

Supplementary Materials: Assignment of the CD Cotton Effect to the Chiral Center in Pseurotins, and the Stereochemical Revision of Pseurotin A₂

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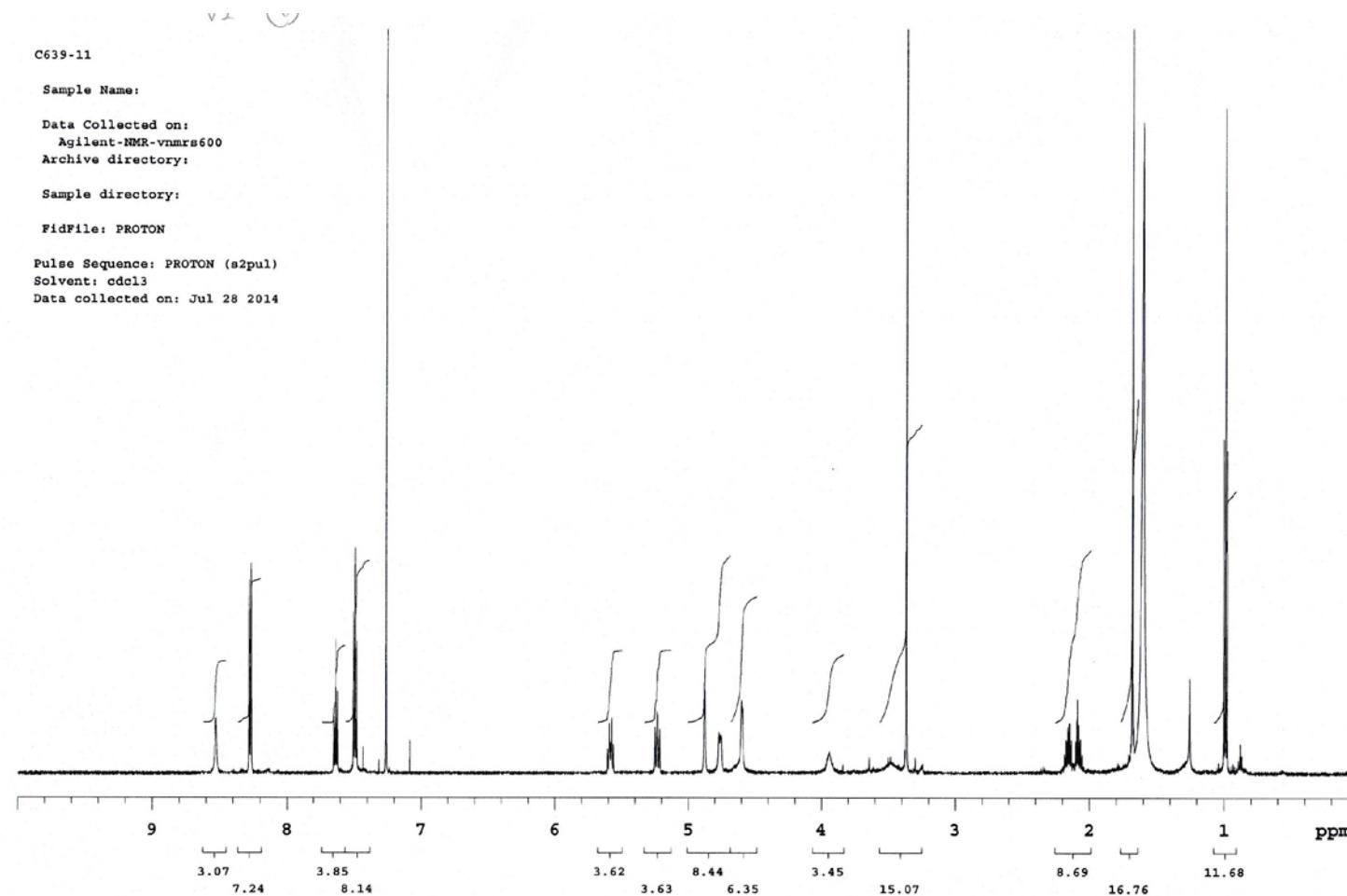


Figure S1. ^1H NMR spectrum in CDCl_3 of pseurotin A₁ (**1**).

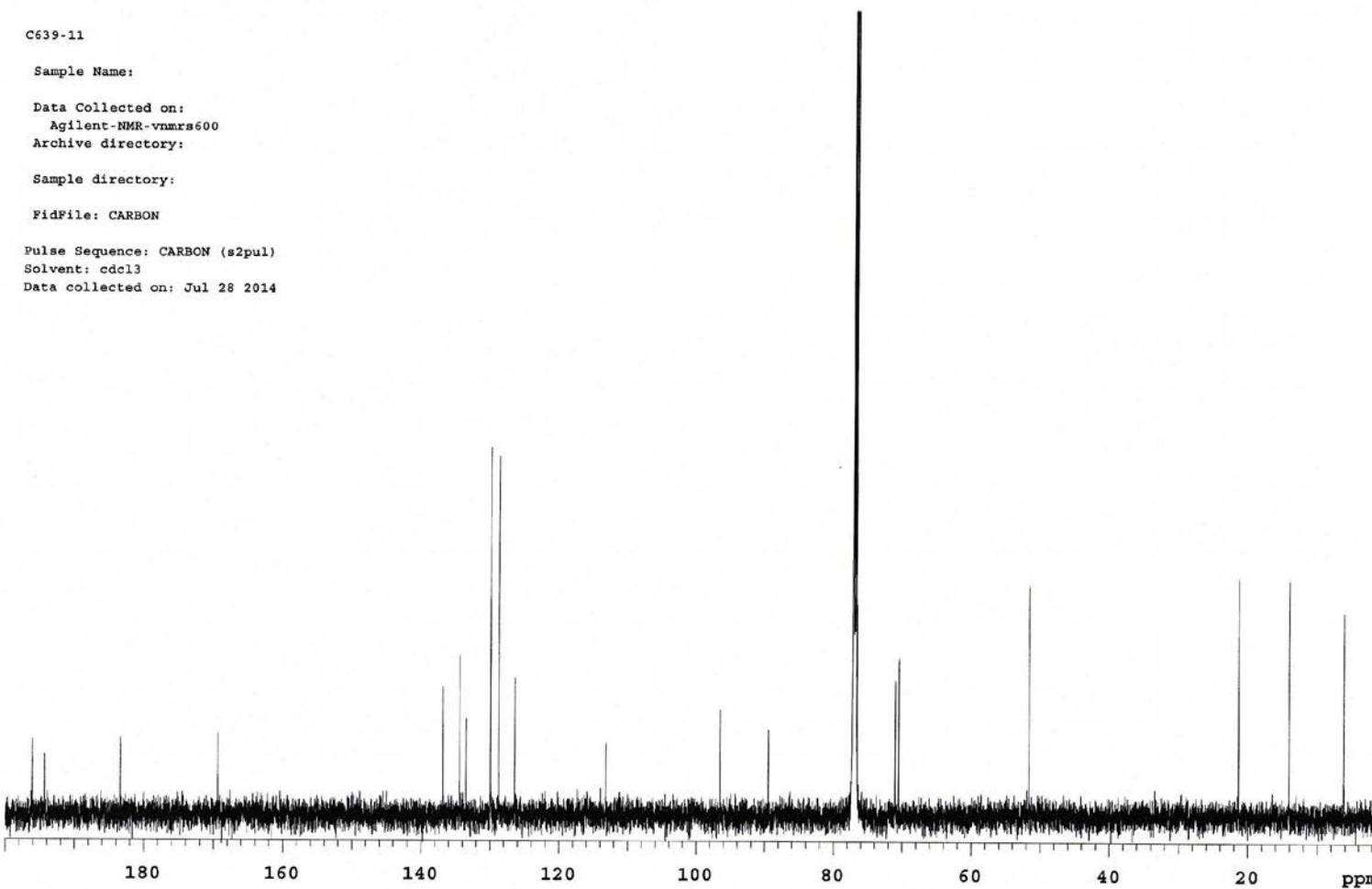


Figure S2. ^{13}C NMR spectrum in CDCl_3 of pseurotin A₁ (**1**).

