Supporting Information

for

Decandrinin, an unprecedented C_9-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.

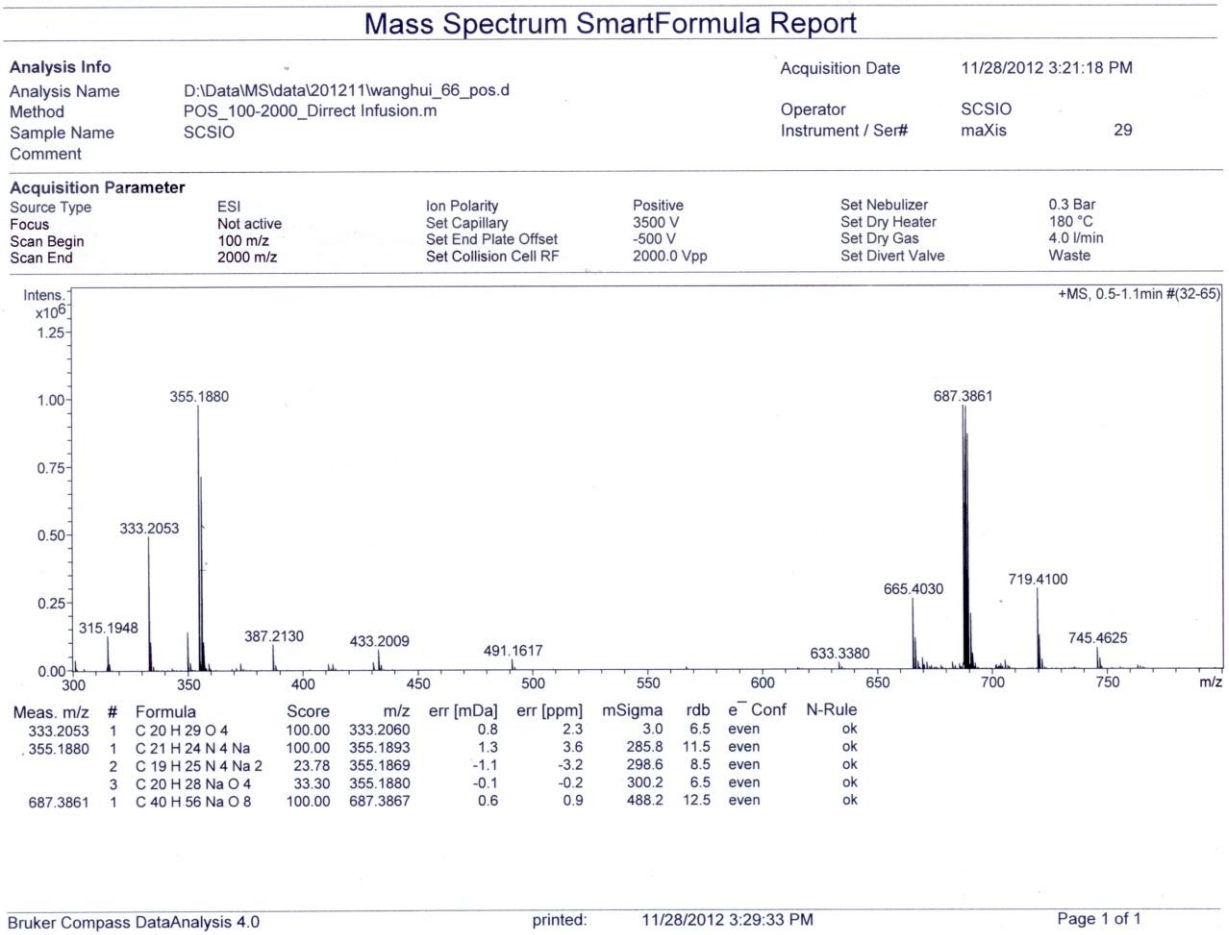


Figure S1: HRMS (ESI) spectrum of decandrinin (**1**) (MeOH)

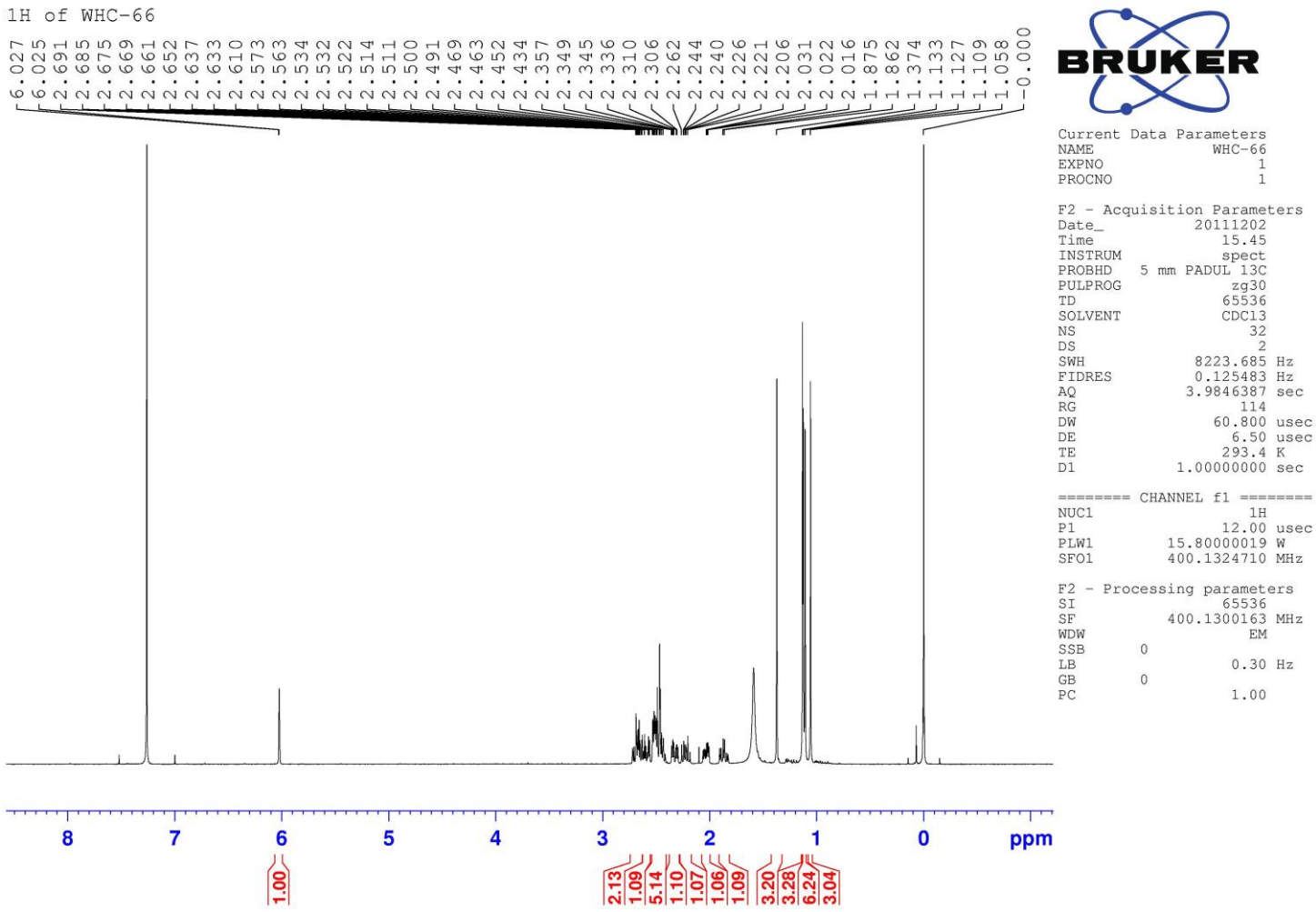


Figure S2A: ^{1}H NMR spectrum of decandrinin (**1**) (400 MHz, $CDCl_3$)

