

Supporting Information

for

Decandrinin, an unprecedented C₉-spiro-fused 7,8-*seco-ent*-abietane from the Godavari mangrove *Ceriops decandra*

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**HRMS (ESI) and NMR spectra of decandrinin (1), NOE interactions for the
B97D/TZVP-optimized structure diagnostic for the 9-epimer of decandrinin (1), and
comparison of the calculated ORD with the experimental one.**

Mass Spectrum SmartFormula Report

Analysis Info		Acquisition Date	11/28/2012 3:21:18 PM
Analysis Name	D:\Data\MS\data\201211\wanghui_66_pos.d	Operator	SCSIO
Method	POS_100-2000_Dirrect Infusion.m	Instrument / Ser#	maXis 29
Sample Name	SCSIO		
Comment			

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Not active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	100 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	2000 m/z	Set Collision Cell RF	2000.0 Vpp	Set Divert Valve	Waste

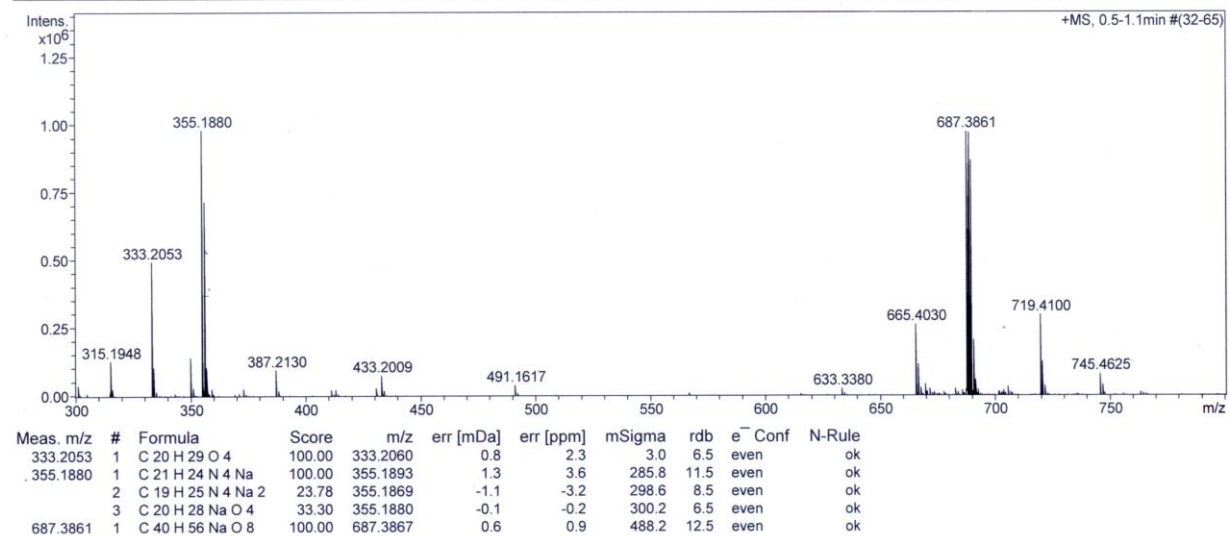


Figure S1: HRMS (ESI) spectrum of decandrinin (1) (MeOH)

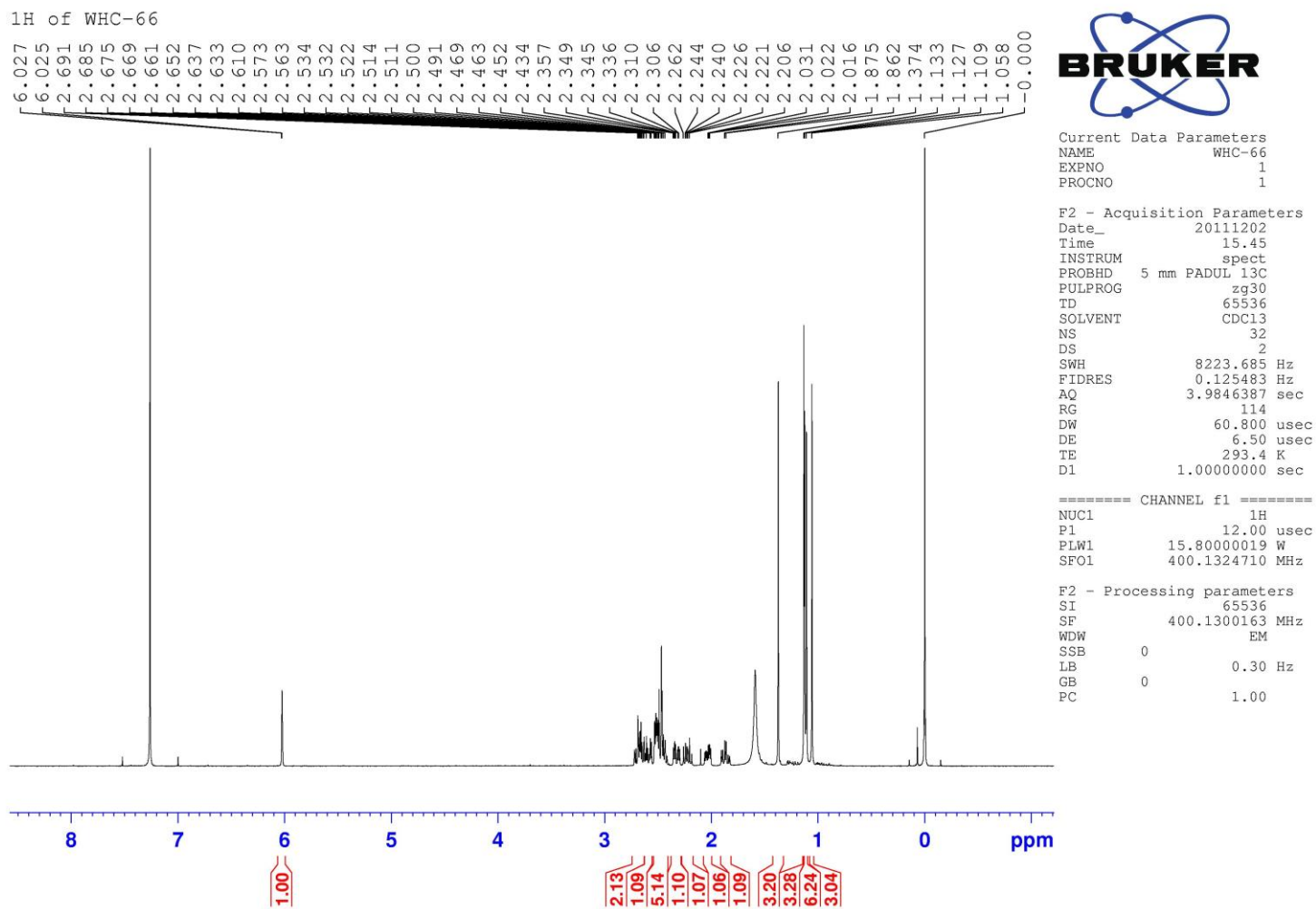


Figure S2A: ¹H NMR spectrum of decandrinin (**1**) (400 MHz, CDCl₃)

