

Title of Manuscript: Iridoids and Lignans from *Valeriana jatamansi*

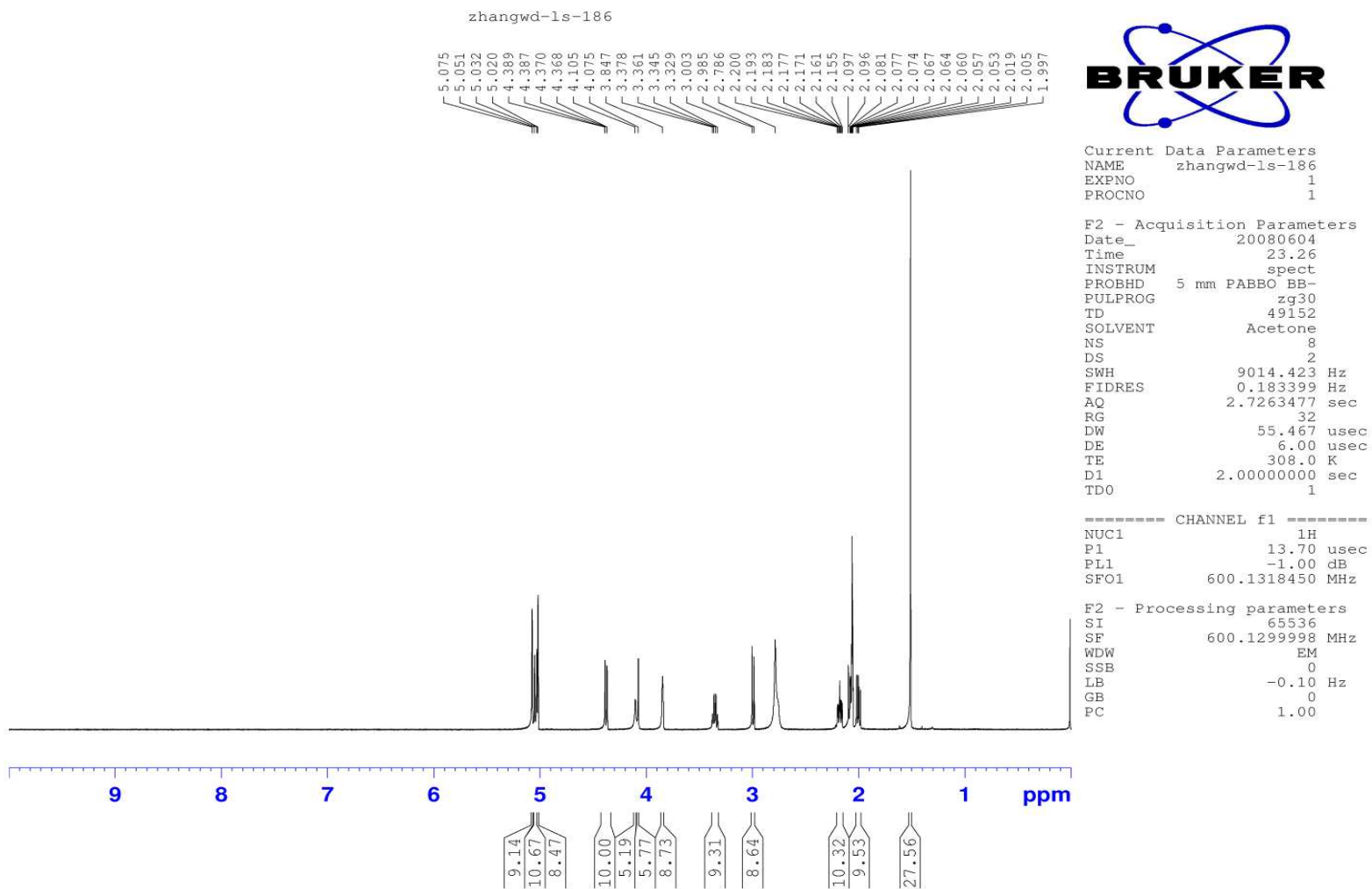
Author list: Sheng Lin, Tao Chen, Xiao-hua Liu, Yun-Heng Shen, Hui-Liang Li, Lei Shan, Run-Hui Liu, Xi-Ke Xu, Wei-Dong Zhang*, Hui Wang*

Supporting Information Available

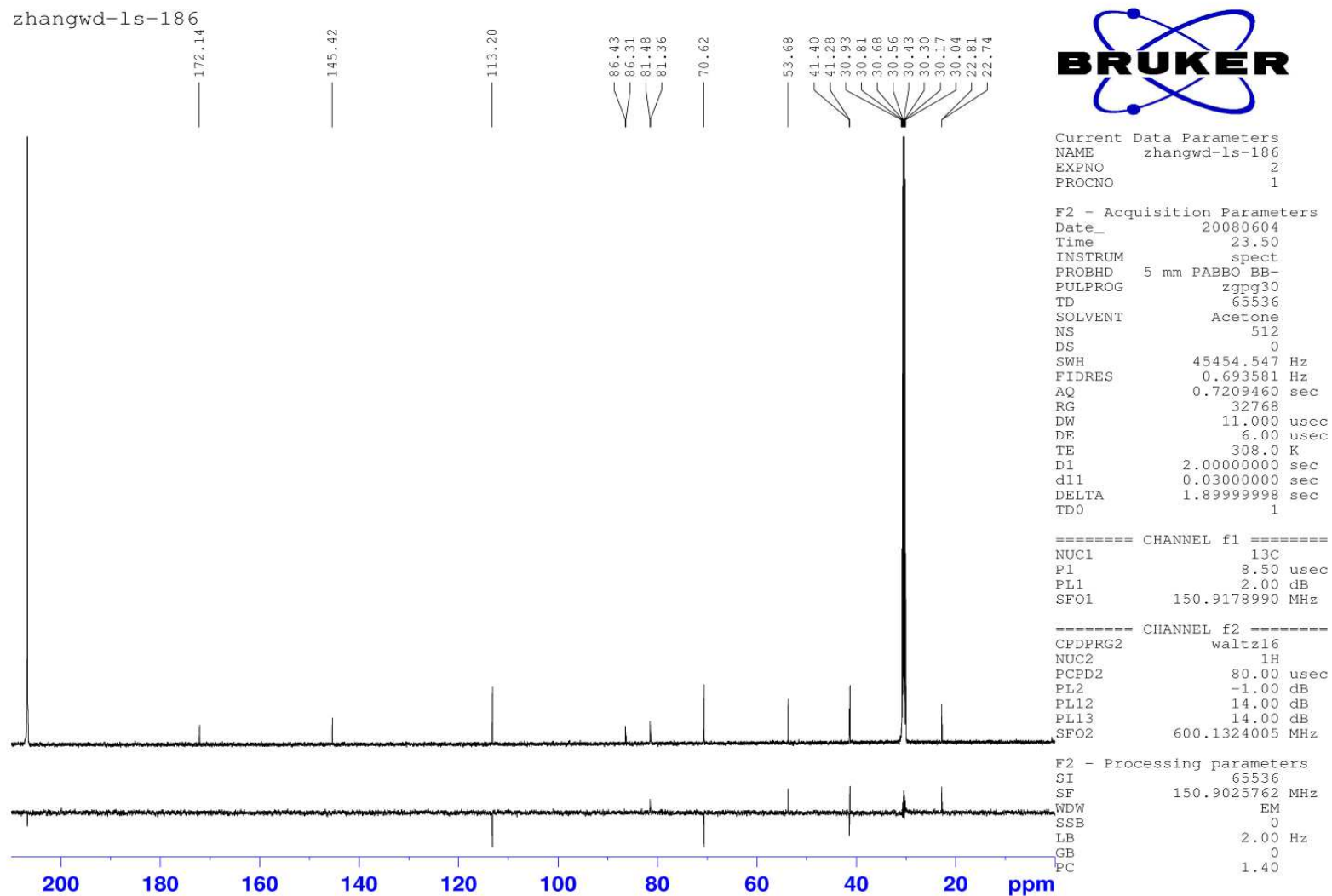
* To whom correspondence should be addressed. Fax: 86-21-65495819. E-mail: wdzhangY@hotmail.com

The List of Contents

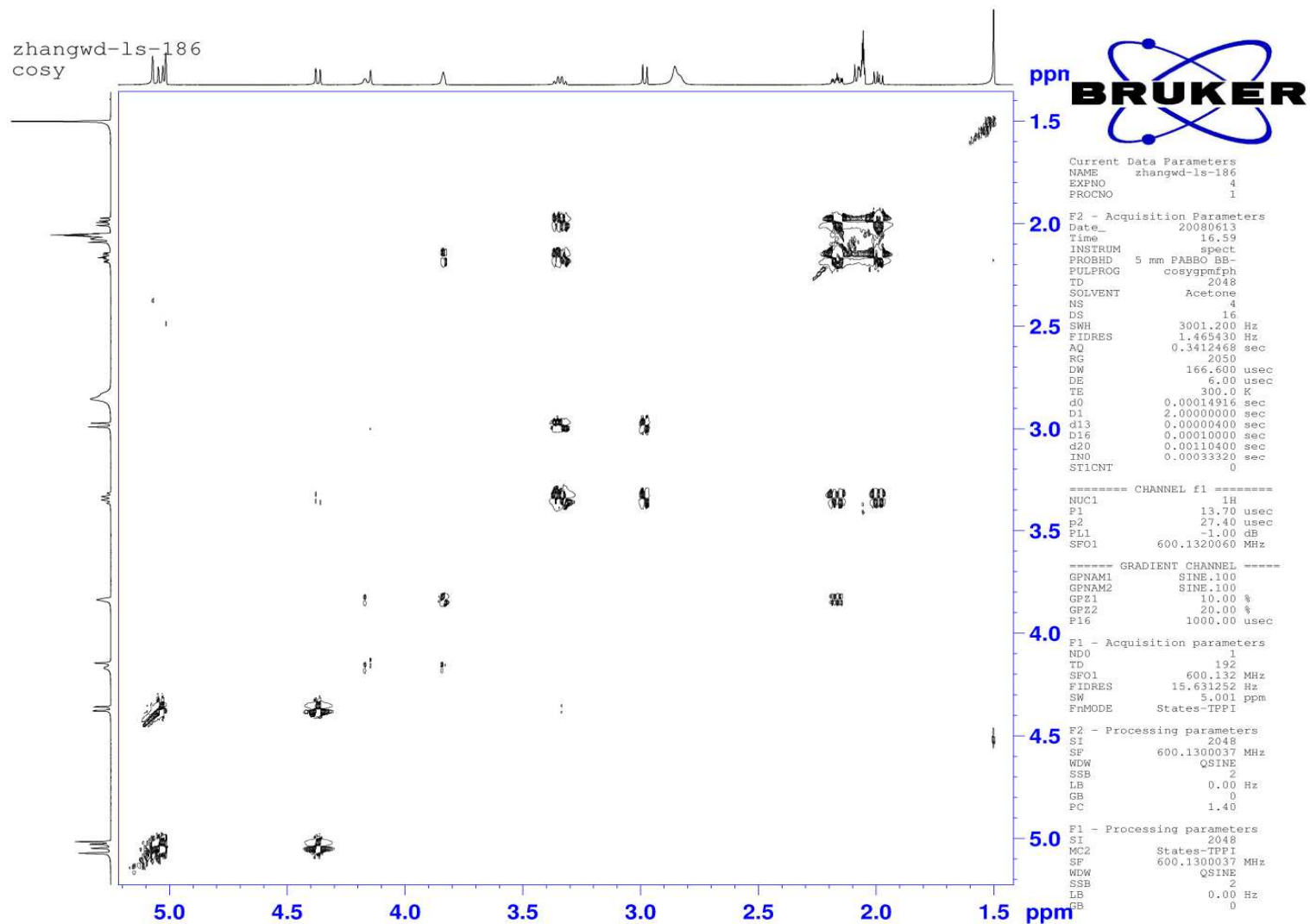
no.	Contents	Page
1	The ^1H NMR Spectrum of Jatamanin A (1) in $\text{Me}_2\text{CO}-d_6$	S3
2	The ^{13}C NMR and DEPT Spectra of Jatamanin A (1) in $\text{Me}_2\text{CO}-d_6$	S4
3	The $^1\text{H}-^1\text{H}$ COSY Spectrum of Jatamanin A (1) in $\text{Me}_2\text{CO}-d_6$	S5
4	The HSQC Spectrum of Jatamanin A (1) in $\text{Me}_2\text{CO}-d_6$	S6
5	The HMBC Spectrum of Jatamanin A (1) in $\text{Me}_2\text{CO}-d_6$	S7
6	The NOESY Spectrum of Jatamanin A (1) in $\text{Me}_2\text{CO}-d_6$	S8
7	The ^1H NMR Spectrum of Jatamanin B (2) in $\text{Me}_2\text{CO}-d_6$	S9
8	The ^{13}C NMR and DEPT Spectra of Jatamanin B (2) in $\text{Me}_2\text{CO}-d_6$	S10
9	The $^1\text{H}-^1\text{H}$ COSY Spectrum of Jatamanin B (2) in $\text{Me}_2\text{CO}-d_6$	S11
10	The HSQC Spectrum of Jatamanin B (2) in $\text{Me}_2\text{CO}-d_6$	S12
11	The HMBC Spectrum of Jatamanin B (2) in $\text{Me}_2\text{CO}-d_6$	S13
12	The NOESY Spectrum of Jatamanin B (2) in $\text{Me}_2\text{CO}-d_6$	S14
13	The ^1H NMR Spectrum of Jatamanin C (3) in $\text{Me}_2\text{CO}-d_6$	S15
14	The ^{13}C NMR Spectrum of Jatamanin C (3) in $\text{Me}_2\text{CO}-d_6$	S16
15	The DEPT Spectrum of Jatamanin C (3) in $\text{Me}_2\text{CO}-d_6$	S17
16	The ^1H NMR Spectrum of Jatamanin D (4) in $\text{Me}_2\text{CO}-d_6$	S18
17	The ^{13}C NMR and DEPT Spectra of Jatamanin D (4) in $\text{Me}_2\text{CO}-d_6$	S19
18	The ^1H NMR Spectrum of Jatamanin E (5) in $\text{Me}_2\text{CO}-d_6$	S20
19	The ^{13}C NMR and DEPT Spectra of Jatamanin E (5) in $\text{Me}_2\text{CO}-d_6$	S21
20	The ^1H NMR Spectrum of Jatamanin F (6) in $\text{Me}_2\text{CO}-d_6$	S22
21	The ^{13}C NMR and DEPT Spectra of Jatamanin F (6) in $\text{Me}_2\text{CO}-d_6$	S23
22	The ^1H NMR Spectrum of Jatamanin G (7) in $\text{Me}_2\text{CO}-d_6$	S24
23	The ^1H NMR Spectrum of Jatamanins H (8) and I (9) in $\text{Me}_2\text{CO}-d_6$	S25
24	The ^{13}C NMR and DEPT Spectra of Jatamanins H (8) and I (9) in $\text{Me}_2\text{CO}-d_6$	S26
25	The $^1\text{H}-^1\text{H}$ COSY Spectrum of Jatamanins H (8) and I (9) in $\text{Me}_2\text{CO}-d_6$	S27
26	The HSQC Spectrum of Jatamanins H (8) and I (9) in $\text{Me}_2\text{CO}-d_6$	S28
27	The HMBC Spectrum of Jatamanins H (8) and I (9) in $\text{Me}_2\text{CO}-d_6$	S29
28	The NOESY Spectrum of Jatamanins H (8) and I (9) in $\text{Me}_2\text{CO}-d_6$	S30
29	The ^1H NMR Spectrum of Jatamanin J (10) in MeOD	S31
30	The ^{13}C NMR and DEPT Spectra of Jatamanin J (10) in MeOD	S32
31	The ^1H NMR Spectrum of Jatamanin K (11) in $\text{Me}_2\text{CO}-d_6$	S33
32	The ^{13}C NMR and DEPT Spectra of Jatamanin K (11) in $\text{Me}_2\text{CO}-d_6$	S34
33	The ^1H NMR Spectrum of Jatamanin L (12) in $\text{Me}_2\text{CO}-d_6$	S35
34	The ^{13}C NMR and DEPT Spectra of Jatamanin L (12) in $\text{Me}_2\text{CO}-d_6$	S36
35	The ^1H NMR Spectrum of Jatamanin M (13) in $\text{Me}_2\text{CO}-d_6$	S37
36	The ^{13}C NMR and DEPT Spectra of Jatamanin M (13) in $\text{Me}_2\text{CO}-d_6$	S38
37	The ^1H NMR Spectrum of Compound 14 in $\text{Me}_2\text{CO}-d_6$	S39
38	The ^{13}C NMR and DEPT Spectra of Compound 14 in $\text{Me}_2\text{CO}-d_6$	S40
39	Crystal data and structure refinement for Jatamanin A (1)	S41



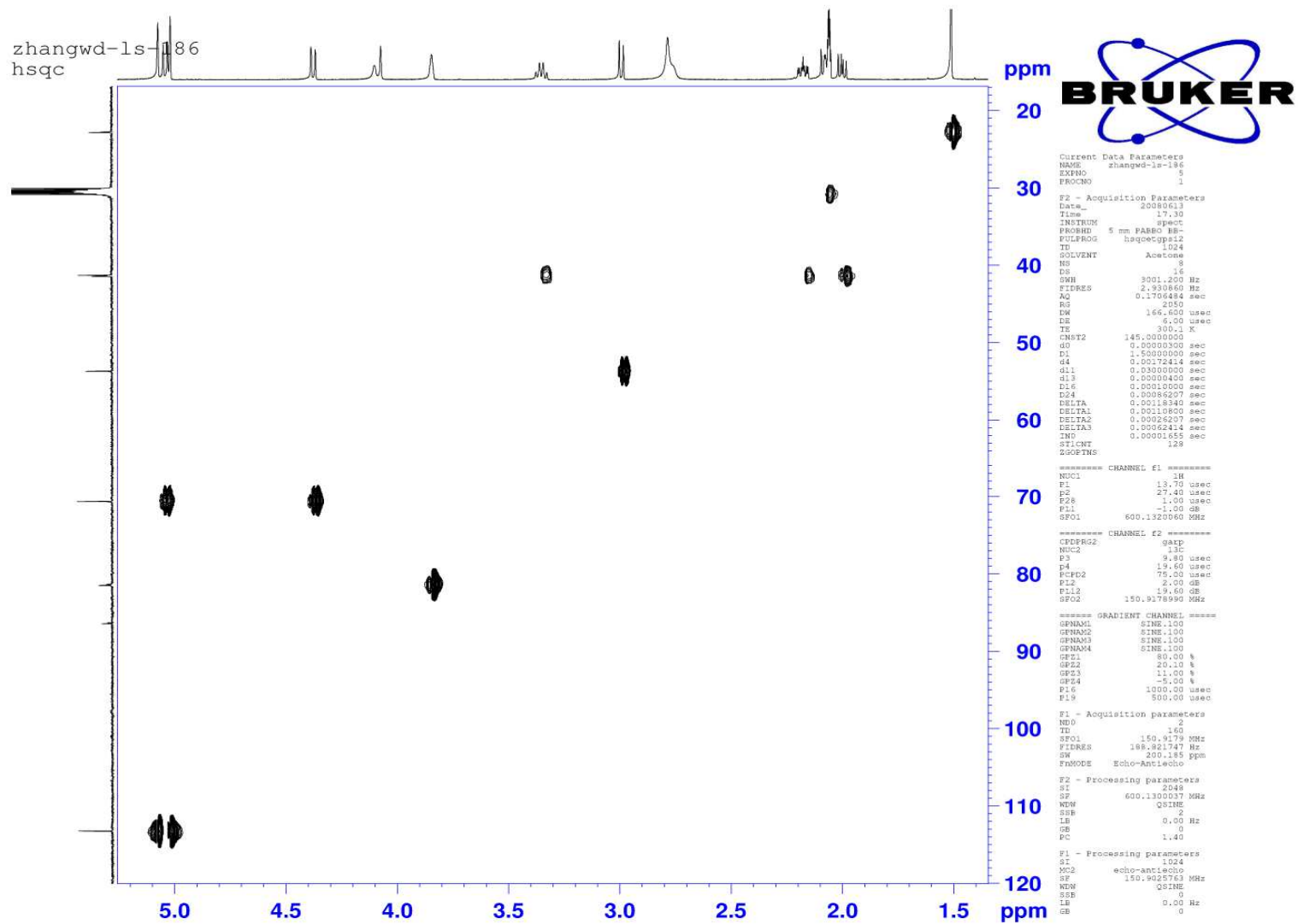
The ^1H NMR Spectrum of Jatamanin A (1) in $\text{Me}_2\text{CO}-d_6$