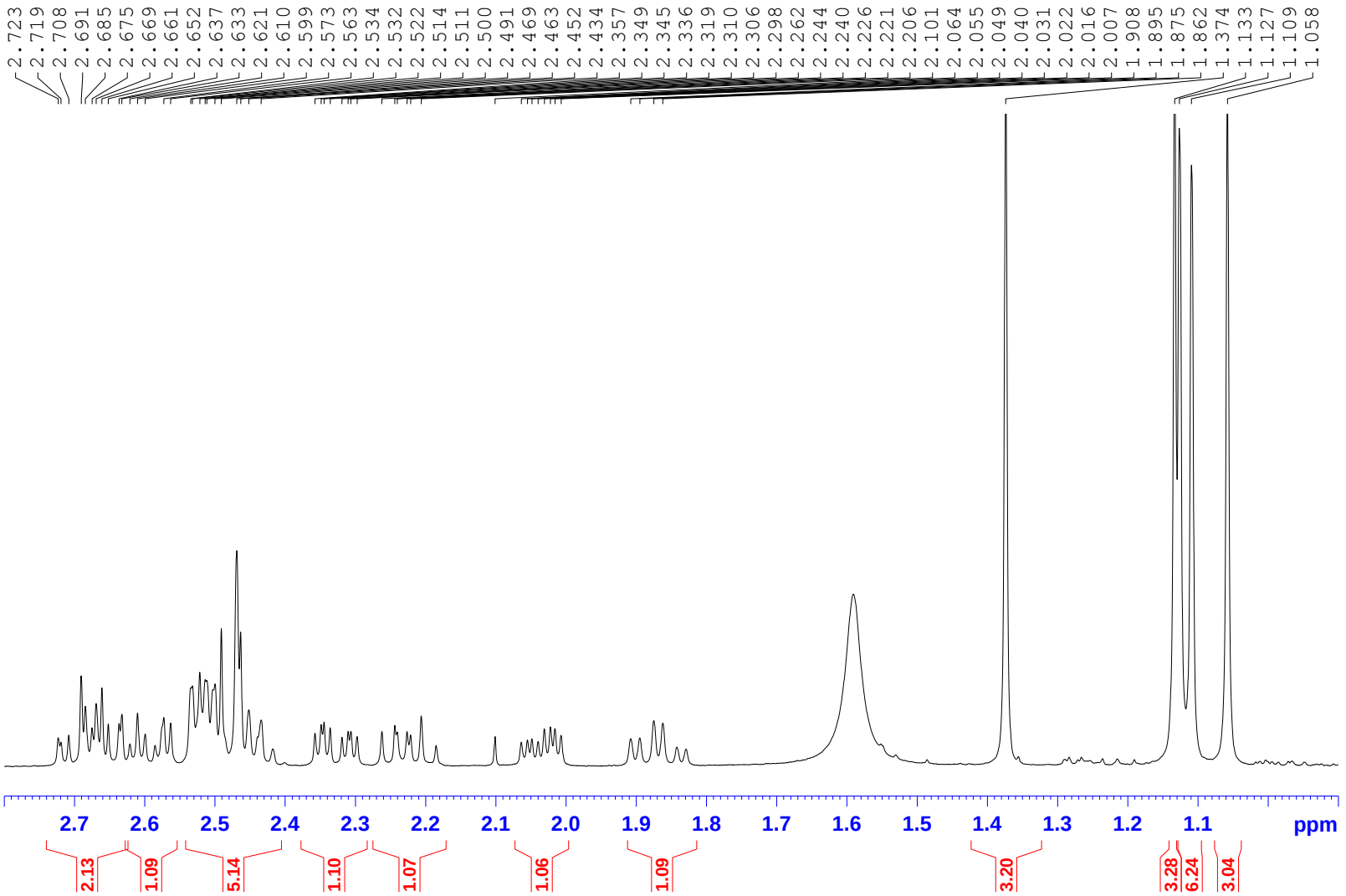


Figure S2B: Enlargement of area 1.0–2.7 ppm

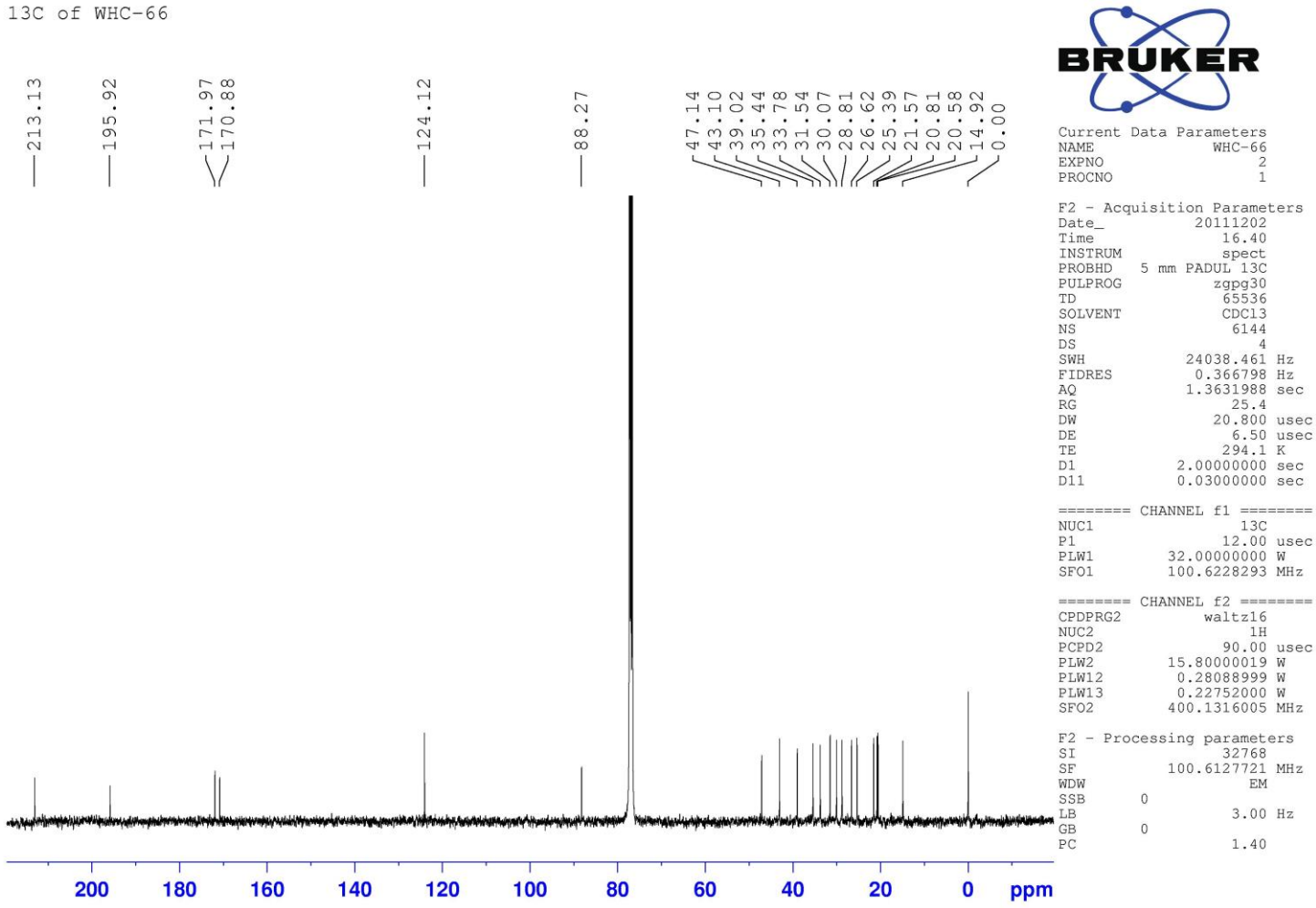


