

Hypocoprins A-C: New Sesquiterpenoids from the Coprophilous

Fungus *Hypocopra rostrata* (Xylariales)

Dinith R. Jayanetti,[†] Qun Yue,[‡] Gerald F. Bills,[‡] and James B. Gloer^{*,†}

[†]Department of Chemistry, University of Iowa, Iowa City, IA 52242

[‡]Texas Therapeutics Institute, The Brown Foundation Institute of Molecular Medicine,

University of Texas Health Science Center at Houston, 1881 East Road, Houston, TX, 77054

List of Supporting Information

Figure S1. *Hypocopra rostrata* TTI-0009. A. Ascomata and mycelia pseudostroma on horse dung (Bar = 2 mm). B. Ascomata and mycelia pseudostroma on horse dung (Bar = 1 mm). C. Conidiomata on horse dung (Bar = 5 mm). D. Conidia and conidiogenous cells (Bar = 10 μ m). E. Ascospores (bar = 20 μ m). F. Ascomata and conidiomata on malt yeast extract agar (Bar = 1 cm).

Figure S2. Consensus neighbor-joining analysis of the ITS rDNA region selected fungi of the Xylariaceae. Numbers at branch points indicate bootstrap support percentages. *Hypocopra rostrata* TTI-0009 is indicated in red. *Daldinia* species were designated as the outgroup.

Figure S3. ¹H NMR Spectrum of Hypocoprin A (**1**, 400 MHz, CDCl₃)

Figure S4. ¹H NMR Spectrum of Hypocoprin A (**1**, 400 MHz, Acetone-*d*₆)

Figure S5. ¹³C NMR Spectrum of Hypocoprin A (**1**, 100 MHz, Acetone-*d*₆)

Figure S6. COSY Spectrum of Hypocoprin A (**1**, 600 MHz, Acetone-*d*₆)

Figure S7. HSQC Spectrum of Hypocoprin A (**1**, 600 MHz, Acetone-*d*₆)

Figure S8. HMBC Spectrum of Hypocoprin A (**1**, 600 MHz, Acetone-*d*₆)

Figure S9. COSY Spectrum of Hypocoprin A (**1**, 600 MHz, Acetone-*d*₆)

Figure S10. ^1H NMR Spectrum of Hypocoprin B (**2**, 400 MHz, CDCl_3)

Figure S11. ^1H NMR Spectrum of Hypocoprin C (**3**, 400 MHz, Acetone- d_6)

Figure S12. ^{13}C NMR Spectrum of Hypocoprin C (**3**, 100 MHz, Acetone- d_6)

Figure S13. Observed chemical shift differences ($\Delta\delta = \delta_S - \delta_R$, ppm; 400 MHz) for the *R*- and *S*-MTPA esters of **1**. Only H's affording notable $\Delta\delta$ values are labelled.