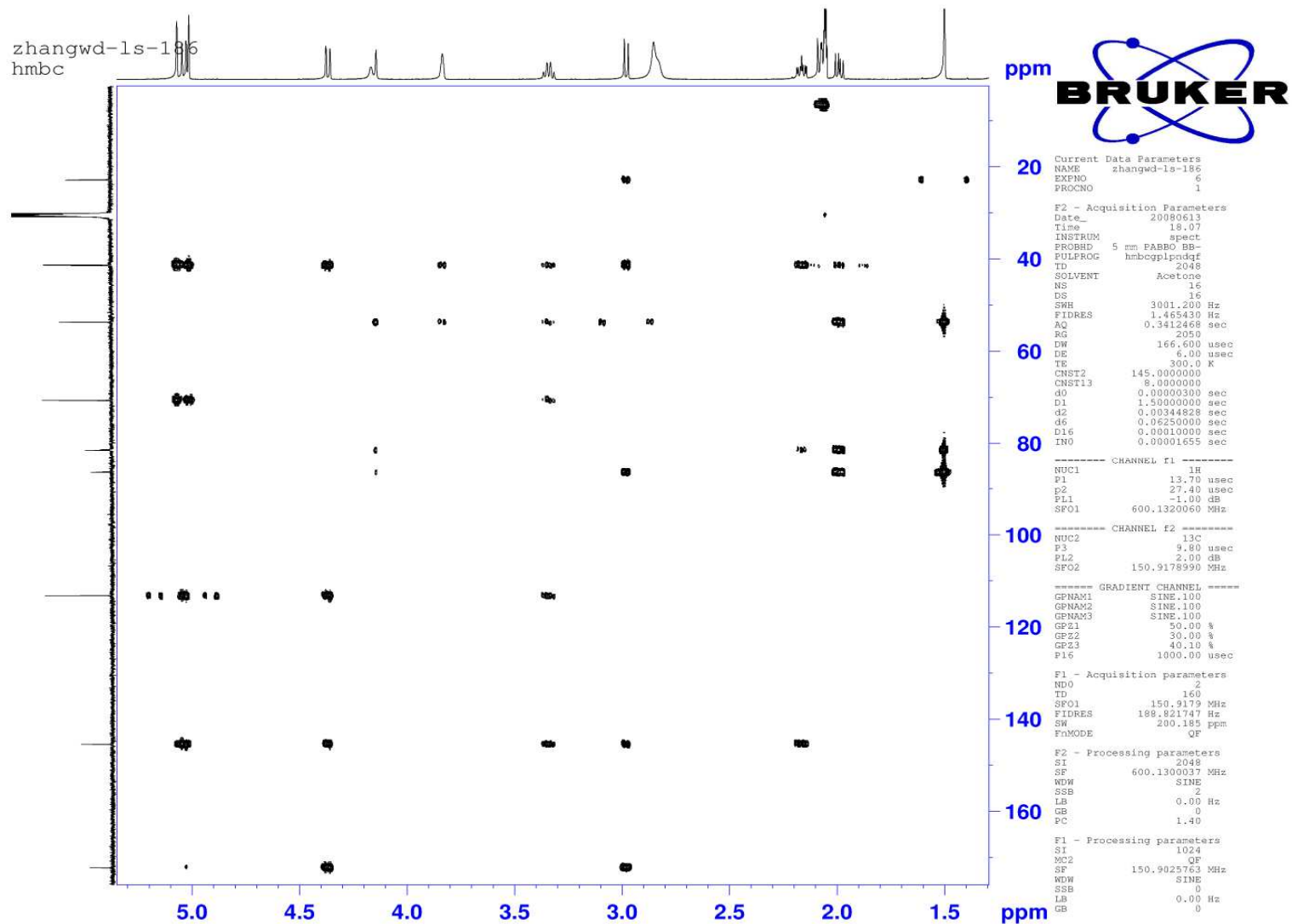
The ^{13}C NMR and DEPT Spectra of Jatamanin A (1) in $\text{Me}_2\text{CO}-d_6$



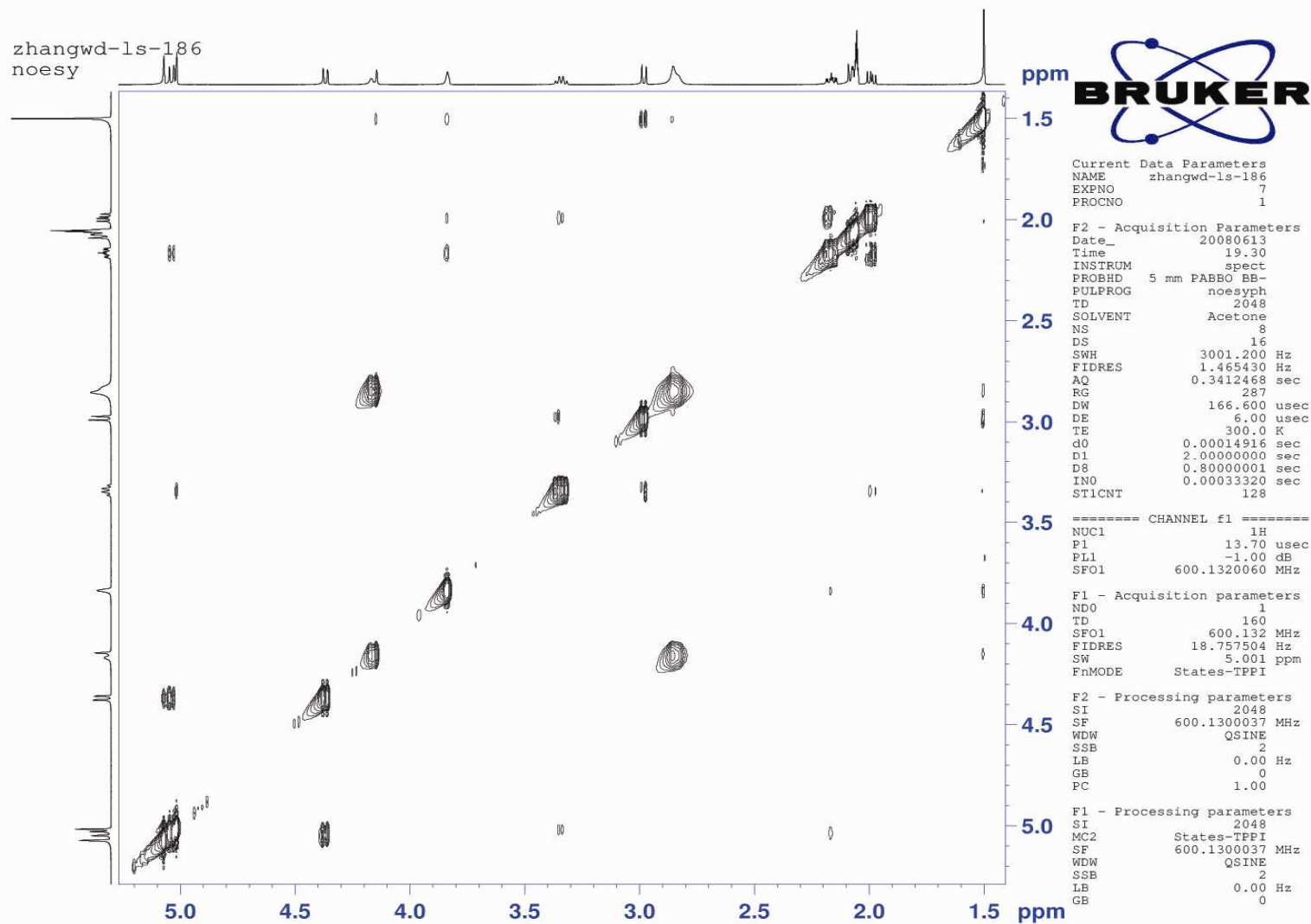
The ^1H - ^1H COSY Spectrum of Jatamanin A (1) in $\text{Me}_2\text{CO}-d_6$



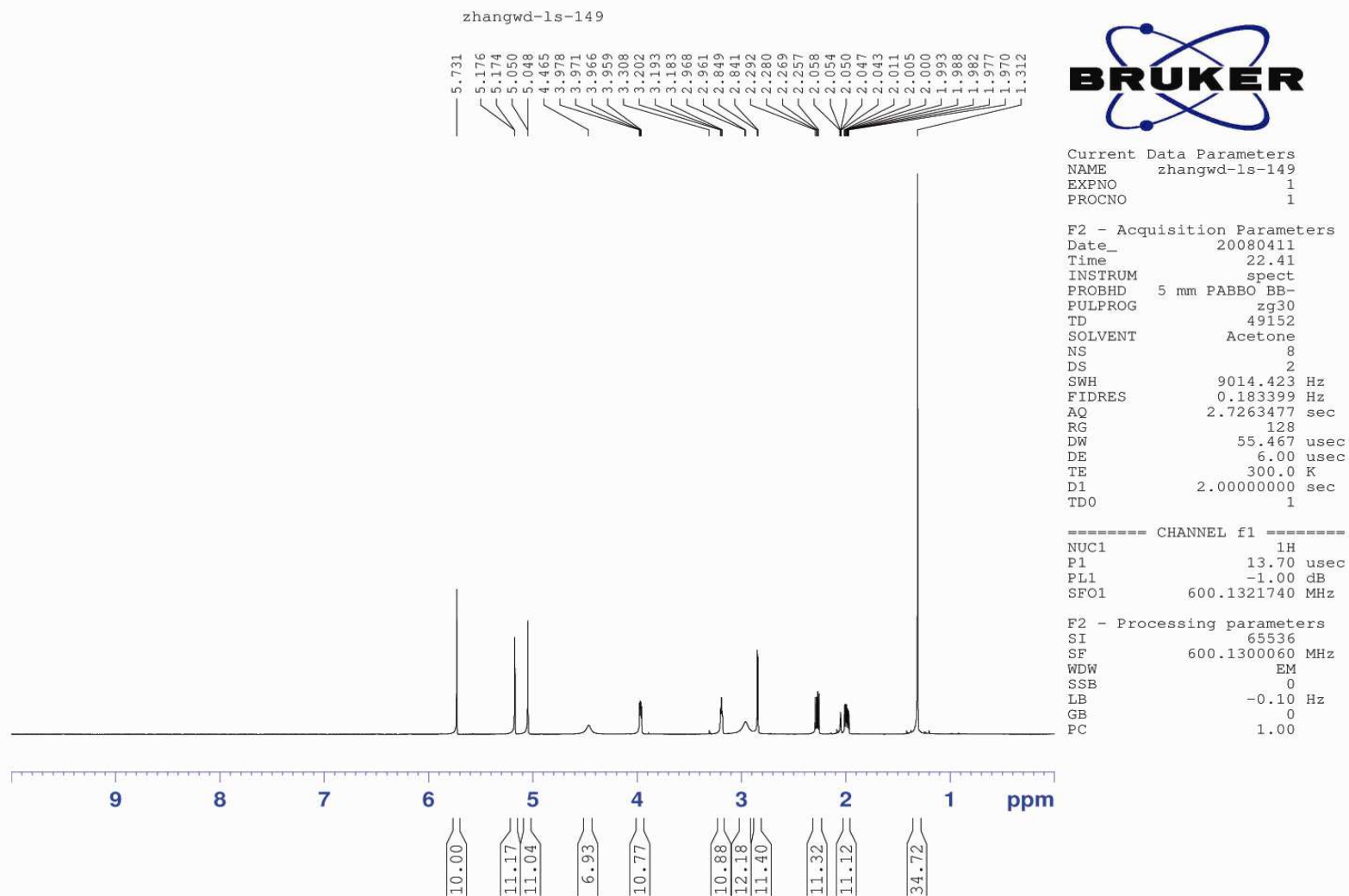
The HSQC Spectrum of Jatamanin A (1) in Me₂CO-d₆



The HMBC Spectrum of Jatamanin A (1) in $\text{Me}_2\text{CO}-d_6$

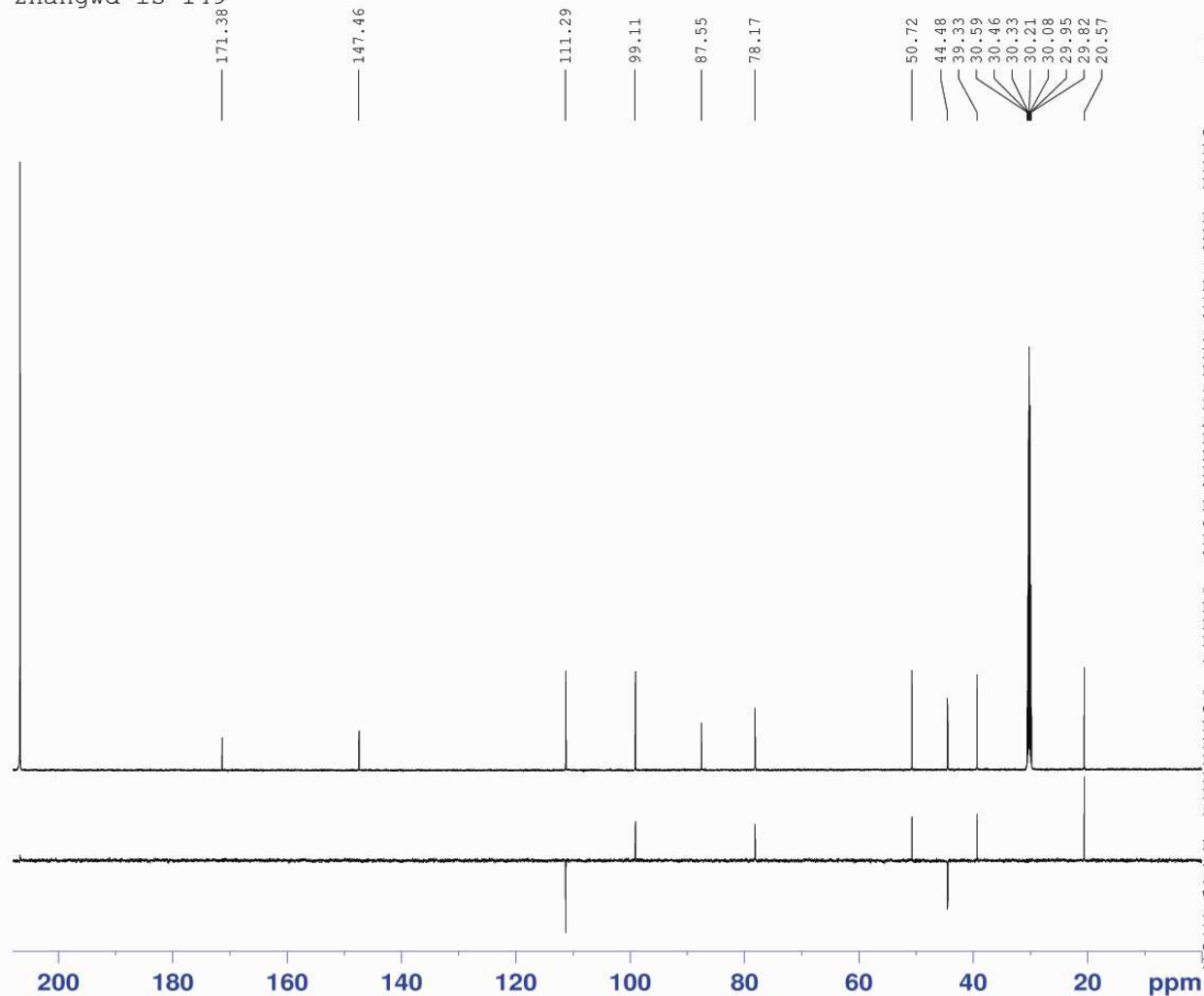


The NOESY Spectrum of Jatamanin A (1) in $\text{Me}_2\text{CO}-d_6$



The ^1H NMR Spectrum of Jatamanin B (2) in $\text{Me}_2\text{CO}-d_6$

zhangwd-ls-149



Current Data Parameters
NAME zhangwd-ls-149
EXPNO 2
PROCNO 1

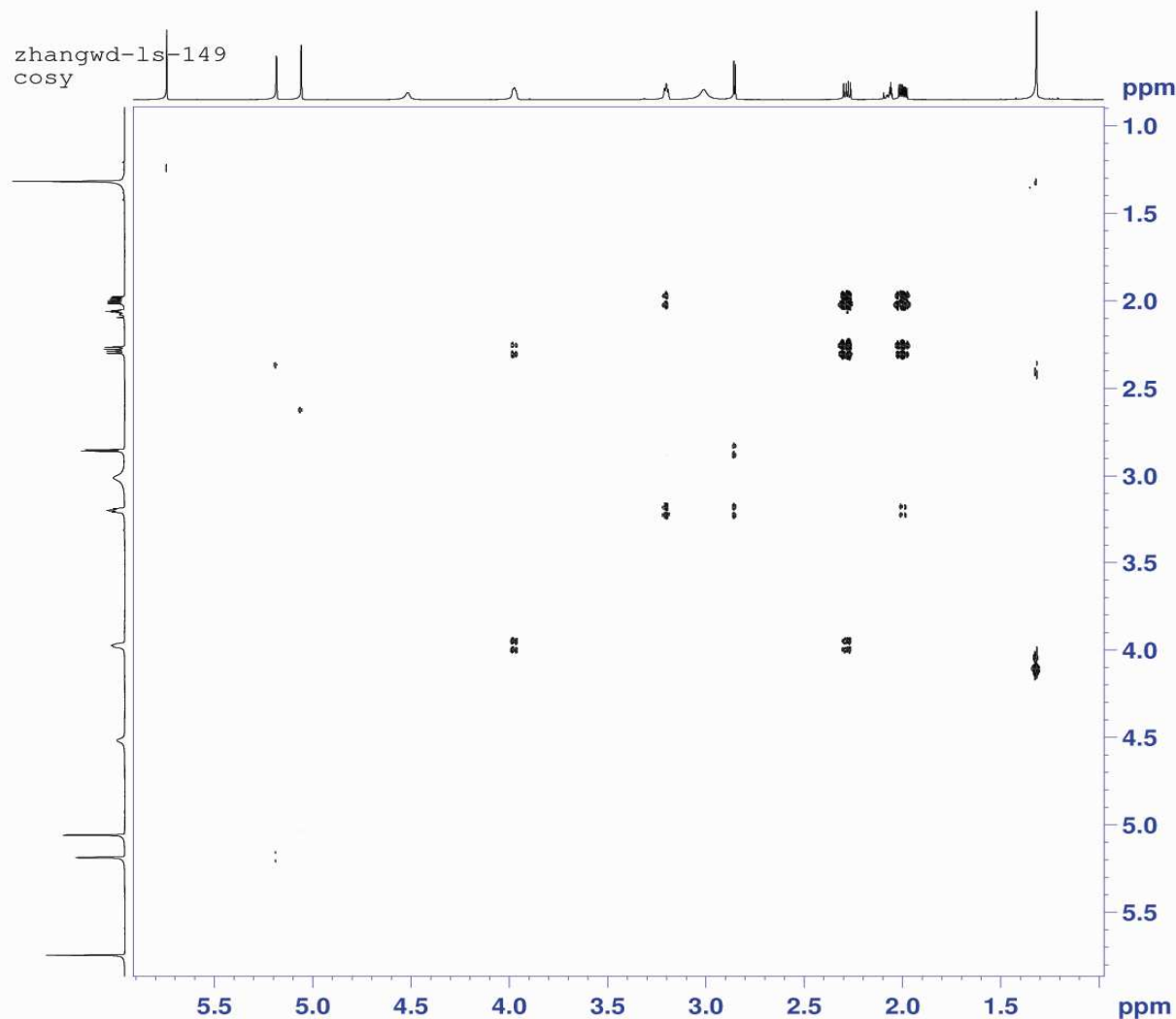
F2 - Acquisition Parameters
Date_ 20080411
Time 22.52
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 242
DS 0
SWH 45454.547 Hz
FIDRES 0.693581 Hz
AQ 0.7209460 sec
RG 32768
DW 11.000 usec
DE 6.00 usec
TE 300.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
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 600.1324005 MHz

F2 - Processing parameters
SI 65536
SF 150.9026234 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

The ^{13}C NMR and DEPT Spectra of Jatamanin B (2) in $\text{Me}_2\text{CO}-d_6$



Current Data Parameters
NAME zhangwd-ls-149
EXPNO 4
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080715
Time 12.33
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpmph
TD 2048
SOLVENT Acetone
NS 4
DS 16
SWH 3597.122 Hz
FIDRES 1.756407 Hz
AQ 0.2847220 sec
RG 2050
DW 139.000 usec
DE 6.00 usec
TE 297.9 K
d0 0.00012156 sec
D1 2.00000000 sec
d13 0.00000400 sec
D16 0.00010000 sec
d20 0.00110400 sec
IN0 0.00027800 sec
ST1CNT 0