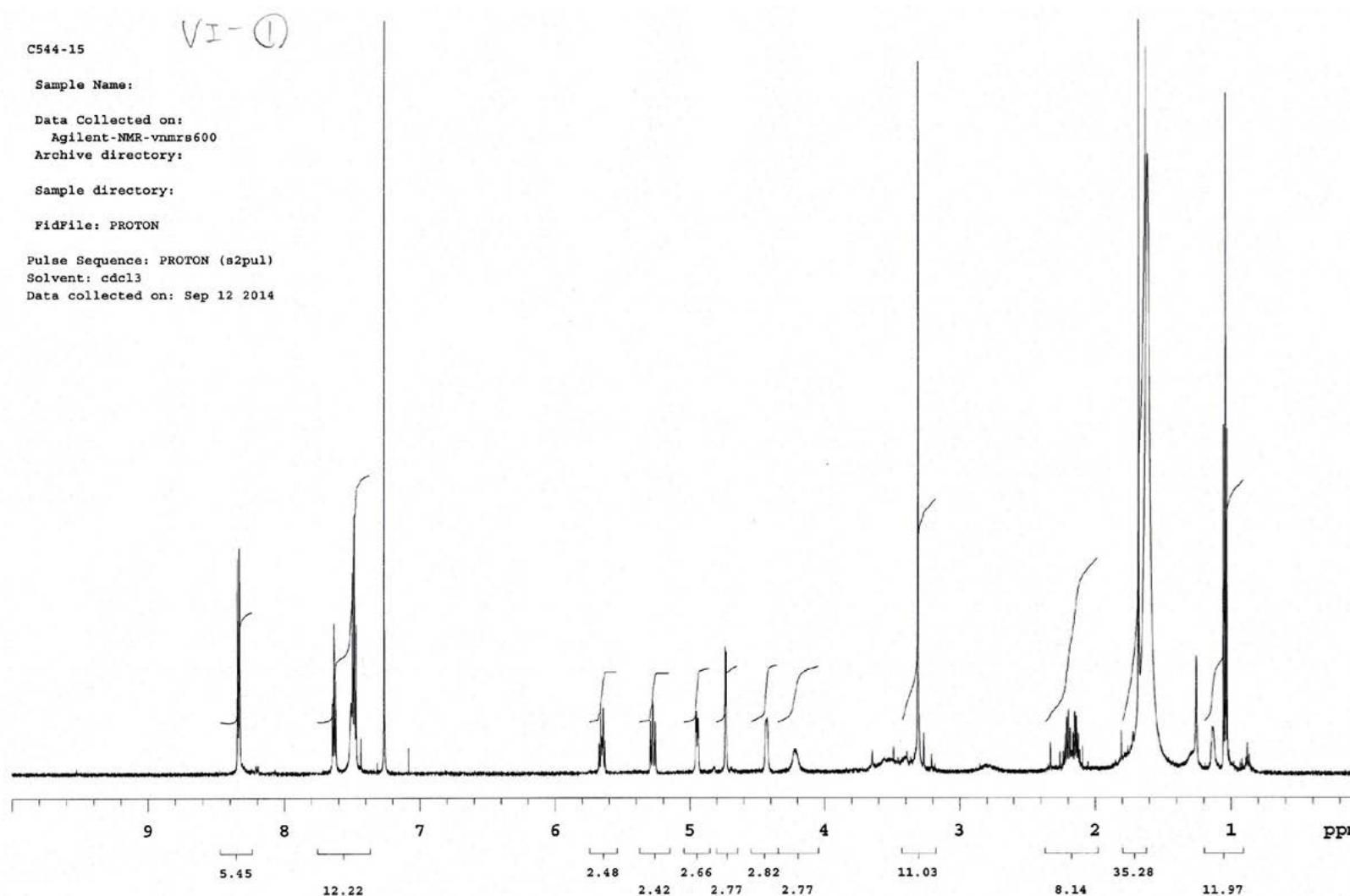


Figure S3. ^1H NMR spectrum in CDCl_3 of pseurotin A₂ (**4**).

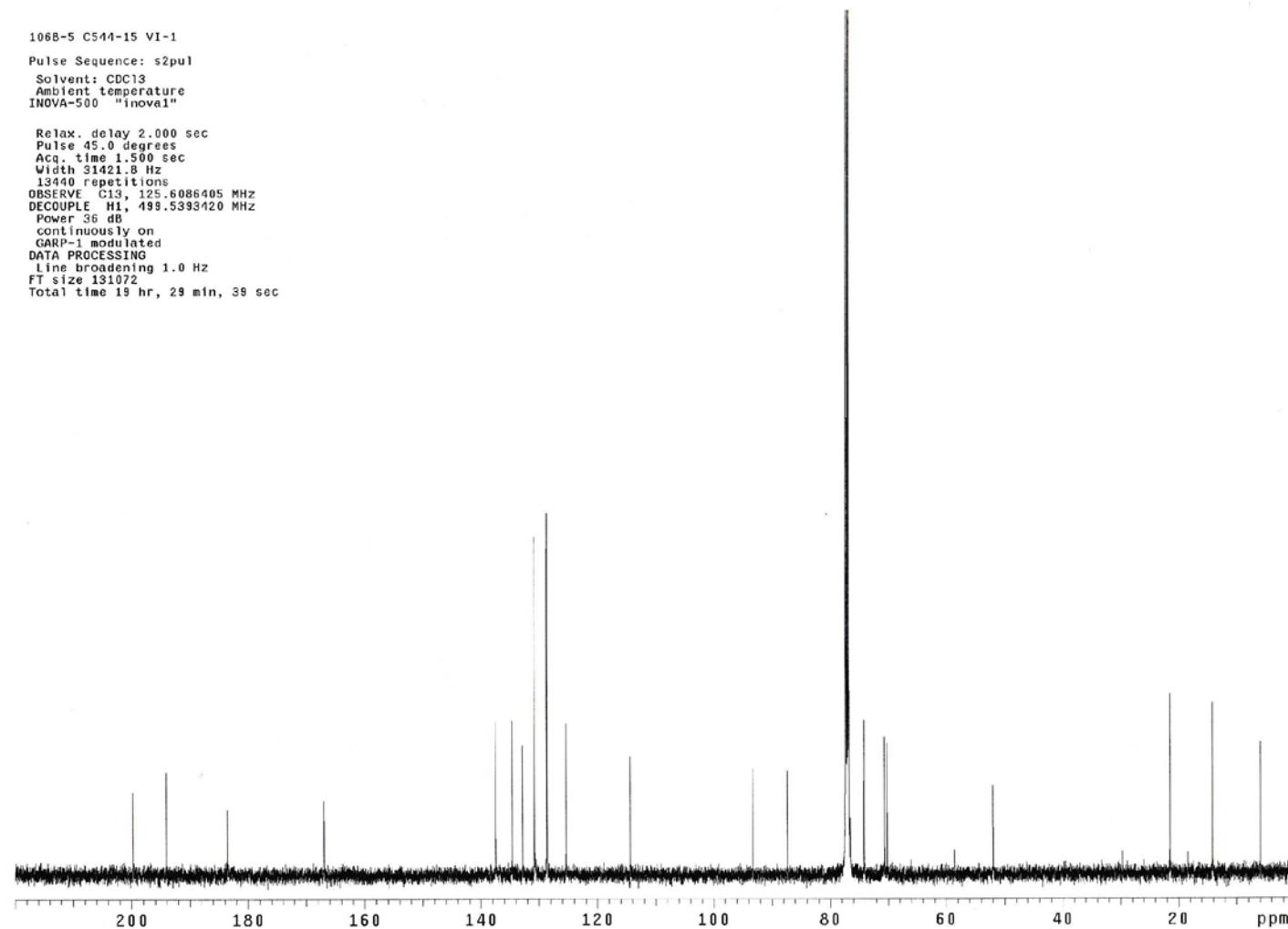


Figure S4. ¹³C NMR spectrum in CDCl₃ of pseurotin A₂ (**4**).