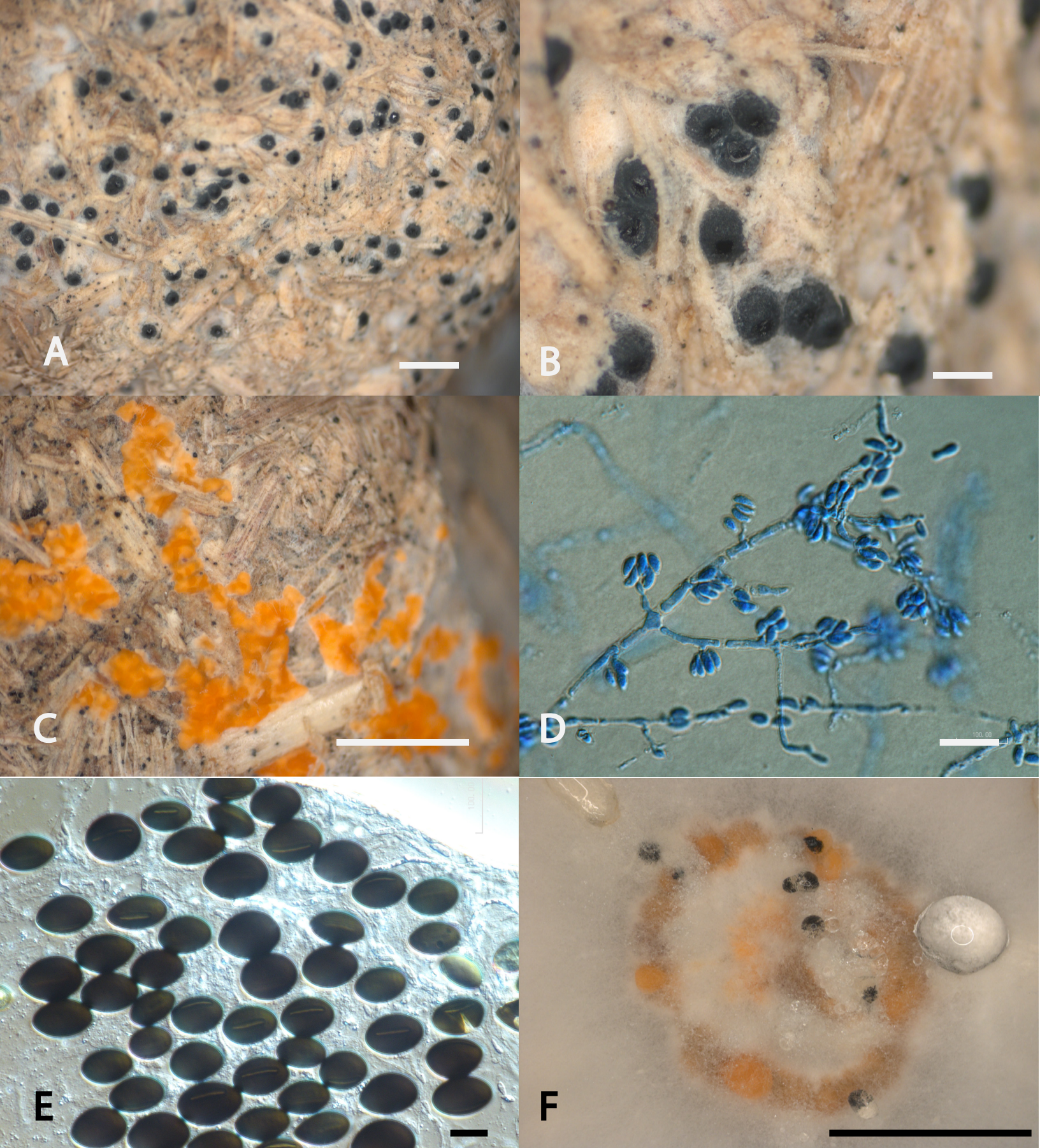


Figure S1. *Hypocopa rostrata* TTI-0009. A. Ascomata and mycelia pseudostroma on horse dung (Bar = 2 mm). B. Ascomata and mycelia pseudostroma on horse dung (Bar = 1 mm). C. Conidiomata on horse dung (Bar = 5 mm). D. Conidia and conidiogenous cells (Bar = 10 μ m). E. Ascospores (bar = 20 μ m). F. Ascomata and conidiomata on malt yeast extract agar (Bar = 1 cm)

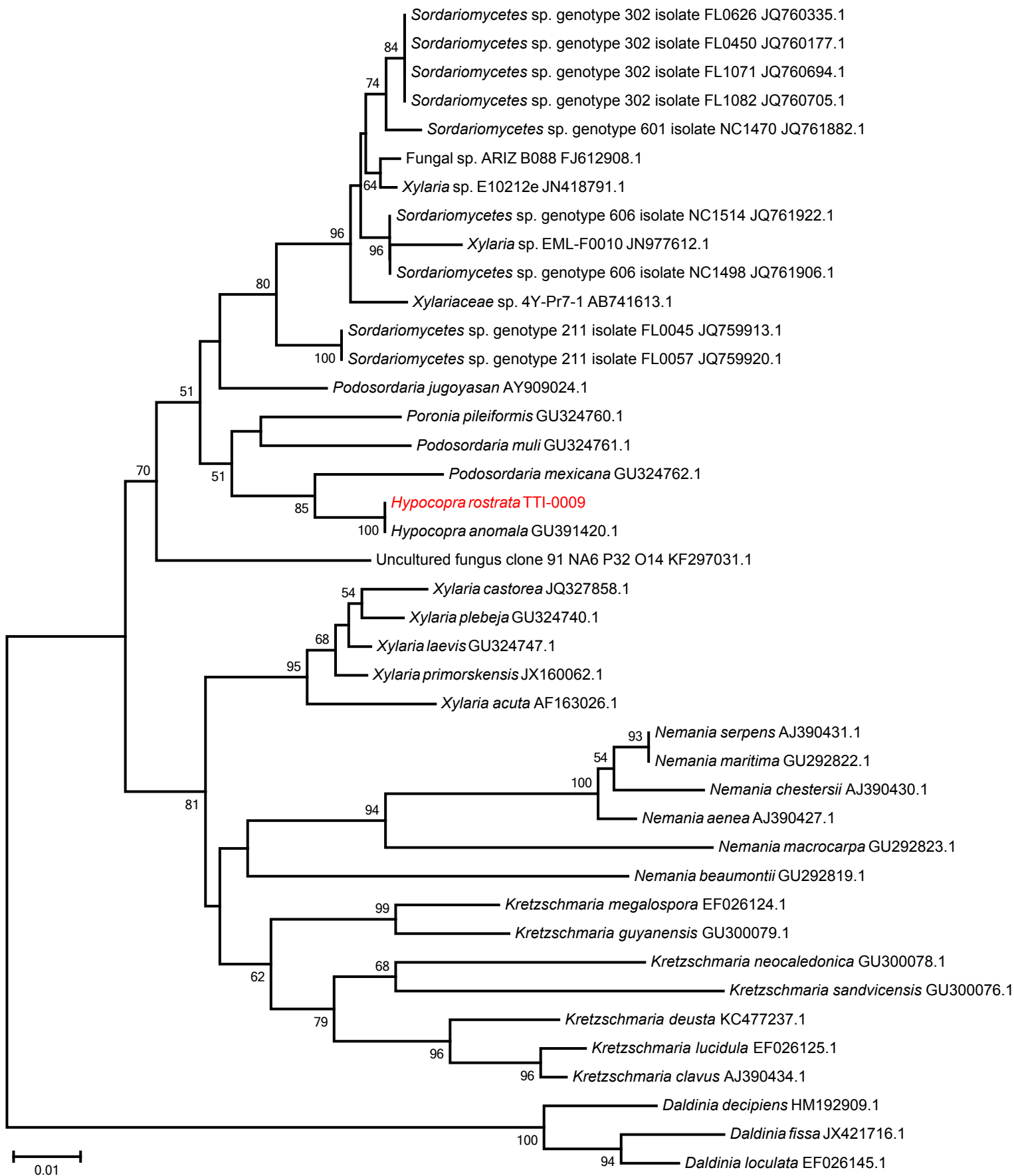


Figure S2. Consensus neighbor-joining analysis of the ITS rDNA region selected fungi of the Xylariaceae. Numbers at branch points indicate bootstrap support percentages. *Hypocopa rostrata* TTI-0009 is indicated in red. *Daldinia* species were designated as the outgroup.