===== CHANNEL f1 =====
NUC1 1H
P1 13.70 usec
p2 27.40 usec
PL1 -1.00 dB
SFO1 600.1319456 MHz

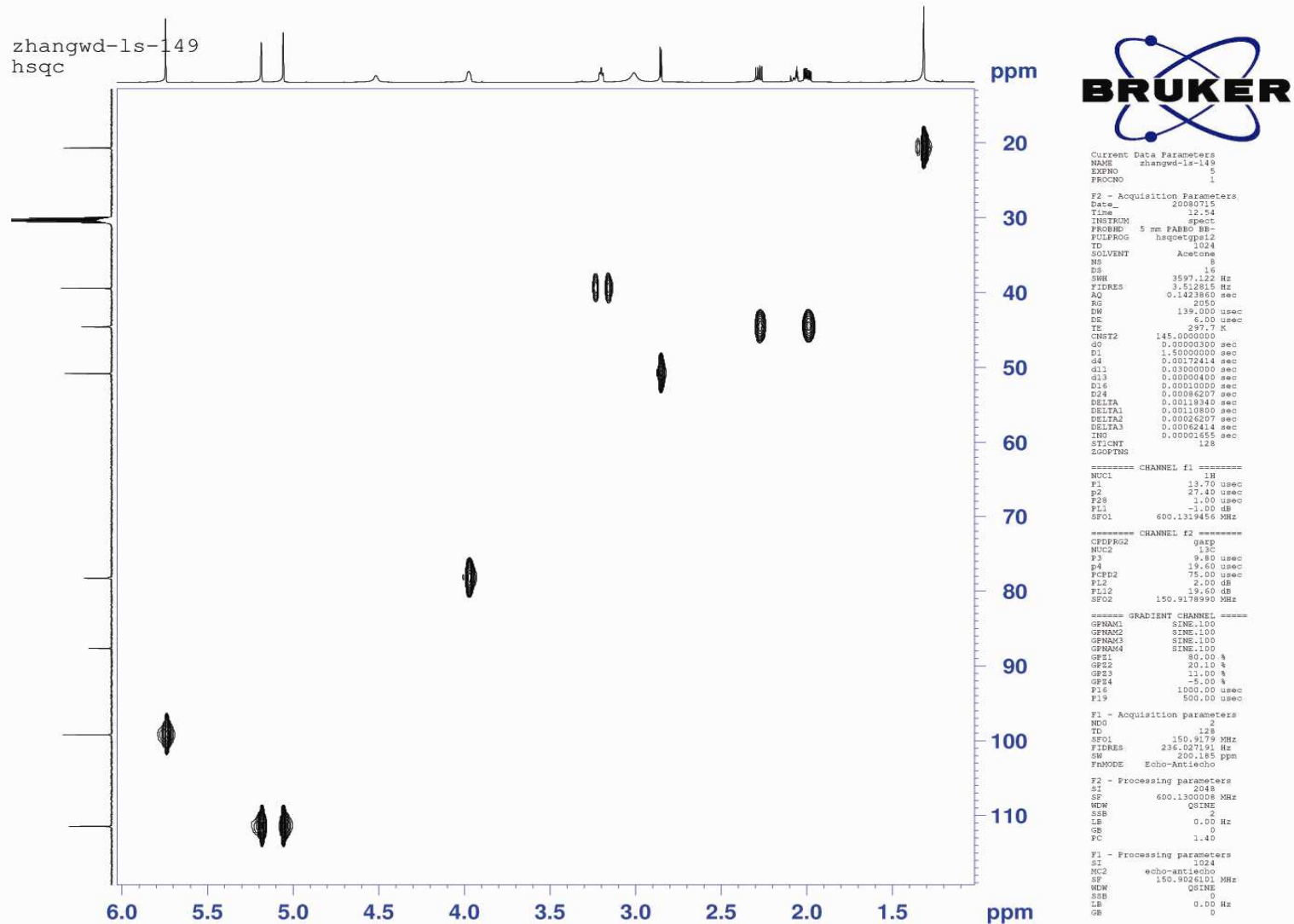
===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec

F1 - Acquisition parameters
ND0 1
TD 128
SFO1 600.1319 MHz
FIDRES 28.102518 Hz
SW 5.994 ppm
FMODE States-TPPI

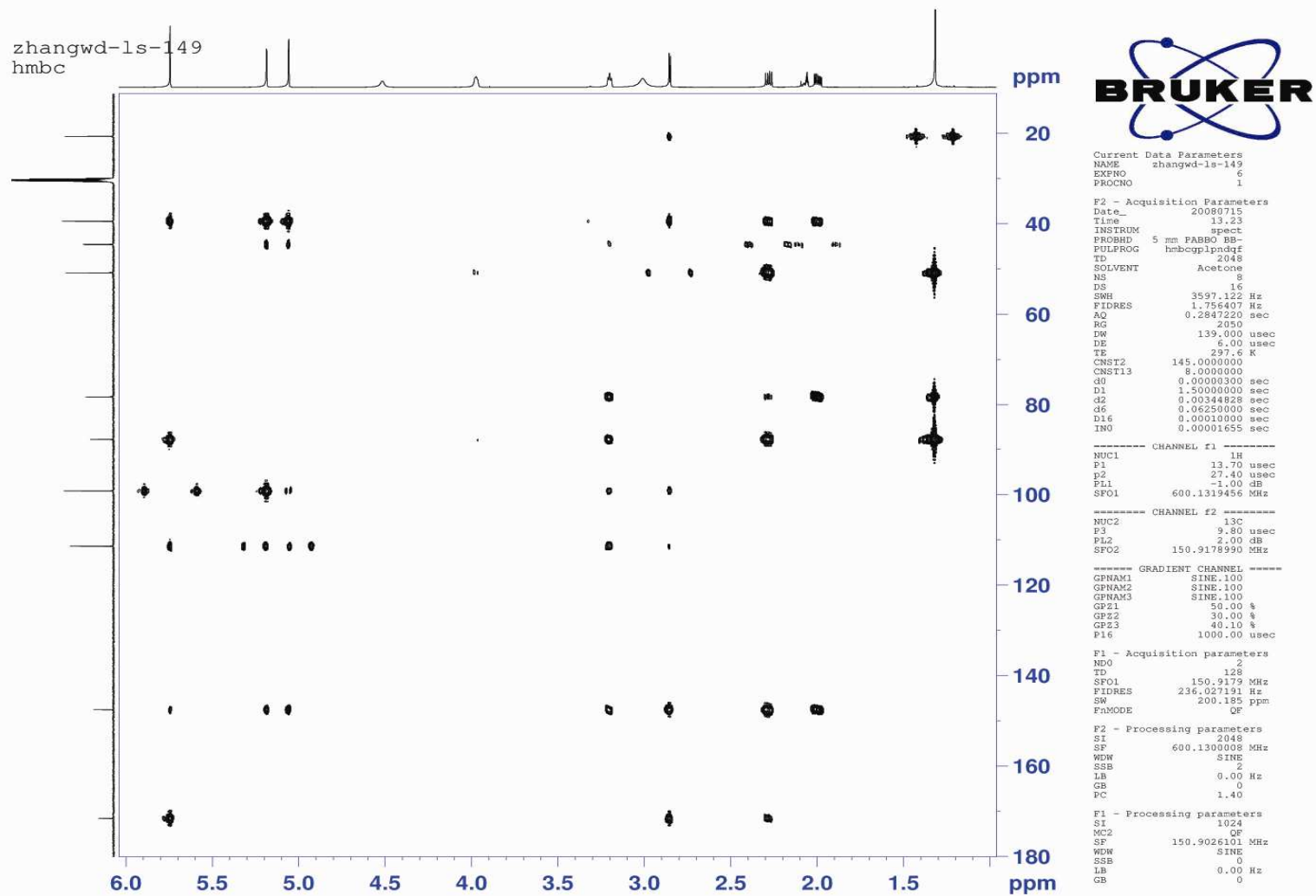
F2 - Processing parameters
SI 2048
SF 600.1300008 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40

F1 - Processing parameters
SI 2048
MC2 States-TPPI
SF 600.1300008 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0

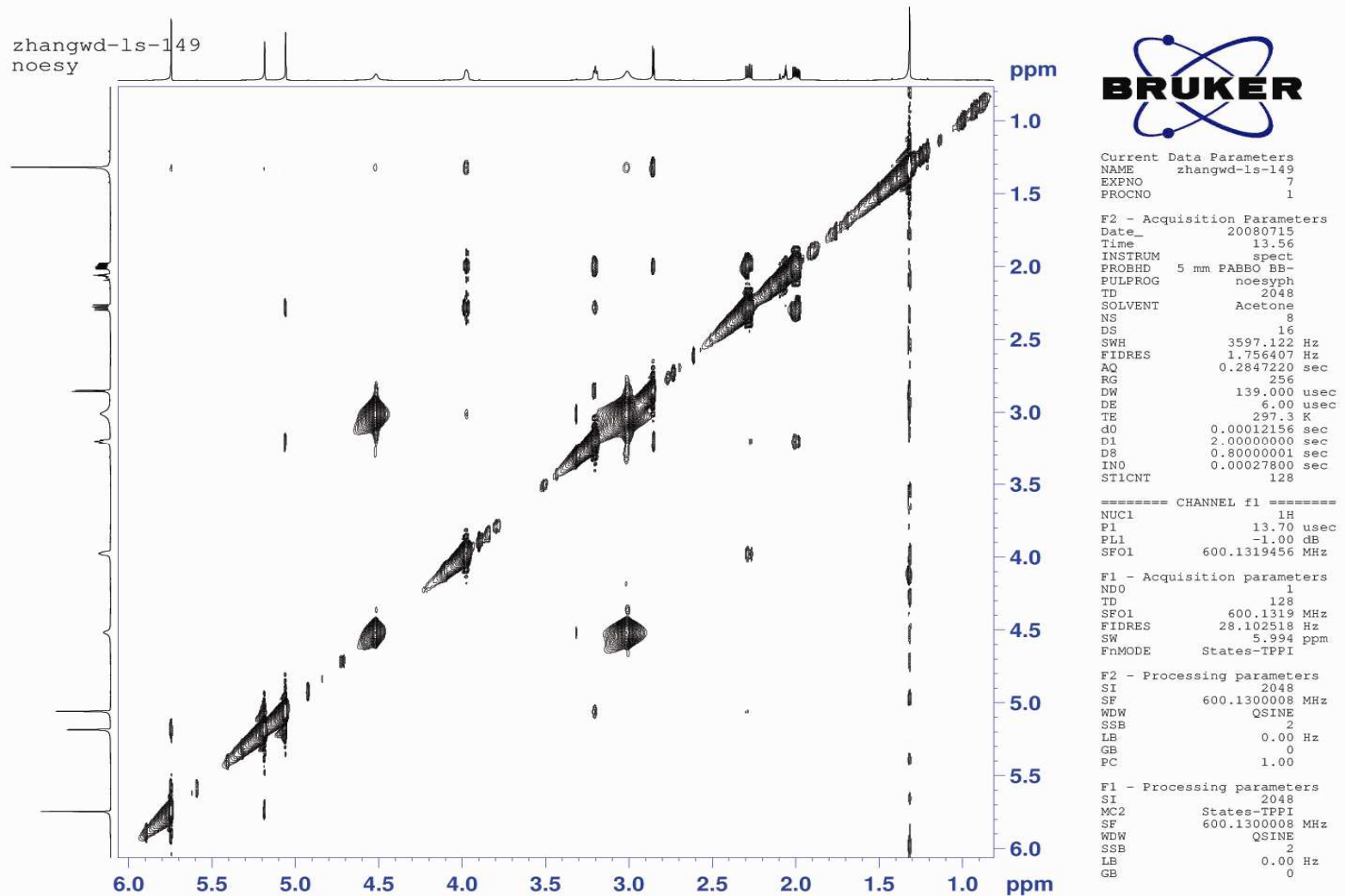
The ^1H - ^1H COSY Spectrum of Jatamanin B (2) in $\text{Me}_2\text{CO}-d_6$



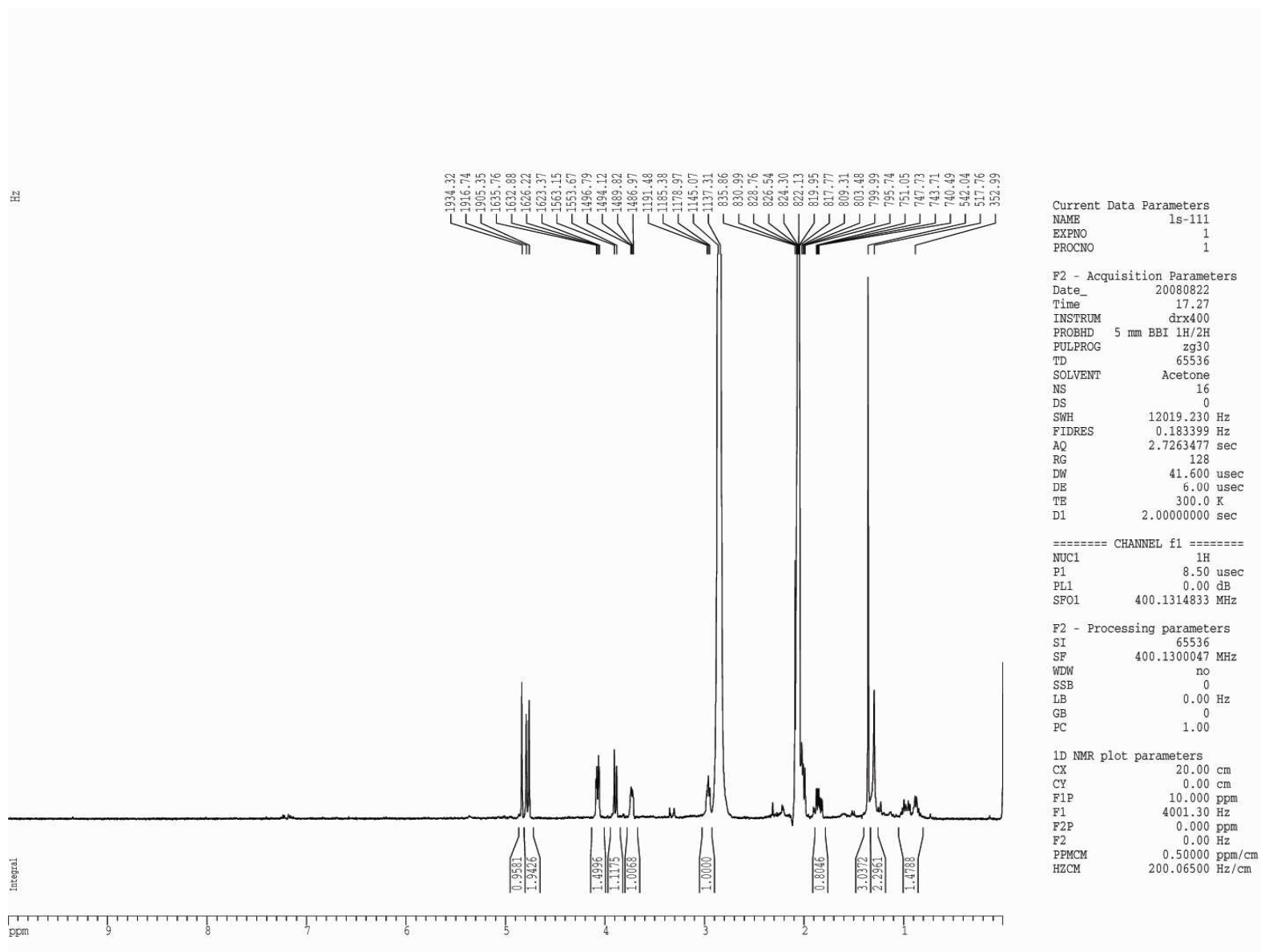
The HSQC Spectrum of Jatamanin B (2) in Me₂CO-*d*₆



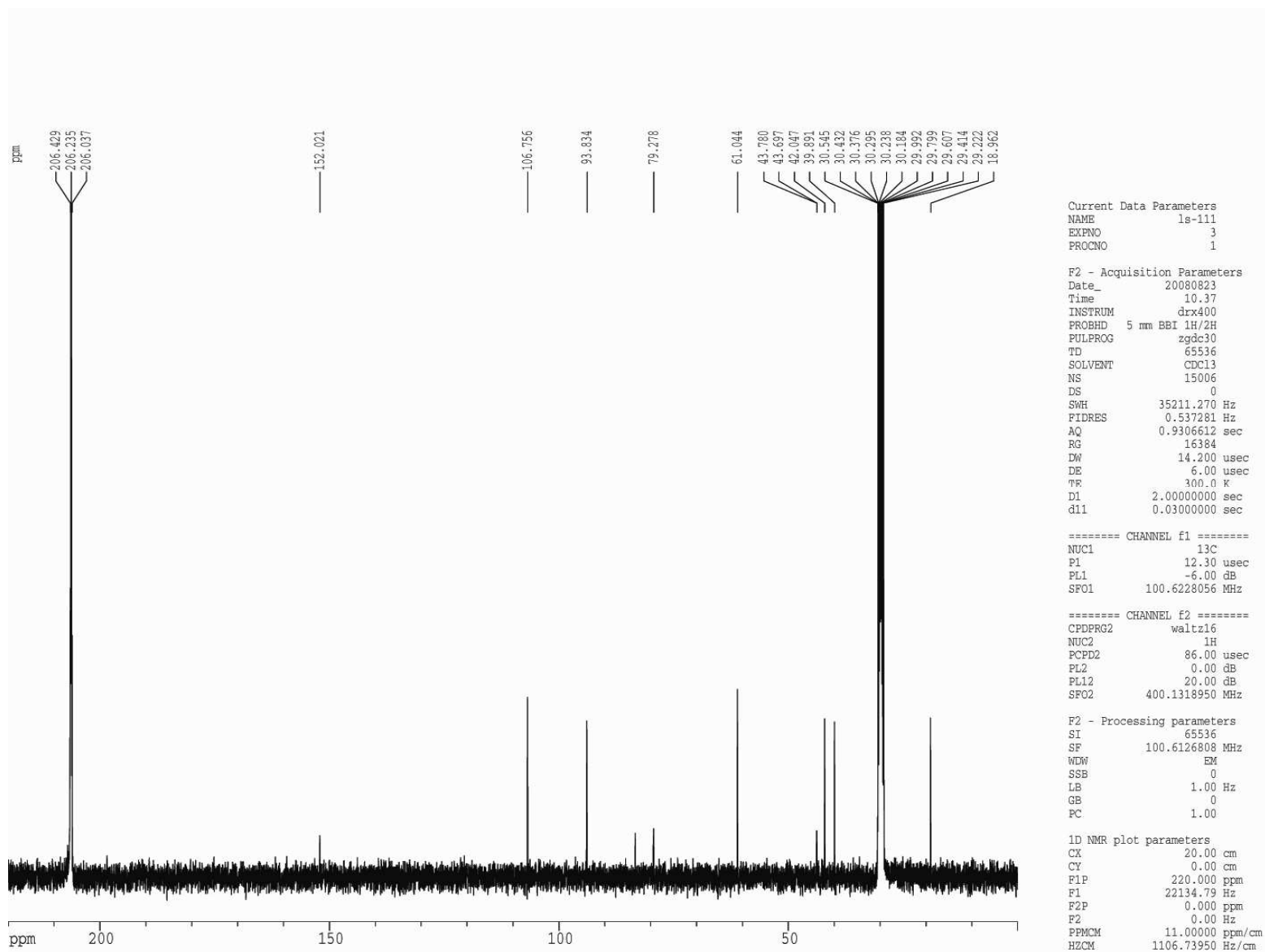
The HMBNMR Spectrum of Jatamanin B (2) in $\text{Me}_2\text{CO}-d_6$