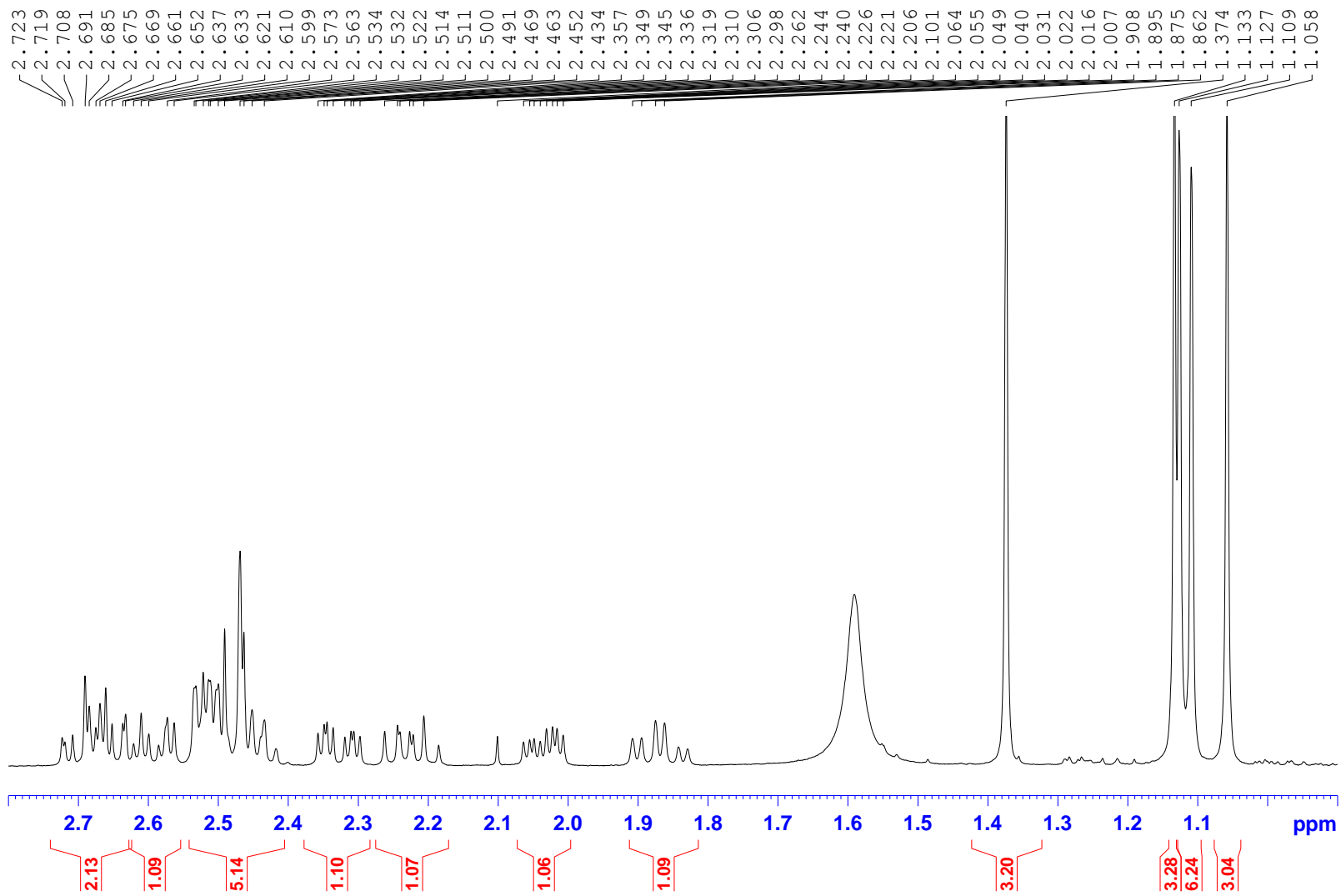
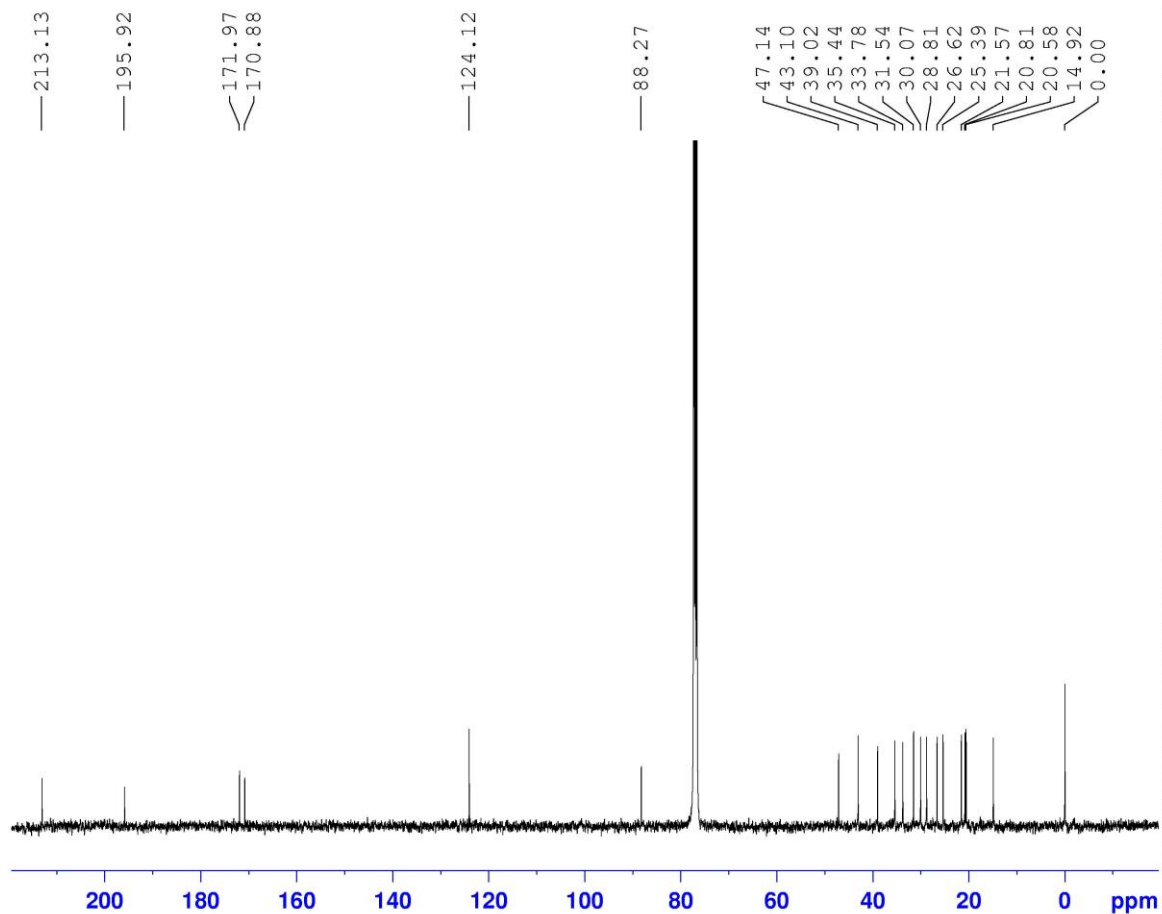