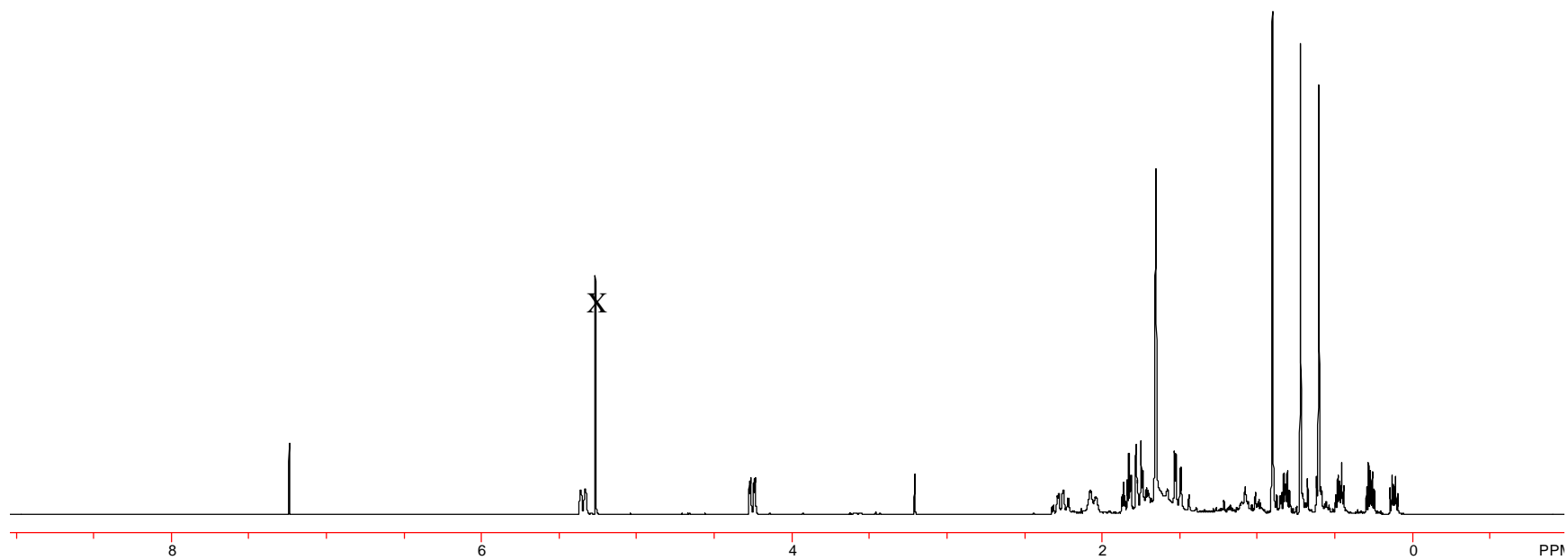


Figure S3. ^1H NMR Spectrum of Hypocoprin A (1, 400 MHz, CDCl_3)

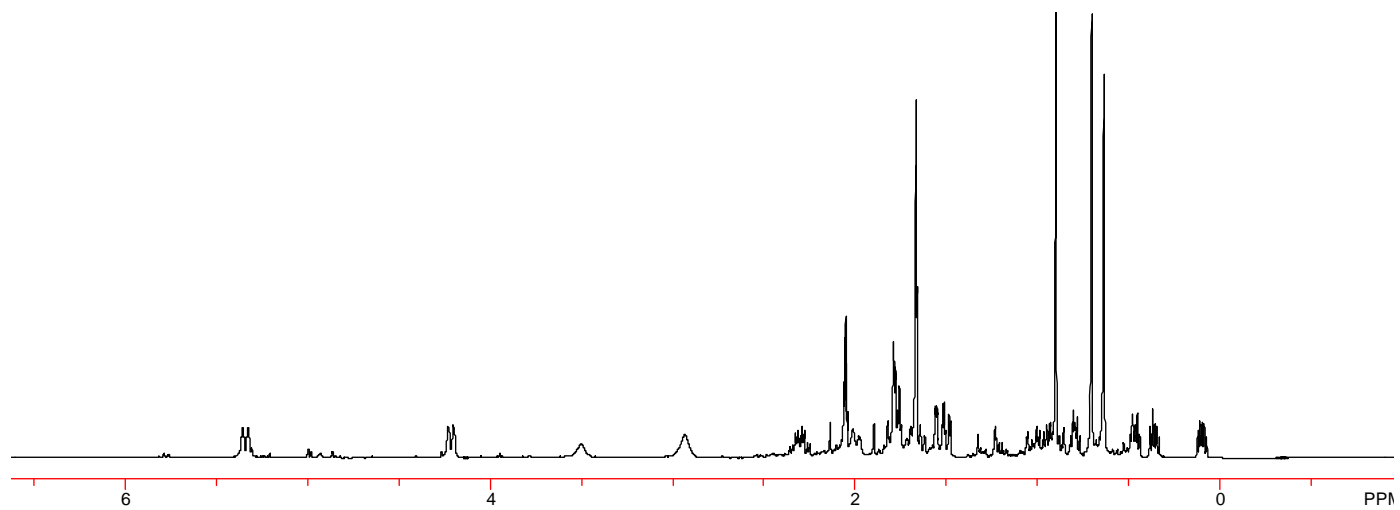


Figure S4. ^1H NMR Spectrum of Hypocoprins A (**1**, 400 MHz, $\text{Acetone-}d_6$)