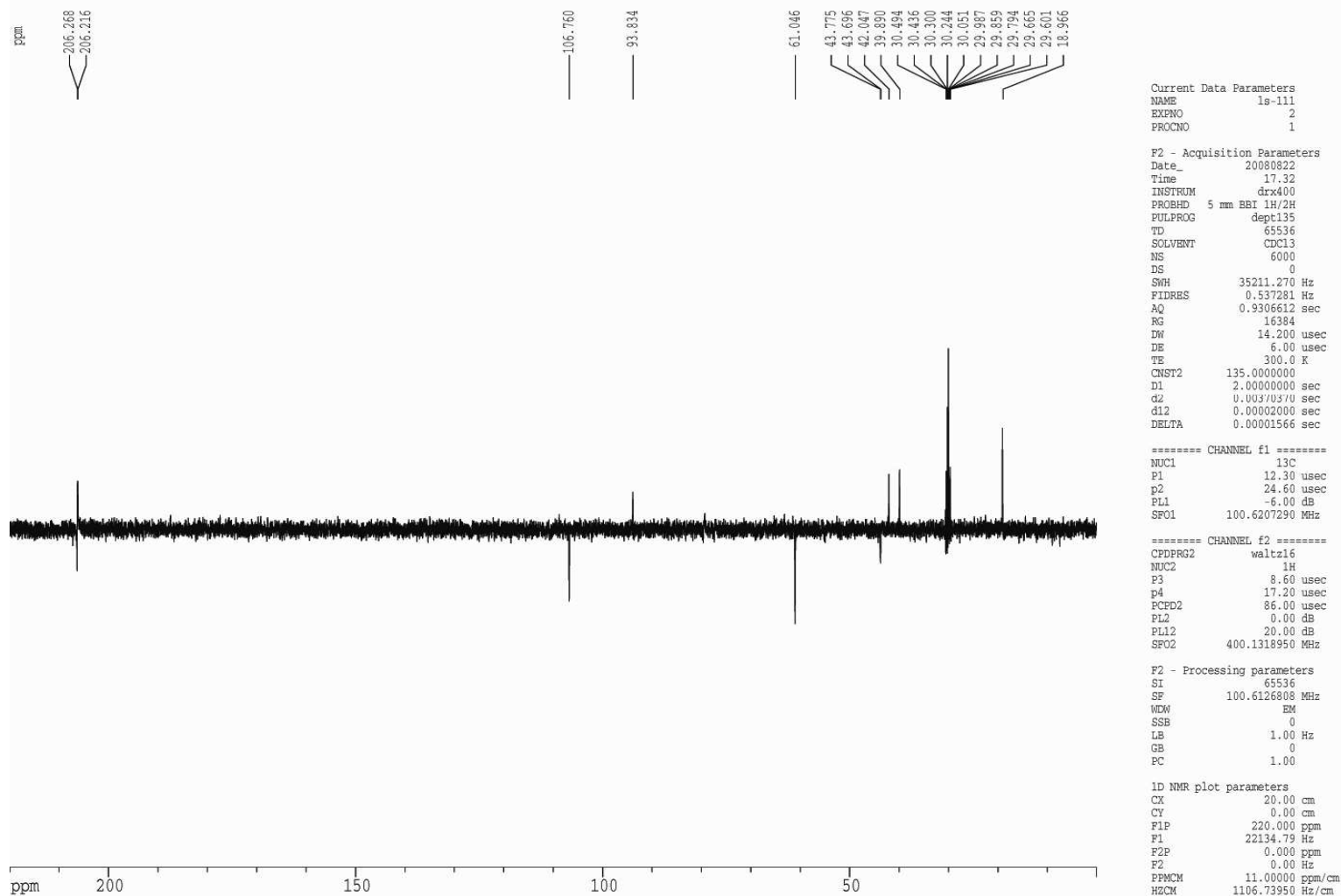
The NOESY Spectrum of Jatamanin B (2) in $\text{Me}_2\text{CO}-d_6$



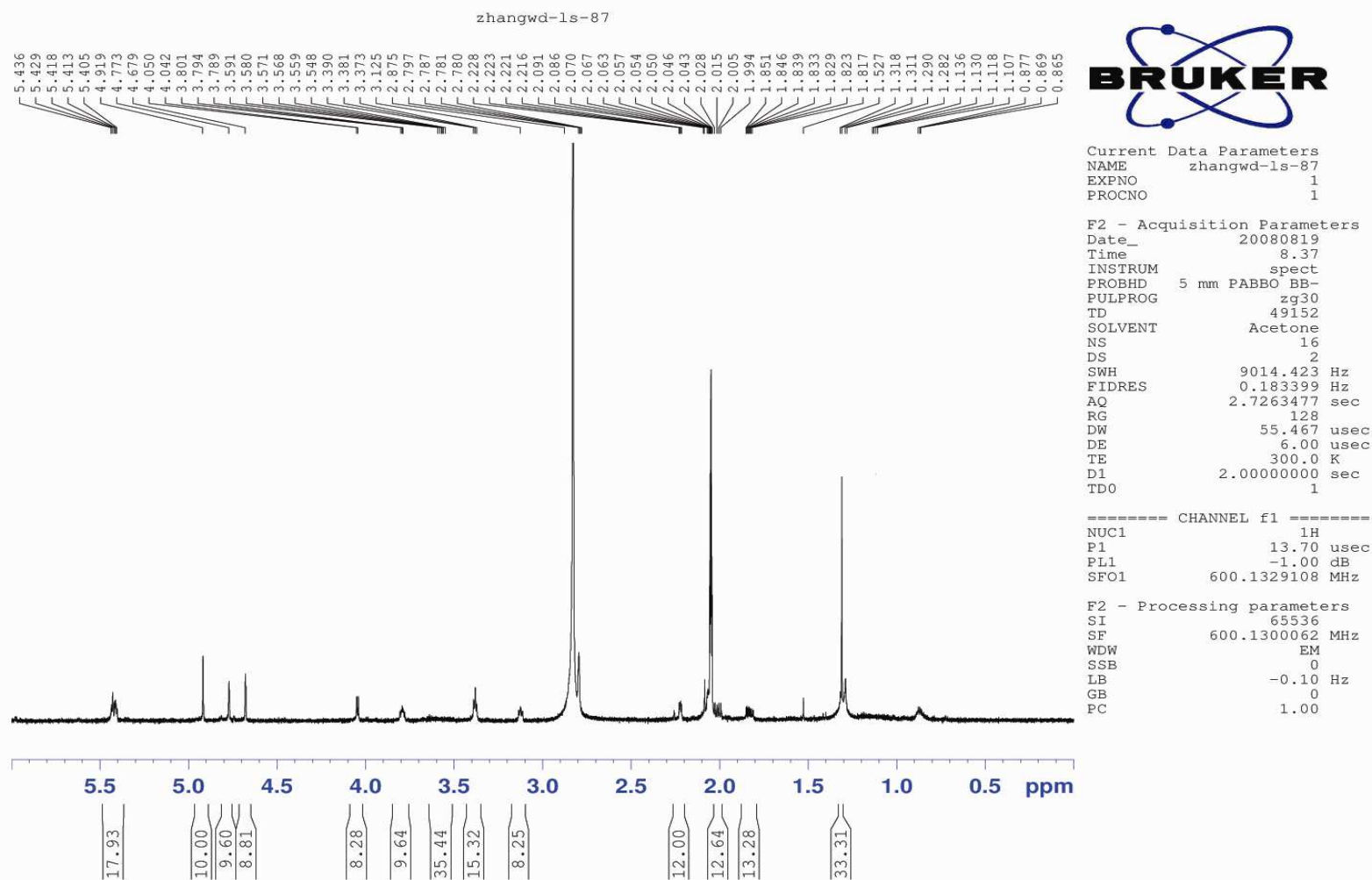
The ^1H NMR Spectrum of Jatamanin C (3) in $\text{Me}_2\text{CO}-d_6$



The ^{13}C NMR Spectrum of Jatamanin C (3) in $\text{Me}_2\text{CO}-d_6$

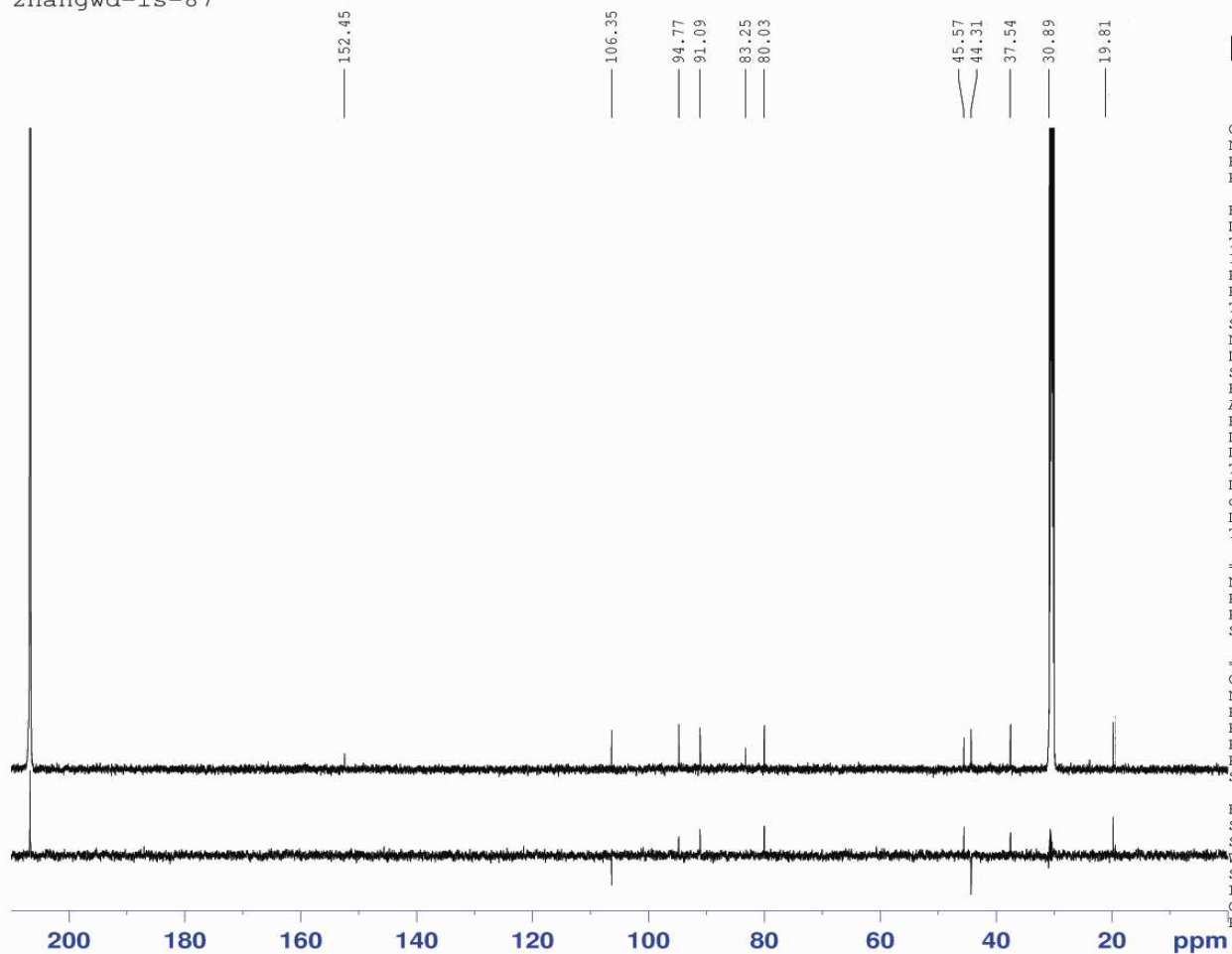


The DEPT Spectrum of Jatamanin C (3) in Me₂CO-*d*₆



The ^1H NMR Spectrum of Jatamanin D (4) in $\text{Me}_2\text{CO}-d_6$

zhangwd-ls-87



Current Data Parameters
NAME zhangwd-ls-87
EXPNO 2
PROCNO 1

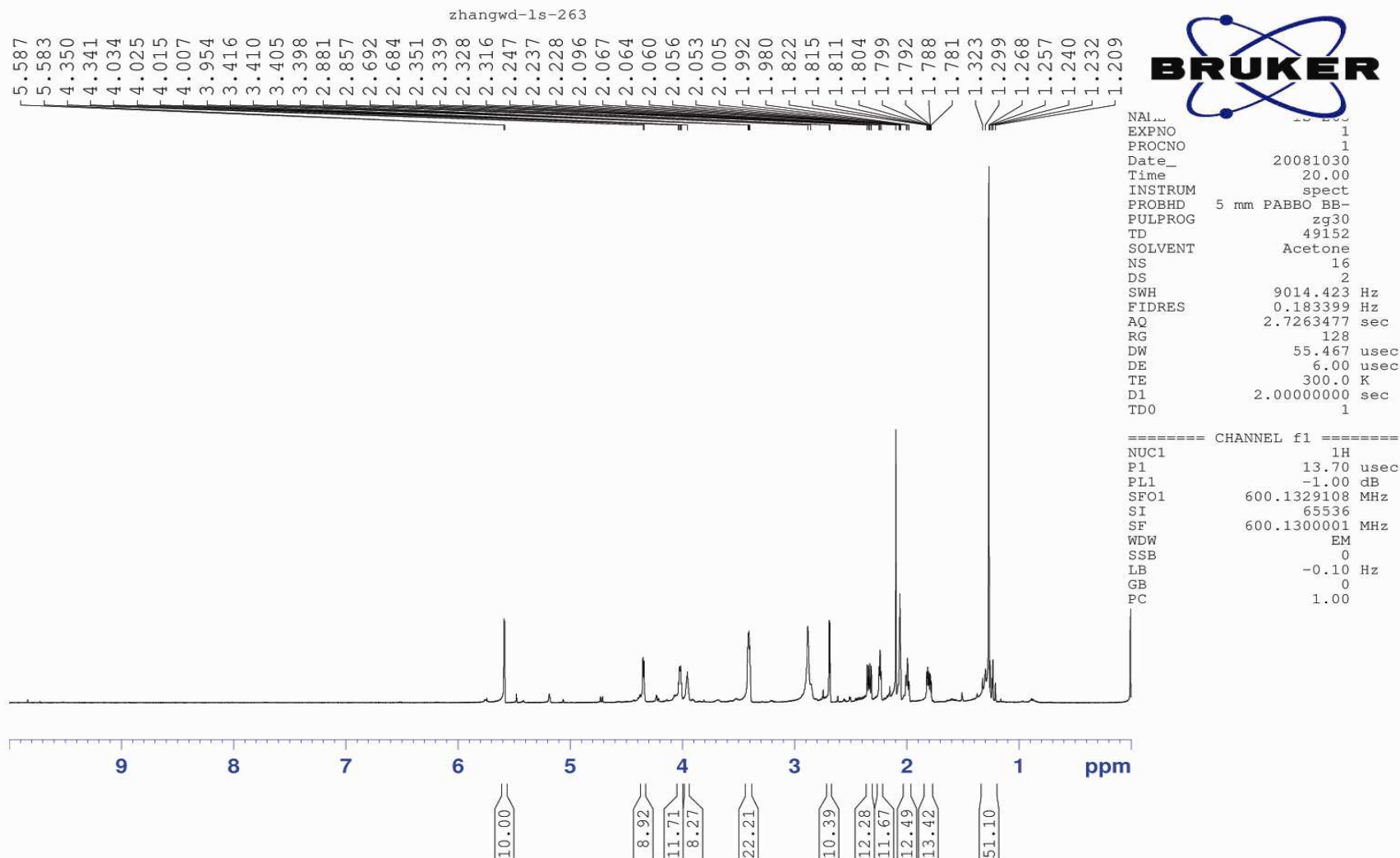
F2 - Acquisition Parameters
Date_ 20080819
Time 11.05
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 3194
DS 0
SWH 45454.547 Hz
FIDRES 0.693581 Hz
AQ 0.7209460 sec
RG 32768
DW 11.000 usec
DE 6.00 usec
TE 300.3 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TD0 1

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

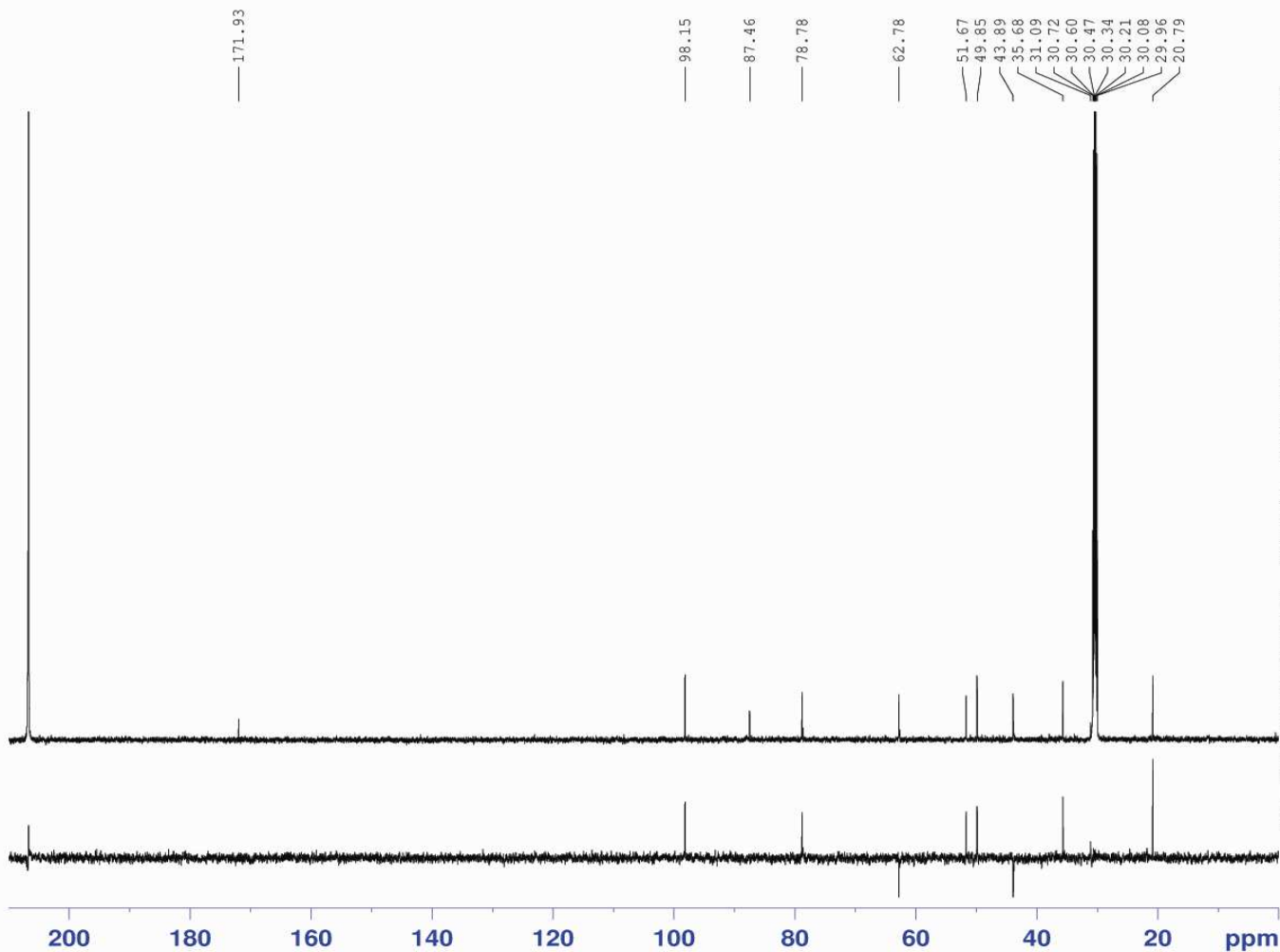
F2 - Processing parameters
SI 65536
SF 150.9025884 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