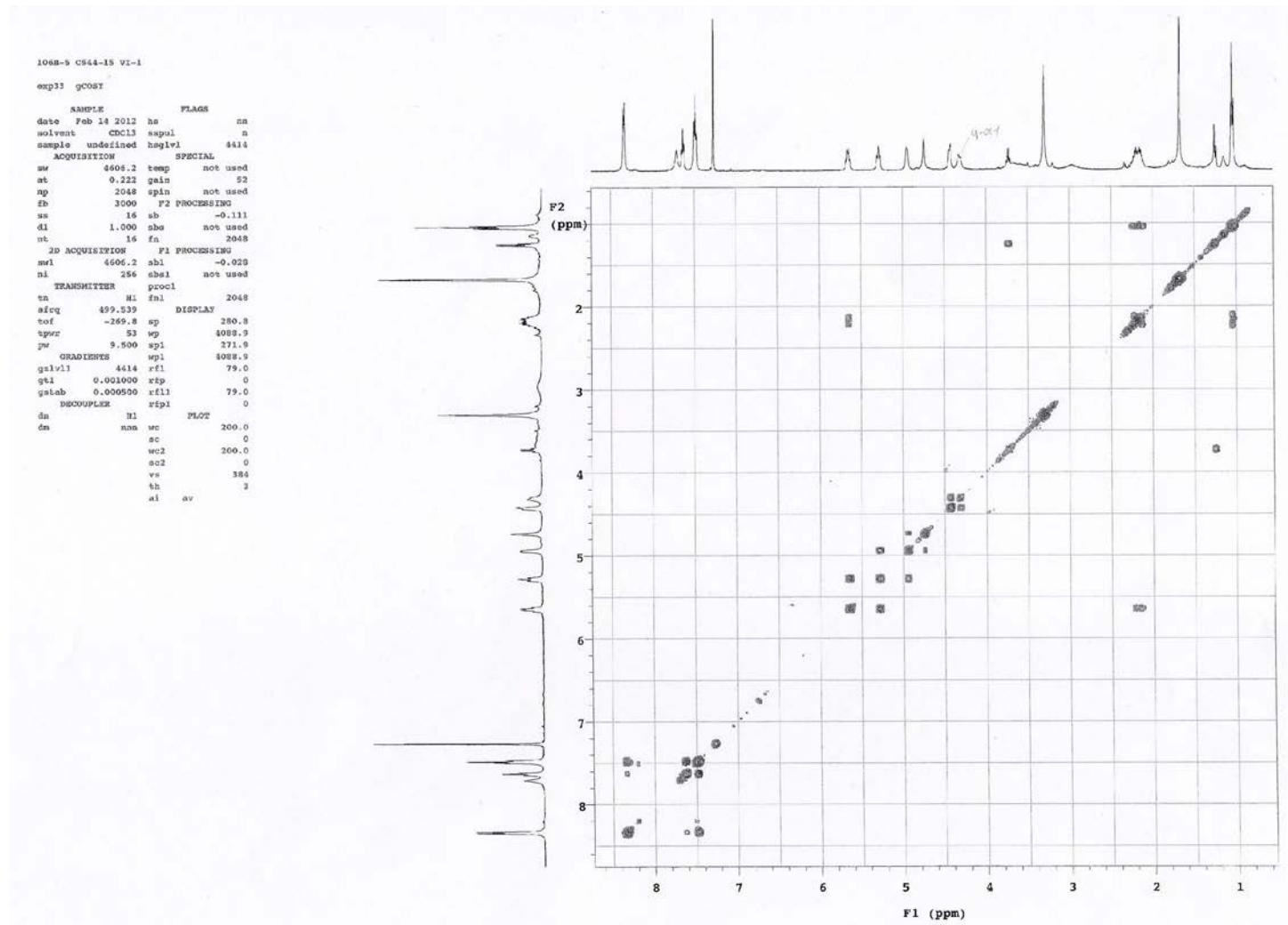


Figure S5. 2D NMR spectra of pseurotin A₂ (**4**) (¹H–¹H COSY).

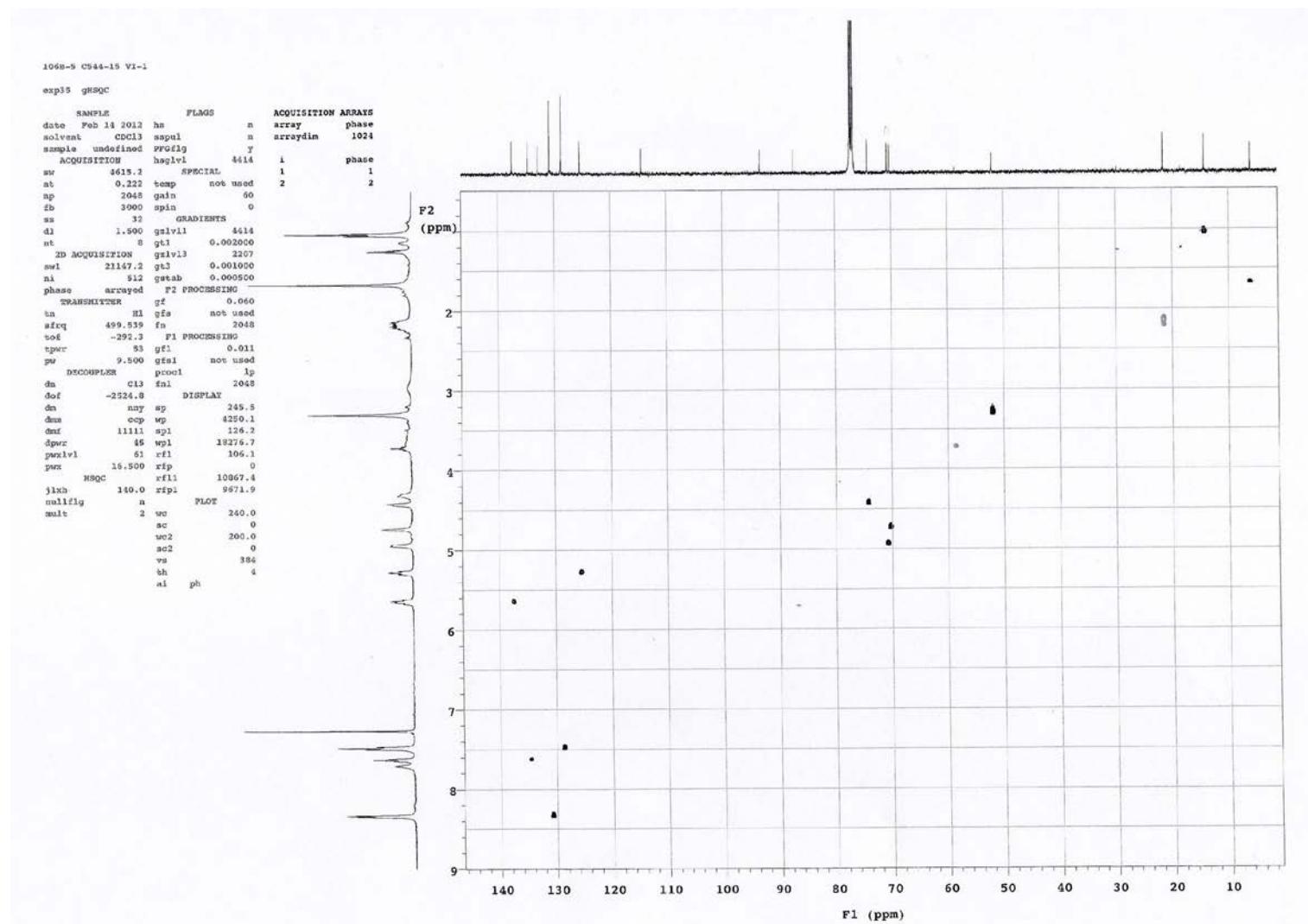


Figure S6. 2D NMR spectra of pseurotin A₂ (**4**) (HMQC).