Figure S2B: Enlargement of area 1.0–2.7 ppm

13C of WHC-66



Current Data Parameters
NAME WHC-66
EXPNO 2
PROCNO 1

F2 - Acquisition Parameters
Date_ 20111202
Time 16.40
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG zgpg30
TD 65536
SOLVENT CDCl3
NS 6144
DS 4
SWH 24038.461 Hz
FIDRES 0.366798 Hz
AQ 1.3631988 sec
RG 25.4
DW 20.800 usec
DE 6.50 usec
TE 294.1 K
D1 2.0000000 sec
D11 0.0300000 sec

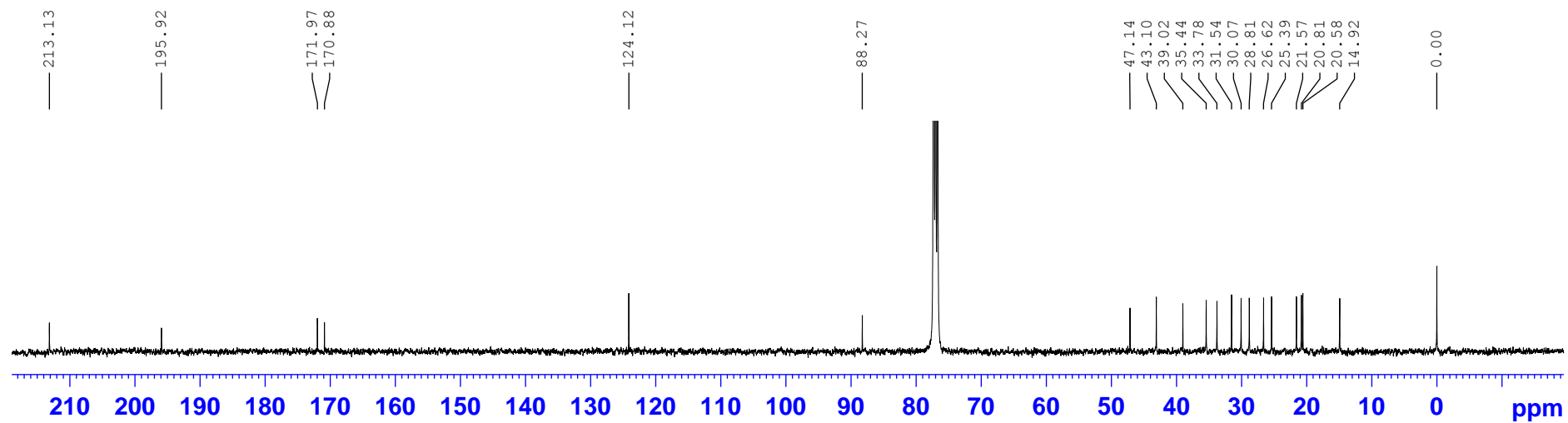
==== CHANNEL f1 =====
NUC1 13C
P1 12.00 usec
PLW1 32.0000000 W
SFO1 100.6228293 MHz

==== CHANNEL f2 =====
CPDPRG2 waltz16
NUC2 1H
PCPD2 90.00 usec
PLW2 15.80000019 W
PLW12 0.28088999 W
PLW13 0.22752000 W
SFO2 400.1316005 MHz

F2 - Processing parameters
SI 32768
SF 100.6127721 MHz
WDW EM
SSB 0
LB 3.00 Hz
GB 0
PC 1.40

Figure S3: ¹³C NMR spectrum of decandrinin (1) (400 MHz, CDCl₃)

^{13}C of WHC-66



DEPT135 of WHC-66

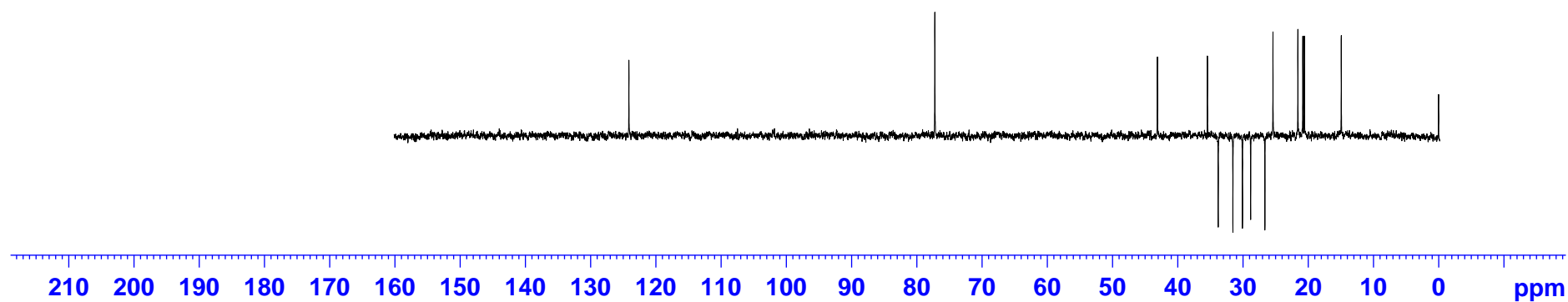
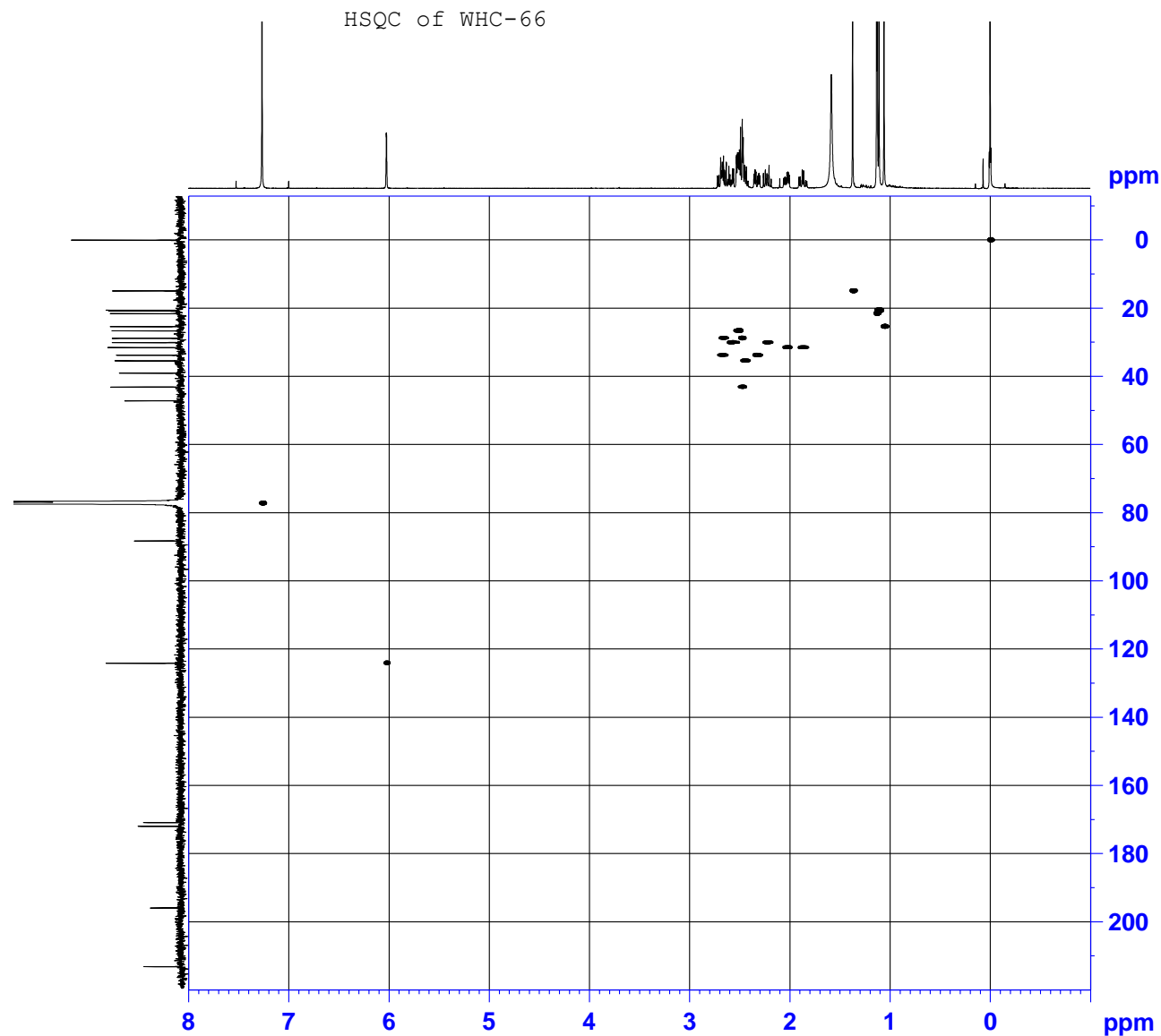