The ^{13}C and DEPT Spectra of Jatamanin D (4) in $\text{Me}_2\text{CO}-d_6$



The ^1H NMR Spectrum of Jatamanin E (5) in $\text{Me}_2\text{CO}-d_6$

zhangwd-1s-263

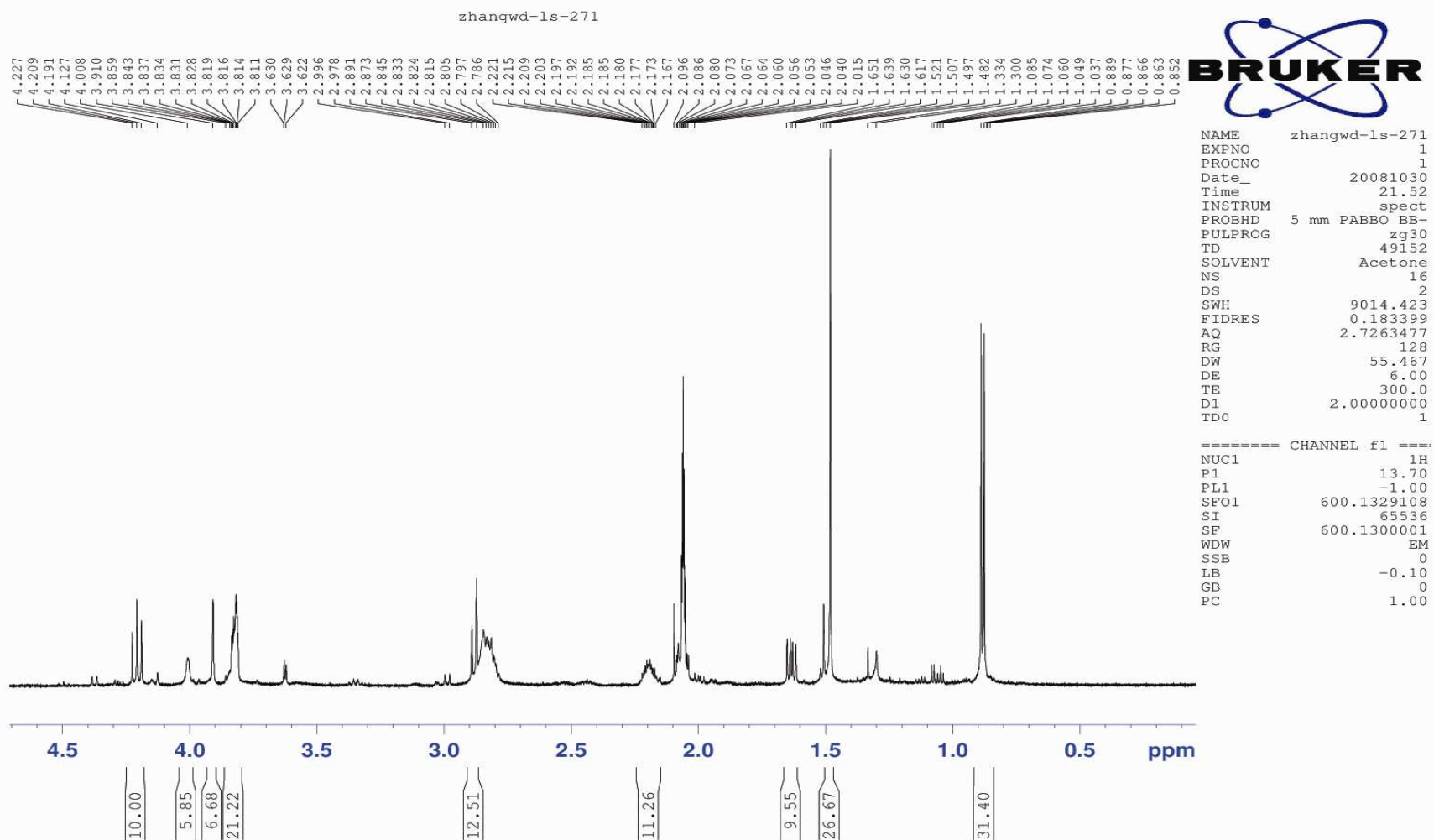


NAME 1s-263
 EXPNO 2
 PROCNO 1
 Date_ 20081030
 Time 20.12
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT Acetone
 NS 400
 DS 4
 SWH 45454.547 Hz
 FIDRES 0.693581 Hz
 AQ 0.7209460 sec
 RG 32768
 DW 11.000 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

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

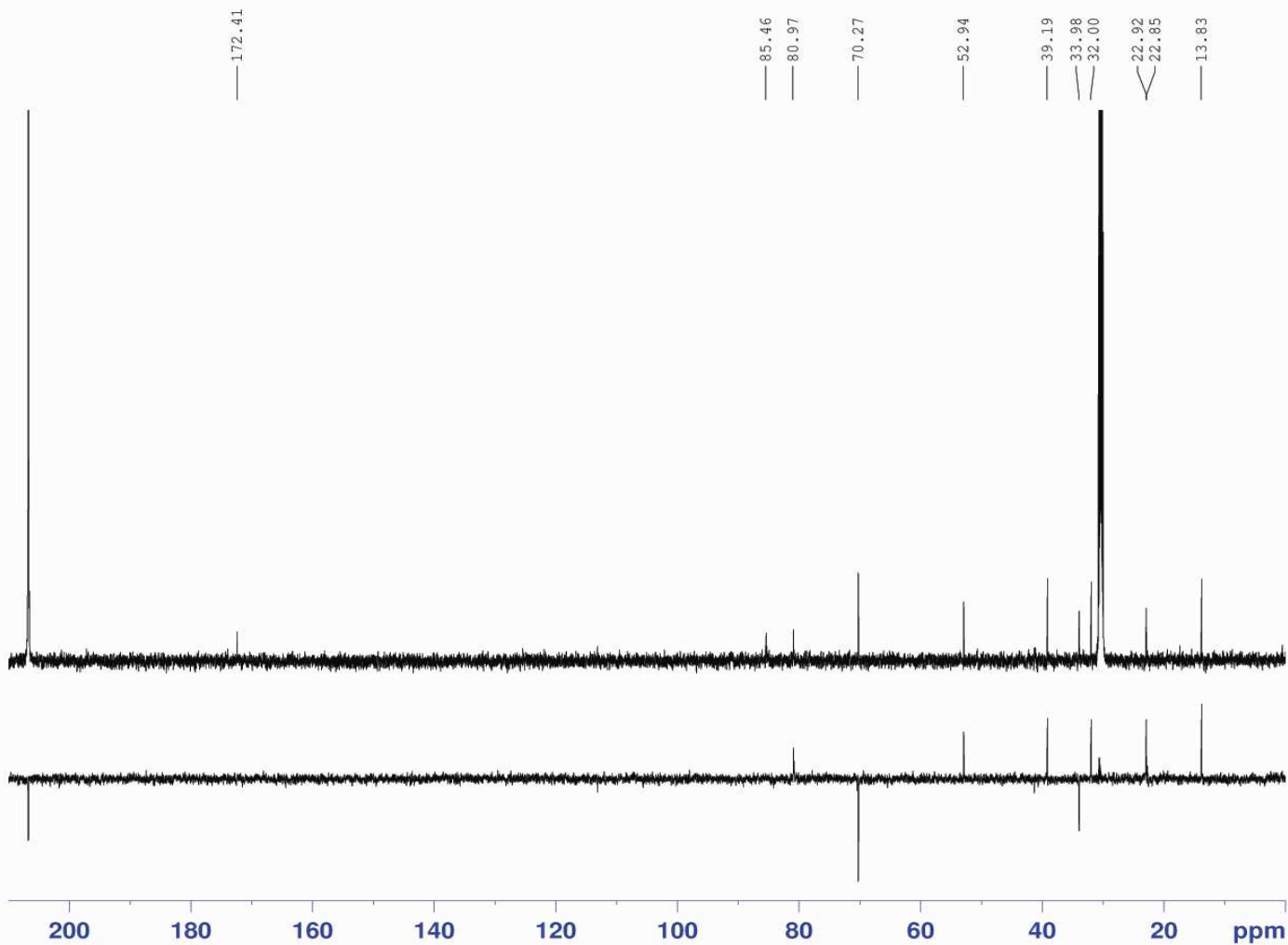
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 14.00 dB
 PL13 14.00 dB
 SFO2 600.1324005 MHz
 SI 65536
 SF 150.9025966 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

The ^{13}C NMR and DEPT Spectra of Jatamanin E (5) in $\text{Me}_2\text{CO}-d_6$



The ^1H NMR Spectrum of Jatamanin F (6) in $\text{Me}_2\text{CO}-d_6$

zhangwd-ls-271

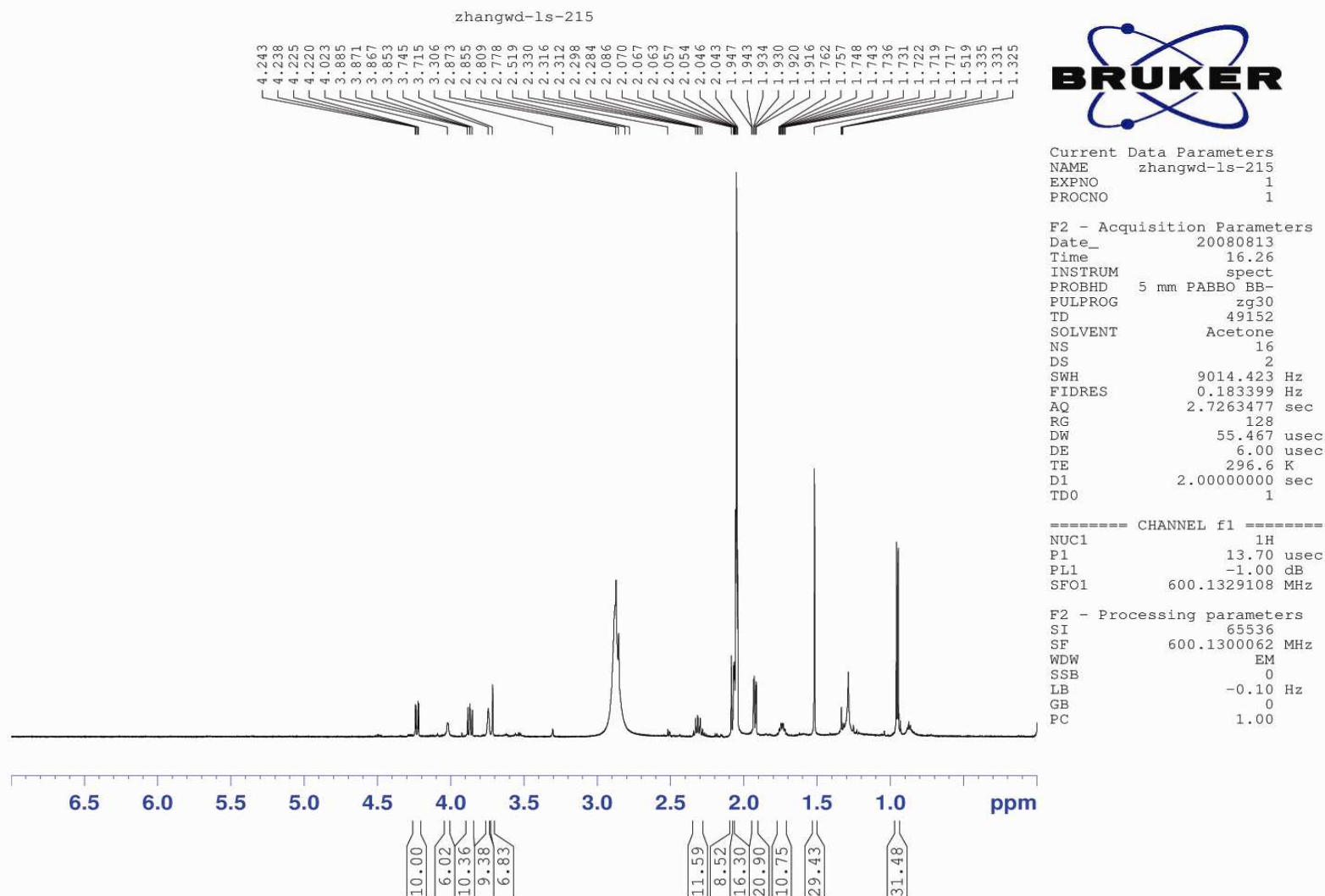


NAME zhangwd-ls-271
EXPNO 2
PROCNO 1
Date_ 20081030
Time 22.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 247
DS 4
SWH 45454.547 Hz
FIDRES 0.693581 Hz
AQ 0.7209460 se
RG 32768
DW 11.000 us
DE 6.00 us
TE 300.0 K
D1 2.00000000 se
d11 0.03000000 se
DELTA 1.89999998 se
TD0 1

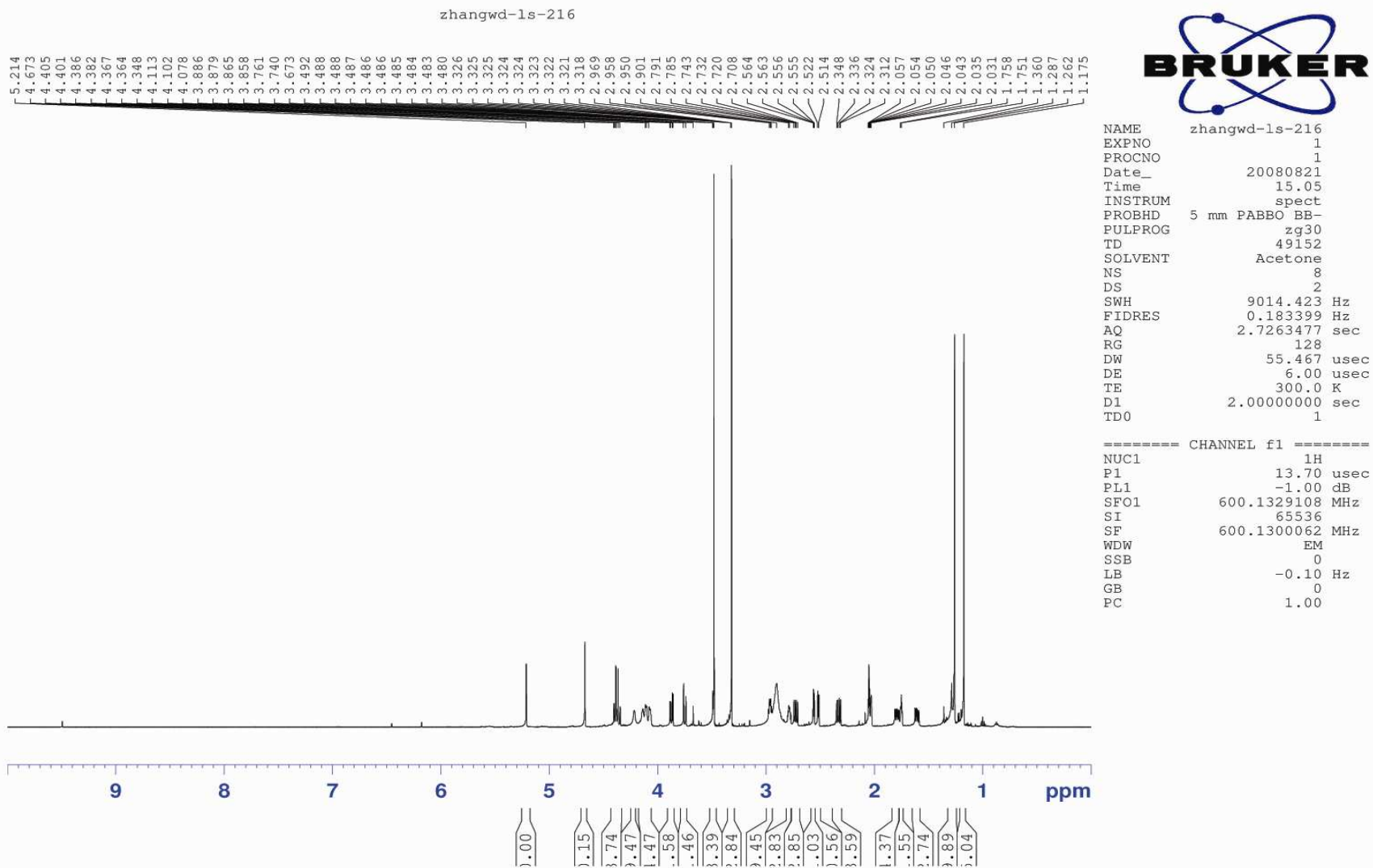
===== CHANNEL f1 =====
NUC1 13C
P1 8.50 us
PL1 2.00 dB
SFO1 150.9178990 MH

===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00 us
PL2 -1.00 dB
PL12 14.00 dB
PL13 14.00 dB
SFO2 600.1324005 MH
SI 65536
SF 150.9025893 MH
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

The ^{13}C NMR and DEPT Spectra of Jatamanin F (6) in $\text{Me}_2\text{CO}-d_6$

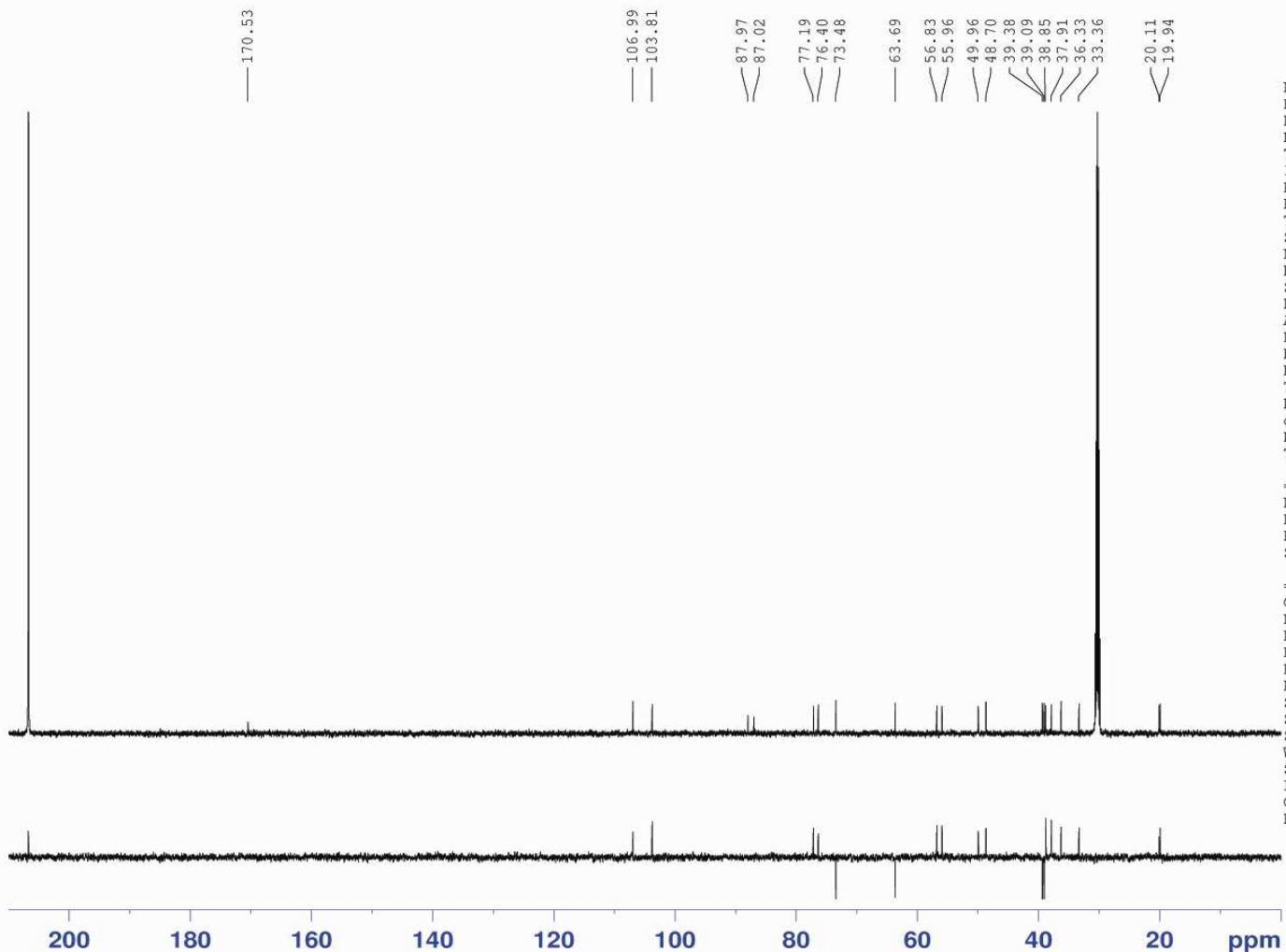


The ^1H NMR Spectrum of Jatamanin G (7) in $\text{Me}_2\text{CO}-d_6$



The ^1H NMR Spectrum of Jatamanins H (8) and I (9) in $\text{Me}_2\text{CO}-d_6$

zhangwd-ls-216



NAME zhangwd-ls-216
EXPNO 2
PROCNO 1
Date_ 20080821
Time 15.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 72
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 300.9 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
SI 65536
SF 150.9026056 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

The ^{13}C NMR and DEPT Spectra of Jatamanins H (8) and I (9) in $\text{Me}_2\text{CO}-d_6$