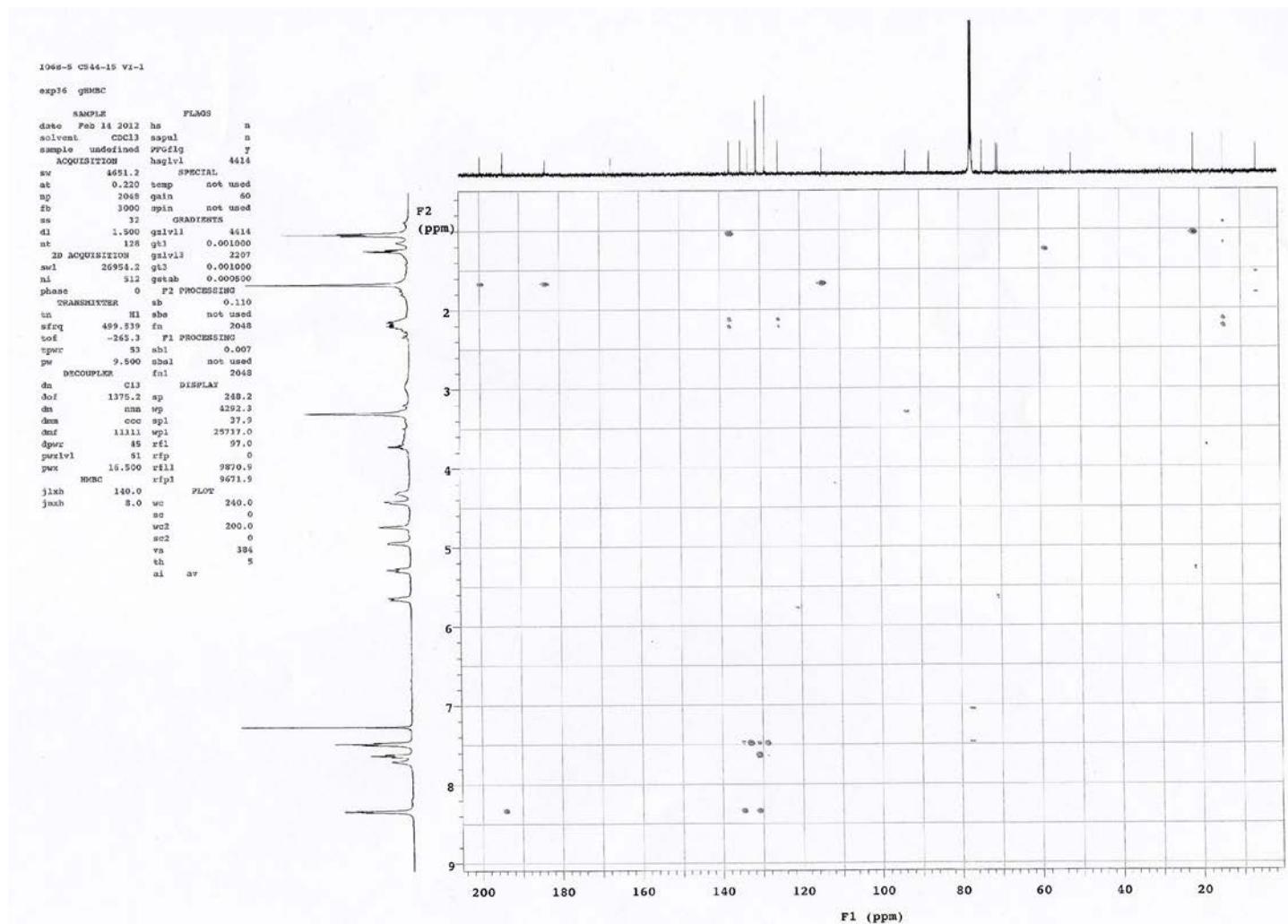


Figure S7. 2D NMR spectra of pseurotin A₂ (4) (HMBC).

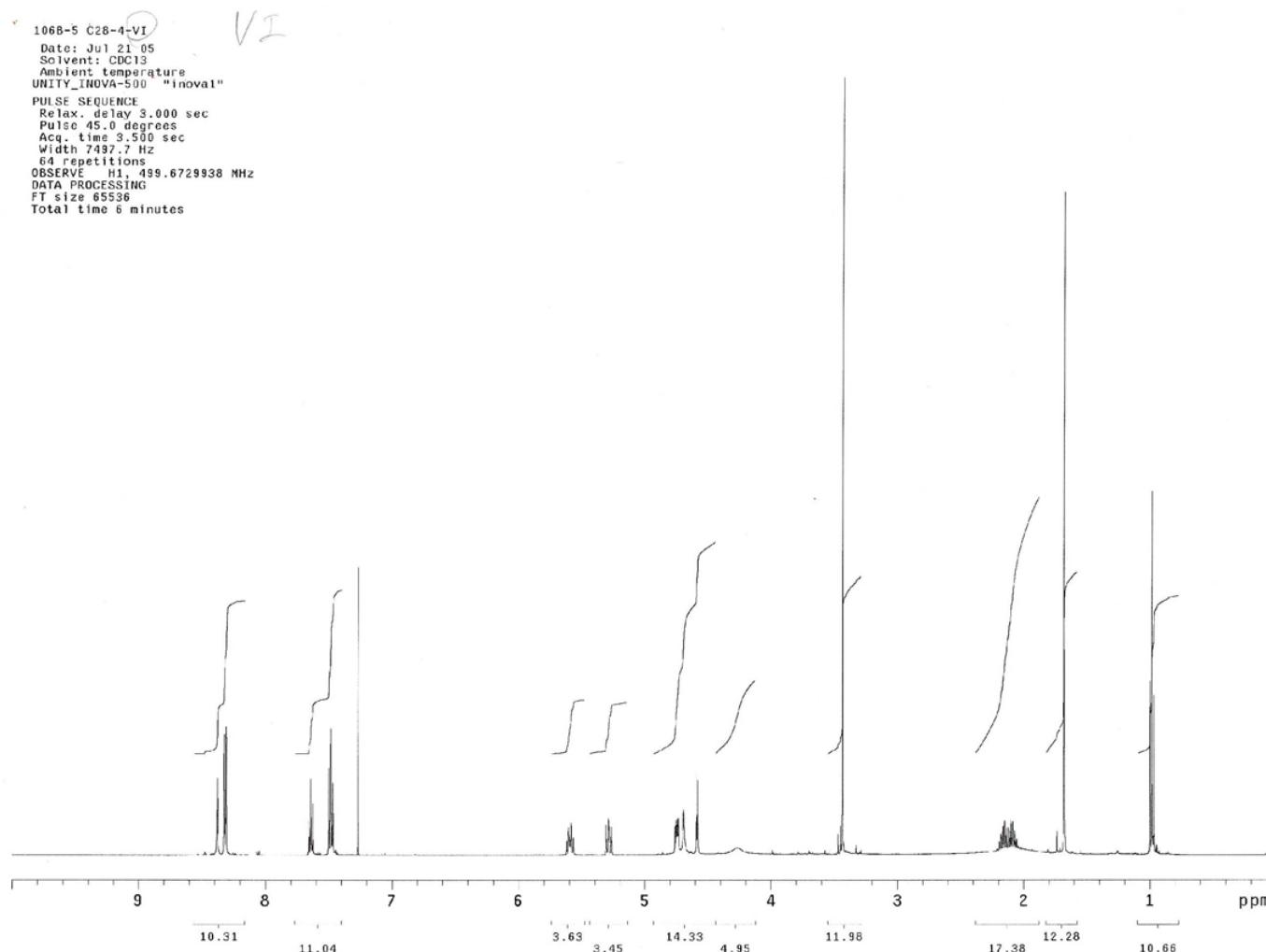


Figure S8. ¹H NMR spectrum in CDCl₃ of pseurotin A (3).

