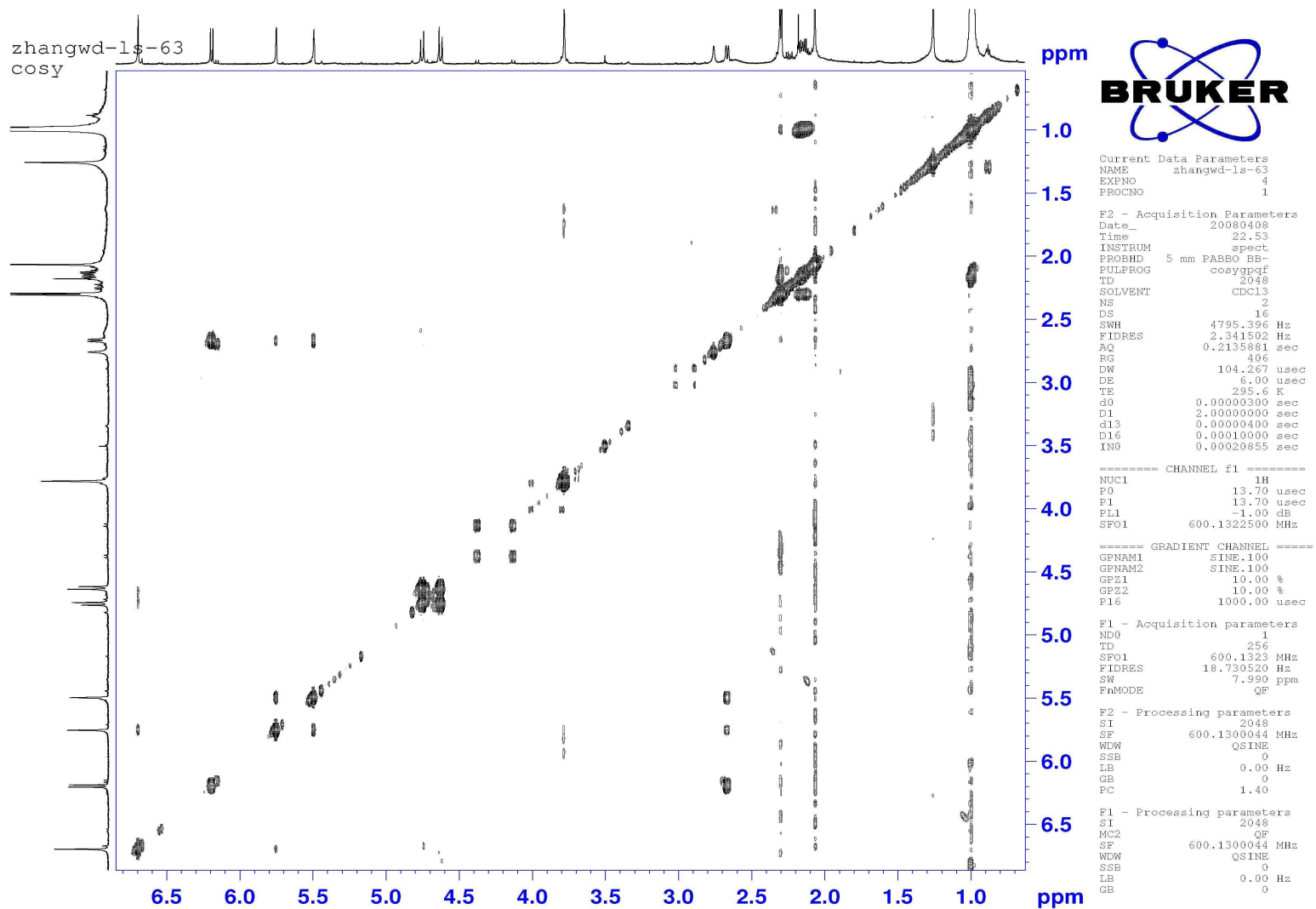
F2 - Acquisition Parameters
 Date_ 20080408
 Time 22.52
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 0
 SWH 45454.547 Hz
 FIDRES 0.693581 Hz
 AQ 0.7209460 sec
 RG 32768
 DW 11.000 usec
 DE 6.00 usec
 TE 296.9 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

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

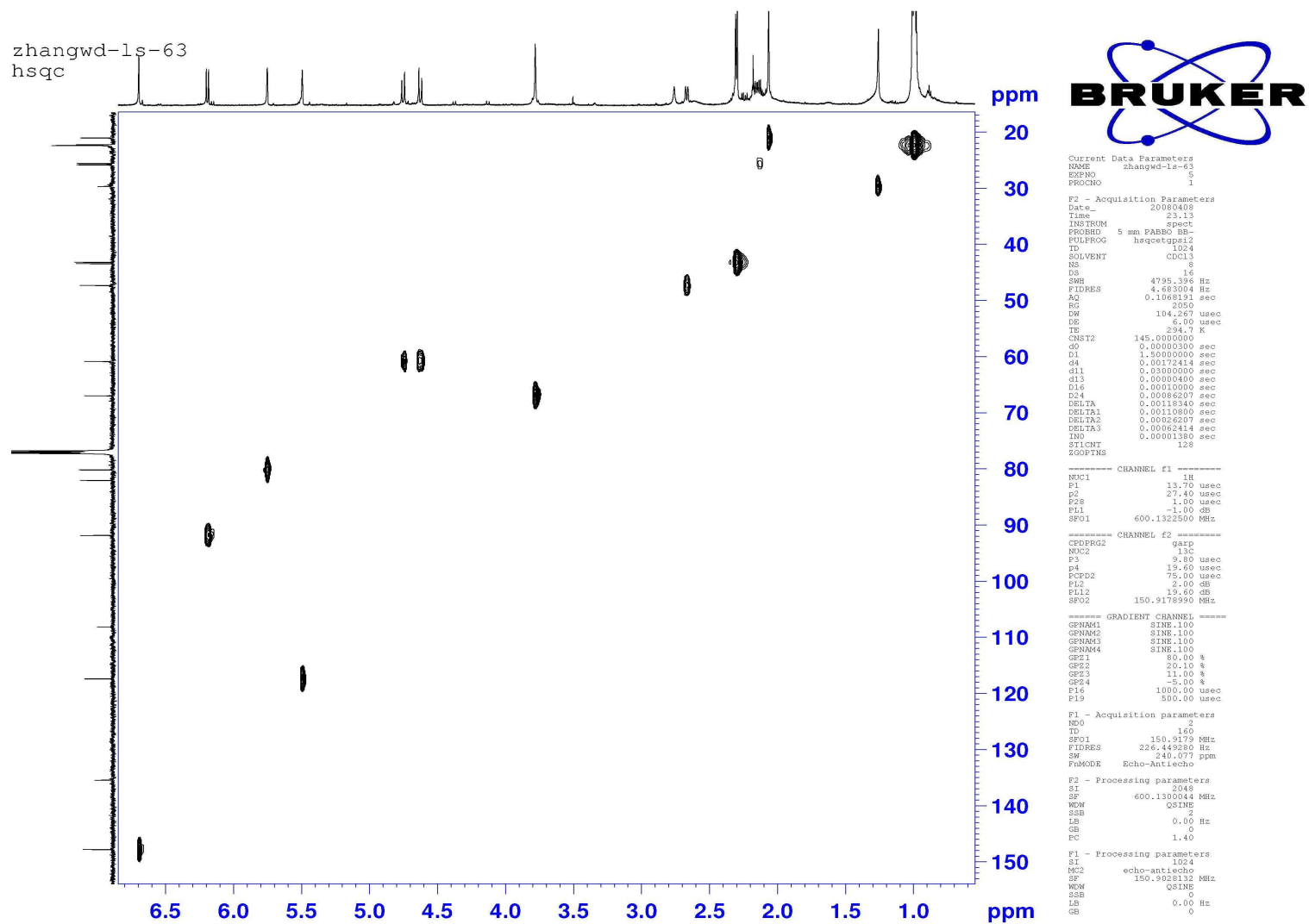
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 14.00 dB
 PL13 14.00 dB
 SFO2 600.1324005 MHz

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

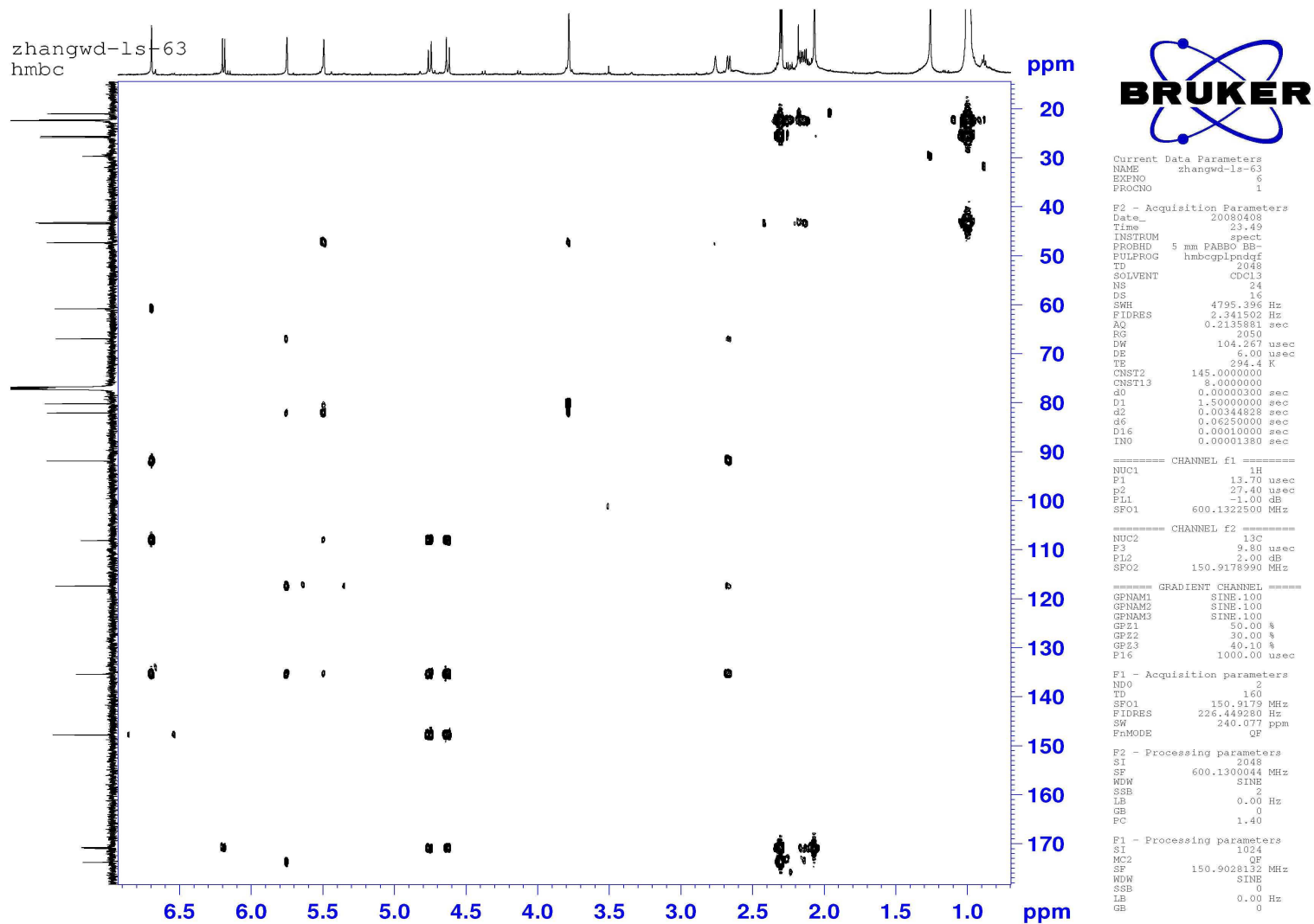
S66. The ^{13}C NMR and DEPT Spectra (150 MHz, CDCl_3) of Jatamanvaltrate K (11)