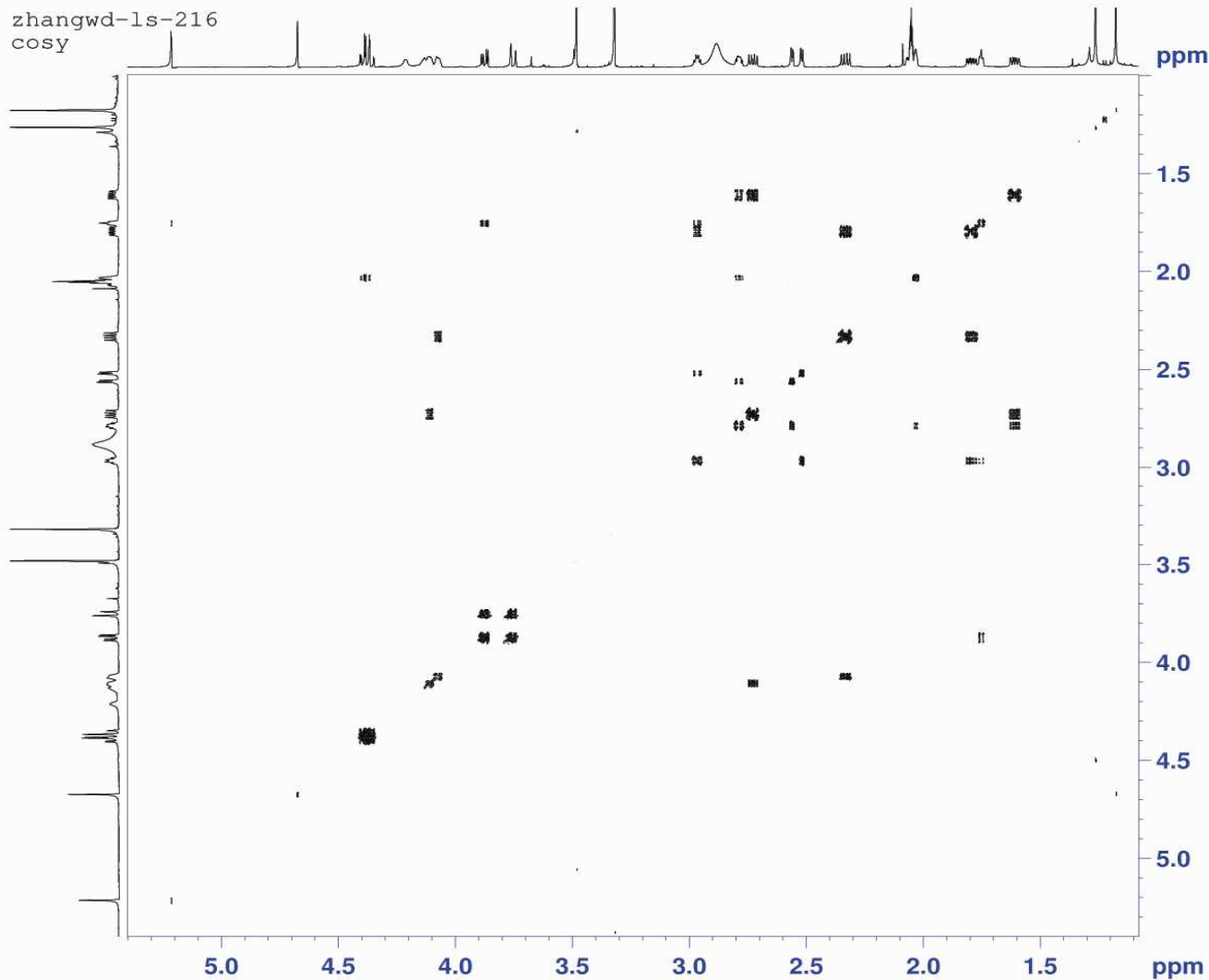
zhangwd-ls-216
cosy



NAME zhangwd-ls-216
EXPNO 4
PROCNO 1
Date_ 20081015
Time 16.01
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG cosygpmfph
TD 4096
SOLVENT Acetone
NS 1
DS 32
SWH 3001.200 Hz
FIDRES 0.732715 Hz
AQ 0.6824436 sec
RG 2050
DW 166.600 usec
DE 6.00 usec
TE 300.0 K
d0 0.00014916 sec
d1 2.00000000 sec
d13 0.00000400 sec
d16 0.00010000 sec
d20 0.00110400 sec
IN0 0.00033320 sec
ST1CNT 0

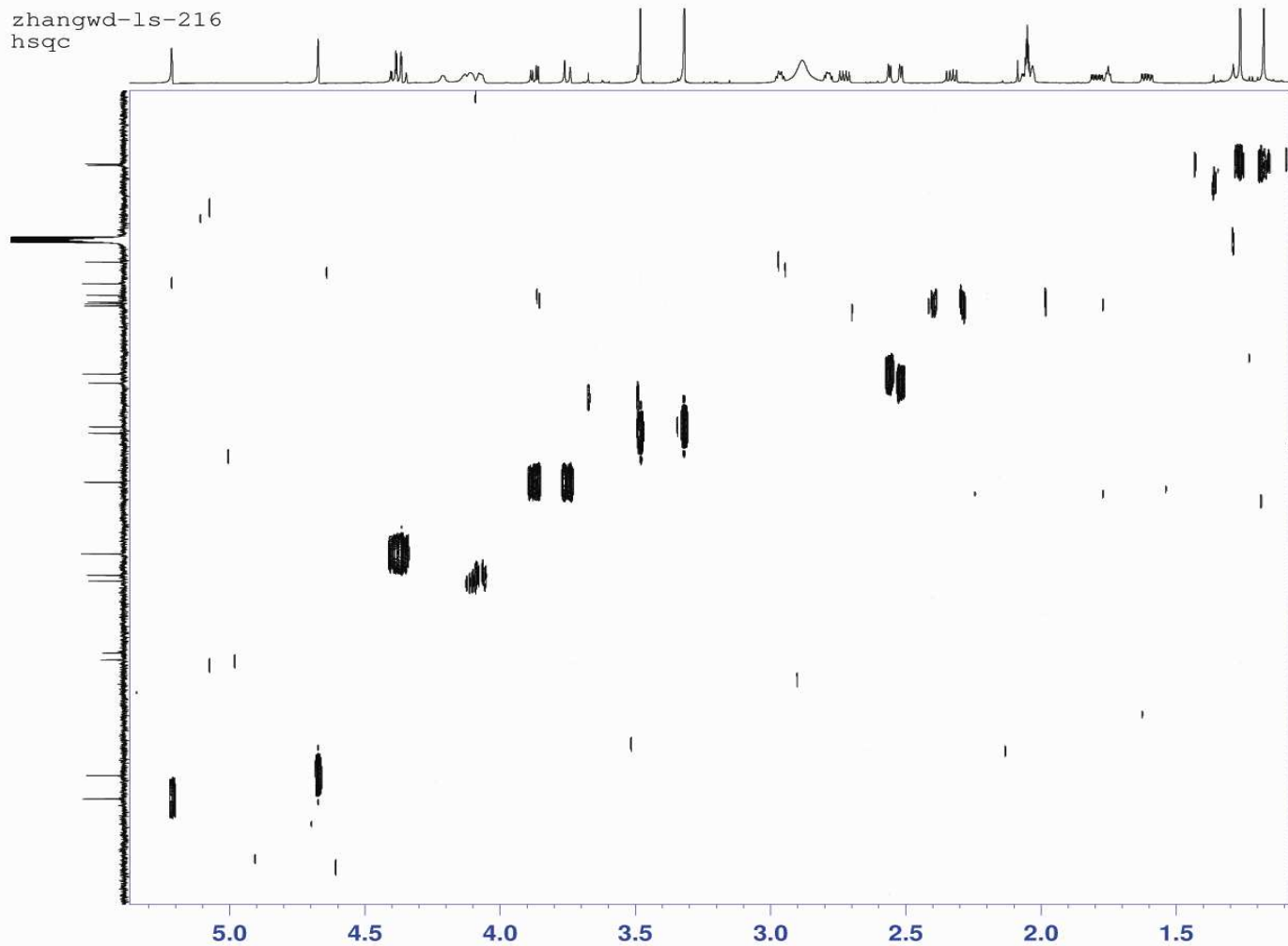
===== CHANNEL f1 =====
NUC1 1H
P1 13.70 usec
p2 27.40 usec
PL1 -1.00 dB
SFO1 600.1319110 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPZ1 10.00 %
GPZ2 20.00 %
P16 1000.00 usec
ND0 1
TD 360
SFO1 600.1319 MHz
FIDRES 8.336668 Hz
SW 5.001 ppm
FMODE States-TPPI
SI 2048
SF 600.1300060 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0
PC 1.40
SI 2048
MC2 States-TPPI
SF 600.1300060 MHz
WDW QSINE
SSB 2
LB 0.00 Hz
GB 0



The ^1H - ^1H COSY Spectrum of Jatamanins H (8) and I (9) in $\text{Me}_2\text{CO}-d_6$

zhangwd-1s-216
hsqc



EXPNO 5
PROCNO 1
Date_ 20081015
Time 16.19
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG hsqcetgps12
TD 2048
SOLVENT Acetone
NS 16
DS 32
SWH 3001.200 Hz
FIDRES 1.465430 Hz
AQ 0.3412468 sec
RG 2050
DM 166.600 usec
DE 6.00 usec
TE 300.1 K
CNS2 145.0000000 sec
d0 0.00000300 sec
d1 1.50000000 sec
d4 0.00172414 sec
d11 0.03000000 sec
d13 0.00000400 sec
d16 0.00010000 sec
D24 0.00086207 sec
DELTA 0.00118340 sec
DELTA1 0.00110800 sec
DELTA2 0.00026207 sec
DELTA3 0.00062414 sec
IN0 0.00001655 sec
ST1CNT 0
ZGPTNS

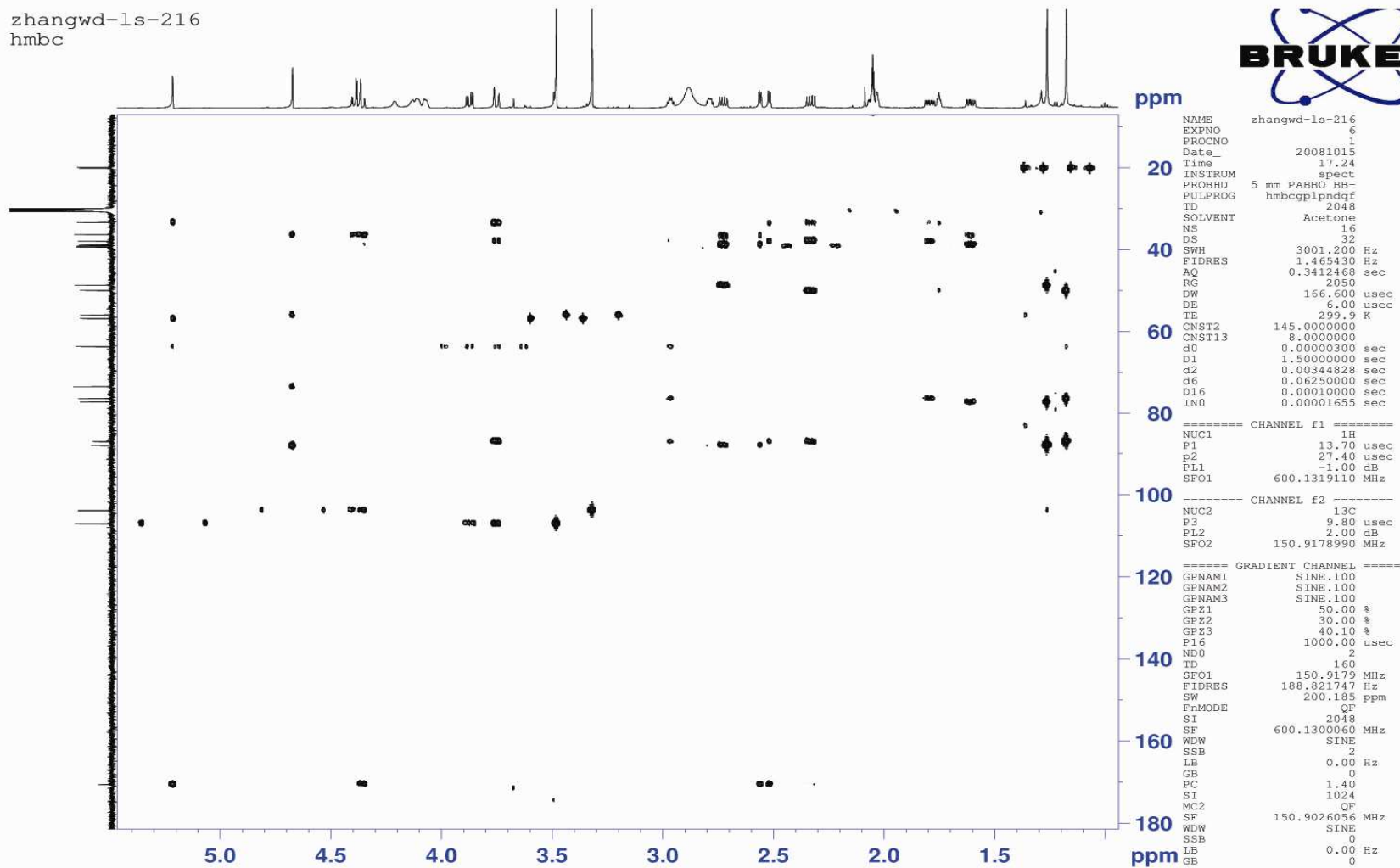
===== CHANNEL f1 =====
NUC1 1H
P1 13.70 usec
P2 27.40 usec
P28 1.00 usec
PL1 -1.00 dB
SFO1 600.1319110 MHz

===== CHANNEL f2 =====
CPDPRG2 garp
NUC2 13C
P3 9.80 usec
P4 19.60 usec
PCPD2 75.00 usec
PL2 2.00 dB
PL12 19.60 dB
SFO2 150.9178990 MHz

===== GRADIENT CHANNEL =====
GPNAM1 SINE.100
GPNAM2 SINE.100
GPNAM3 SINE.100
GPNAM4 SINE.100
GPZ1 80.00 %
GPZ2 20.10 %
GPZ3 11.00 %
GPZ4 -5.00 %
F16 1000.00 usec
F19 500.00 usec
NO0 2
TD 128
SFO1 150.9179 MHz
FIDRES 236.027191 Hz
SW 200.185 ppm
FMODE Echo-Antiecho
SI 2048
SF 600.1300060 MHz
WDW QSINE
SSB 0
LB 0.0 Hz
GB 0
FC 1.40
SI 1024
MC2 echo-antiecho
SF 150.9026056 MHz
WDW QSINE
SSB 0
LB 0.00 Hz
GB 0

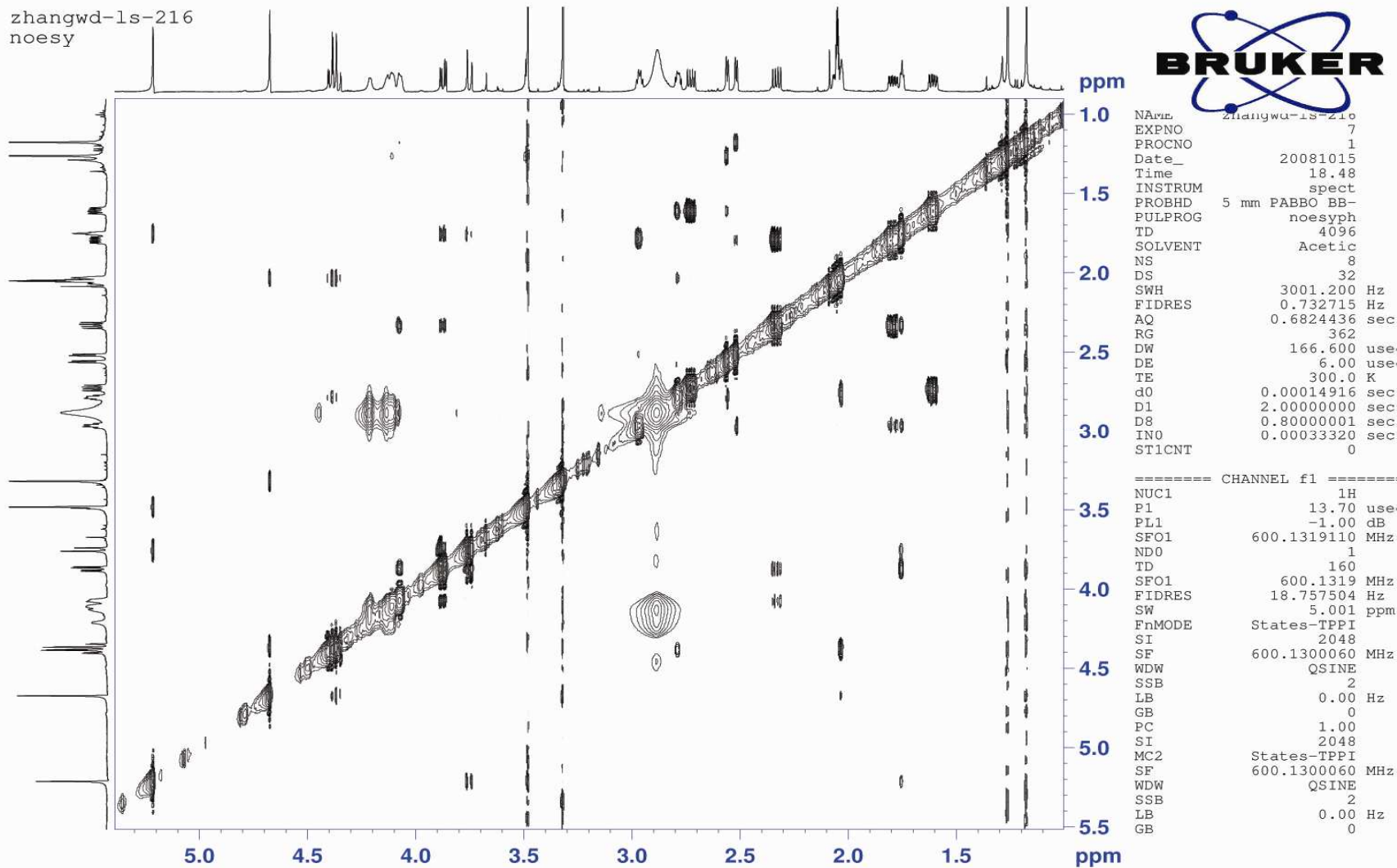
The HSQC Spectrum of Jatamanins H (8) and I (9) in $\text{Me}_2\text{CO}-d_6$