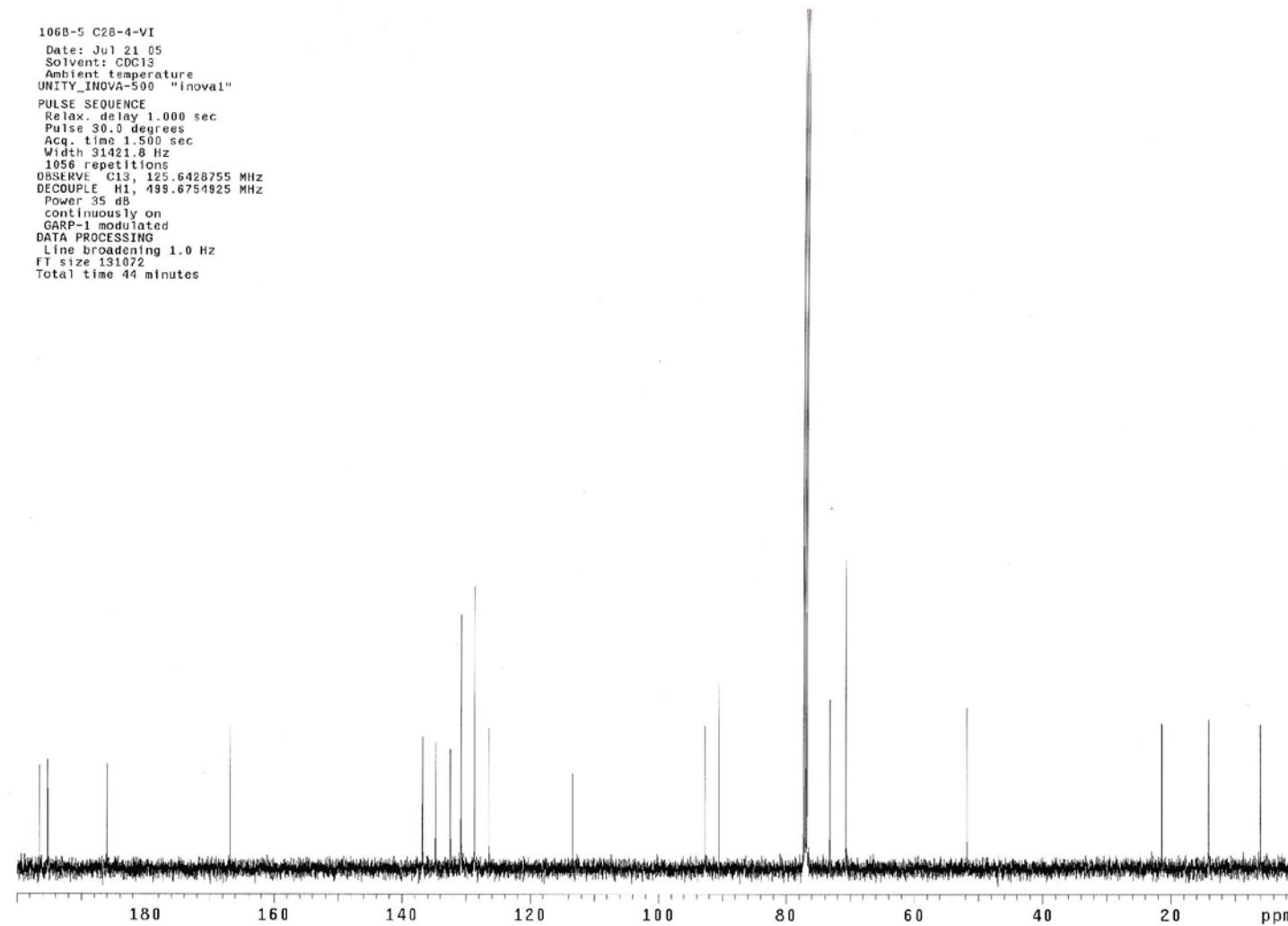


Figure S9. ¹³C NMR spectrum in CDCl₃ of pseurotin A (3).

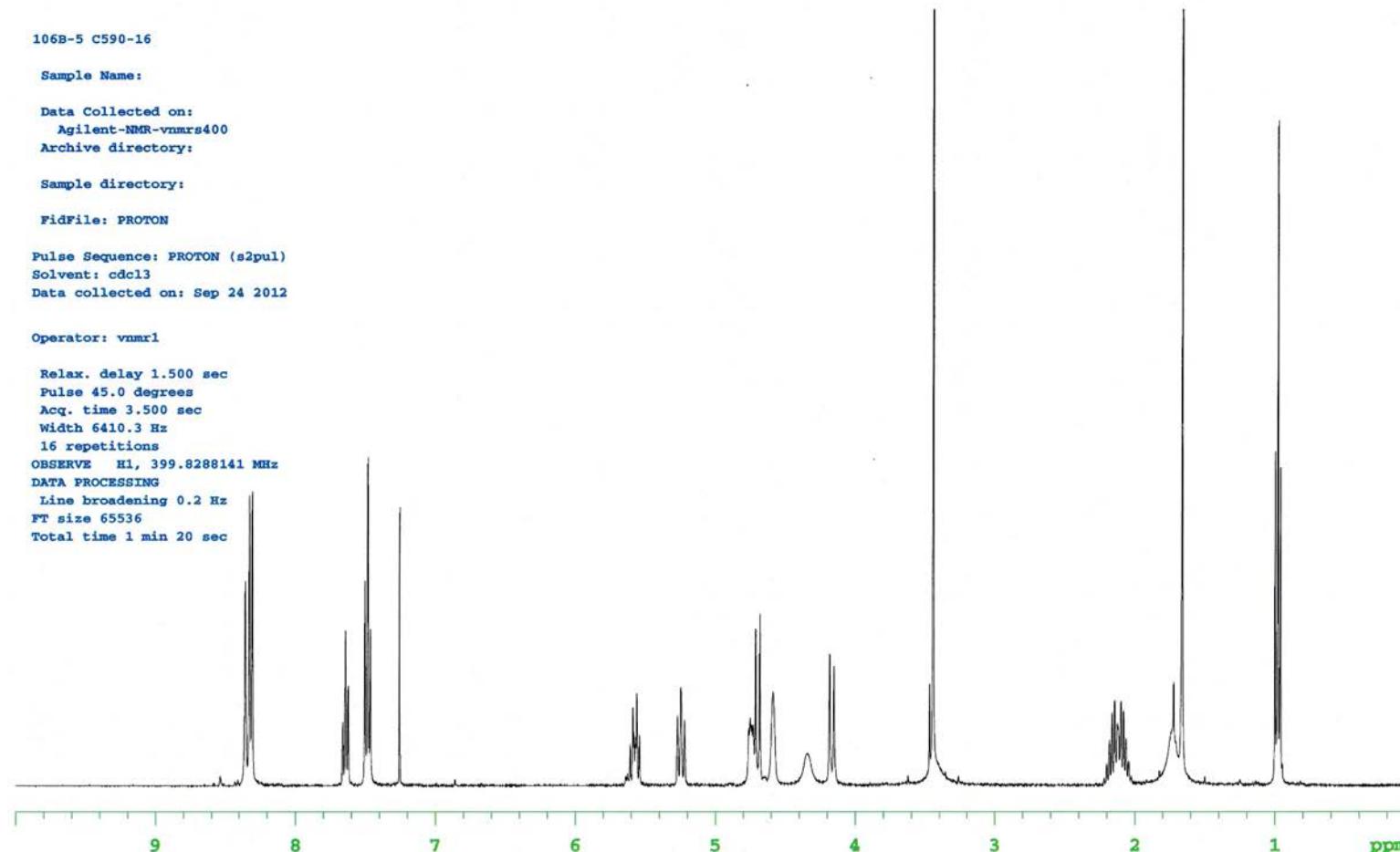


Figure S10. ¹H NMR spectrum in CDCl₃ of pseurotin A (3) (400 MHz).