Figure S3: ^{13}C NMR spectrum of decandrinin (**1**) (400 MHz, $CDCl_3$)

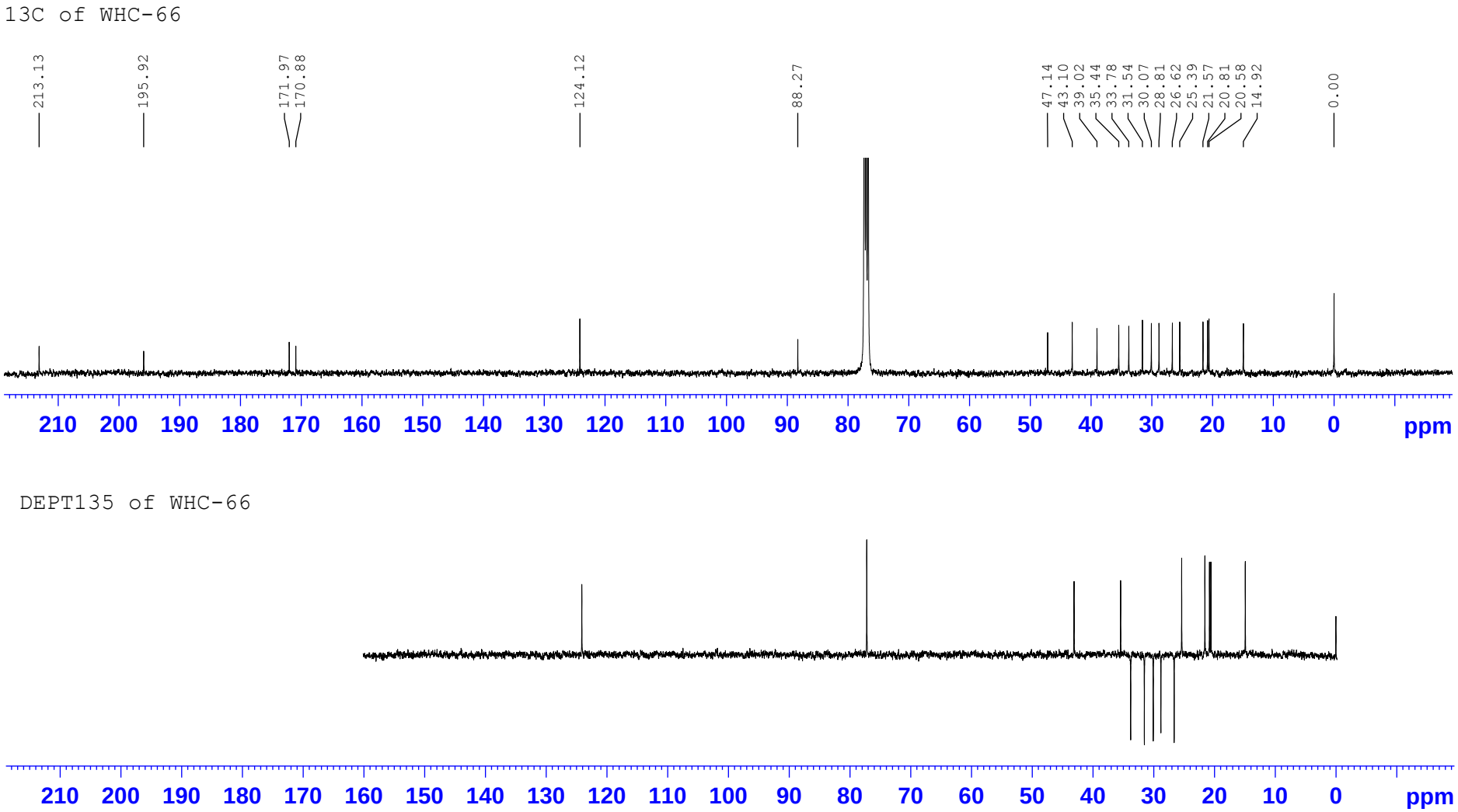
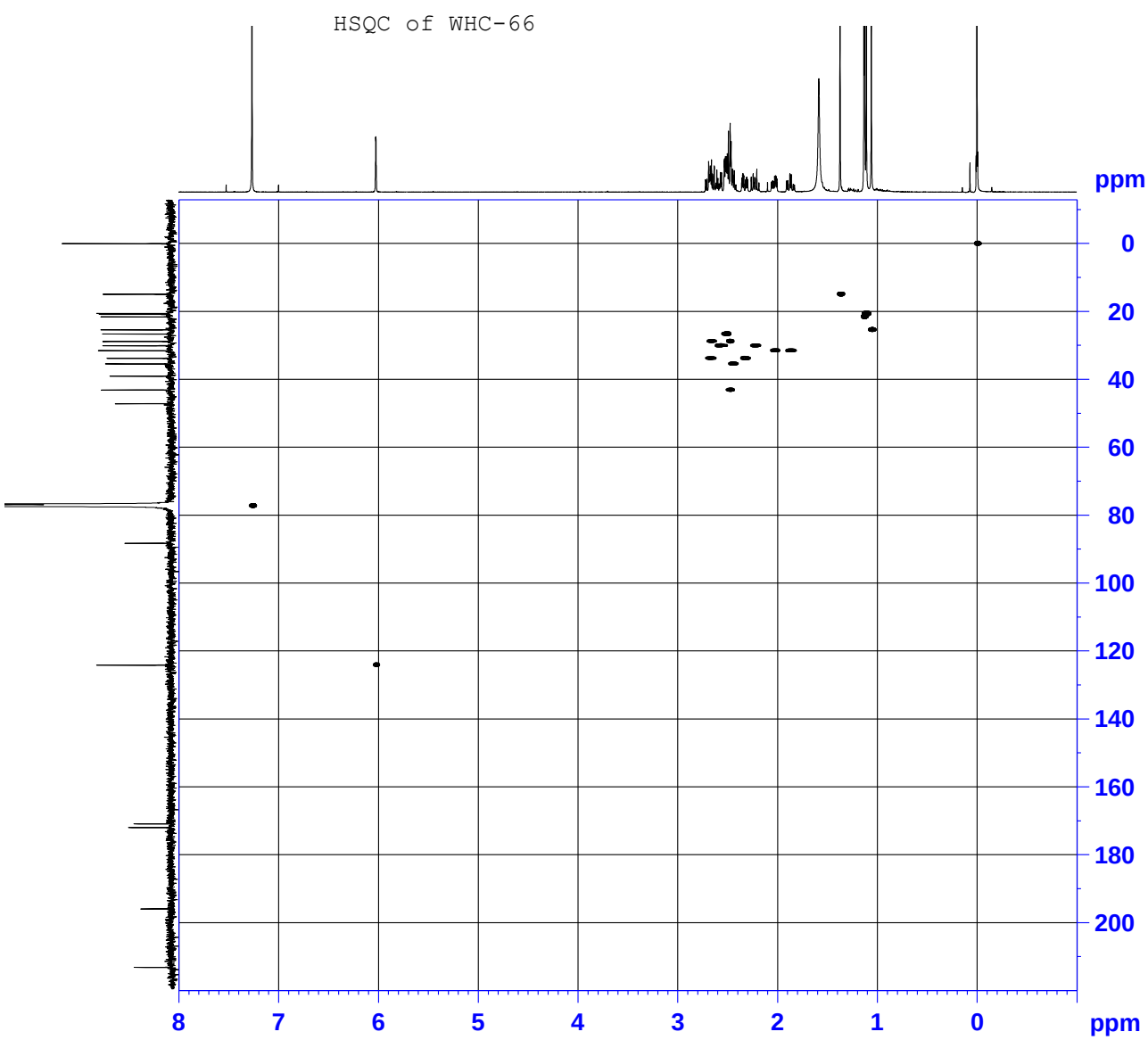