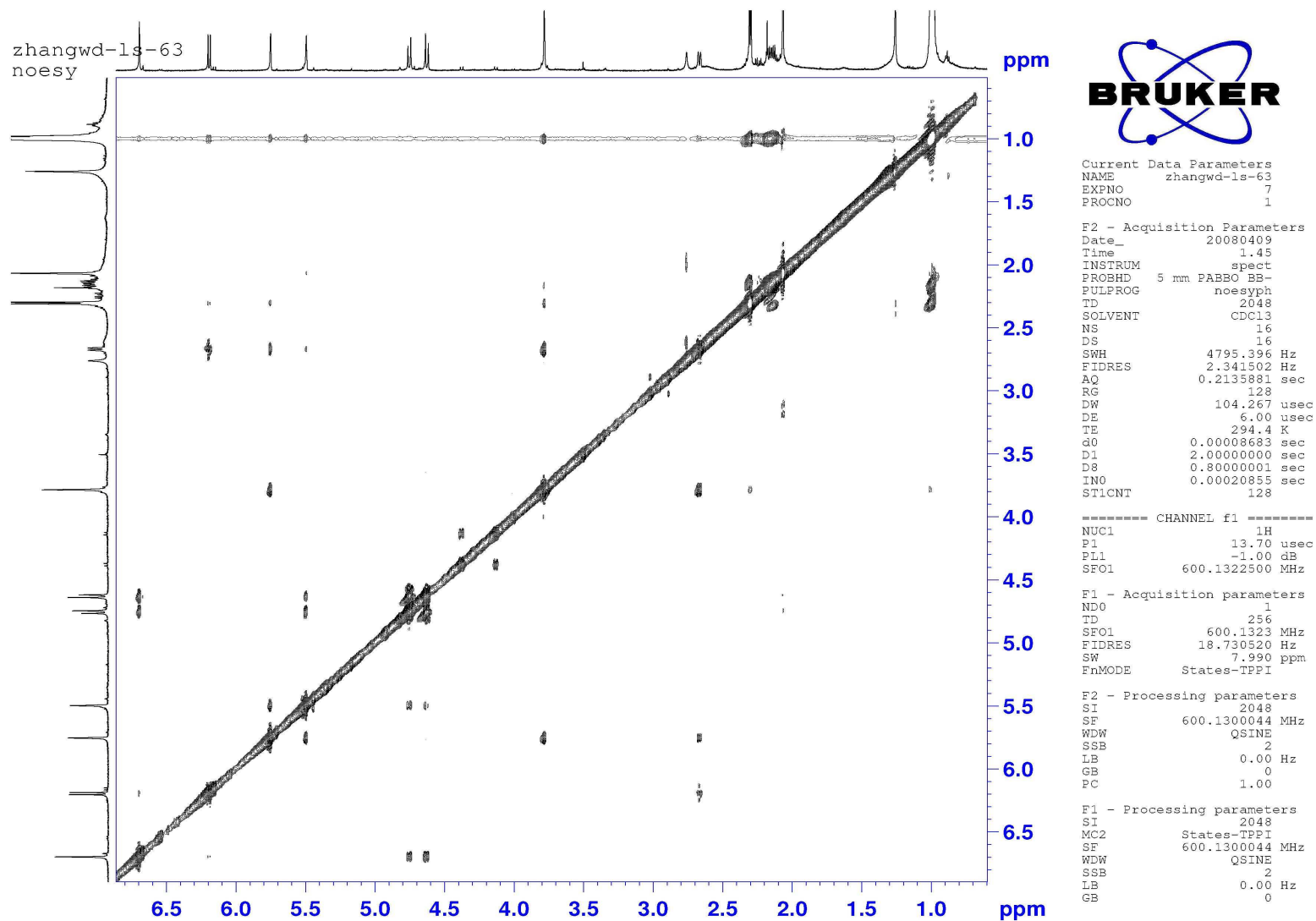
S67. The ^1H - ^1H COSY Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate K (11)



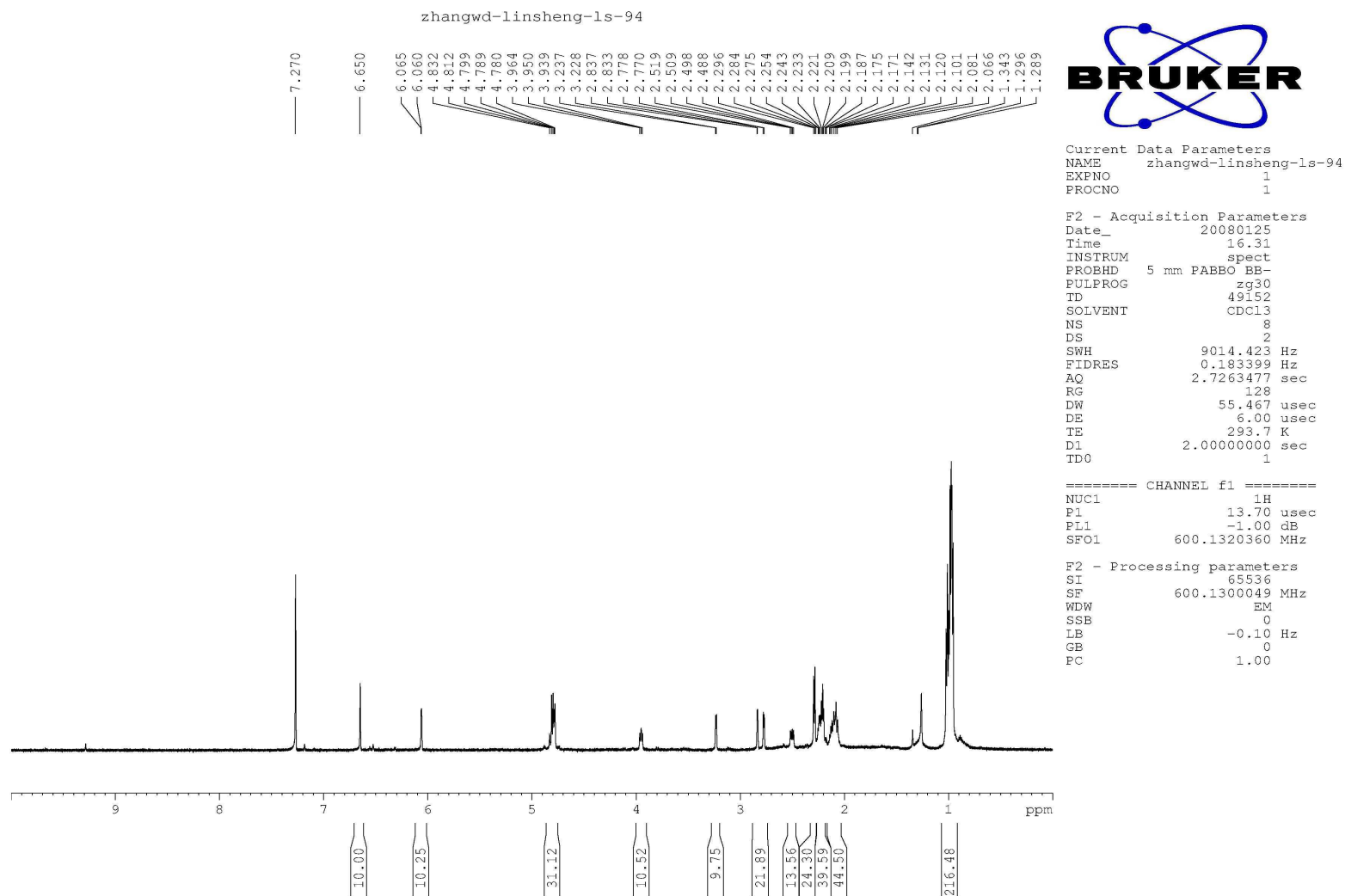
S68. The HSQC Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate K (11)



S69. The HMBC Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate K (11)

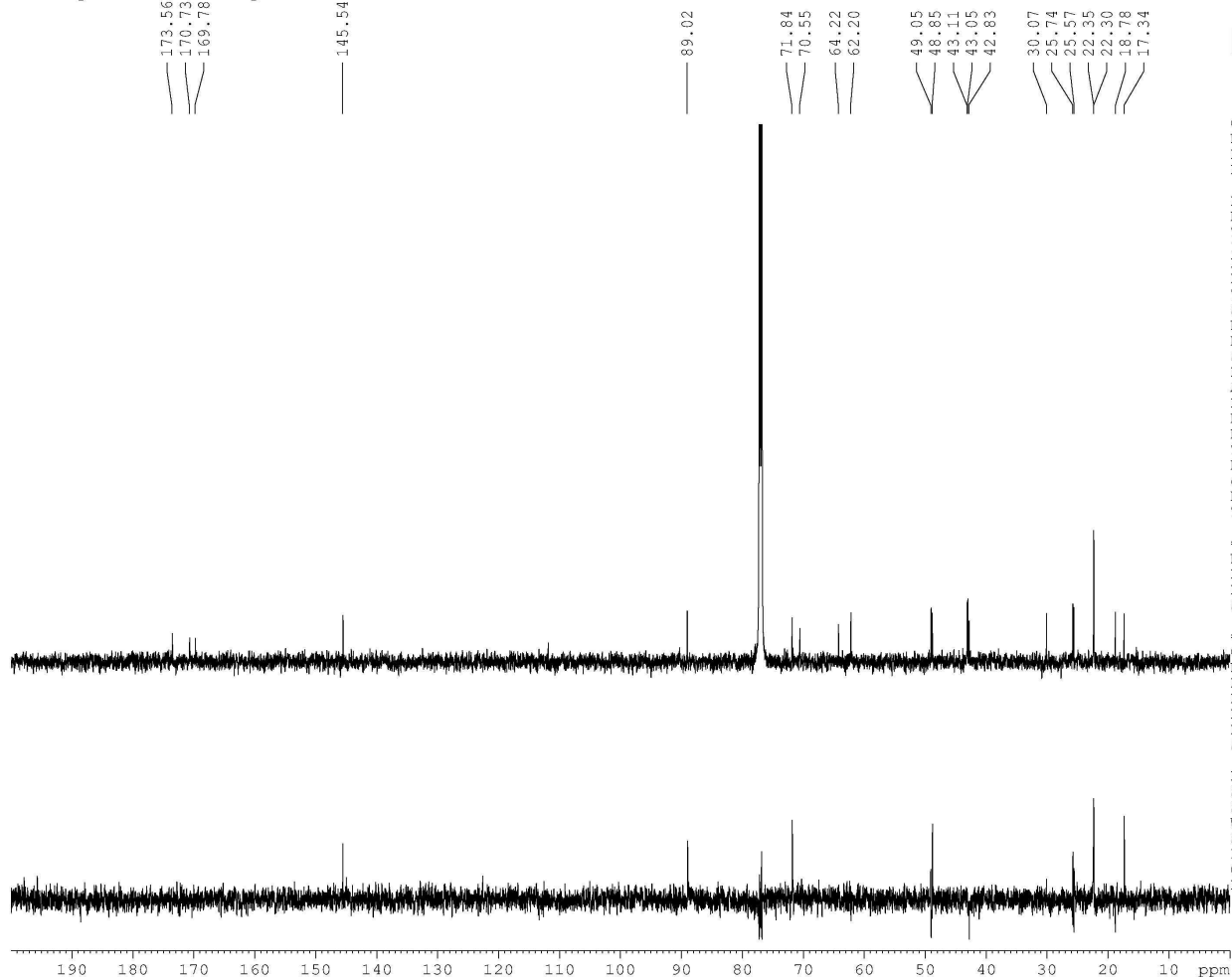


S70. The NOESY Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate K (11)