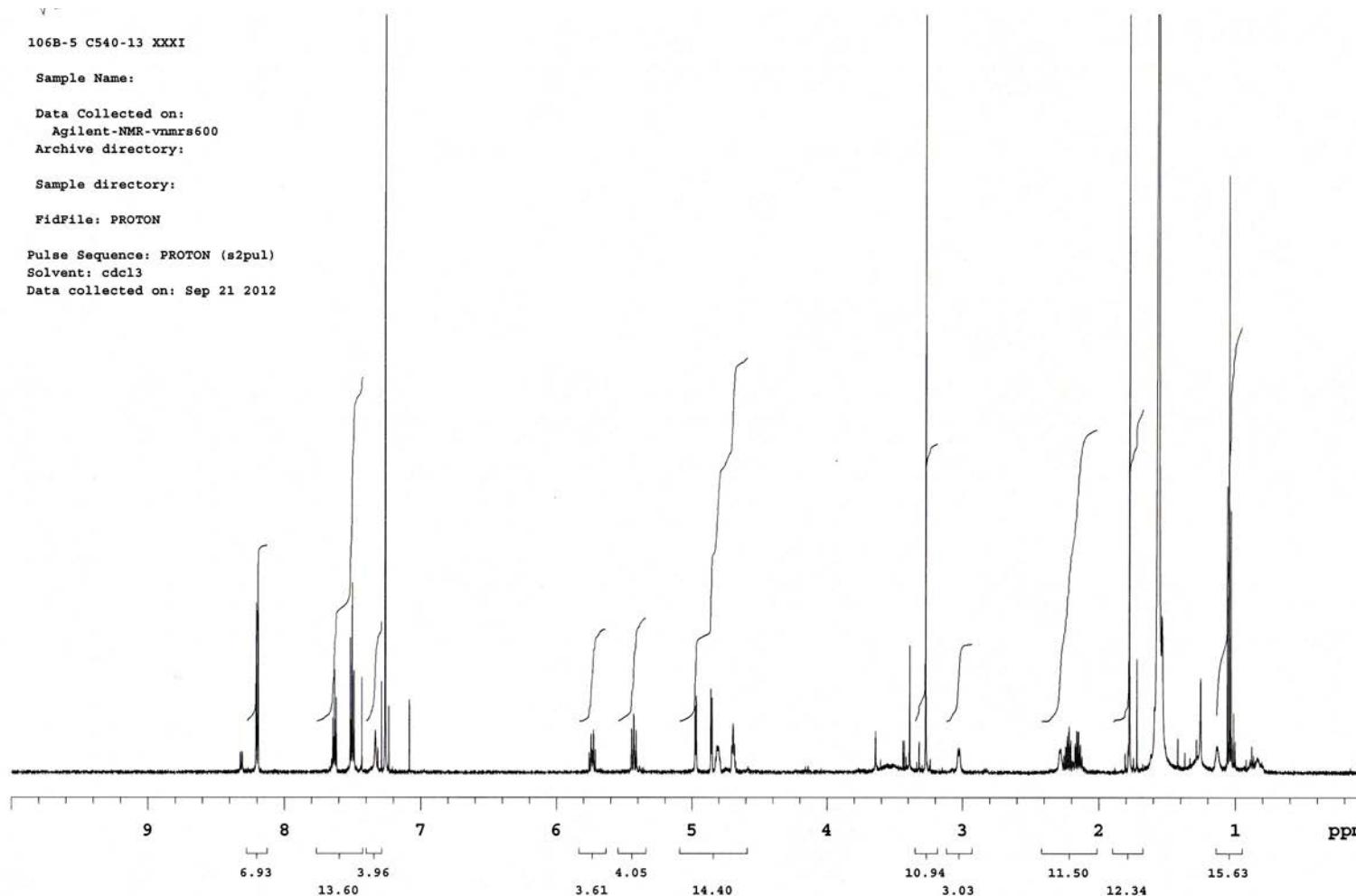


Figure S11. ^1H NMR spectrum in CDCl_3 of **5** (8-epimer of **3**).

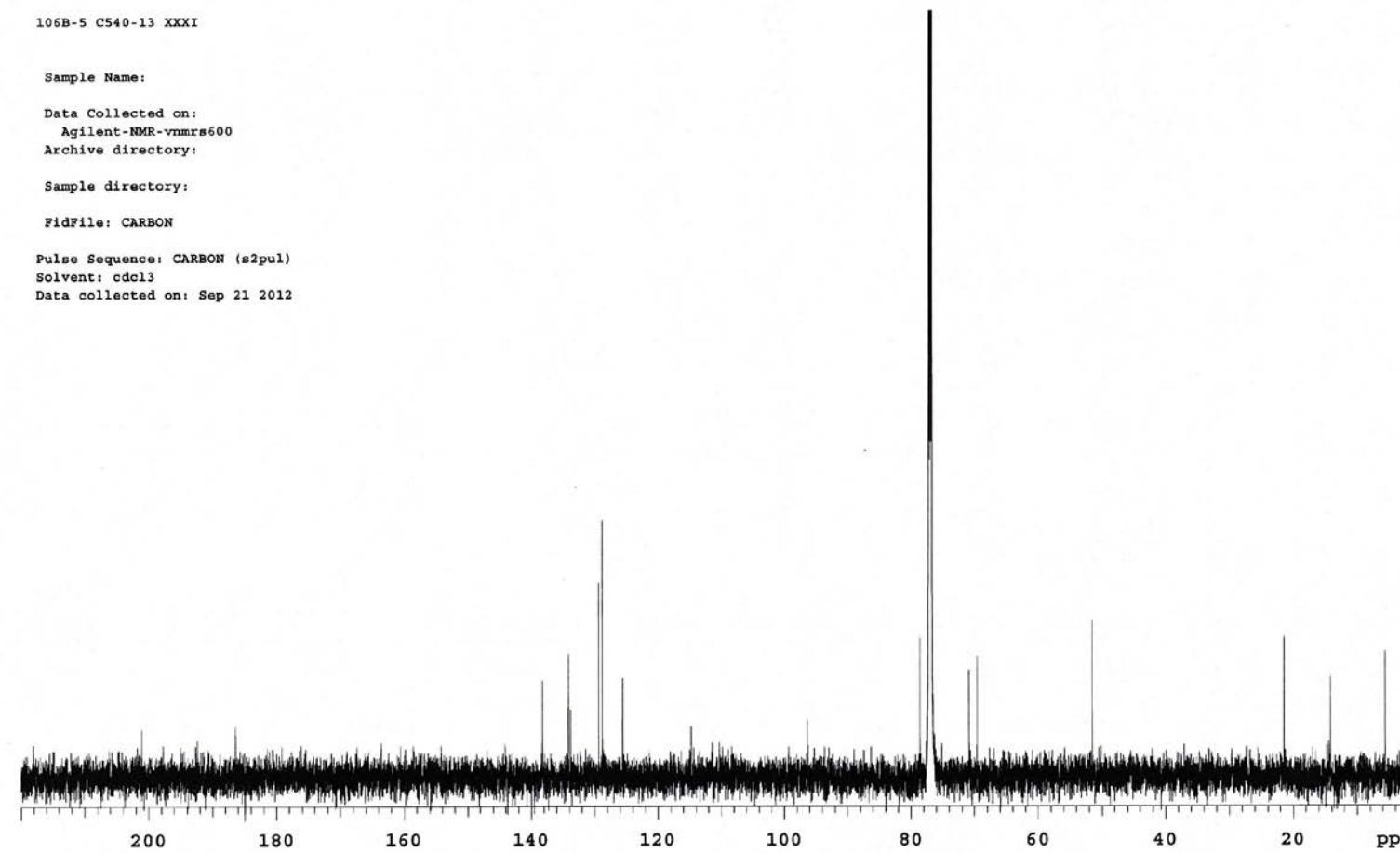


Figure S12. ^{13}C NMR spectrum in CDCl_3 of **5** (8-epimer of **3**).