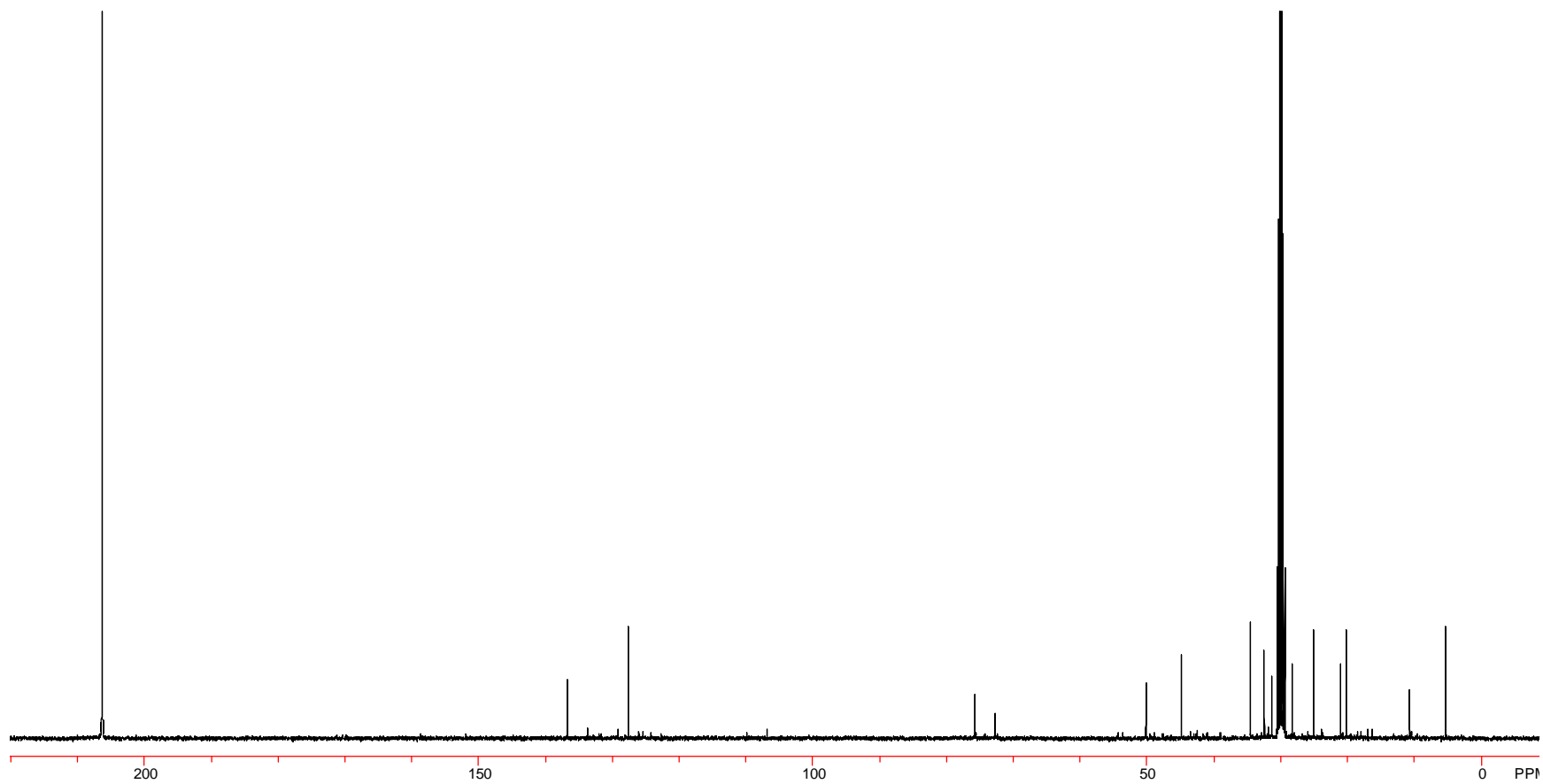


Figure S5. ^{13}C NMR Spectrum of Hypocoprin A (**1**, 100 MHz, Acetone- d_6)