zhangwd-ls-216
hmbc

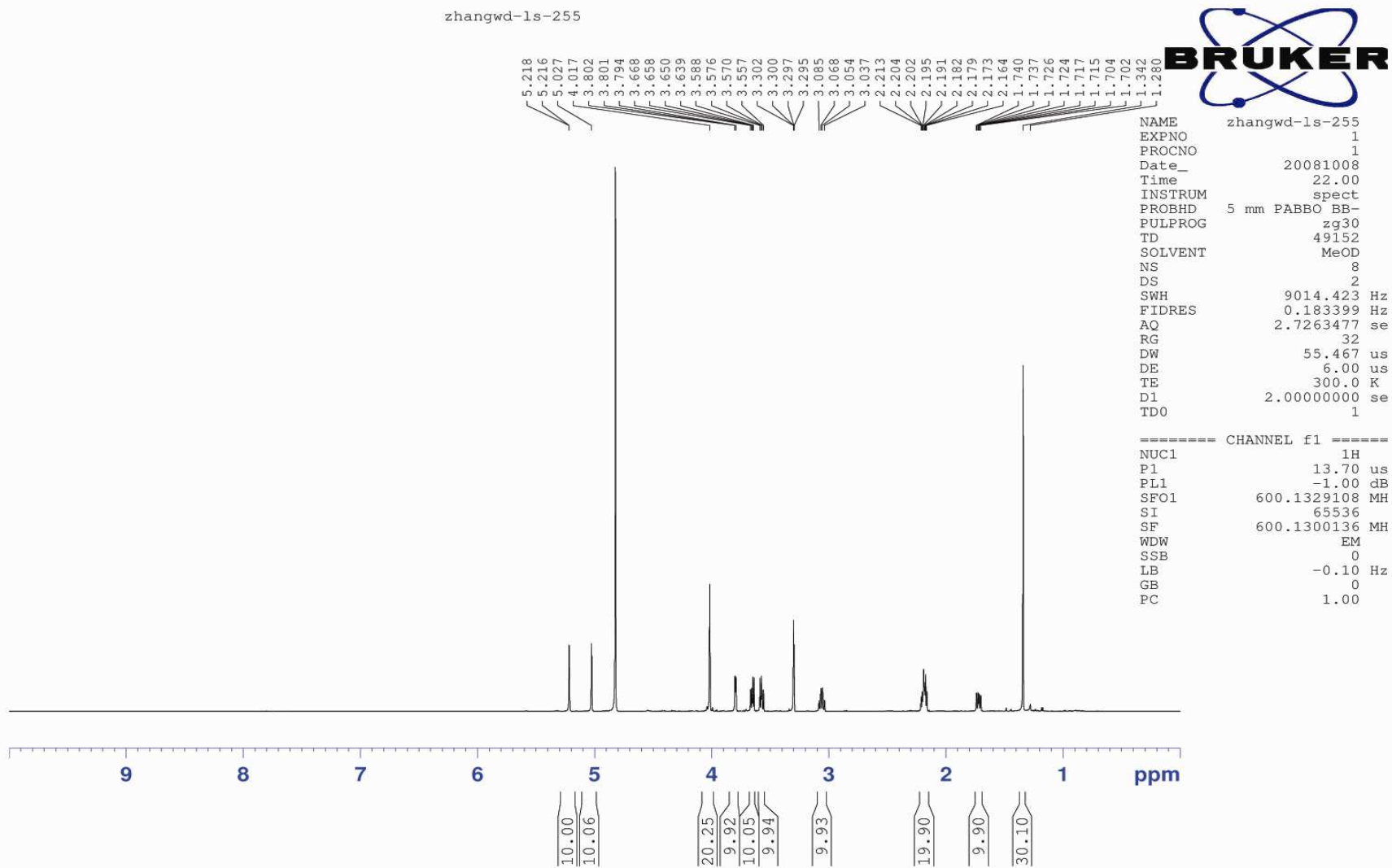


The HMBC Spectrum of Jatamanins H (8) and I (9) in $\text{Me}_2\text{CO}-d_6$

zhangwd-ls-216
noesy

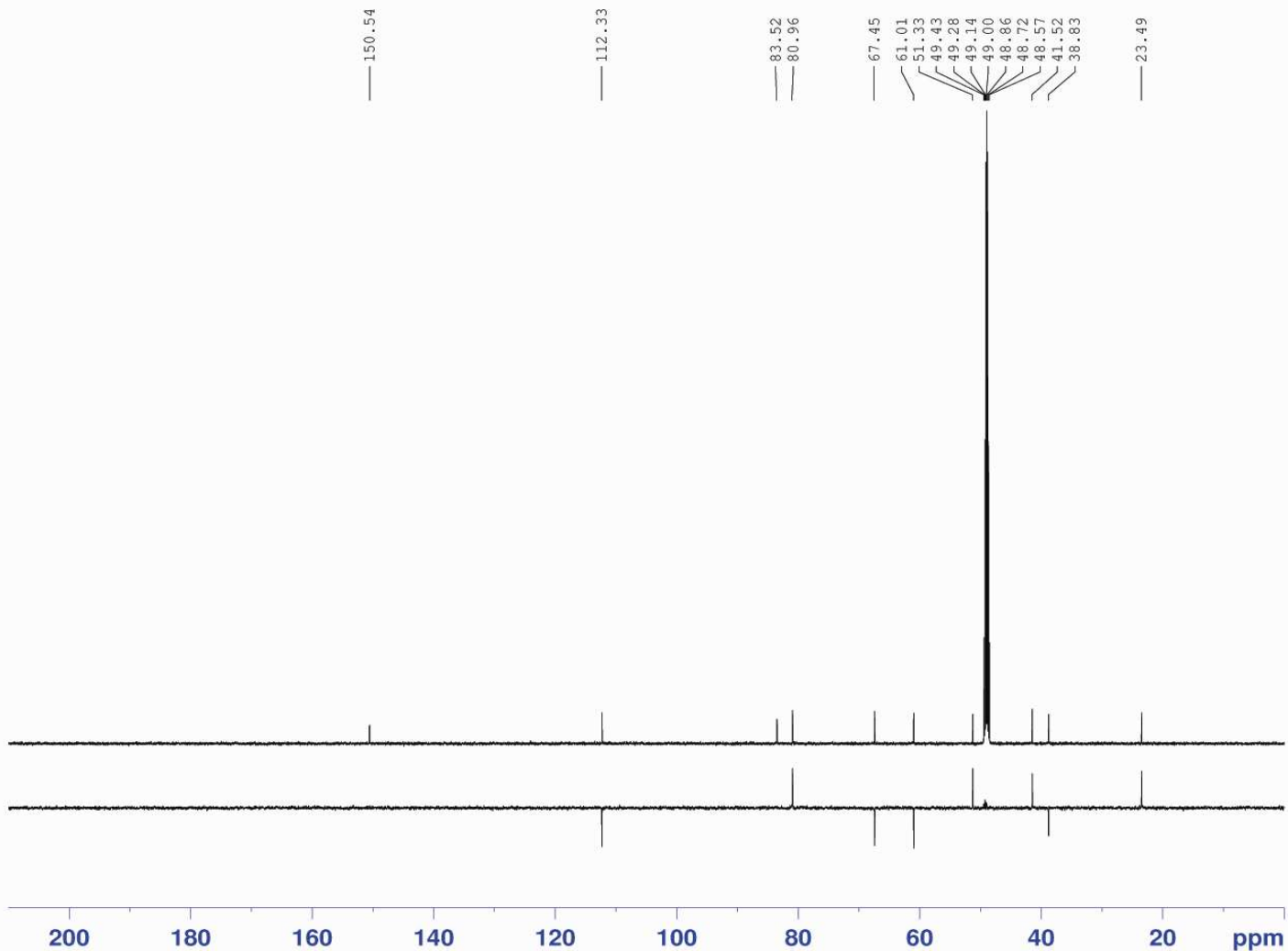


The NOESY Spectrum of Jatamanins H (8) and I (9) in Me₂CO-*d*₆



The ^1H NMR Spectrum of Jatamanin J (10) in MeOD

zhangwd-ls-255

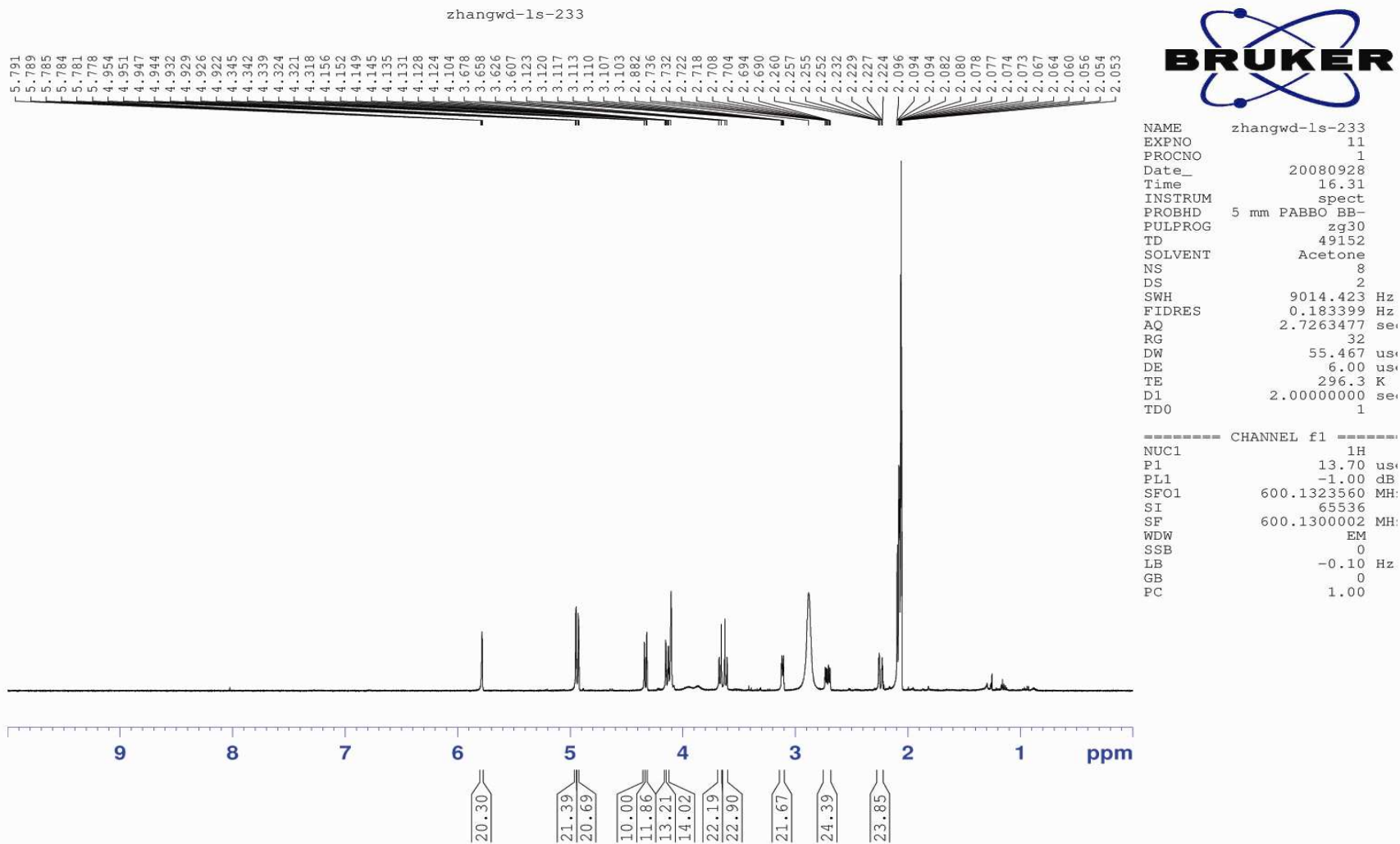


NAME zhangwd-ls-255
 EXPNO 2
 PROCNO 1
 Date_ 20081008
 Time 22.08
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT MeOD
 NS 167
 DS 0
 SWH 45454.547 Hz
 FIDRES 0.693581 Hz
 AQ 0.7209460 sec
 RG 32768
 DW 11.000 usec
 DE 6.00 usec
 TE 300.1 K
 D1 2.00000000 sec
 d11 0.03000000 sec
 DELTA 1.89999998 sec
 TD0 1

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

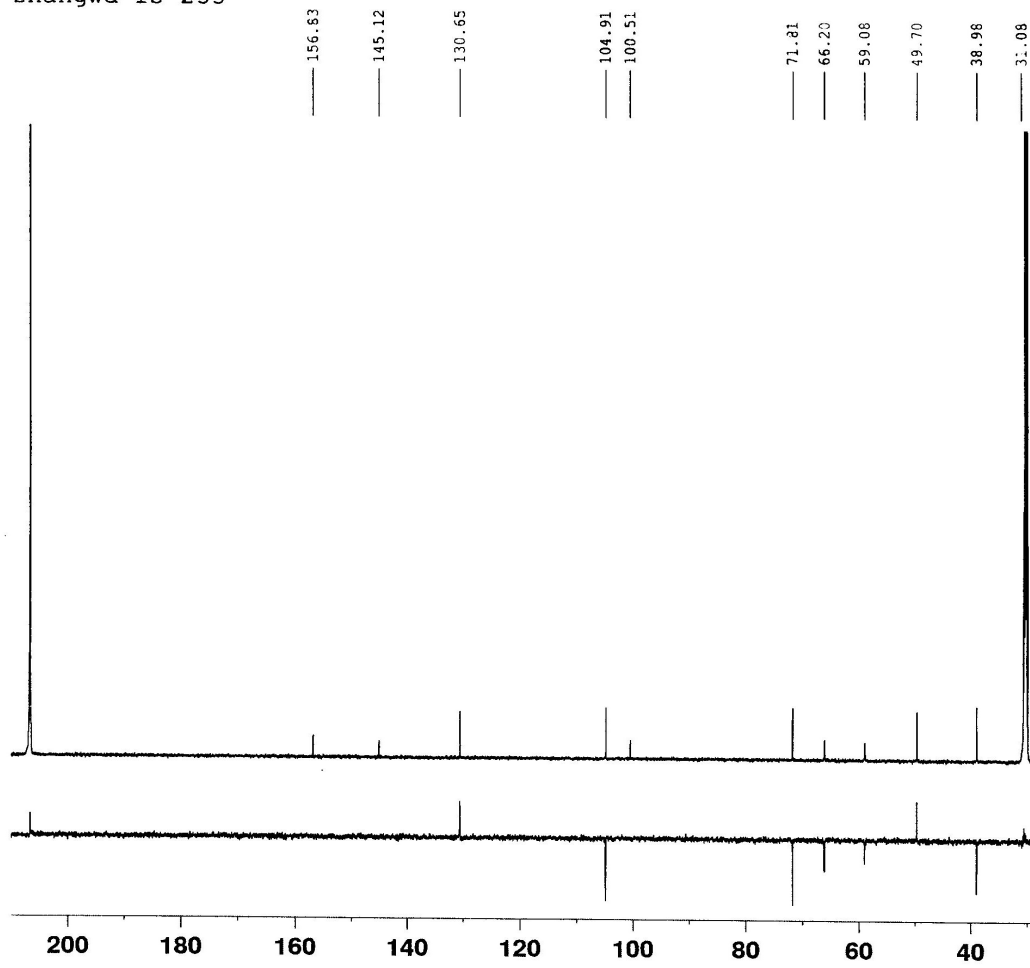
===== CHANNEL f2 =====
 CPDPRG2 waltz16
 NUC2 1H
 PCPD2 80.00 usec
 PL2 -1.00 dB
 PL12 14.00 dB
 PL13 14.00 dB
 SFO2 600.1324005 MHz
 SI 65536
 SF 150.9025969 MHz
 WDW EM
 SSB 0
 LB 2.00 Hz
 GB 0
 PC 1.40

The ^{13}C NMR and DEPT Spectra of Jatamanin J (10) in MeOD



The ^1H NMR Spectrum of Jatamanin K (11) in $\text{Me}_2\text{CO}-d_6$

zhangwd-1s-233



Current Data Parameters
NAME zhangwd-1s-233
EXPNO 2
PROCNO 1

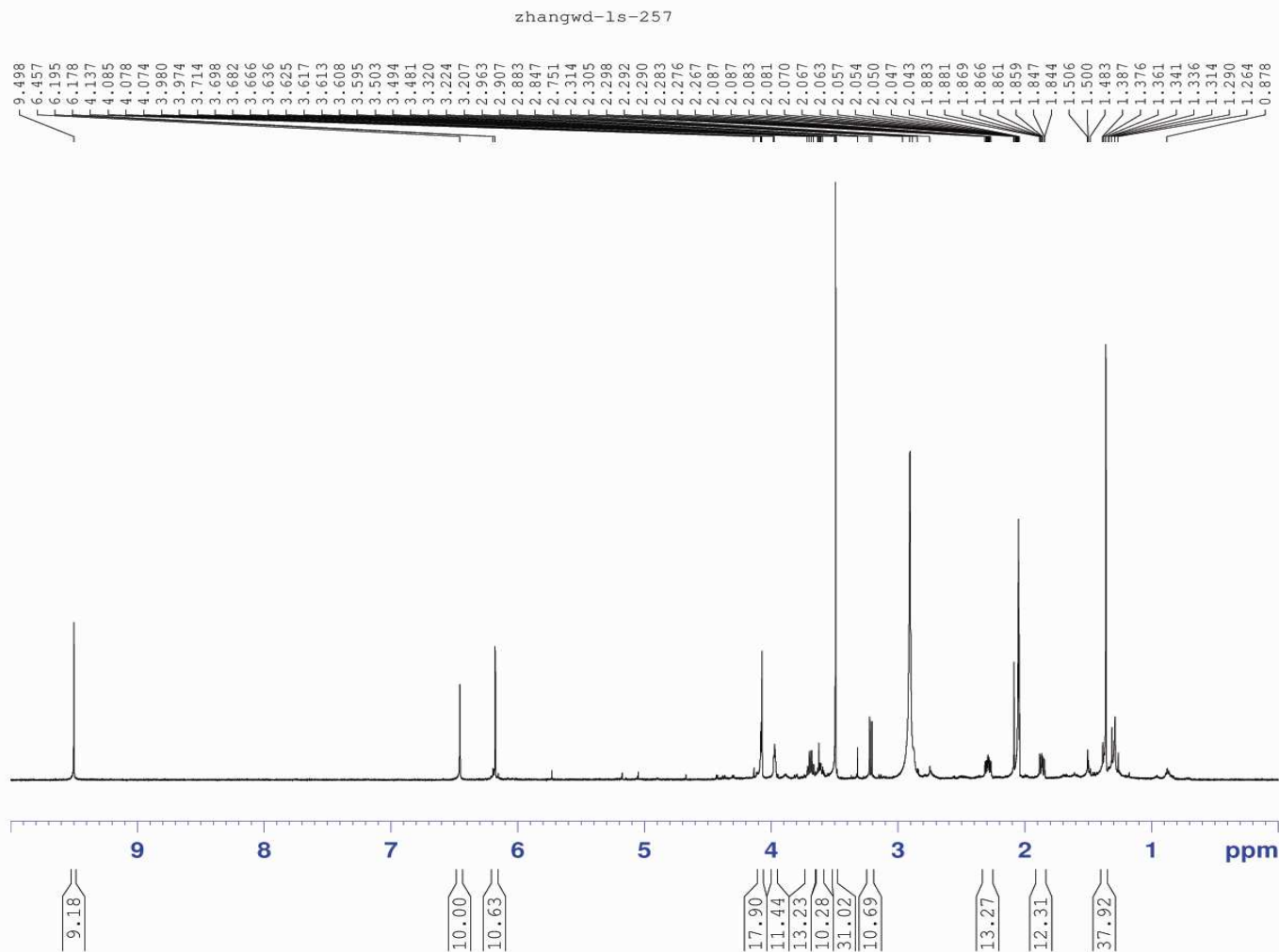
F2 - Acquisition Parameters
Date_ 20080914
Time 17.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 2048
DS 0
SWH 45454.547 Hz
FIDRES 0.693581 Hz
AQ 0.7209460 sec
RG 32768
DW 11.000 usec
DE 6.00 usec
TE 300.1 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
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 150.9025968 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

The ^{13}C NMR and DEPT Spectra of Jatamanin K (11) in $\text{Me}_2\text{CO}-d_6$

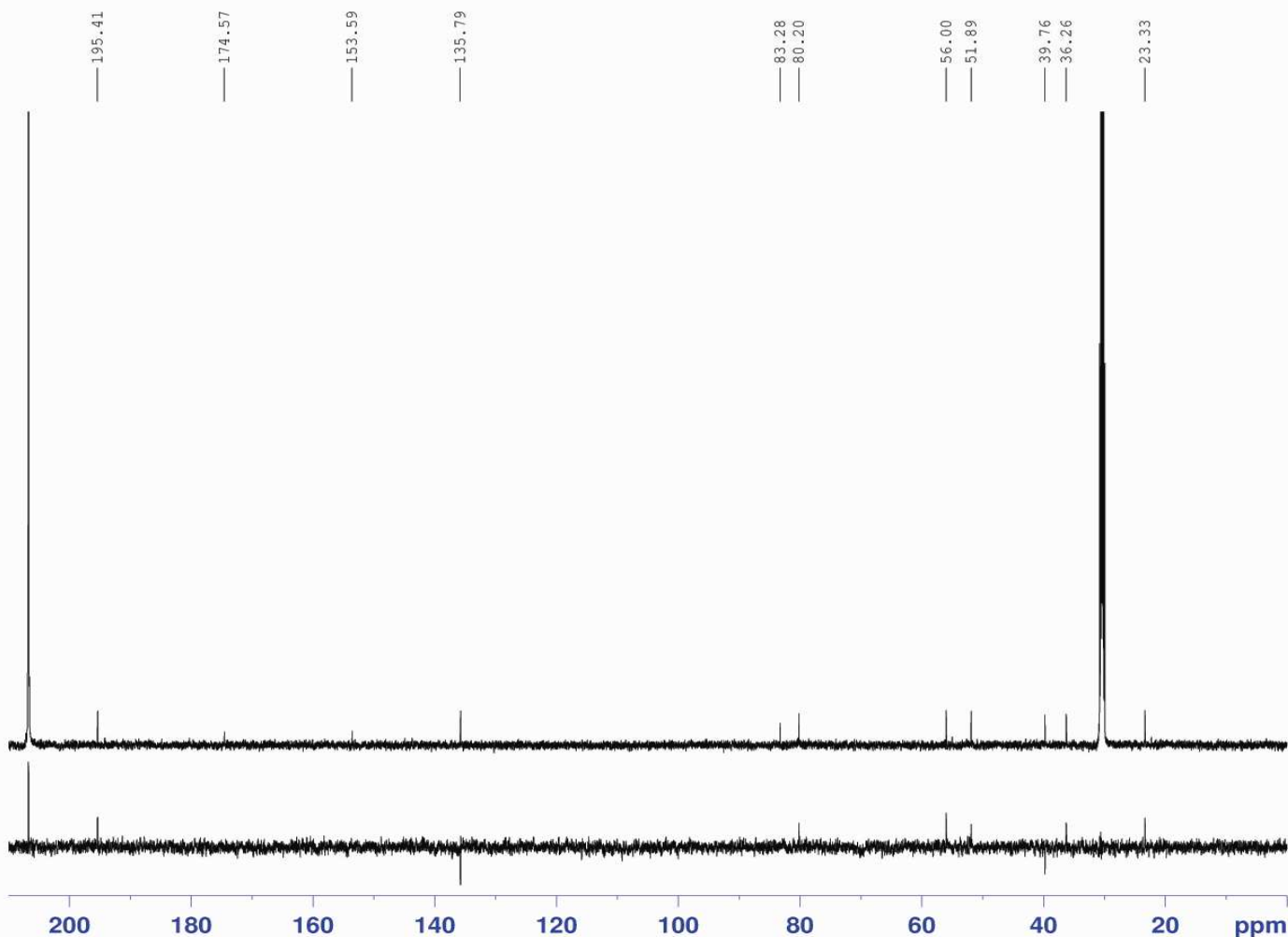


NAME zhangwd-ls-257
 EXPNO 1
 PROCNO 1
 Date_ 20081020
 Time_ 7.44
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 FULPROG zg30
 TD 49152
 SOLVENT Acetone
 NS 8
 DS 2
 SWH 9014.423 Hz
 FIDRES 0.183399 Hz
 AQ 2.7263477 sec
 RG 144
 DW 55.467 usec
 DE 6.00 usec
 TE 300.0 K
 D1 2.00000000 sec
 TD0 1