Figure S4: ^{13}C NMR and DEPT 135 spectra of decandrinin (**1**) (400 MHz, CDCl_3)



Current Data Parameters
NAME WHC-66
EXPNO 6
PROCNO 1

F2 - Acquisition Parameter
Date_ 20111221
Time_ 16.10
INSTRUM spect
PROBHD 5 mm PADUL 13C
PULPROG hsqcetgpsisp2.2
TD 1024
SOLVENT CDCl3
NS 16
DS 32
SWH 6410.256 Hz
FIDRES 6.260016 Hz
AQ 0.0799220 se
RG 203
DW 78.000 us
DE 6.50 us
TE 295.2 K
CNST2 145.000000
CNST17 -0.500000
D0 0.00000300 se
D1 1.50000000 se
D4 0.00172414 se
D11 0.03000000 se
D16 0.00020000 se
D24 0.00089000 se
IN0 0.00003000 se

===== CHANNEL f1 =====
NUC1 1H
P1 11.95 us
P2 23.90 us
P28 1000.00 us
PLW1 15.80000019 W
SFO1 400.1318818 MH
----- CHANNEL f2 -----

Figure S5A: HSQC spectrum of decandrinin (1) (400 MHz, CDCl₃)

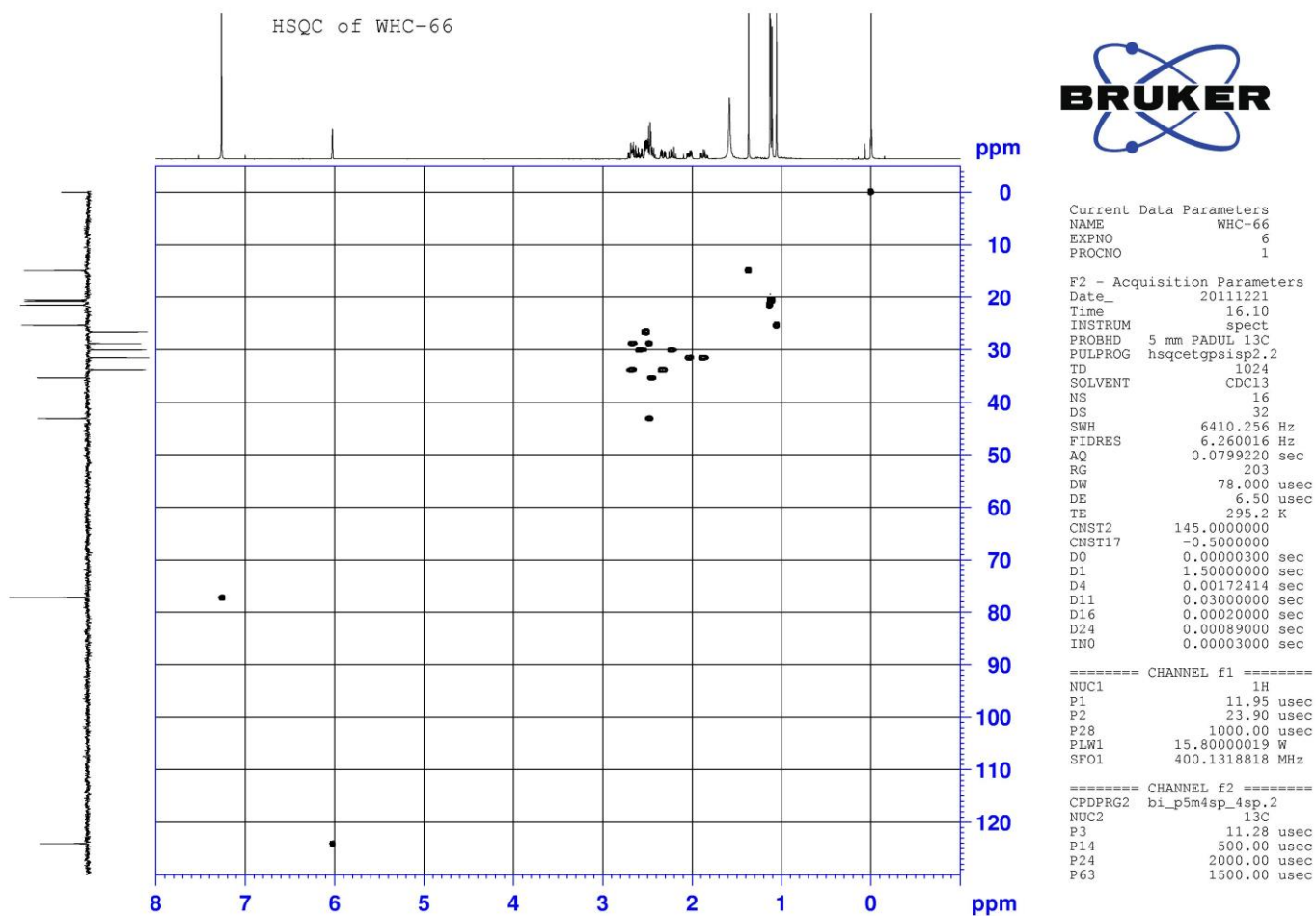
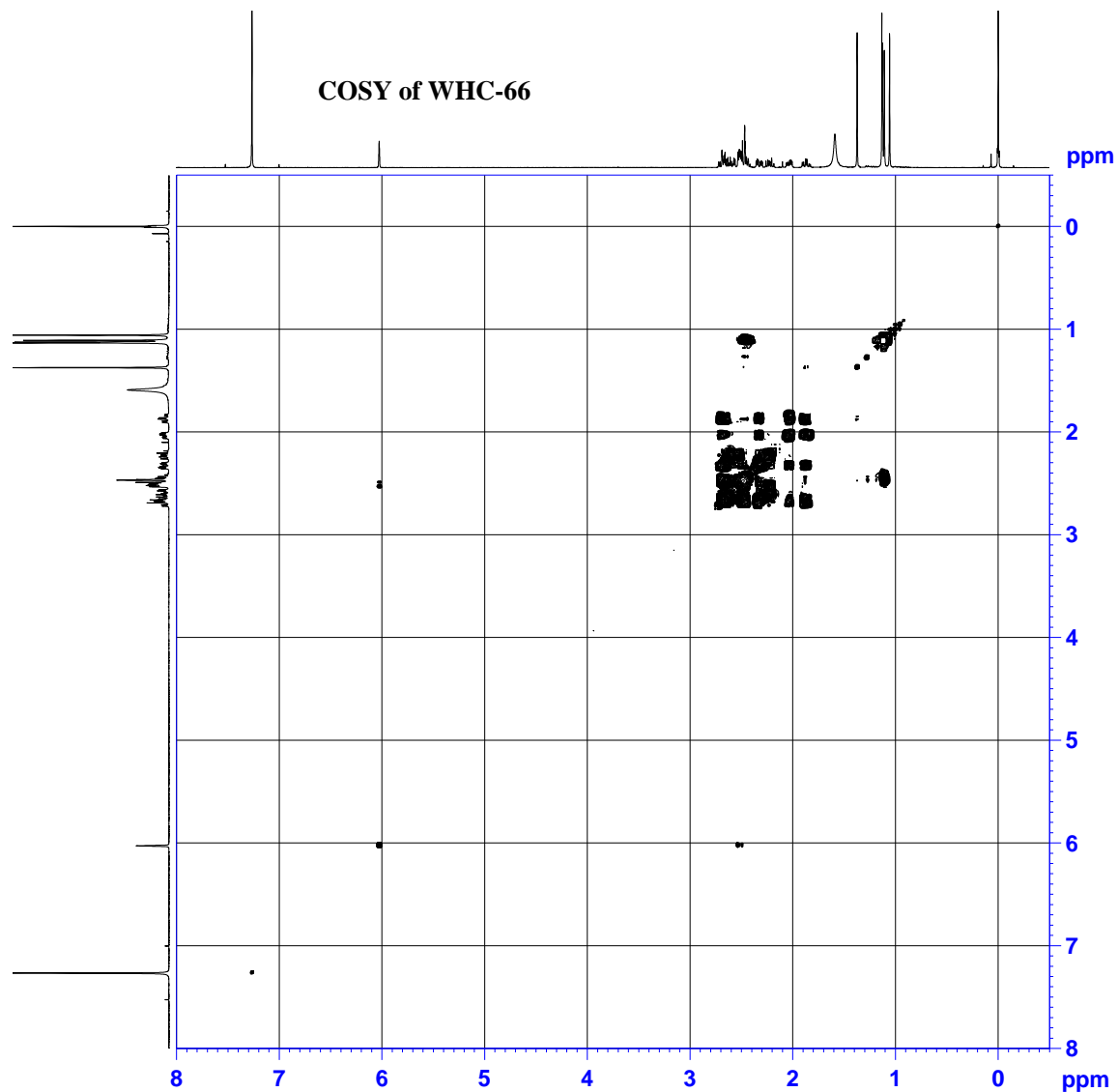