S71. The ^1H NMR Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate L (12)

zhangwd-linsheng-ls-94



Current Data Parameters
 NAME zhangwd-linsheng-ls-94
 EXPNO 2
 PROCNO 1

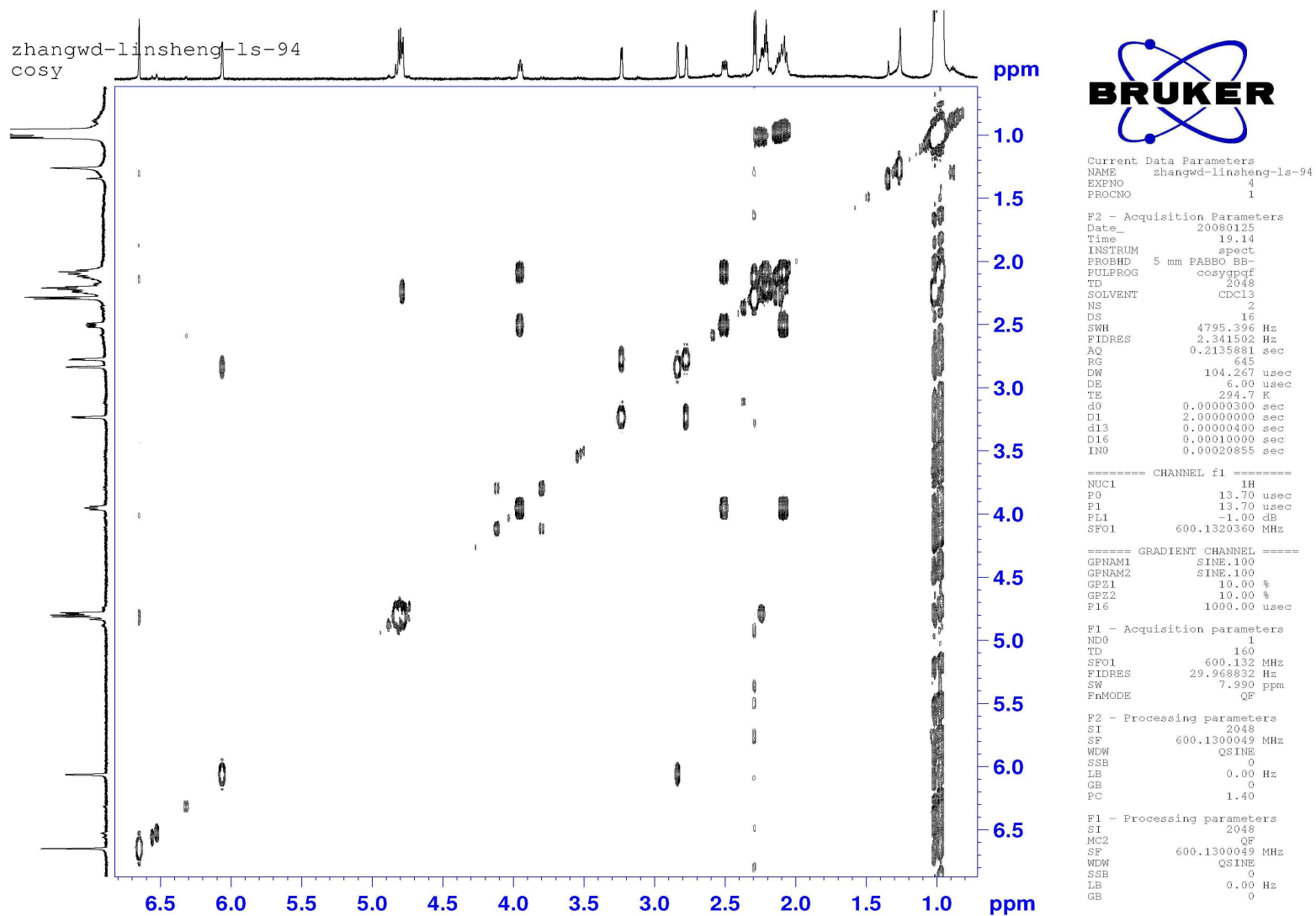
F2 - Acquisition Parameters
 Date_ 20080125
 Time 18.49
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 2048
 DS 2
 SWH 45454.547 Hz
 FIDRES 0.693581 Hz
 AQ 0.7209460 sec
 RG 32768
 DW 11.000 usec
 DE 6.00 usec
 TE 296.7 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

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

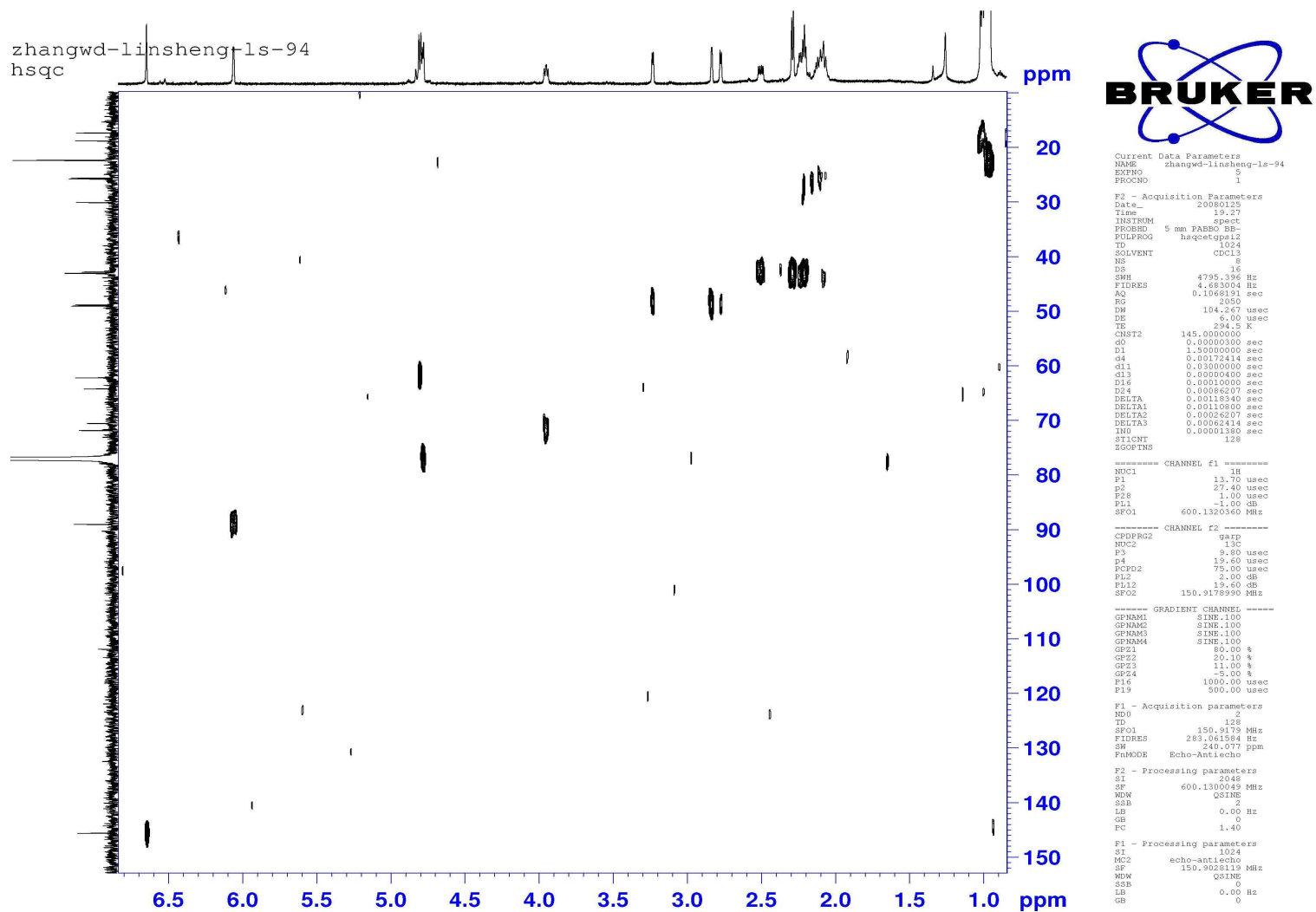
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 14.00 dB
 PL13 14.00 dB
 SFO2 600.1324005 MHz

F2 - Processing parameters
 SI 65536
 SF 150.9028114 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