----- CHANNEL f1 -----
 NUC1 1H
 P1 13.70 usec
 PL1 -1.00 dB
 SFO1 600.1329108 MHz
 SI 65536
 SF 600.1300060 MHz
 WDW EM
 SSB 0
 LB -0.10 Hz
 GB 0
 PC 1.00

The ^1H NMR Spectrum of Jatamanin L (12) in $\text{Me}_2\text{CO}-d_6$

zhangwd-ls-257

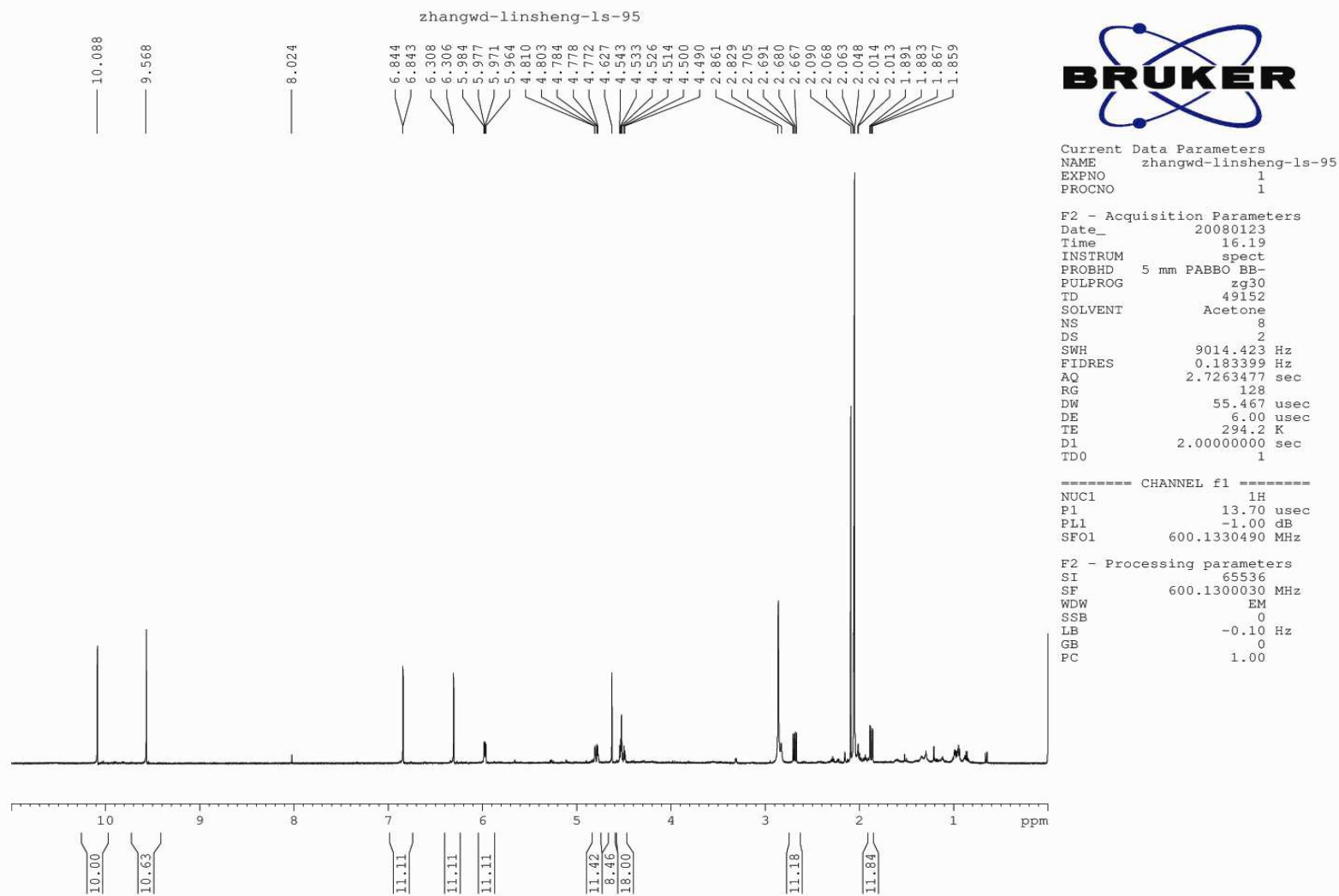


NAME zhangwd-ls-257
EXPNO 2
PROCNO 1
Date_ 20081020
Time 8.07
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 506
DS 4
SWH 45454.547
FIDRES 0.693581
AQ 0.7209460
RG 32768
DW 11.000
DE 6.00
TE 300.0
D1 2.00000000
d11 0.03000000
DELTA 1.89999998
TD0 1

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

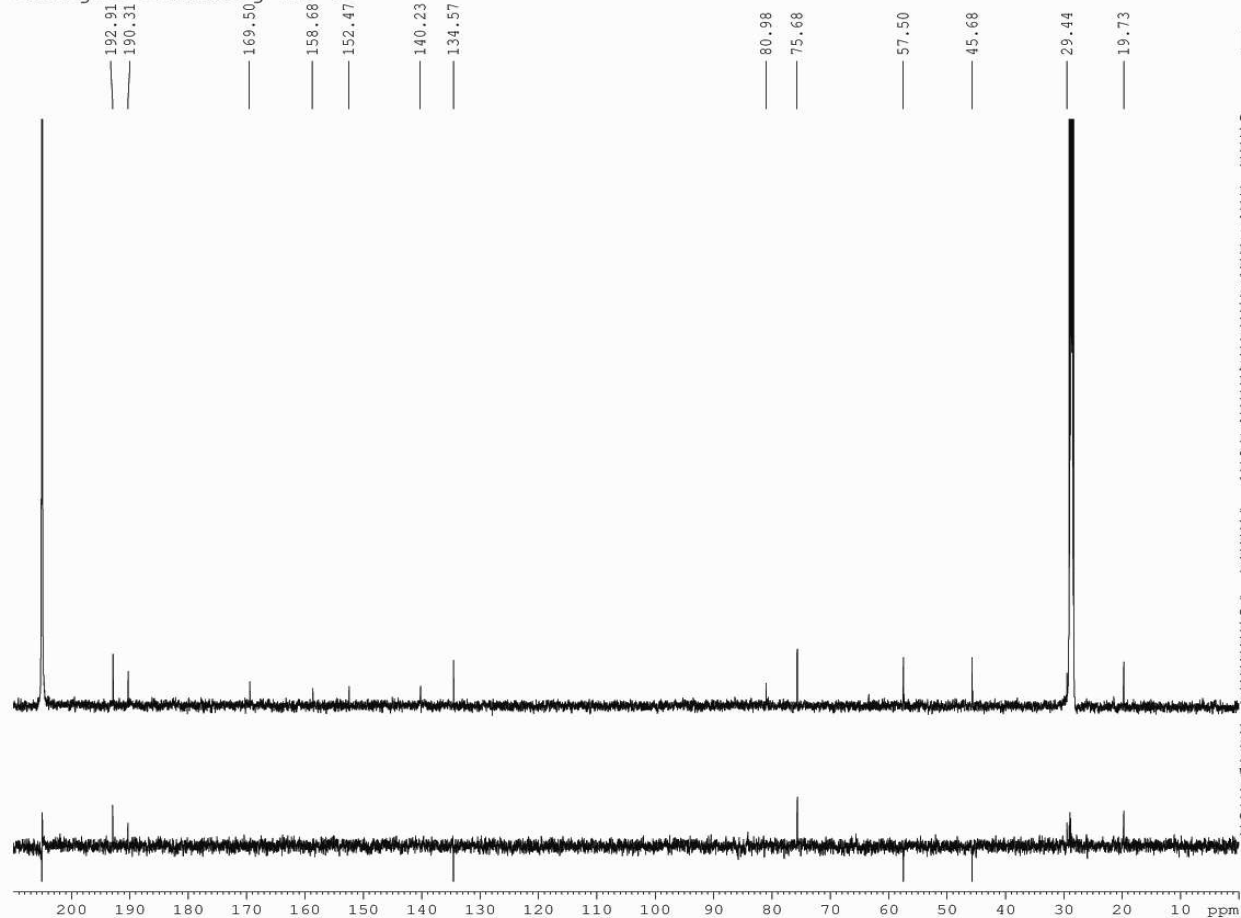
===== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 80.00
PL2 -1.00
PL12 14.00
PL13 14.00
SFO2 600.1324005
SI 65536
SF 150.9025917
WDW EM
SSB 0
LB 2.00
GB 0
PC 1.40

The ^{13}C NMR and DEPT Spectra of Jatamanin L (12) in $\text{Me}_2\text{CO}-d_6$



The ^1H NMR Spectrum of Jatamanin M (13) in $\text{Me}_2\text{CO}-d_6$

zhangwd-linsheng-ls-95



Current Data Parameters
NAME zhangwd-linsheng-ls-95
EXPNO 2
PROCNO 1

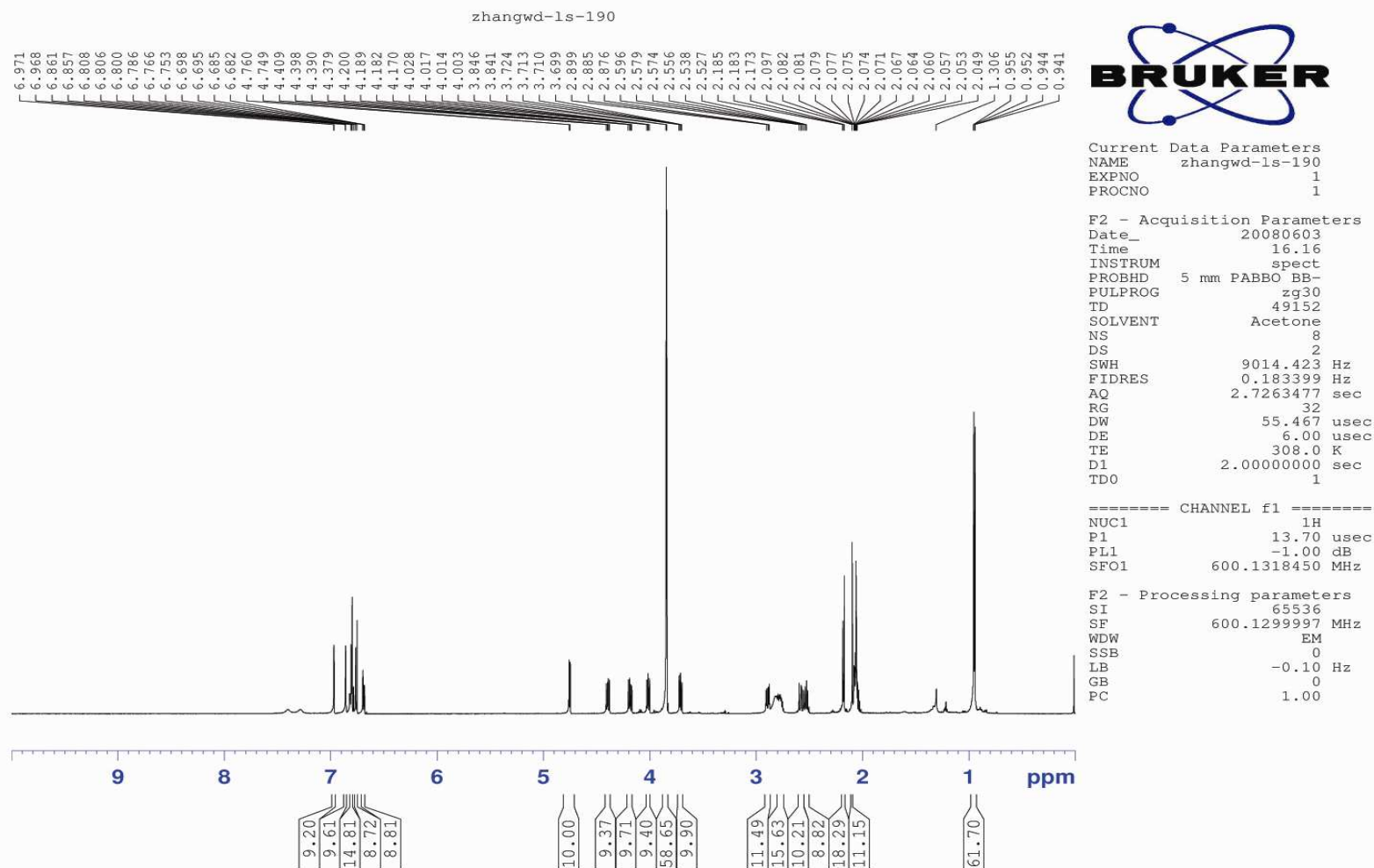
F2 - Acquisition Parameters
Date_ 20080123
Time 16.31
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
NS 872
DS 2
SWH 45454.547 Hz
FIDRES 0.693581 Hz
AQ 0.7209460 sec
RG 32768
DW 11.000 usec
DE 6.00 usec
TE 296.5 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
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

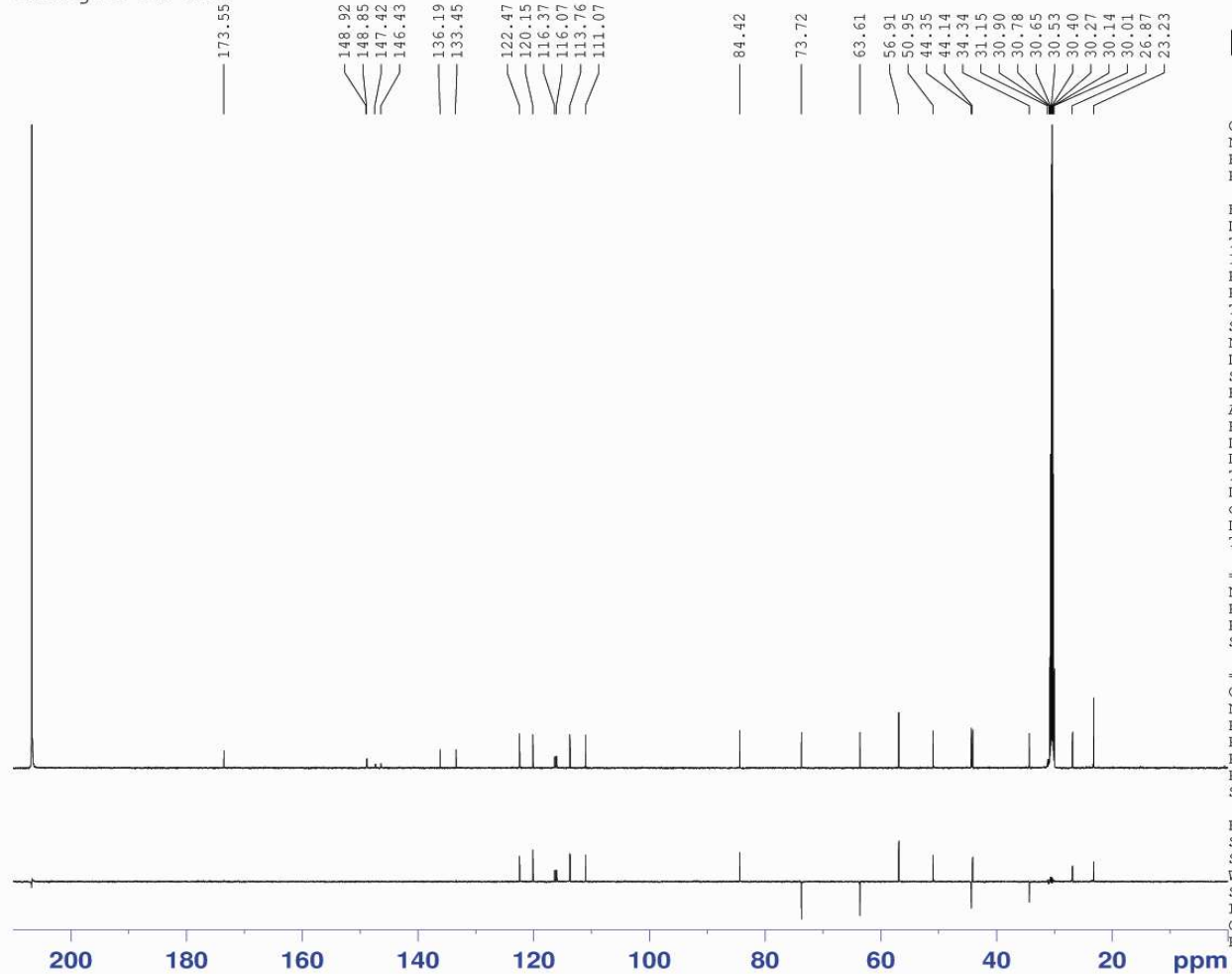
F2 - Processing parameters
SI 65536
SF 150.9028473 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

The ^{13}C NMR and DEPT Spectra of Jatamanin M (13) in $\text{Me}_2\text{CO}-d_6$



The ^1H NMR Spectrum of Compound 14 in $\text{Me}_2\text{CO}-d_6$

zhangwd-ls-190



Current Data Parameters
NAME zhangwd-ls-190
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20080603
Time 17.04
INSTRUM spect
PROBHD 5 mm PABBO BB-
PULPROG zgpg30
TD 65536
SOLVENT Acetone
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 308.0 K
D1 2.00000000 sec
d11 0.03000000 sec
DELTA 1.89999998 sec
TDO 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 150.9025824 MHz
WDW EM
SSB 0
LB 2.00 Hz
GB 0
PC 1.40

The ^{13}C NMR and DEPT Spectra of Compound 14 in $\text{Me}_2\text{CO}-d_6$

Crystal Data and Structure Refinement for Jatamanin A (1)

Empirical formula	C ₁₀ H ₁₄ O ₄
Formula weight	198.09
Temperature	293(2) K
Wavelength	0.71073 Å
Crystal system	Monoclinic
space group	P2(1)
Unit cell dimensions	a= 5.957(14) Å α= 90 ° b= 13.28(3) Å β= 90 ° c= 7.662(17) Å γ= 90 °
Volume	587 (2) Å ³
Z	2
Calculated density	1.320 Mg/m ³
Absorption coefficient	0.109 mm ⁻¹
F(000)	250
Crystal size	0.25 × 0.20 × 0.18 mm ³
Theta range for data collection	3.07 to 25.00 °
Limiting indices	-6<=h<=7 -14<=k<=15 -8<=l<=9
Reflections collected / unique	2385/1835 [R(int) = 0.0406]
Completeness to θ= 24.99 °	99.2 %
Absorption correction	Semi-empirical from equivalents
Max. and min. transmission	0.9806 and 0.9732
Refinement method	Full-matrix least-squares on F ²
Data / restraints / parameters	1835/7/162
Goodness-of-fit on F ²	1.091
Final R indices [I>2σ(I)]	R ₁ = 0.0595, wR ₂ = 0.1501
R indices (all data)	R ₁ = 0.0606, wR ₂ = 0.1517
Absolute structure parameter	1.0(14)