Figure S5B: Enlargement of area (^1H) 0.0–8.0 ppm and (^{13}C) 0–130 ppm



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NAME           WH-66
EXPNO           5
PROCNO          1
Date_          20111221
Time_          14.53
INSTRUM        spect
PROBHD         5 mm PADUL 13C
PULPROG        cosygpmfzf
TD             2048
SOLVENT        CDC13
NS             16
DS             8
SWH            5341.880 Hz
FIDRES         2.608340 Hz
AQ             0.1917428 sec
RG             203
DW             93.600 usec
DE             6.50 usec
TE             294.8 K
D0             0.00000300 sec
D1             2.00000000 sec
D13            0.00000400 sec
D16            0.00020000 sec
IN0            0.00018720 sec

```

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===== CHANNEL f1 =====
NUC1            1H
P1              11.95 usec
ND0             1
TD              128
SFO1            400.1324 MHz
FIDRES          41.733440 Hz
SW              13.350 ppm
FnMODE          QF
SI              1024
SF              400.1300134 MHz
WDW             SINE
SSB             0
LB              0.00 Hz
GB              0
PC              1.40
SI              1024
MC2             QF
SF              400.1300156 MHz
WDW             SINE
SSB             0
LB              0.00 Hz
GB              0

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Figure S6A: ^1H , ^1H COSY spectrum of decandrinin (**1**) (400 MHz, CDCl_3)

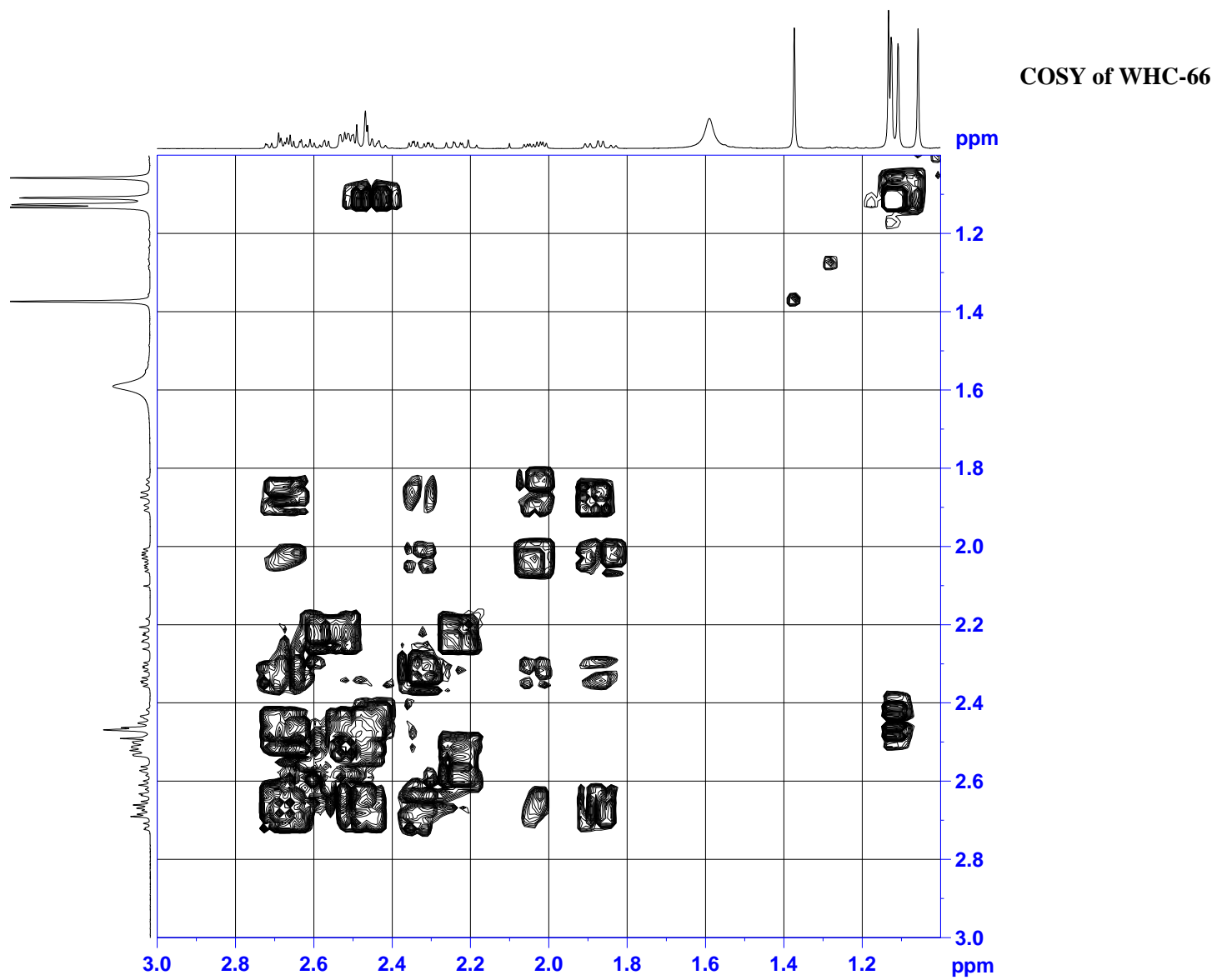


Figure S6B: Enlargement of area 1.0–3.0 ppm

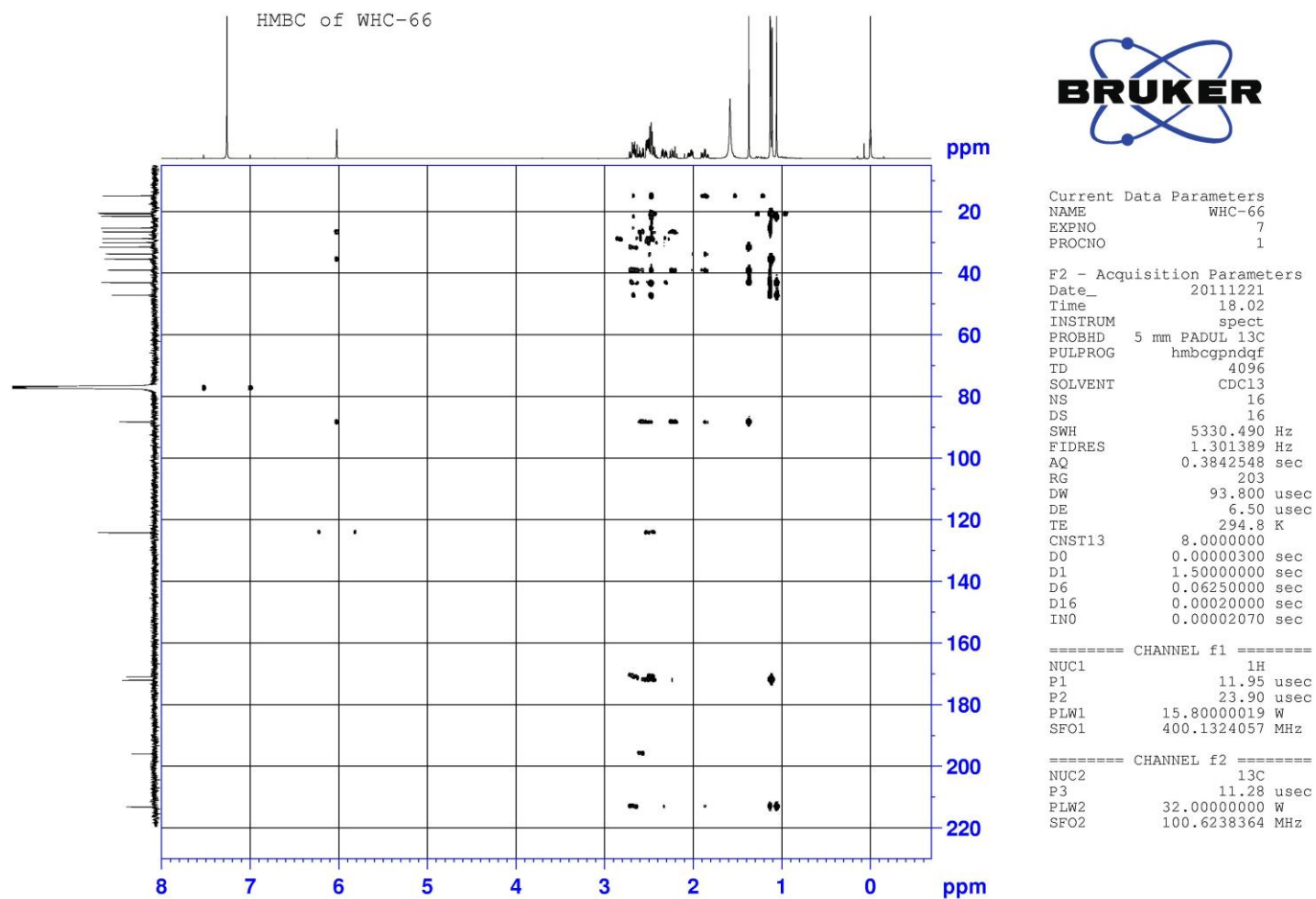


Figure S7A: HMBC spectrum of decandrinin (**1**) (400 MHz, CDCl₃)

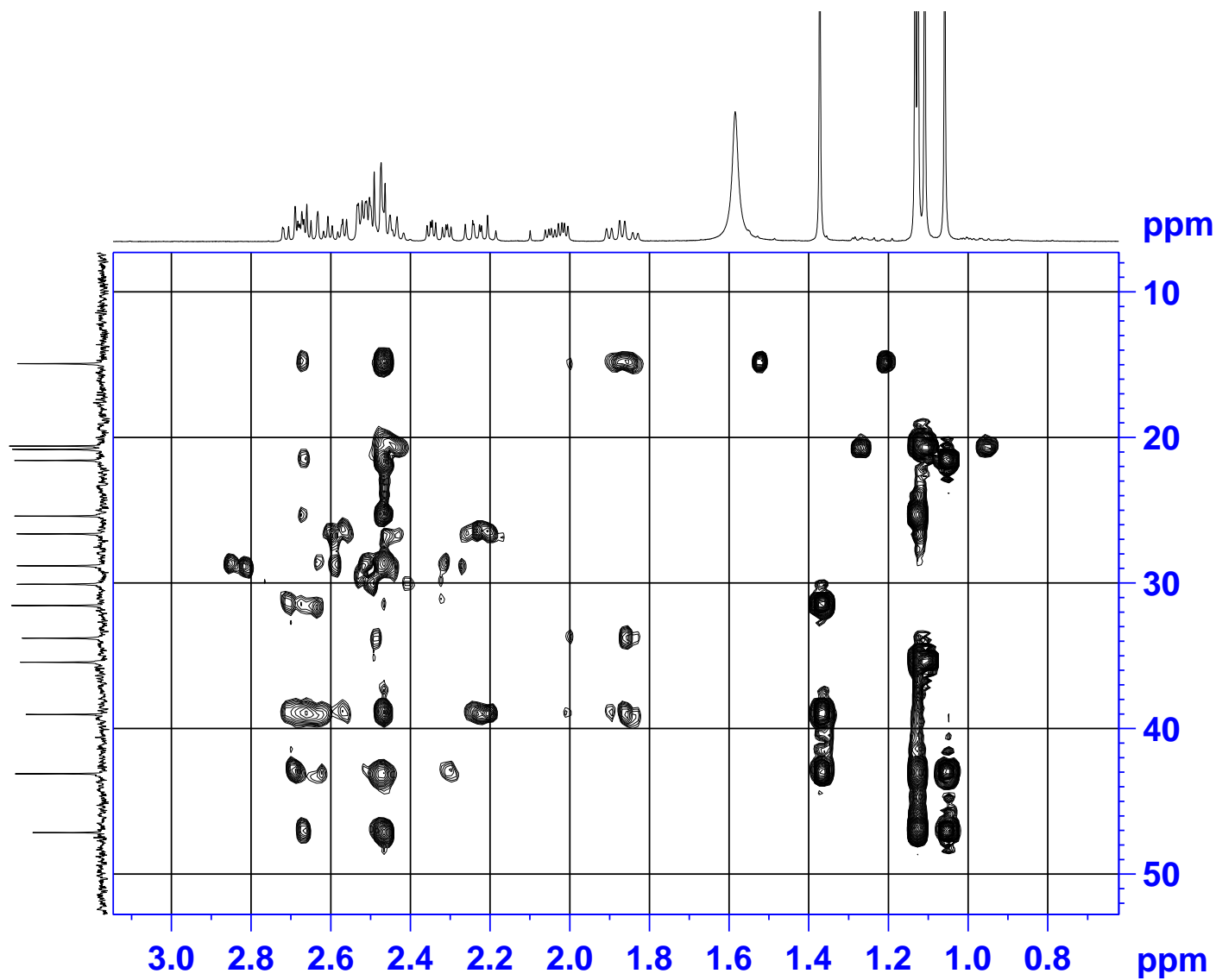


Figure S7B: Enlargement of area (^1H) 0.8–3.0 ppm and (^{13}C) 10–50 ppm

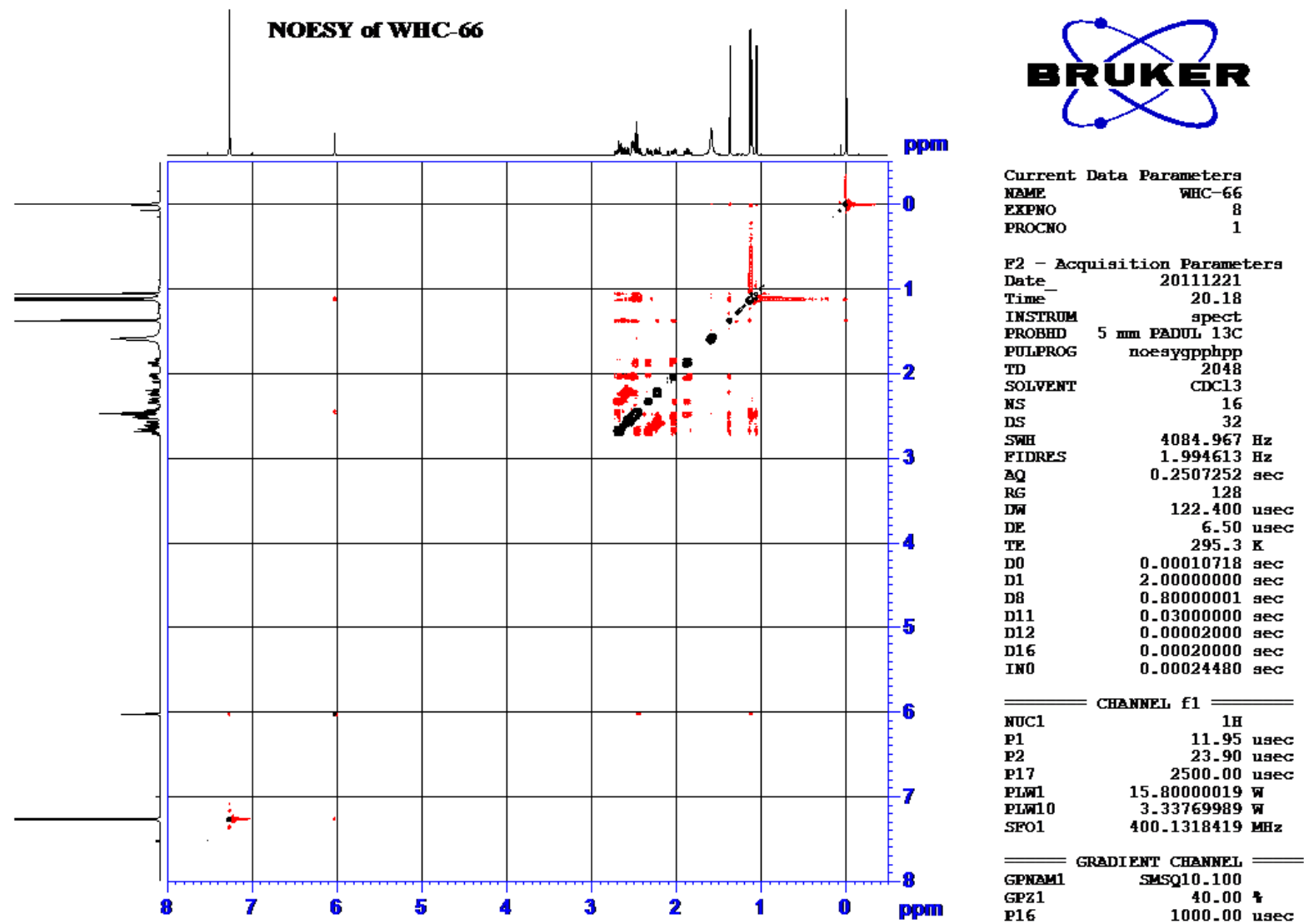