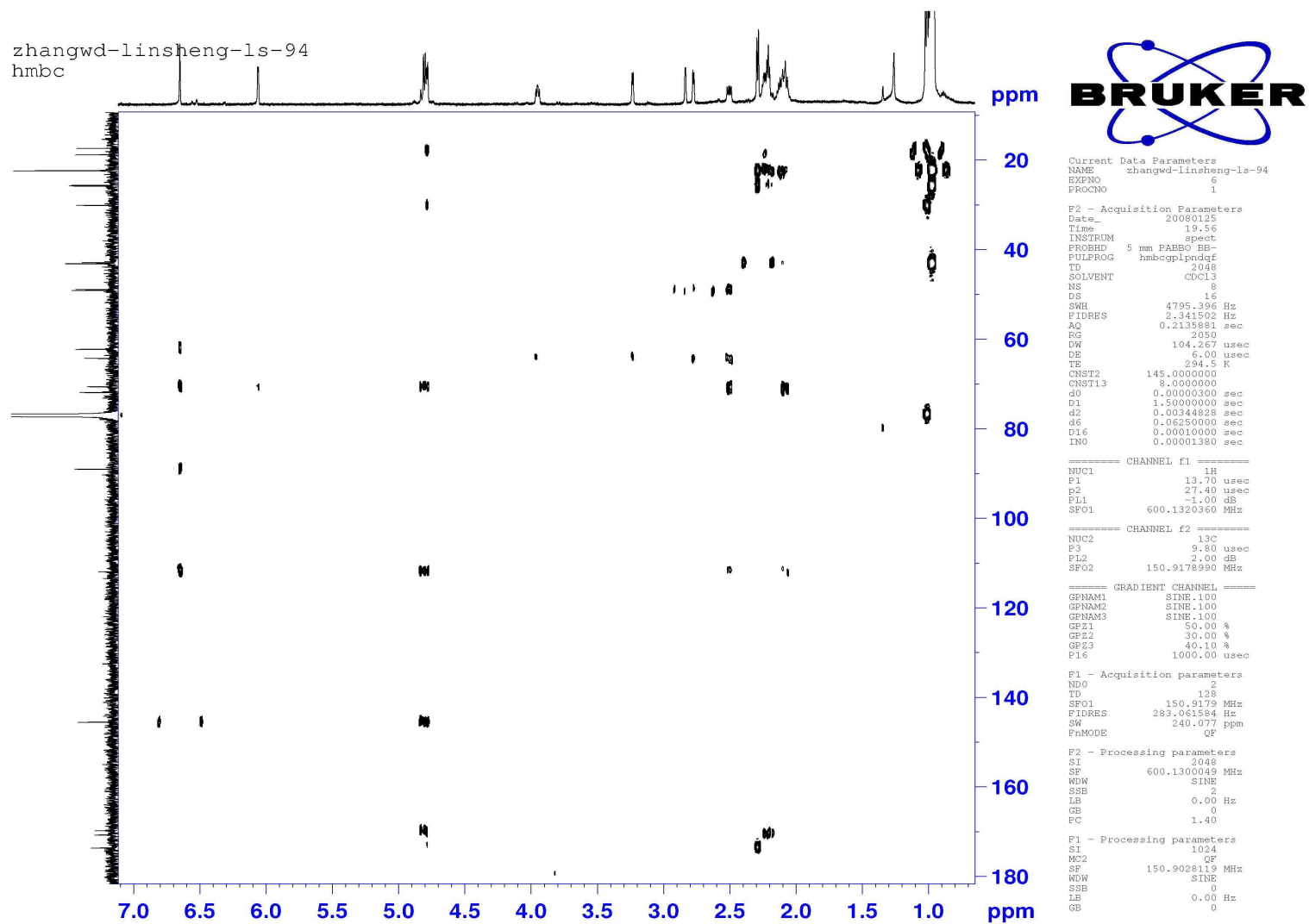
S72. The ^{13}C NMR and DEPT Spectra (150 MHz, CDCl_3) of Jatamanvaltrate L (12)



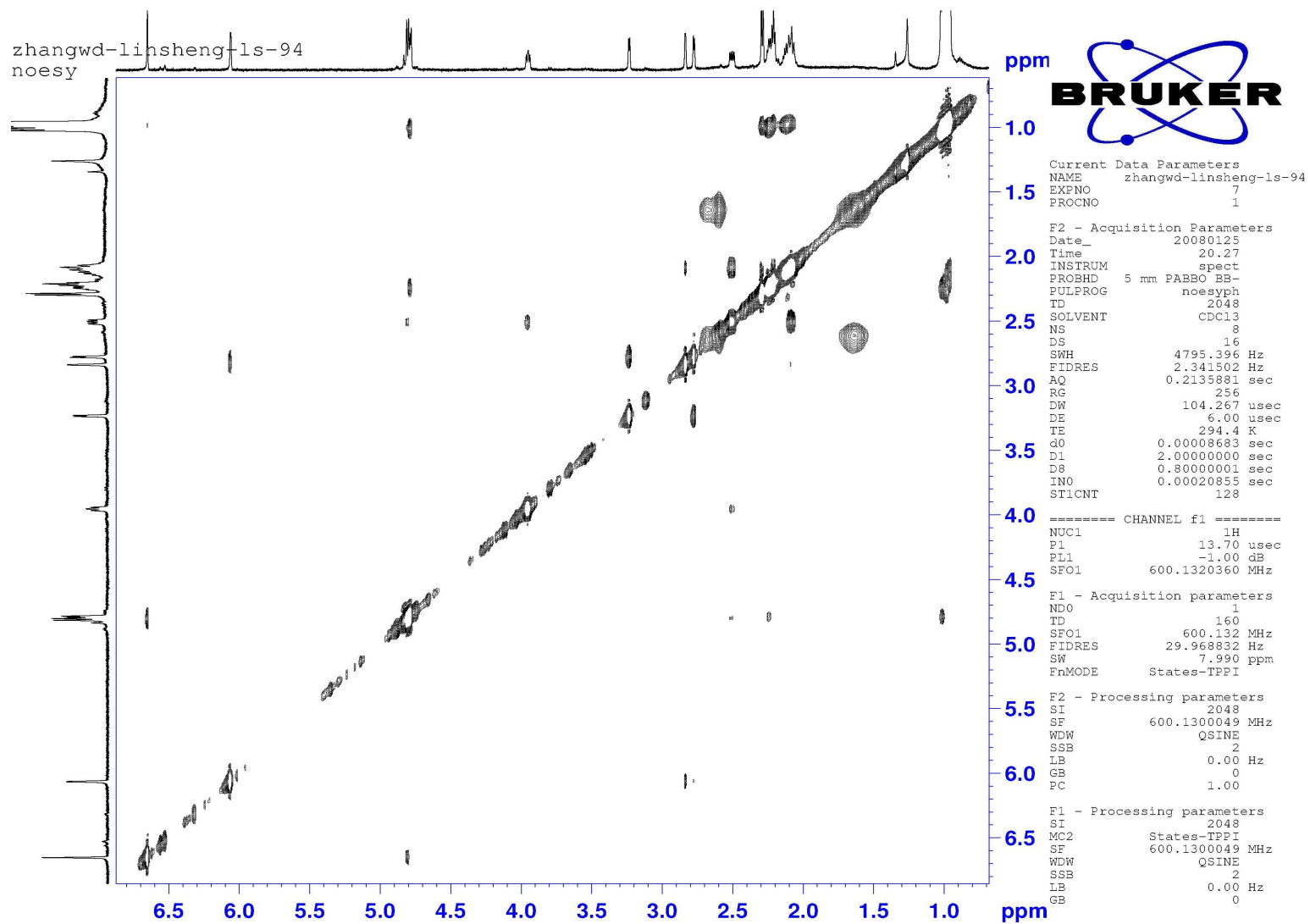
S73. The ^1H - ^1H COSY Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate L (12)



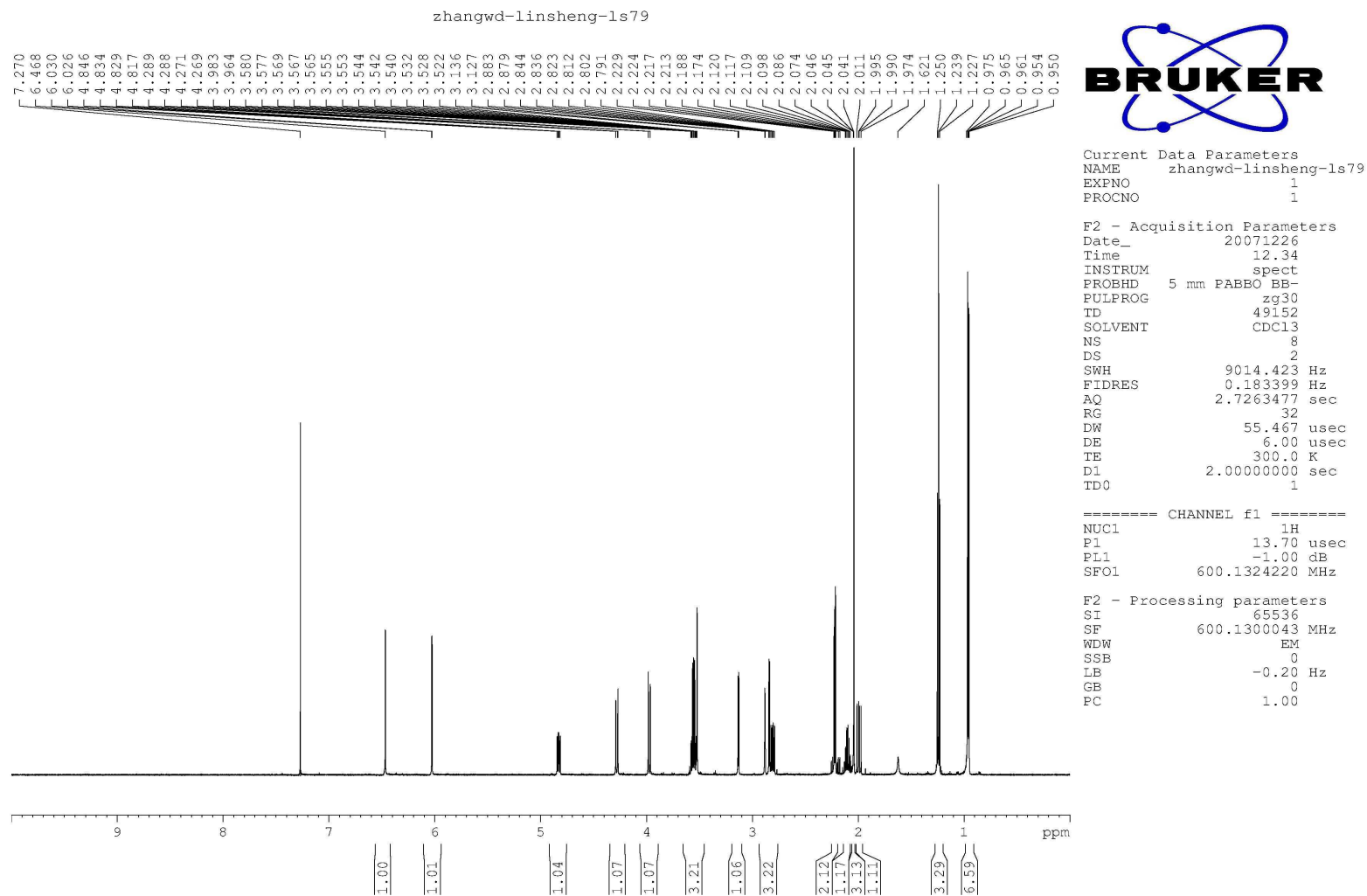
S74. The HSQC Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate L (12)



S75. The HMBC Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate L (12)