Figure S4: ^{13}C NMR and DEPT 135 spectra of decandrinin (**1**) (400 MHz, $CDCl_3$)

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PROCNO                    1

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TD                     1024
SOLVENT              CDCl3
NS                        16
DS                        32
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FIDRES             6.260016 Hz
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RG                      203
DW                   78.000 us
DE                    6.50 us
TE                   295.2 K
CNST2           145.0000000
CNST17           -0.5000000
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 ------
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Figure S5A: HSQC spectrum of decandrinin (**1**) (400 MHz, $CDCl_3$)

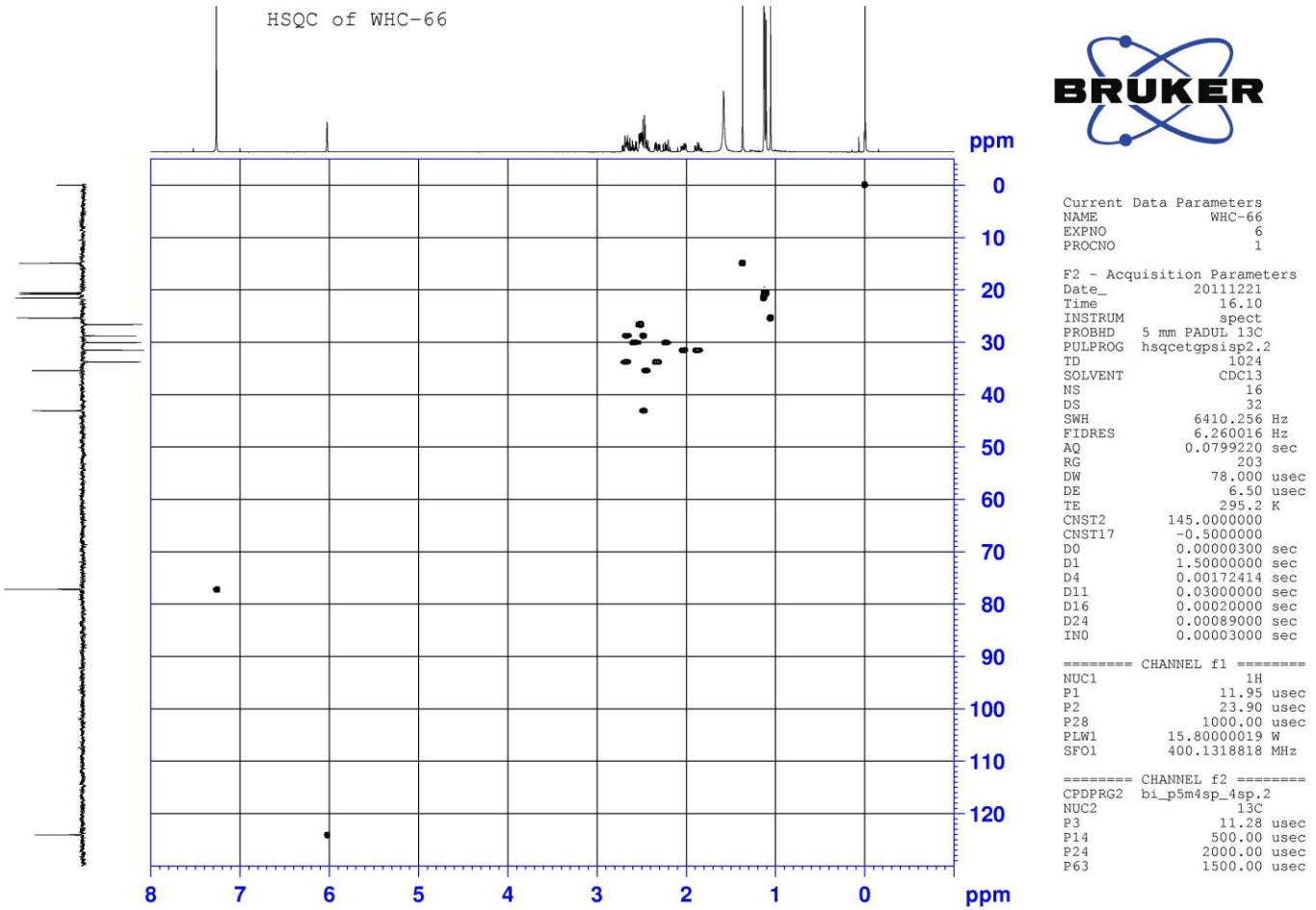
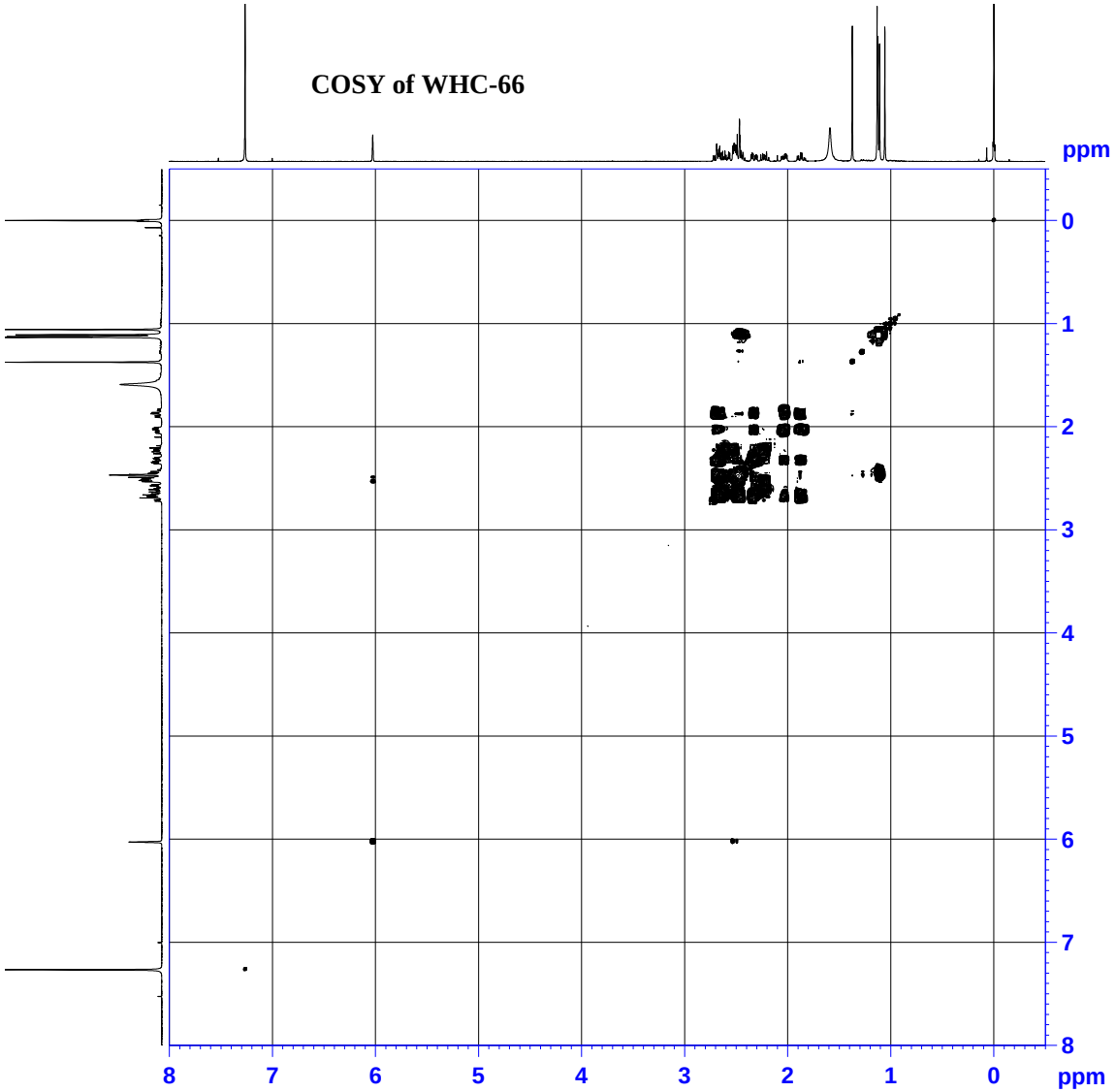
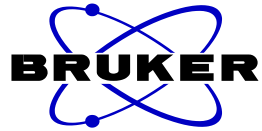