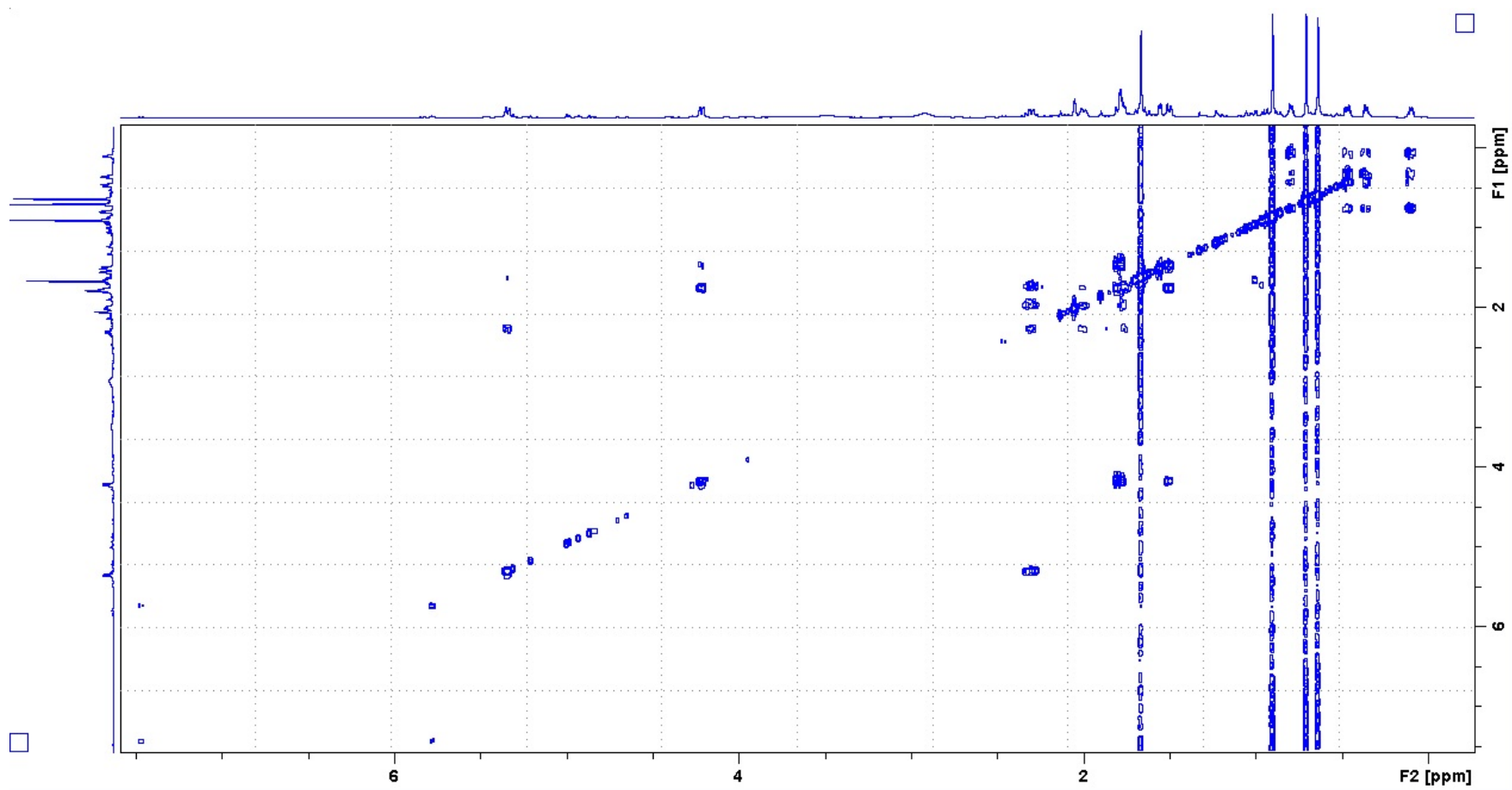


Figure S6. COSY Spectrum of Hypocypin A (**1**, 600 MHz, Acetone-*d*₆)

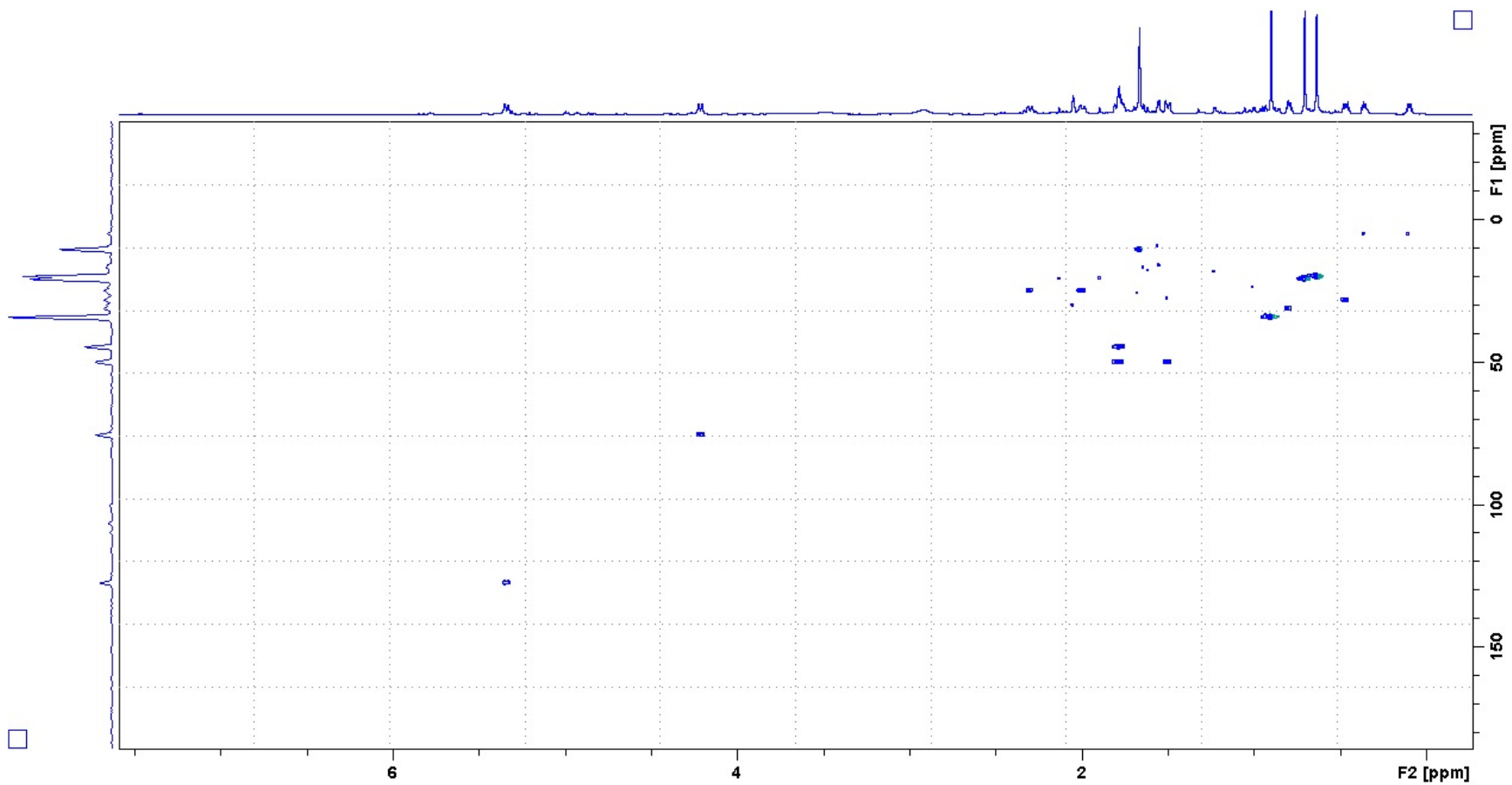


Figure S7. HSQC Spectrum of Hypocopin A (**1**, 600 MHz, Acetone- d_6)