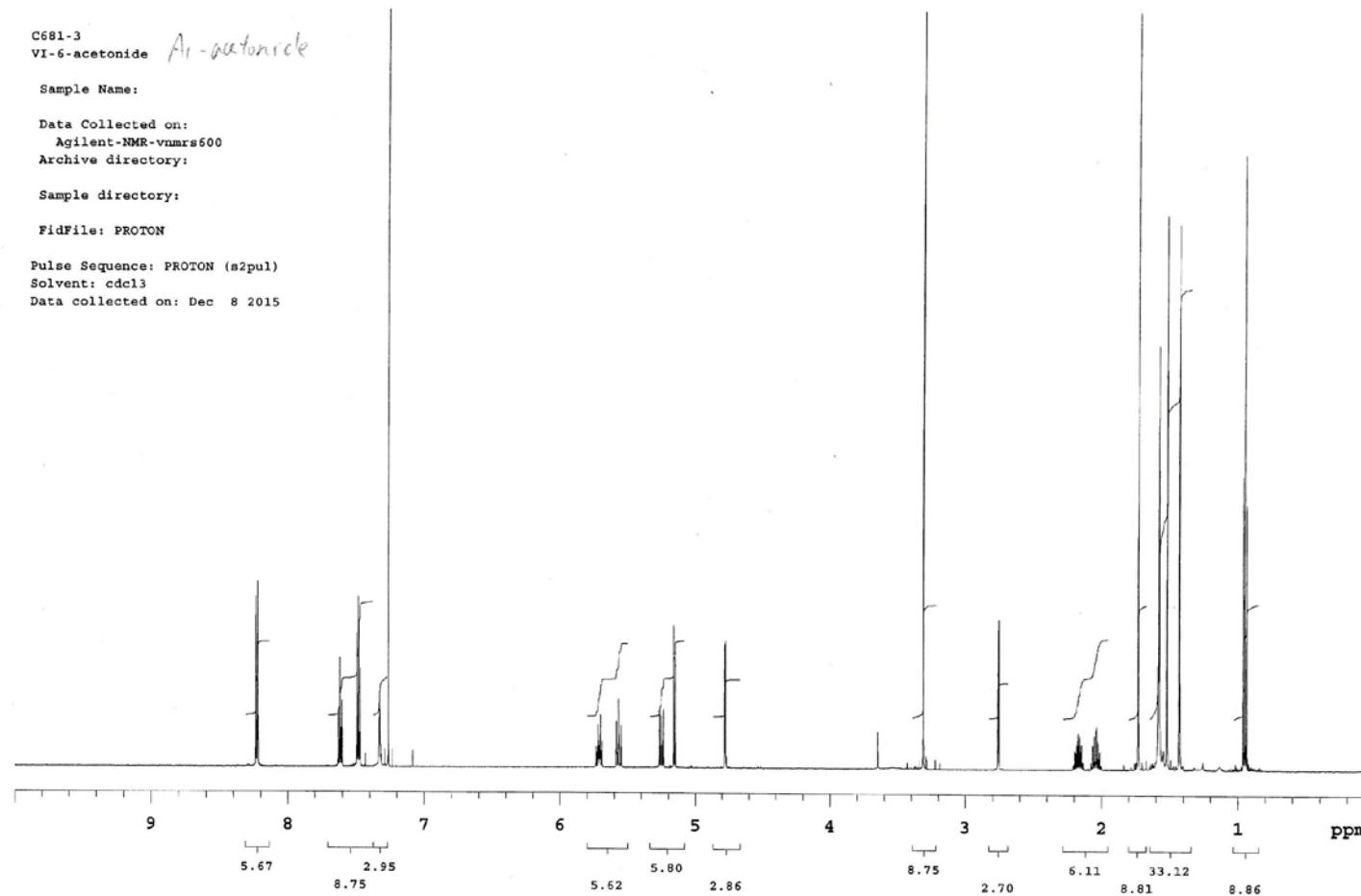


Figure S13. ^1H NMR spectrum in CDCl_3 of **6** (acetonide of **1**).

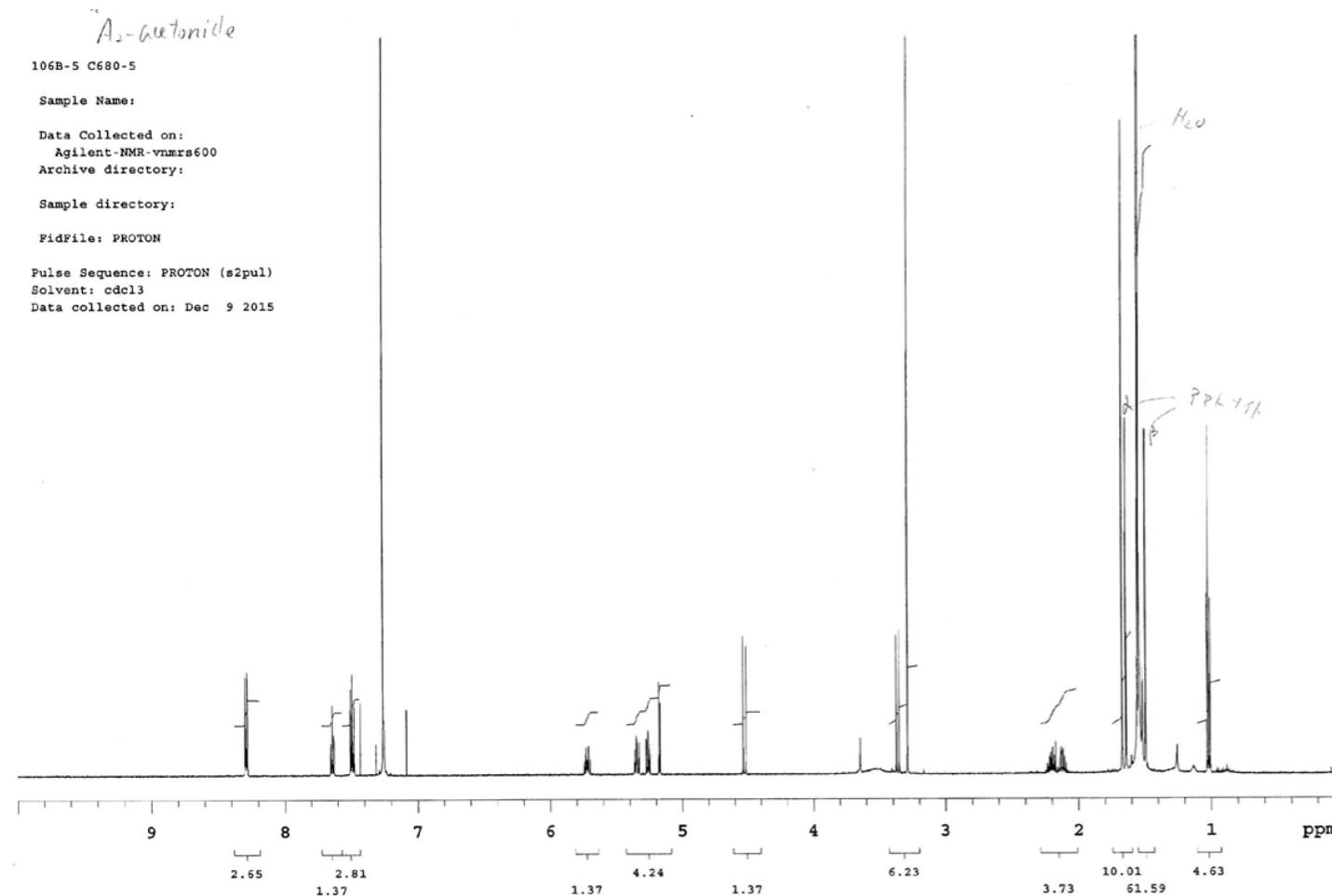


Figure S14. ^1H NMR spectrum in CDCl_3 of 7 (acetonide of 4).