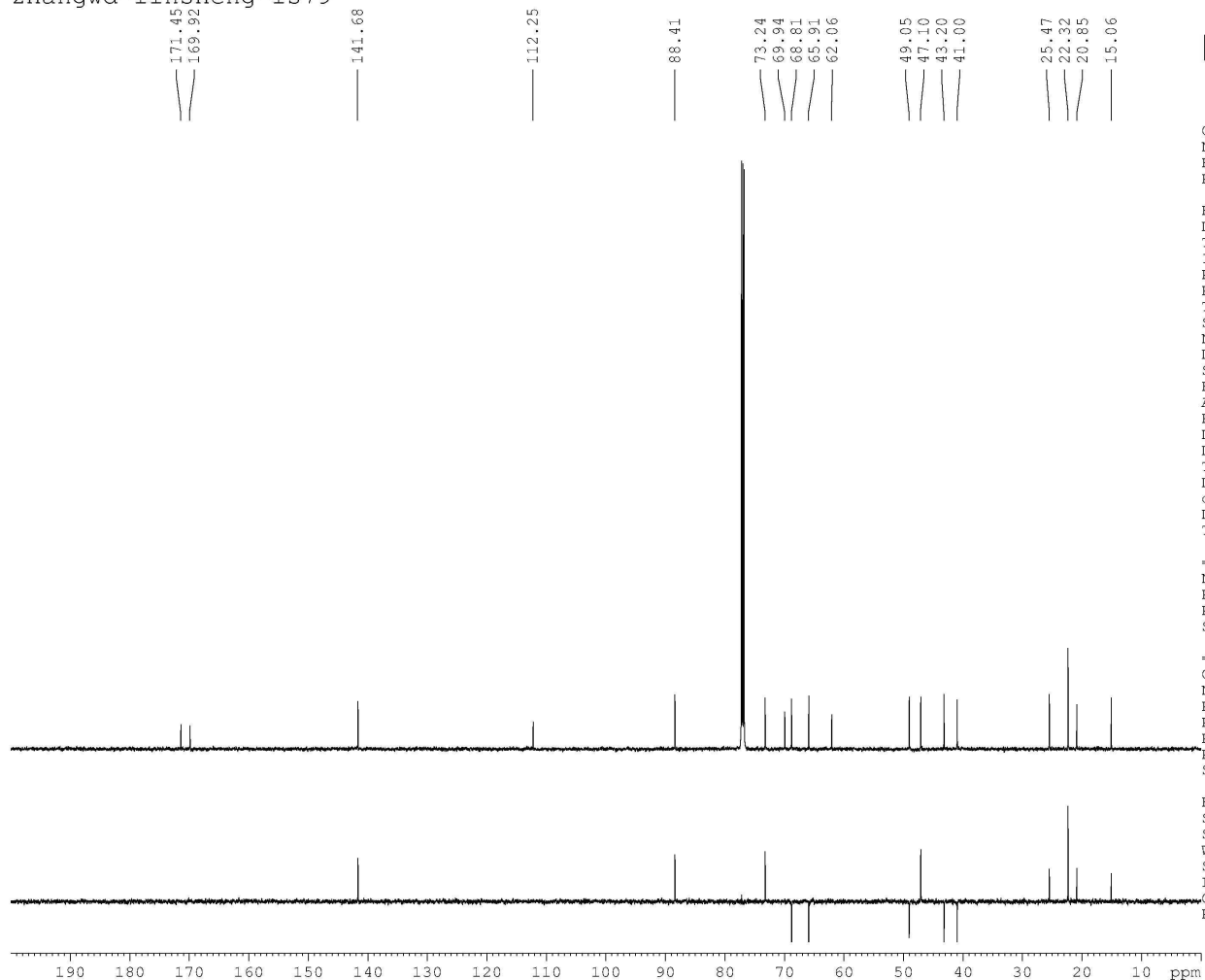


S76. The NOESY Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate L (12)



S77. The ^1H NMR Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate M (13)

zhangwd-linsheng-ls79



Current Data Parameters
NAME zhangwd-linsheng-ls79
EXPNO 2
PROCNO 1

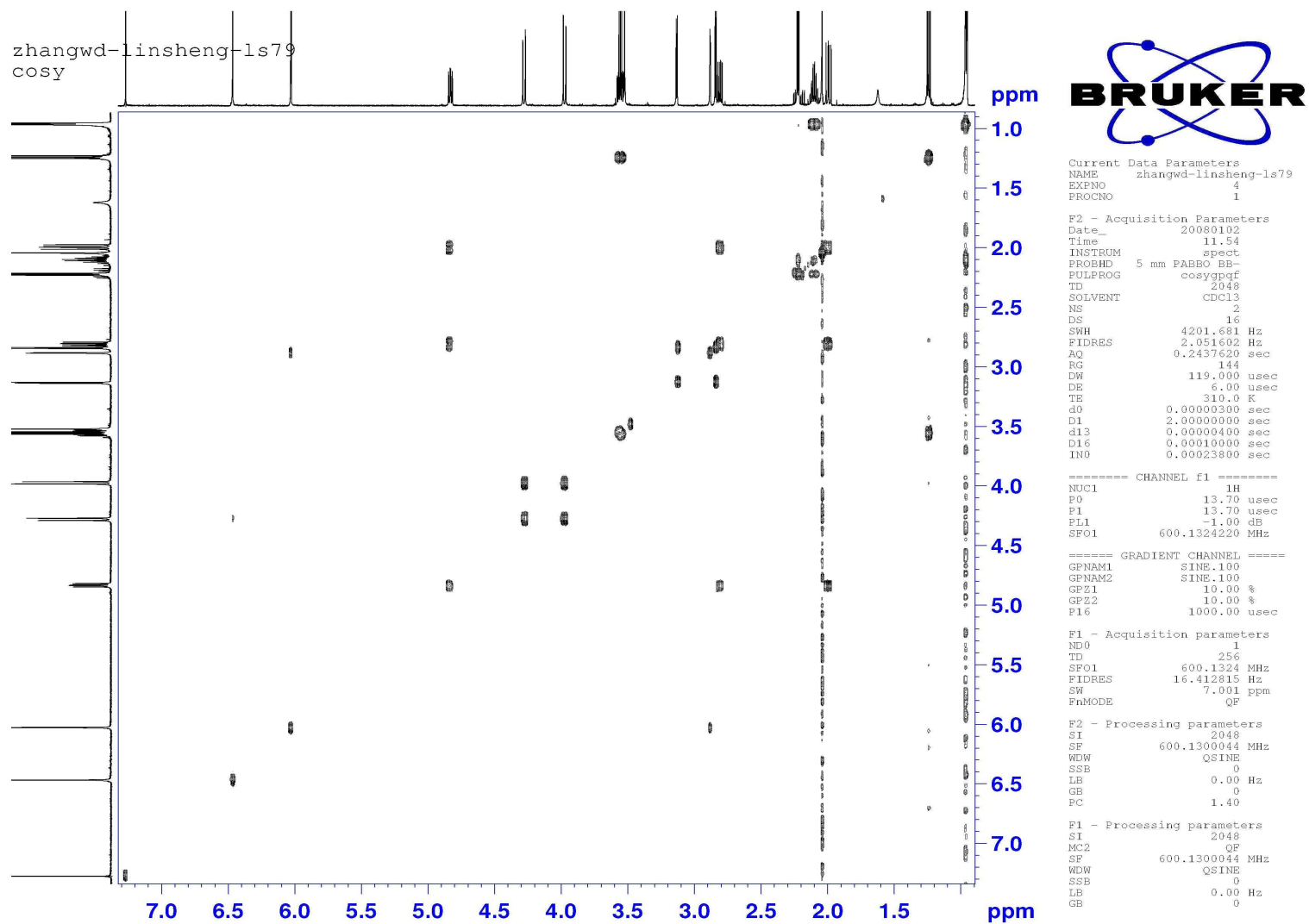
F2 - Acquisition Parameters
Date_ 20071226
Time 12.59
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 512
DS 2
SWH 45454.547 Hz
FIDRES 0.693581 Hz
AQ 0.7209460 sec
RG 32768
DW 11.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

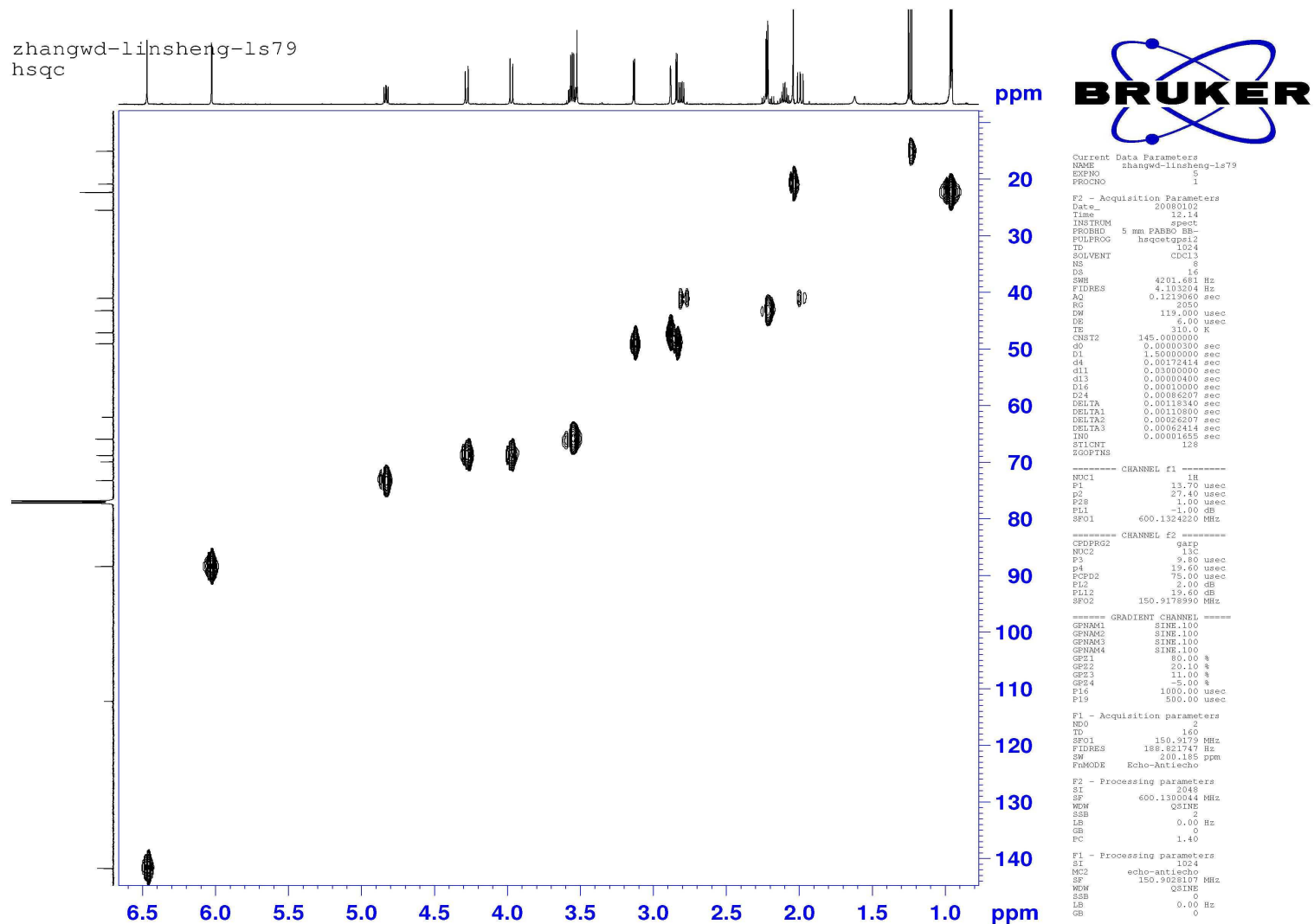
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 usec
PL2 -1.00 dB
PL12 14.00 dB
PL13 14.00 dB
SFO2 600.1324220 MHz