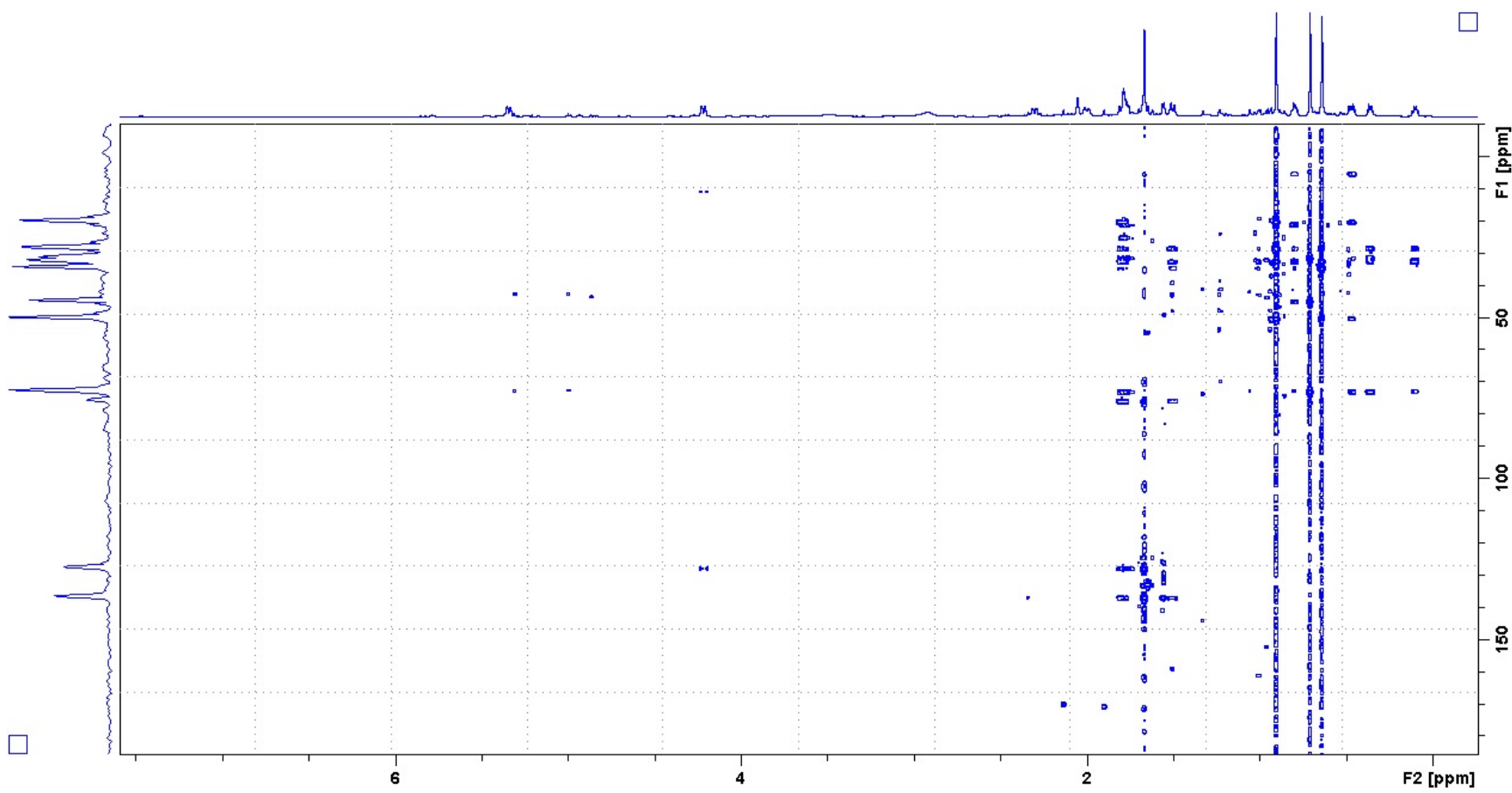


Figure S8. HMBC Spectrum of Hypocopin A (**1**, 600 MHz, Acetone- d_6)