Figure S5B: Enlargement of area (^{1}H) 0.0–8.0 ppm and (^{13}C) 0–130 ppm



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EXPNO                   5
PROCNO                  1
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PULPROG       cosygpmfqf
TD                   2048
SOLVENT             CDCl3
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

======== CHANNEL f1 ========
NUC1                   1H
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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: $^{1}H,^{1}H$ COSY spectrum of decandrinin (**1**) (400 MHz, $CDCl_3$)

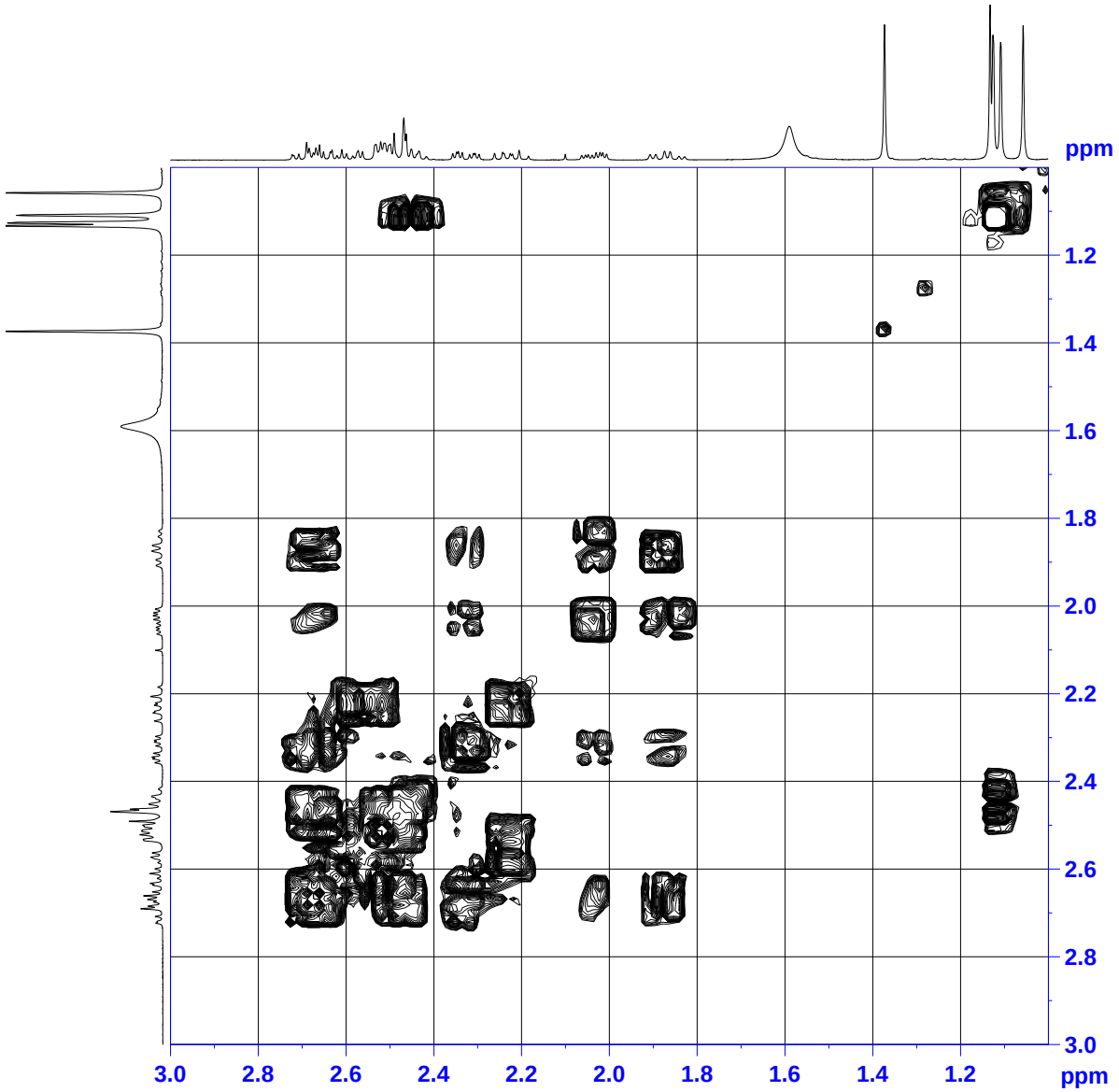

Figure S6B: Enlargement of area 1.0–3.0 ppm

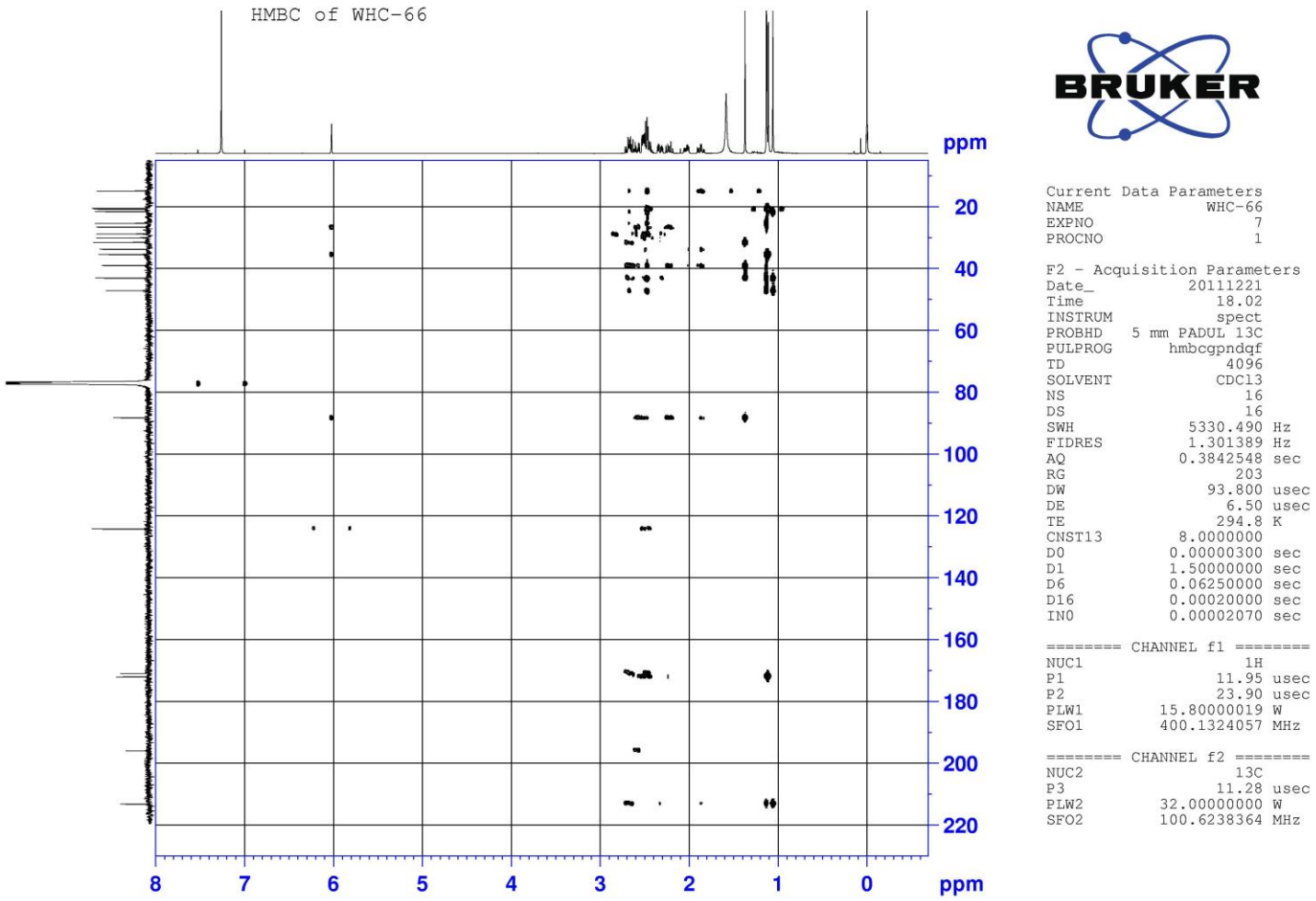

Figure S7A: HMBC spectrum of decandrinin (**1**) (400 MHz, $CDCl_3$)