F2 - Processing parameters
SI 65536
SF 150.9028107 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

S78. The ^{13}C NMR and DEPT Spectra (150 MHz, CDCl_3) of jatamanvaltrate M (13)

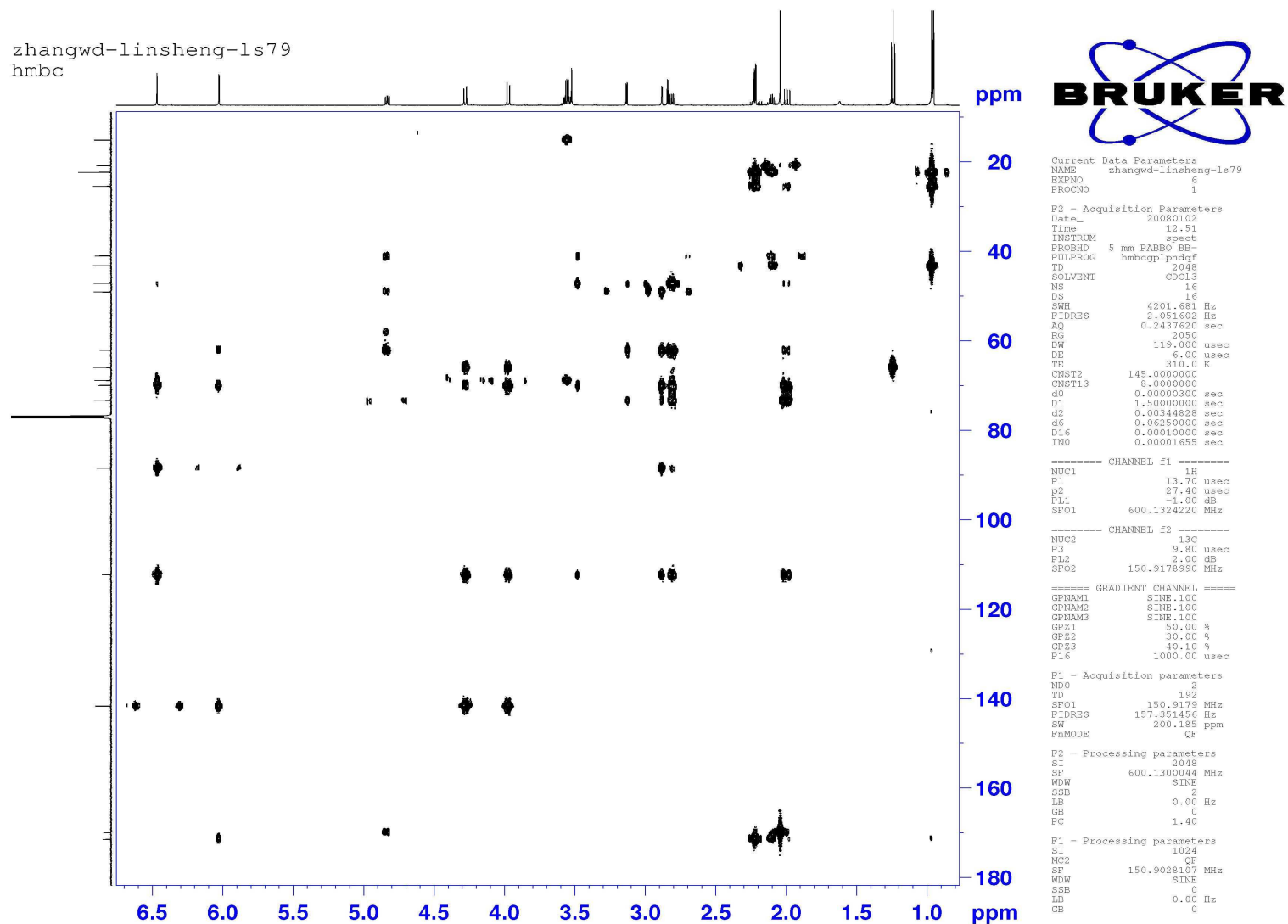


S79. The ^1H - ^1H COSY Spectrum (600 MHz, CDCl_3) of Jatamanvaltrate M (13)

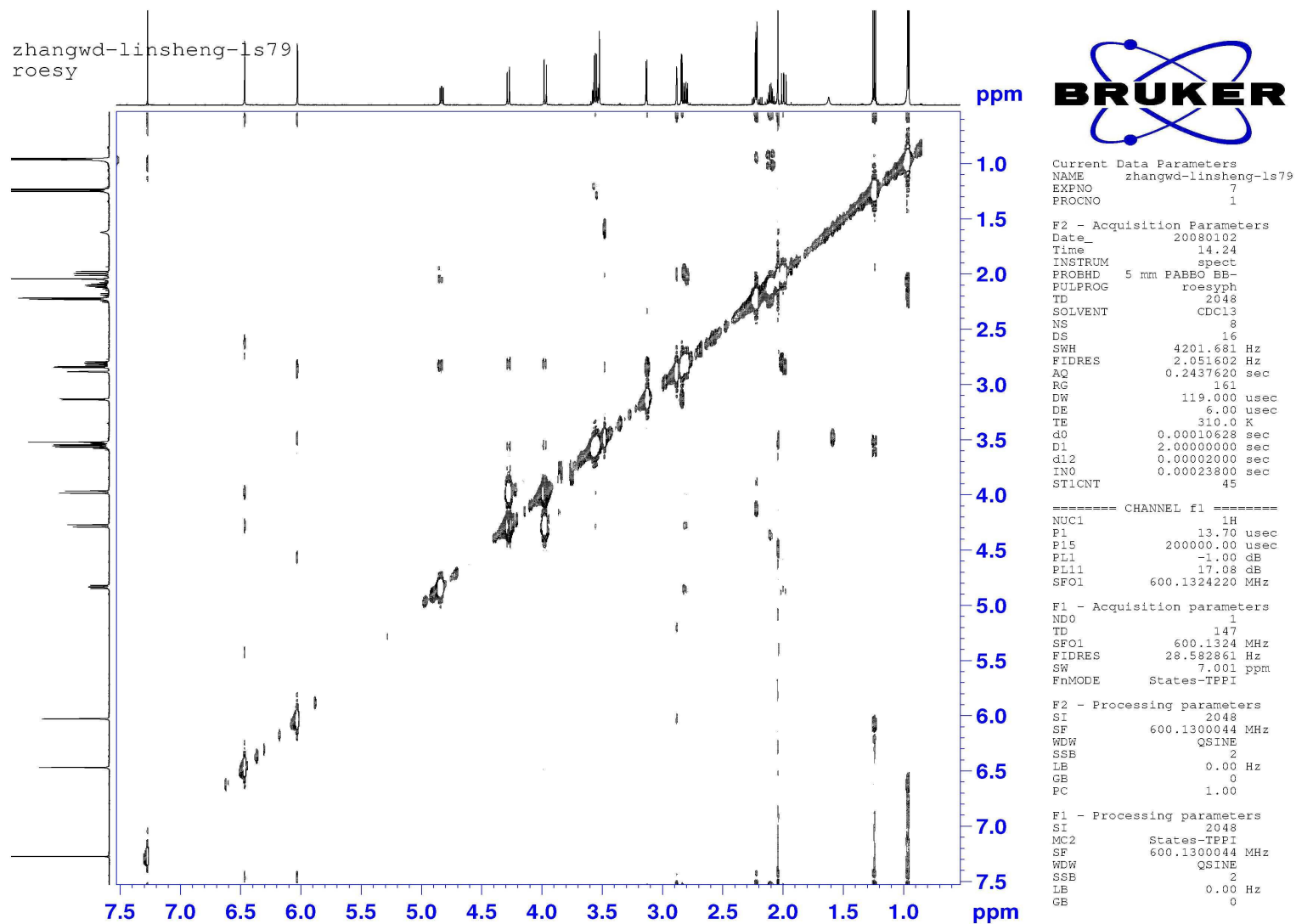


S80. The HSQC Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate M (13)

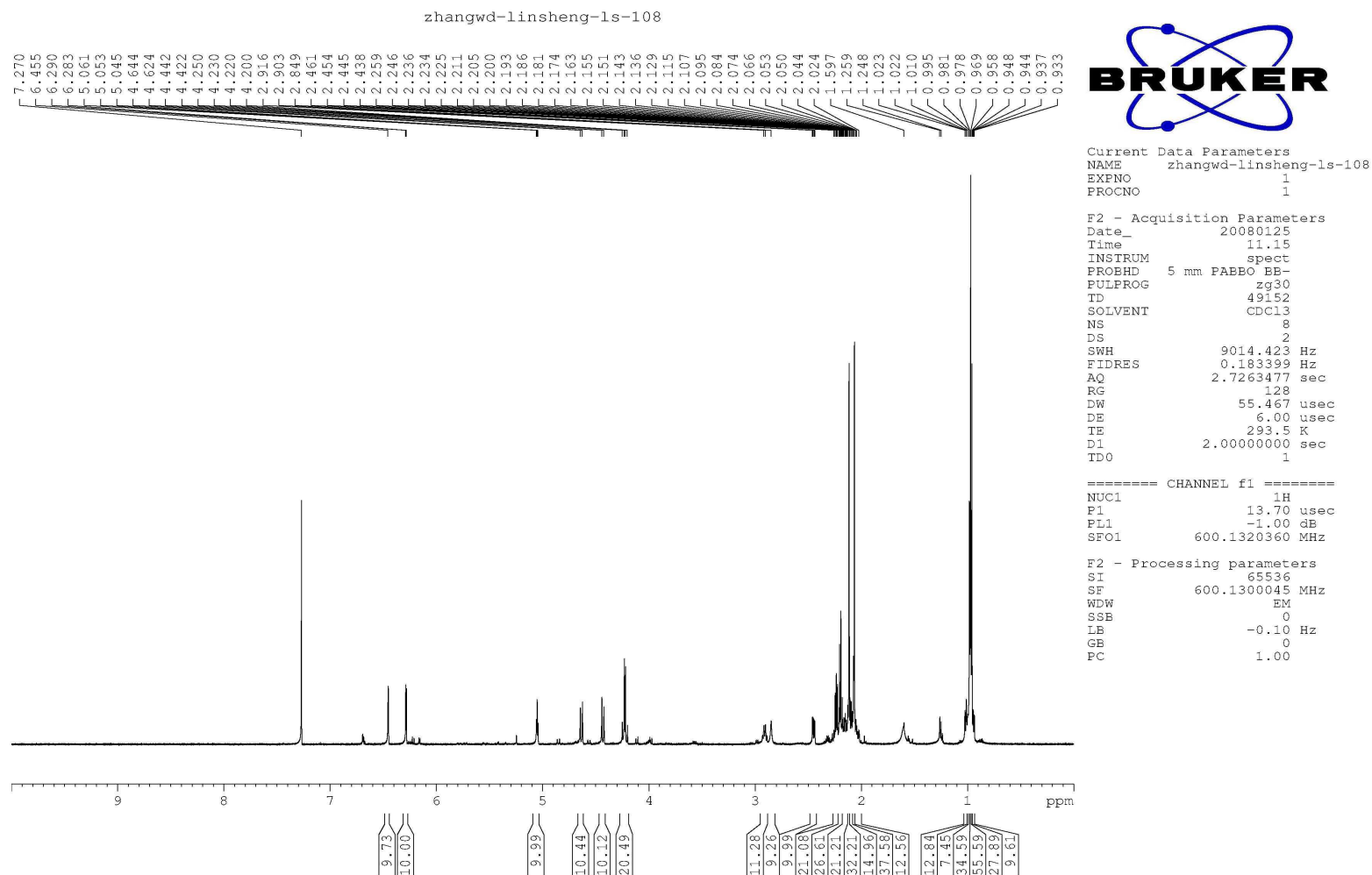
zhangwd-linsheng-ls79
hmbc



S81. The HMBC Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate M (13)