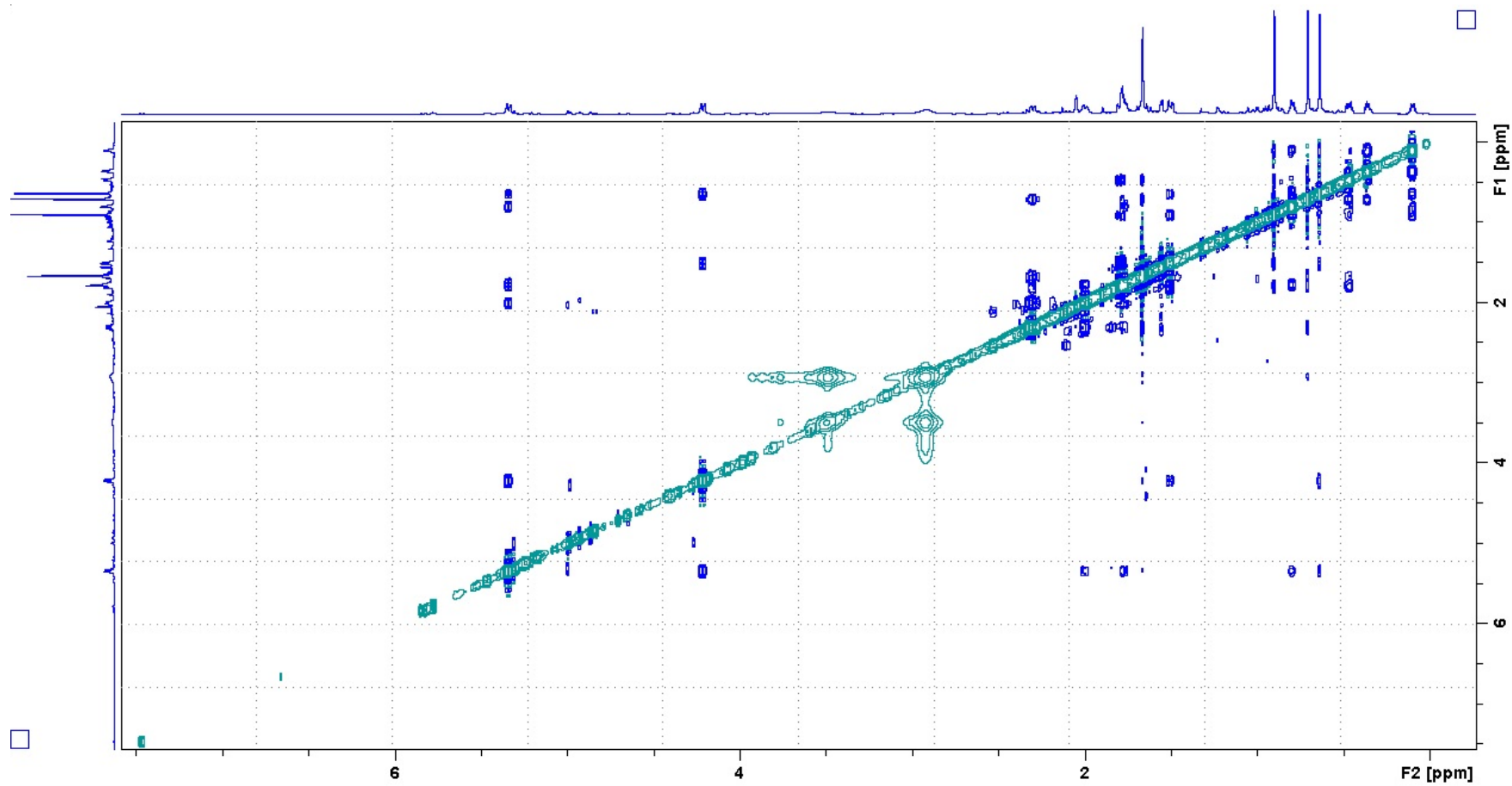


Figure S9. NOESY Spectrum of Hypocoprins A (1, 600 MHz, Acetone-*d*₆)

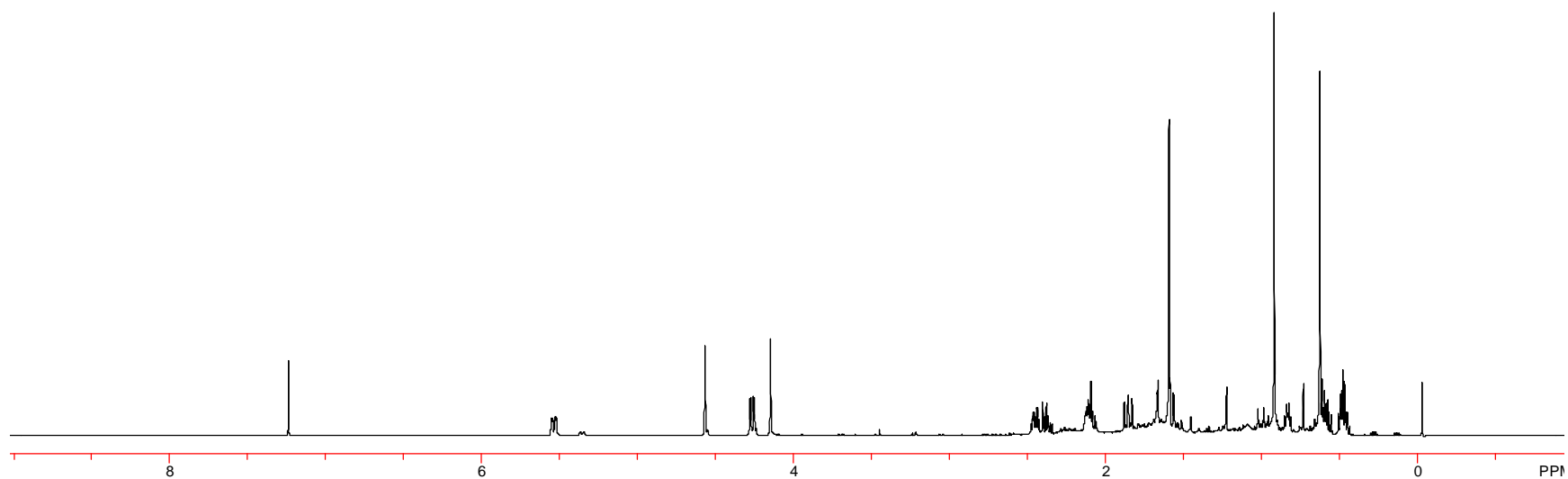


Figure S10. ¹H NMR Spectrum of Hypocoprin B (2, 500 MHz, CDCl₃)