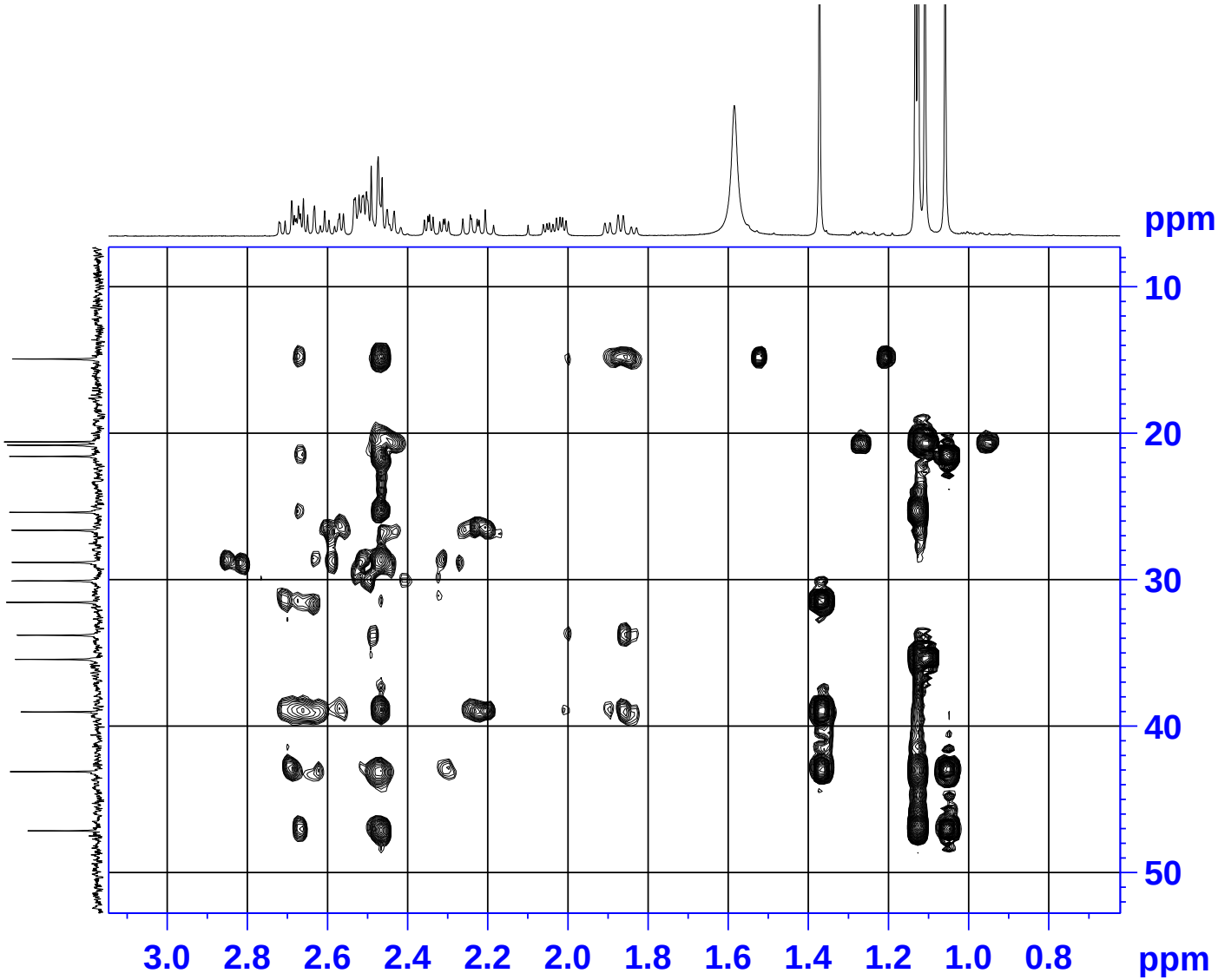

Figure S7B: Enlargement of area (^{1}H) 0.8–3.0 ppm and (^{13}C) 10–50 ppm

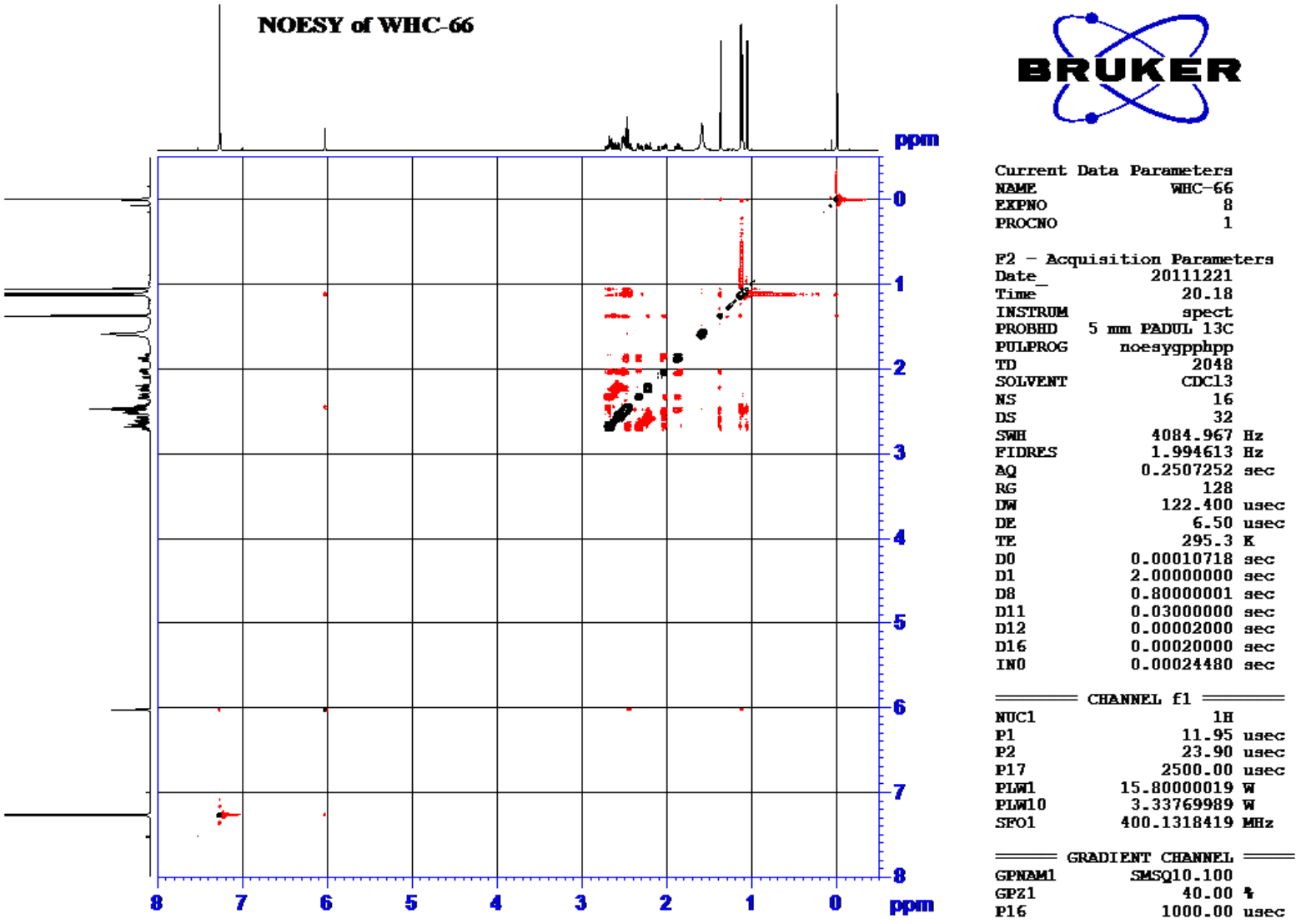

Figure S8A: NOESY spectrum of decandrinin (**1**) (400 MHz, $CDCl_3$)