Figure S8A: NOESY spectrum of decandrinin (**1**) (400 MHz, CDCl₃)

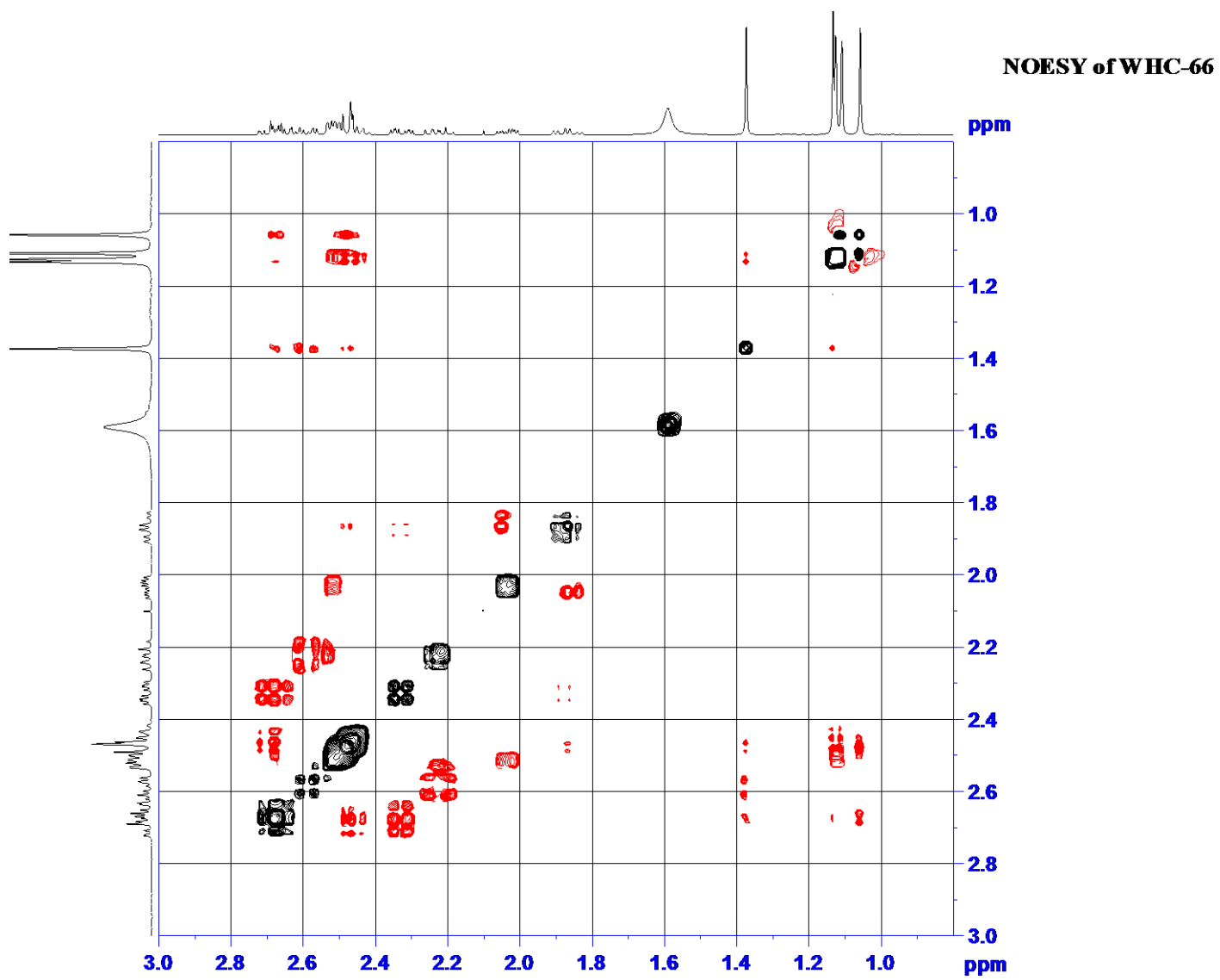


Figure S8B: Enlargement of area 1.0–3.0 ppm

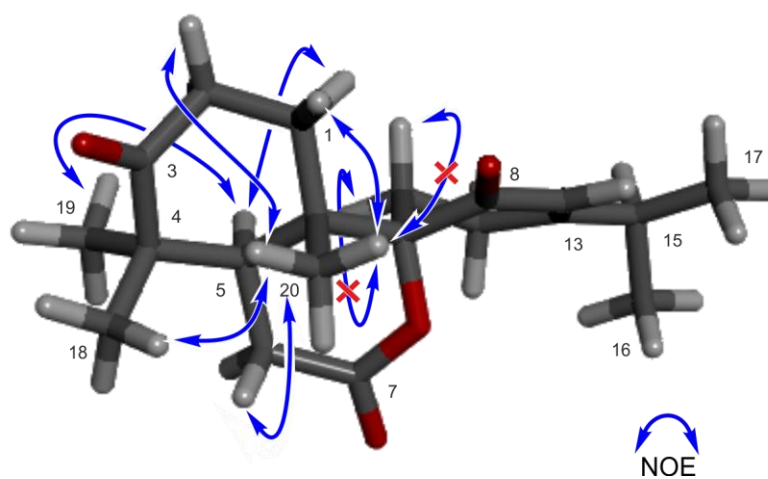


Figure S9: NOE interactions for the B97D/TZVP-optimized structure diagnostic for the (unnatural) 9-epimer of decandrinin (**1**): arbitrarily the 5*R*,9*S*,10*S*-enantiomer is shown.

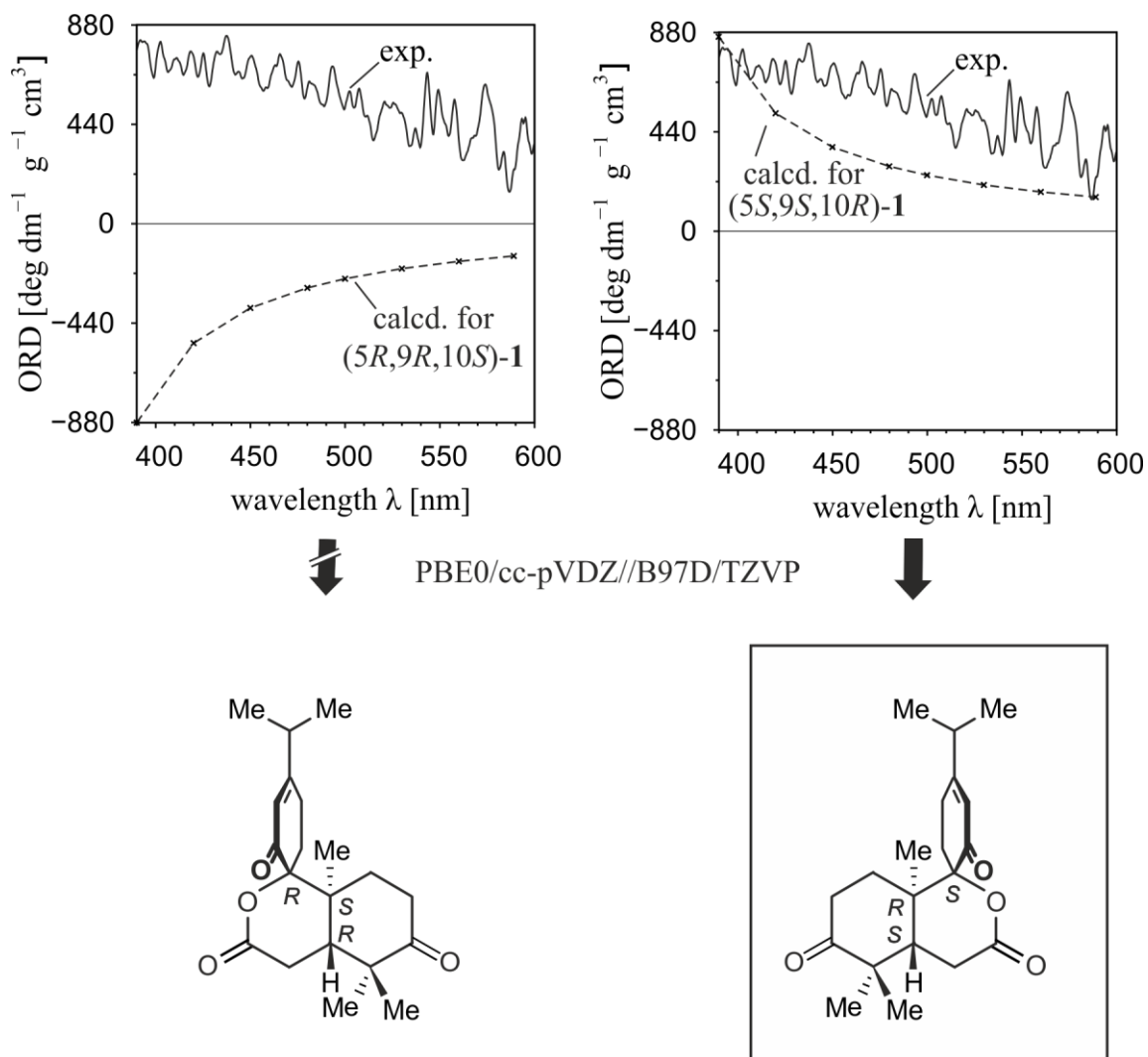


Figure S10: Confirmation of the absolute configuration of decandrinin (**1**) by comparison of the calculated ORD with the experimental one.