

Supporting Information

for

A cyclopeptide and three oligomycin-class polyketides produced by an underexplored actinomycete of the genus *Pseudosporangium*

Shun Saito, Kota Atsumi, Tao Zhou, Keisuke Fukaya, Daisuke Urabe, Naoya Oku, Md. Rokon Ul Karim, Hisayuki Komaki and Yasuhiro Igarashi

Beilstein J. Org. Chem. 2020, 16, 1100-1110. doi:10.3762/bjoc.16.97

Copies of NMR spectra for compounds 1-4

Table of contents

Figure S1. ¹ H NMR spectrum of pseudosporamide (1) (500 MHz, DMSO- <i>d</i> ₆)	S3
Figure S2. 13 C NMR spectrum of 1 (125 MHz, DMSO- d_6)	S4
Figure S3. DEPT135 spectrum of 1 (125 MHz, DMSO- d_6)	S5
Figure S4. ¹ H- ¹ H COSY spectrum of 1 (500 MHz, DMSO- <i>d</i> ₆)	S 6
Figure S5. HSQC spectrum of 1 (500 MHz, DMSO-d ₆)	S 7
Figure S6. HMBC spectrum of 1 (500 MHz, DMSO-d ₆)	S8
Figure S7. ROESY spectrum of 1 (500 MHz, DMSO- d_6)	S 9
Figure S8. HPLC chromatogram of hydrolysate from 1 and comparison to standa	rd amino
acids, derivatized with Marfey's reagent (FDLA)	S10
Figure S9. ¹ H NMR spectrum of 5a (500 MHz, DMSO- <i>d</i> ₆)	S11
Figure S10. ¹ H- ¹ H COSY spectrum of 5a (500 MHz, DMSO- <i>d</i> ₆)	S12
Figure S11. ¹ H NMR spectrum of 5b (500 MHz, DMSO- <i>d</i> ₆)	S13
Figure S12. ¹ H- ¹ H COSY spectrum of 5b (500 MHz, DMSO- <i>d</i> ₆)	S14
Figure S13. ¹ H NMR spectrum of pseudosporamicin A (2) (500 MHz, CDCl ₃)	S15
Figure S14. ¹³ C NMR spectrum of 2 (125 MHz, CDCl ₃)	S16
Figure S15. ¹ H- ¹ H COSY spectrum of 2 (500 MHz, CDCl ₃)	S17
Figure S16. HSQC spectrum of 2 (500 MHz, CDCl ₃)	S18
Figure S17. HMBC spectrum of 2 (500 MHz, CDCl ₃)	S19
Figure S18. NOESY spectrum of 2 (500 MHz, CDCl ₃)	S20
Figure S19. ¹ H NMR spectrum of pseudosporamicin B (3) (500 MHz, CDCl ₃)	S21
Figure S20. ¹³ C NMR spectrum of 3 (125 MHz, CDCl ₃)	S22
Figure S21. ¹ H- ¹ H COSY spectrum of 3 (500 MHz, CDCl ₃)	S23
Figure S22. HSQC spectrum of 3 (500 MHz, CDCl ₃)	S24
Figure S23. HMBC spectrum of 3 (500 MHz, CDCl ₃)	S25
Figure S24. NOESY spectrum of 3 (500 MHz, CDCl ₃)	S26
Figure S25. ¹ H NMR spectrum of pseudosporamicin C (4) (500 MHz, CDCl ₃)	S27
Figure S26. ¹³ C NMR spectrum of 4 (125 MHz, CDCl ₃)	S28
Figure S27. ¹ H- ¹ H COSY spectrum of 4 (500 MHz, CDCl ₃)	S29
Figure S28. HSQC spectrum of 4 (500 MHz, CDCl ₃)	S30
Figure S29. HMBC spectrum of 4 (500 MHz, CDCl ₃)	S31
Figure S30. NOESY spectrum of 4 (500 MHz, CDCl ₃)	S32
Figure S31. COSY, key HMBC and NOESY correlations of 3 and 4	S33

Figure S1. ¹H NMR spectrum of pseudosporamide (1) (500 MHz, DMSO-*d*₆).

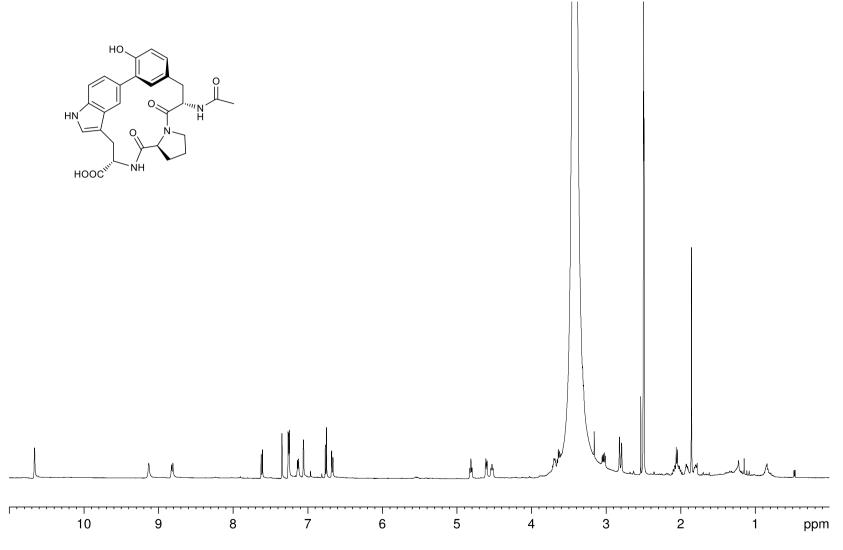


Figure S2. 13 C NMR spectrum of **1** (125 MHz, DMSO- d_6).