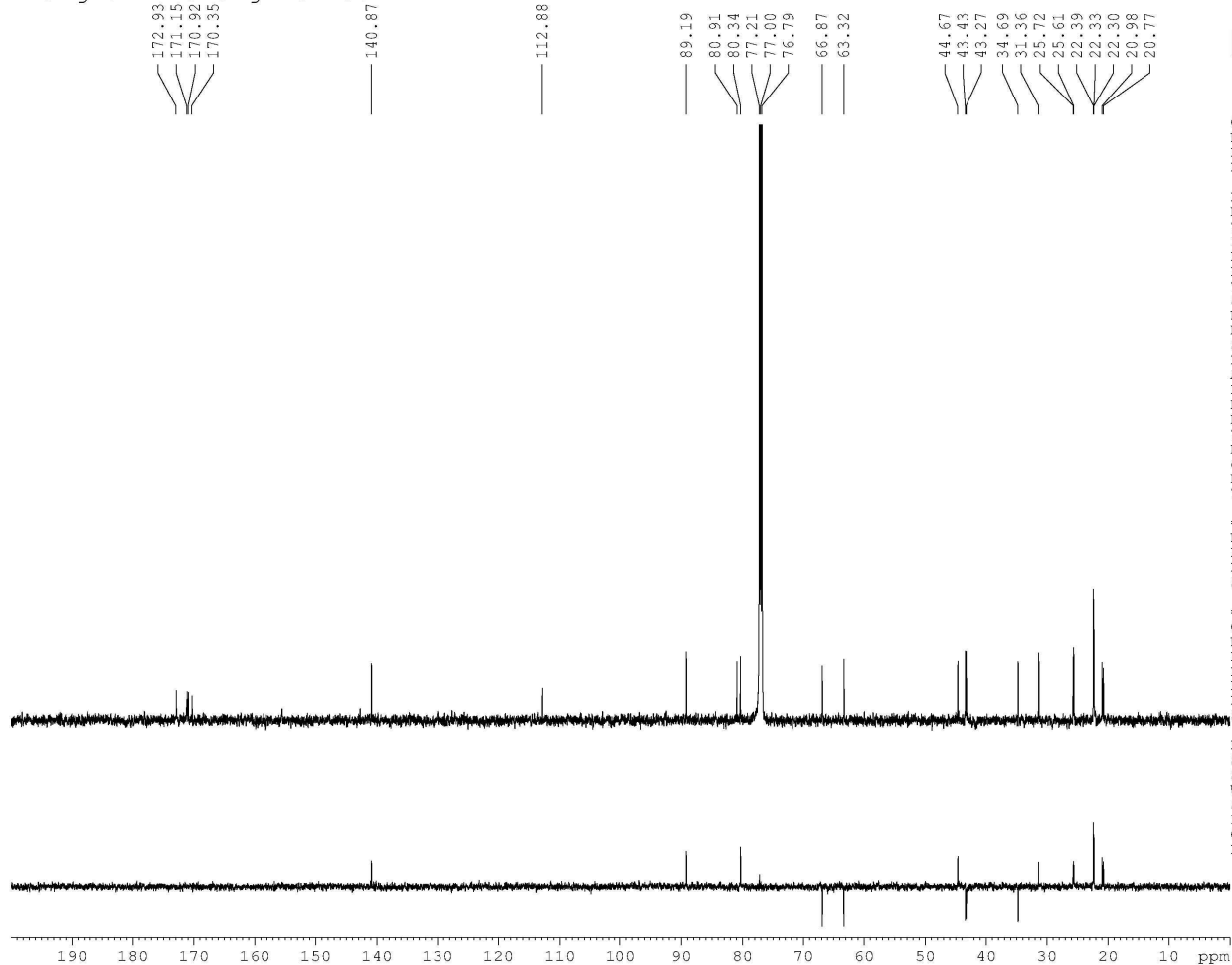


S82. The ROESY Spectrum (600 MHz, CDCl₃) of Jatamanvaltrate M (13)



S83. The ^1H NMR Spectrum (600 MHz, CDCl_3) of Compound (16)

zhangwd-linsheng-ls-108



Current Data Parameters
 NAME zhangwd-linsheng-ls-108
 EXPNO 2
 PROCNO 1

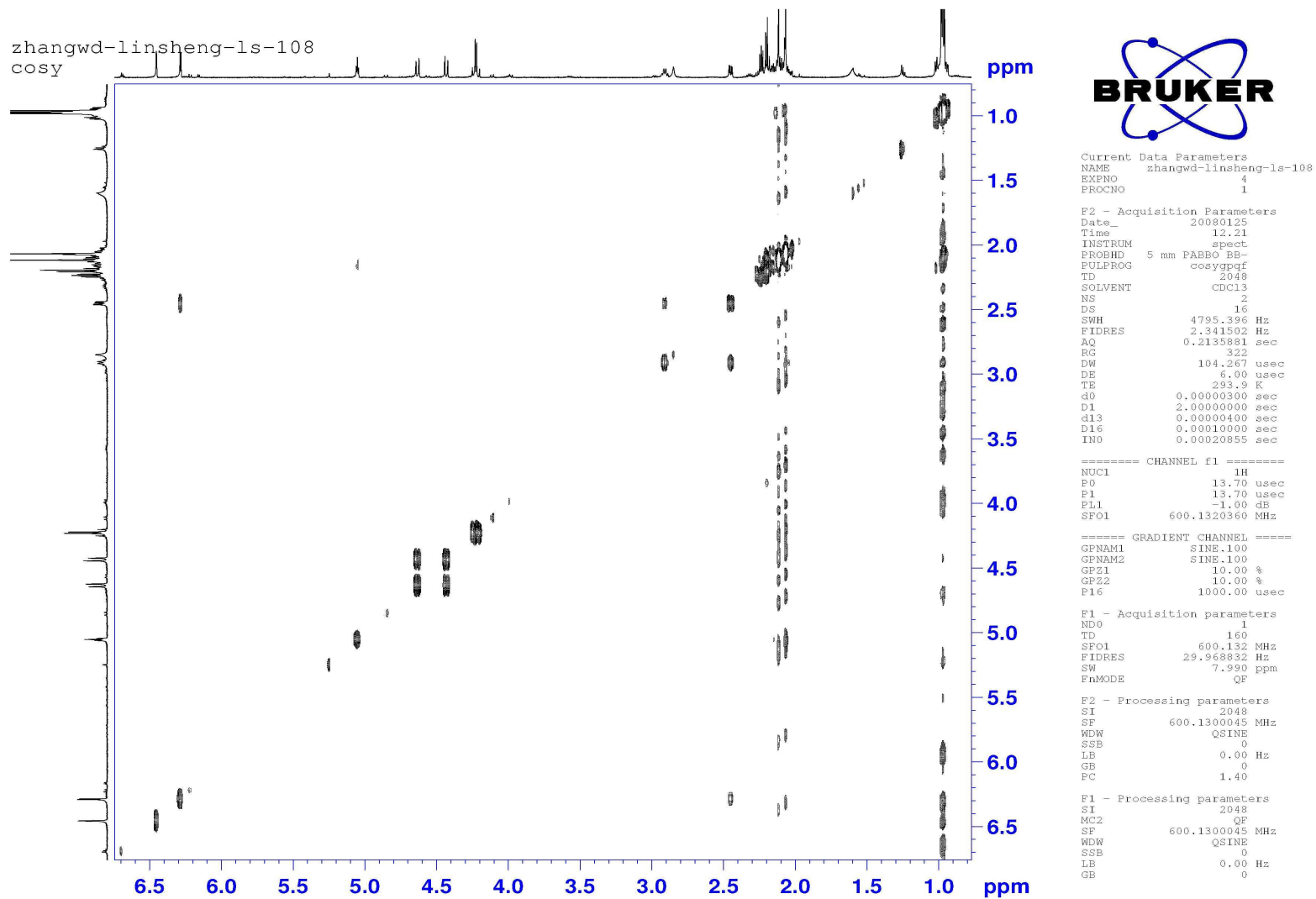
F2 - Acquisition Parameters
 Date_ 20080125
 Time 11.17
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1024
 DS 2
 SWH 45454.547 Hz
 FIDRES 0.693581 Hz
 AQ 0.7209460 sec
 RG 32768
 DW 11.000 usec
 DE 6.00 usec
 TE 295.2 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