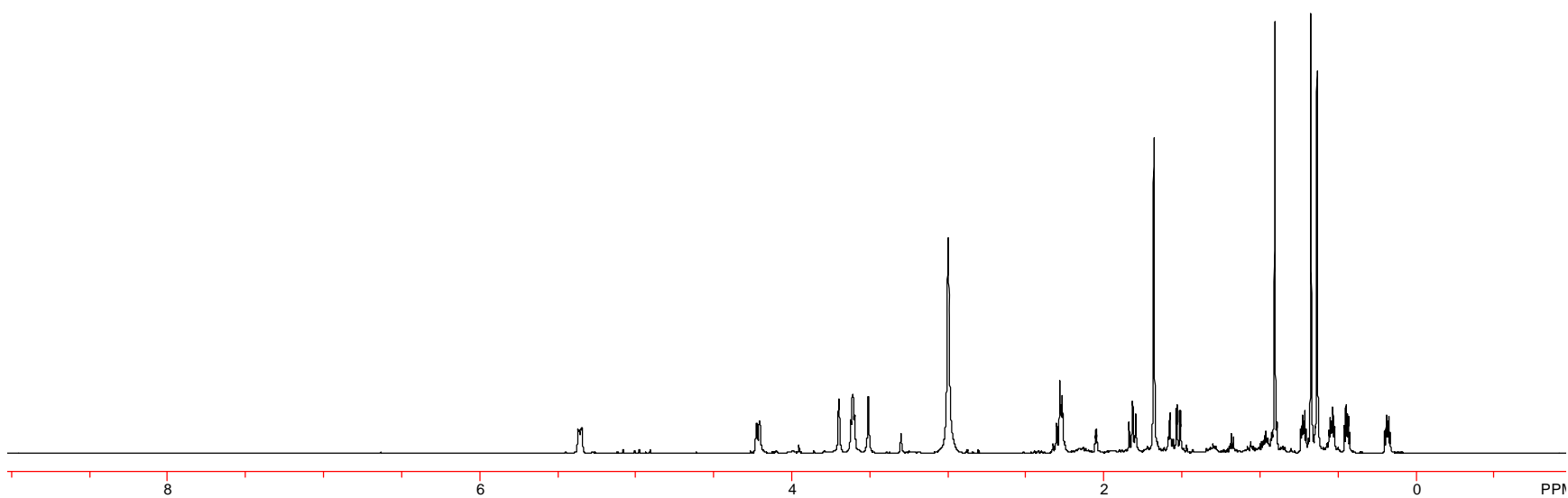


Figure S11. ^1H NMR Spectrum of Hypocopin C (**3**, 400 MHz, Acetone- d_6)

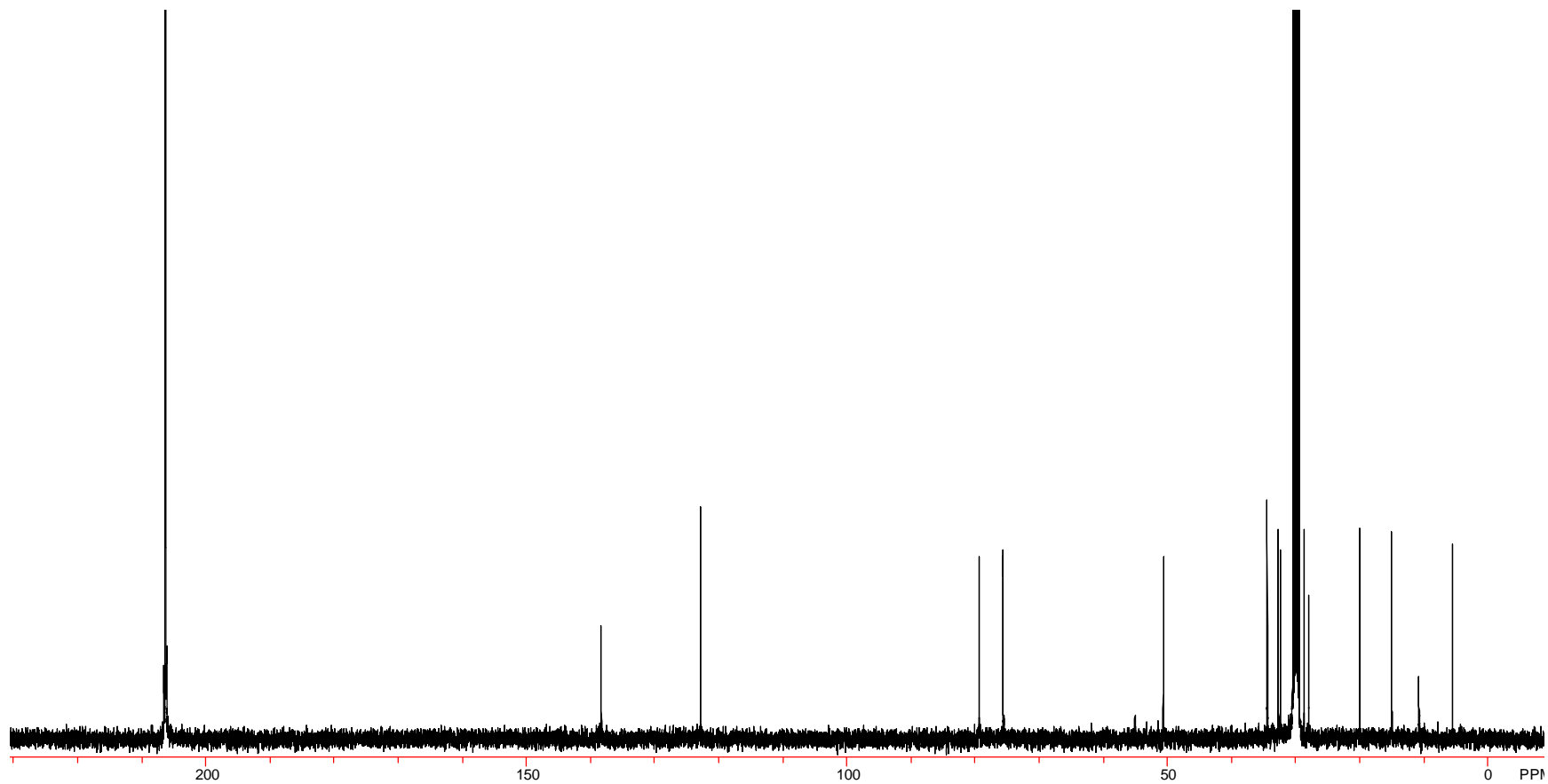


Figure S12. ^{13}C NMR Spectrum of Hypocoprin C (**3**, 100 MHz, $\text{Acetone-}d_6$)

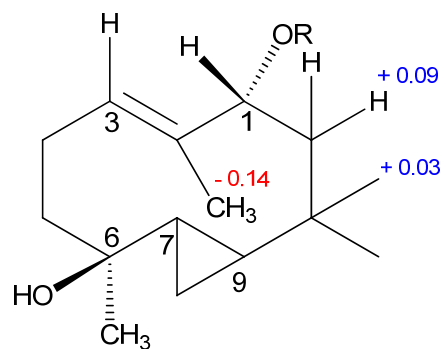


Figure S13. Observed chemical shift differences ($\Delta\delta = \delta_S - \delta_R$, ppm; 400 MHz) for the *R*- and *S*-MTPA esters of **1**. Only H's affording notable $\Delta\delta$ values are labelled.