C681-3
VI-6-acetonide
exp43 NOESY

SAMPLE FLAGS
date Dec 8 2015 hc nn
solvent cdc13 esql y
sample PFG12g y
ACQUISITION basql 6120
sw 5387.9 SPECIAL
st 0.150 temp not used
np 1616 gain 52
tb 4000 spin 0
ss 32 F2 PROCESSING
di 1.300 gf 0.060
nt 16 gfs not used
2D ACQUISITION fn 2048
sw1 5387.9 F1 PROCESSING
ni 256 gfs 0.030
TRANSMITTER Hz proc1 1p
tr 599.898 f1l 2048
sfreq -424.0 DISPLAY
tppr 58 sp 354.5
pw 9.600 wp 4862.8
NOESY 0.800 spl 349.2
mixN 0.800 wpl 4862.8
PRESATURATION rf1 119.1
satmode n rfp 0
wet n rf1l 119.1
DECOUPLER rf1l 0
dn C13 PLOT
ds nnn wc 200.0
sc 0
wc1 200.0
sc2 0
vs 508
th 2
ai cdc ph

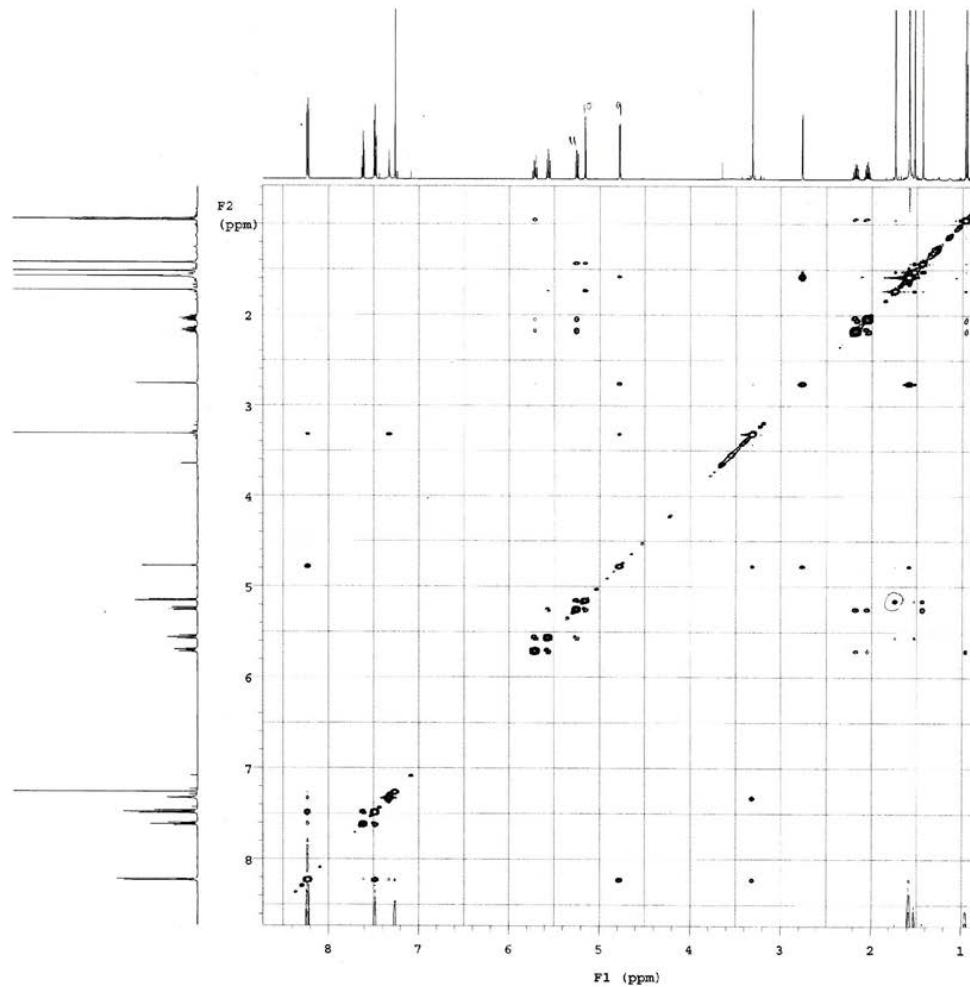


Figure S15. NOESY of **6** (acetonide of **1**).

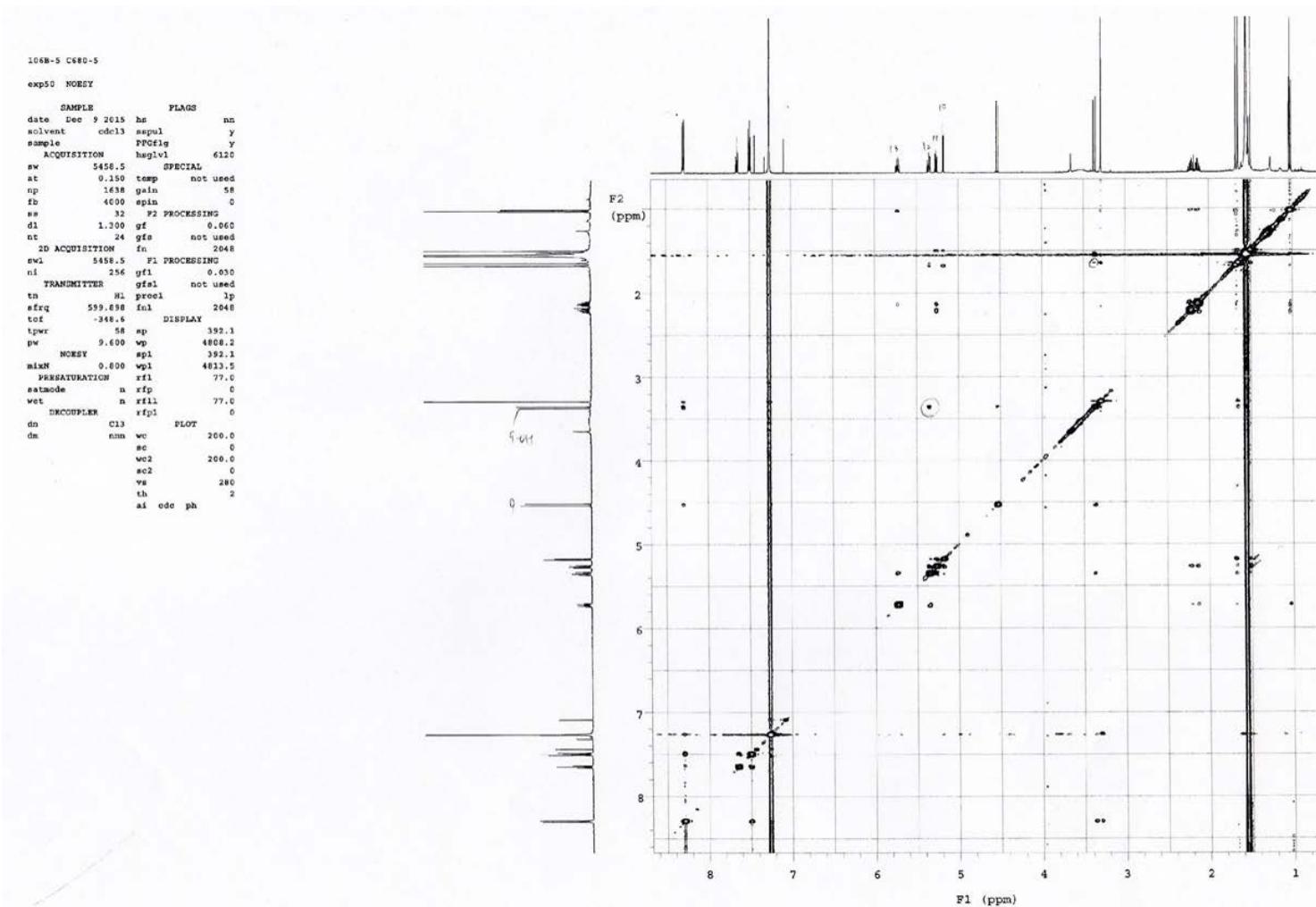


Figure S16. NOESY of 7 (acetonide of 4).