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

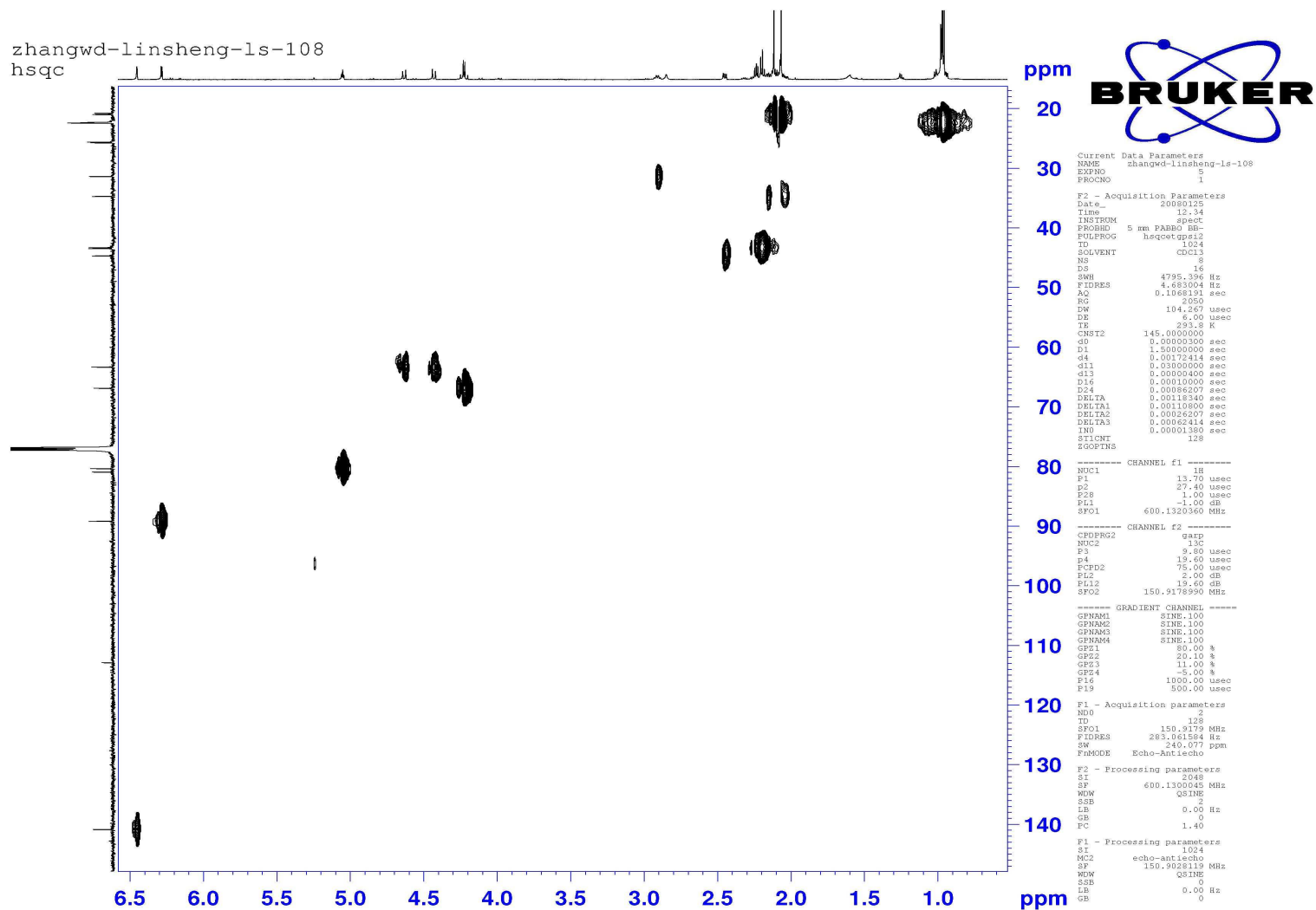
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 14.00 dB
 PL13 14.00 dB
 SFO2 600.1324005 MHz

F2 - Processing parameters
 SI 65536
 SF 150.9028119 MHz
 WDW EM
 SSB 0
 LB 3.00 Hz
 GB 0
 PC 1.40

S84. The ^{13}C NMR and DEPT Spectra (150 MHz, CDCl_3) of Compound (16)

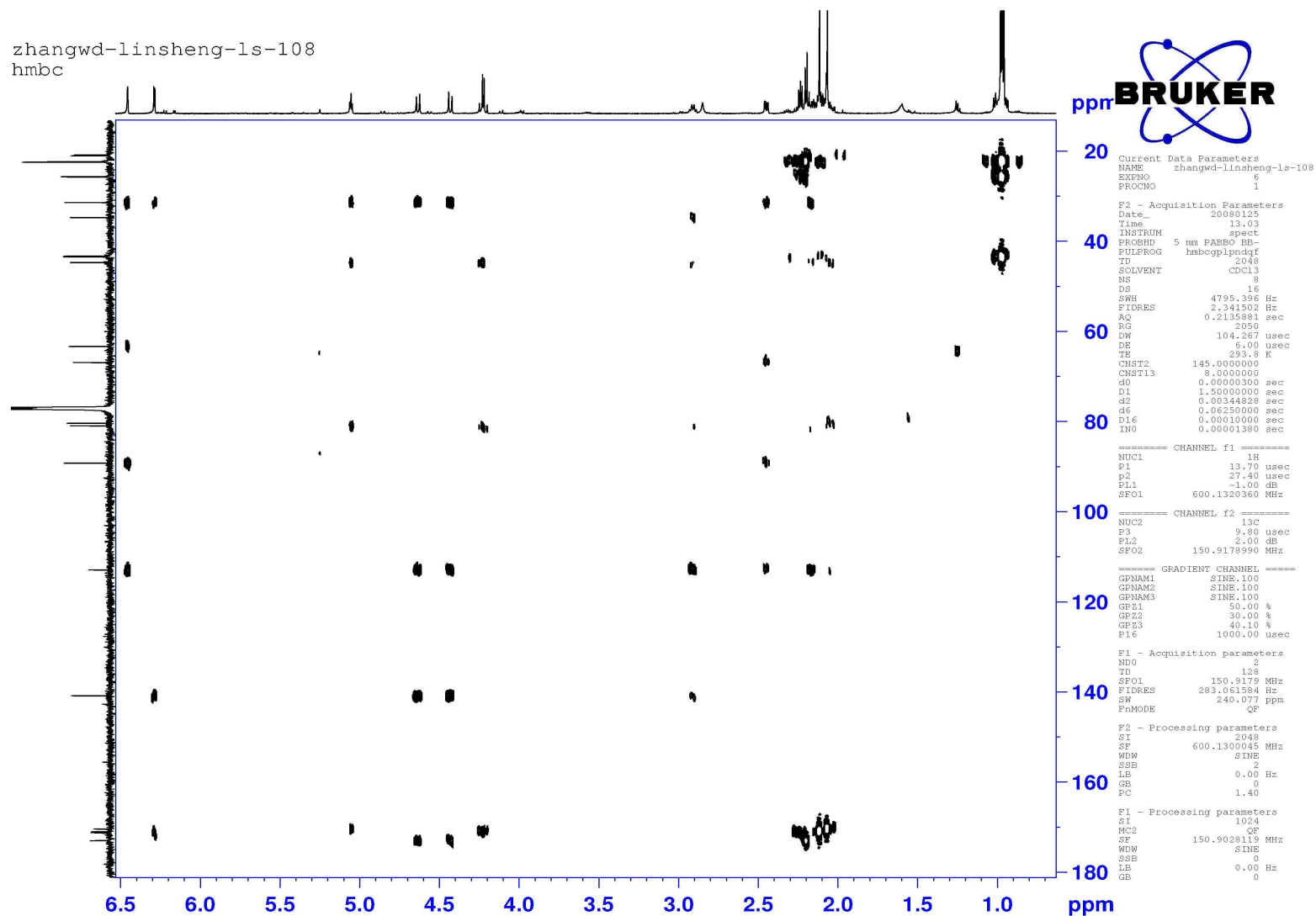


S85. The ^1H - ^1H COSY Spectrum (600 MHz, CDCl_3) of Compound (16)

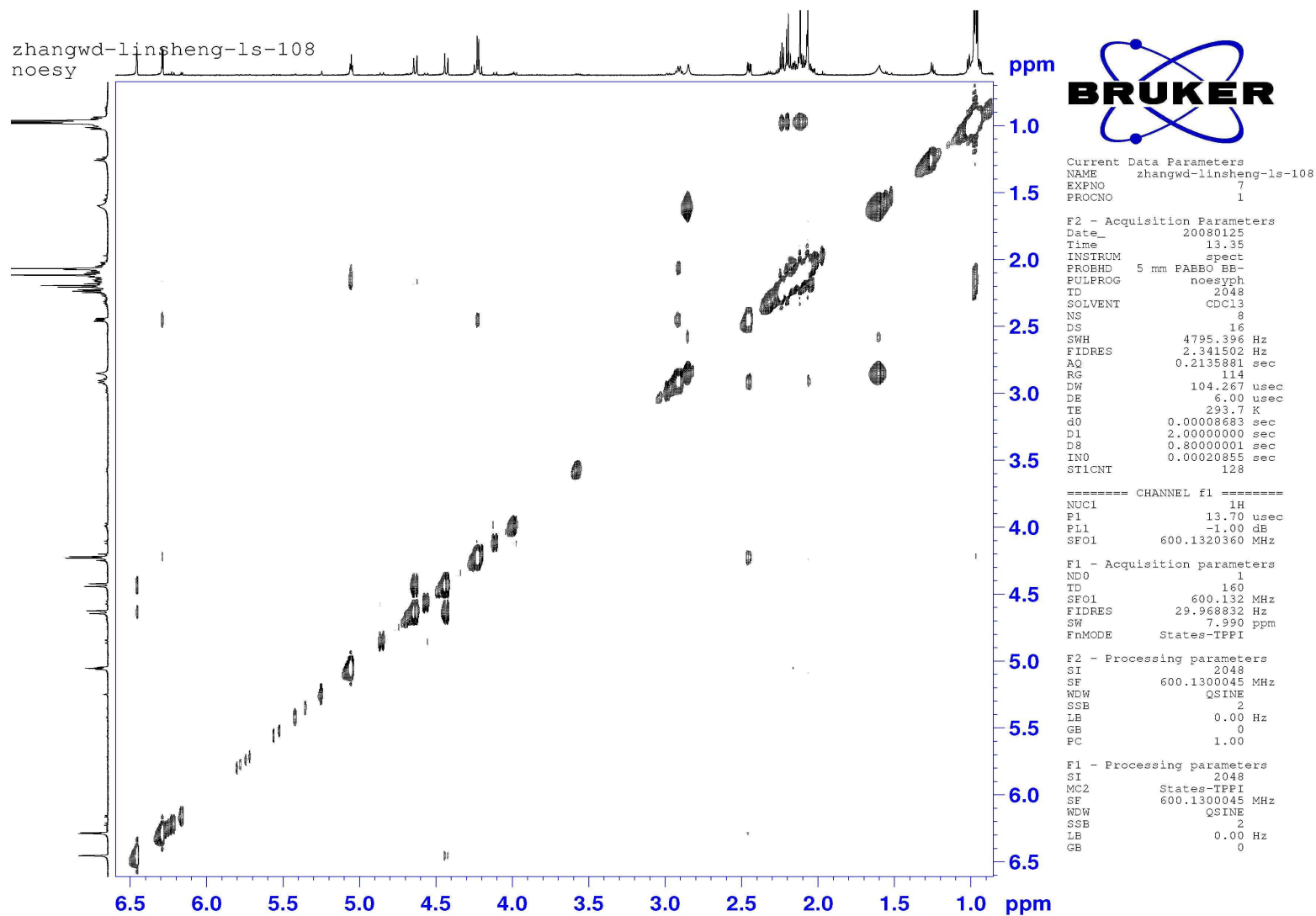


S86. The HSQC Spectrum (600 MHz, CDCl_3) of Compound (16)

zhangwd-linsheng-ls-108
hmbc



S87. The HMBC Spectrum of Compound (16)



S88. The NOESY Spectrum (600 MHz, CDCl₃) of Compound (16)

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

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

^a paclitaxel was used as a positive control