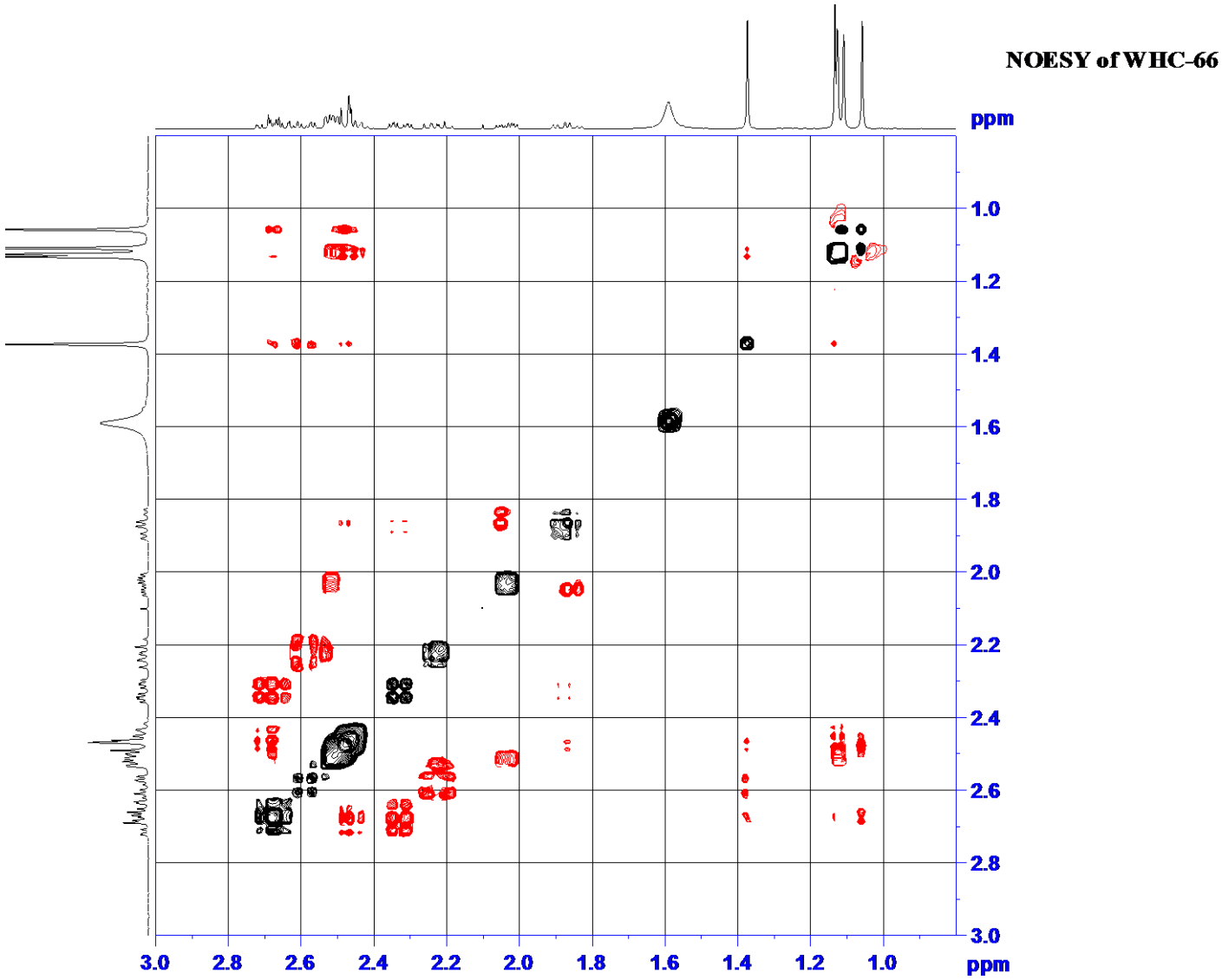

Figure S8B: Enlargement of area 1.0–3.0 ppm

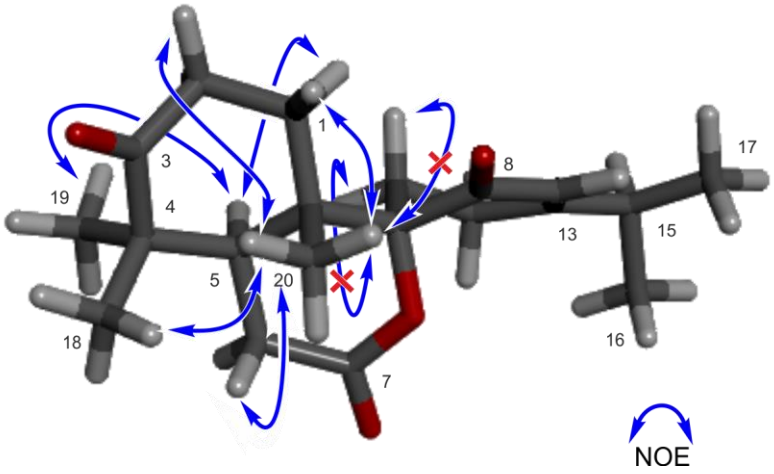

Figure S9: NOE interactions for the B97D/TZVP-optimized structure diagnostic for the (unnatural) 9-epimer of decandrinin (**1**): arbitrarily the 5*R*,9*S*,10*S*-enantiomer is shown.

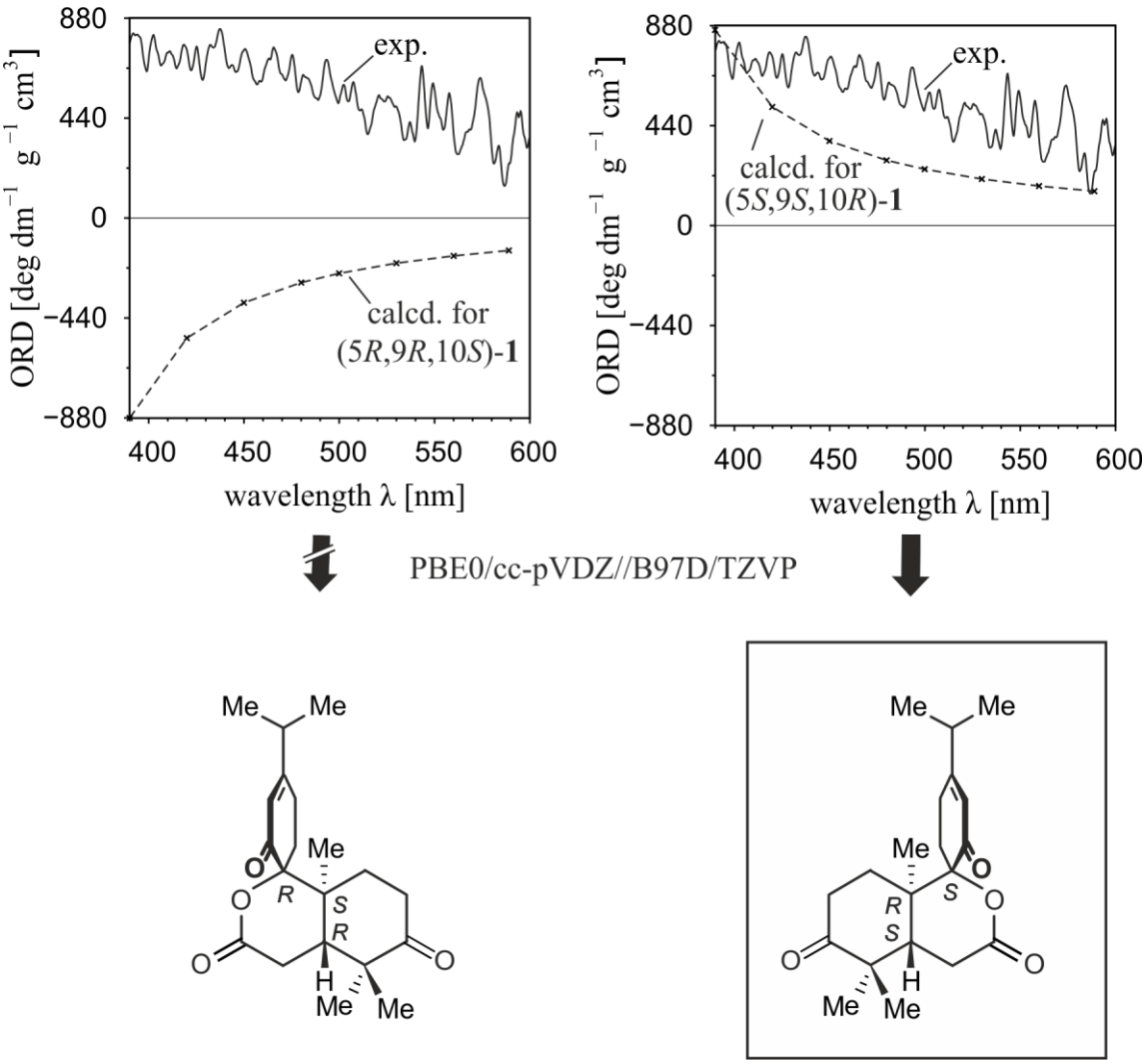

Figure S10: Confirmation of the absolute configuration of decandrinin (**1**) by comparison of the calculated ORD with the experimental one.