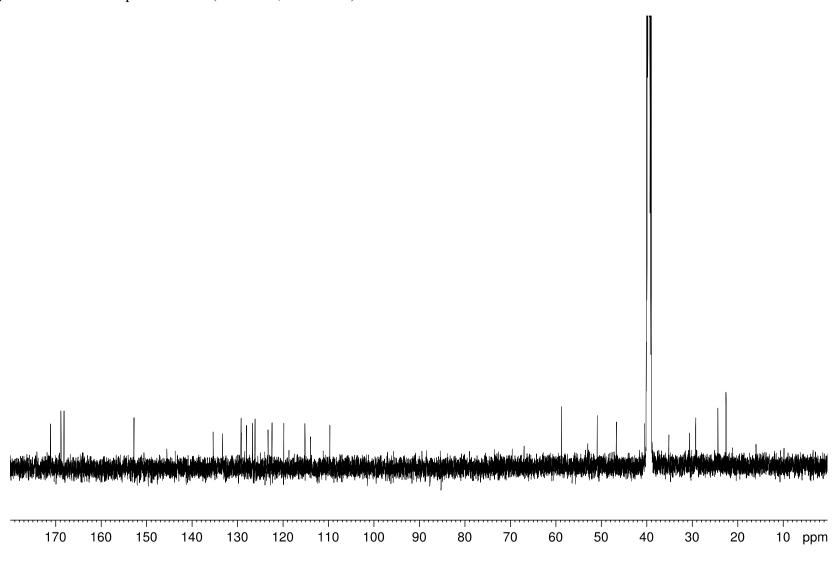


Figure S3. DEPT135 spectrum of **1** (125 MHz, DMSO- d_6).

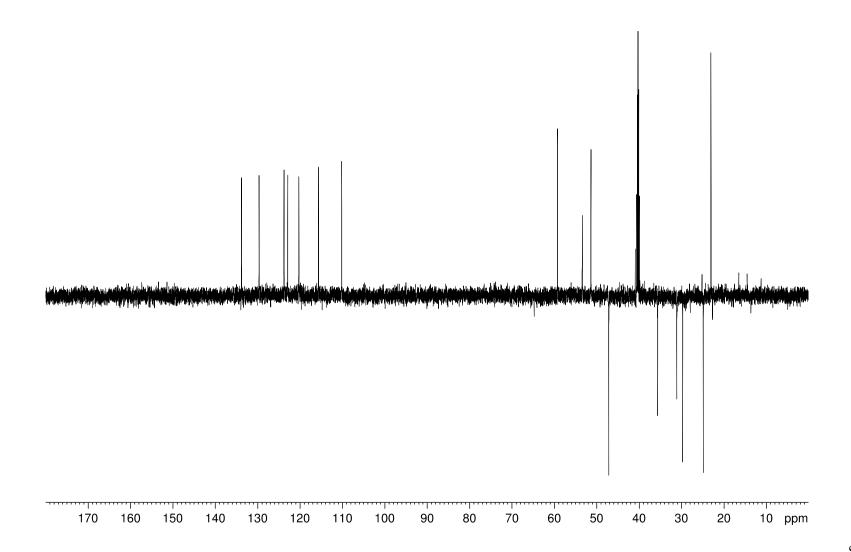


Figure S4. $^{1}\text{H}-^{1}\text{H COSY}$ spectrum of **1** (500 MHz, DMSO- d_{6}).

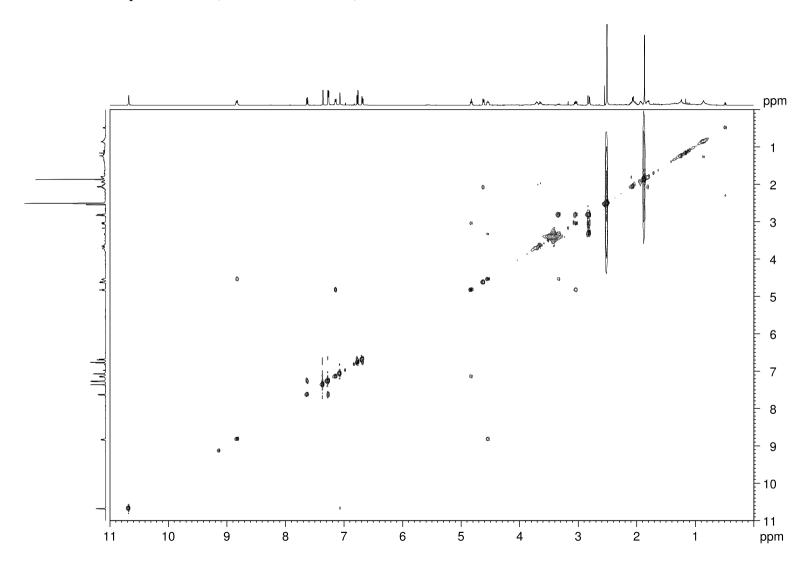


Figure S5. HSQC spectrum of **1** (500 MHz, DMSO-*d*₆).

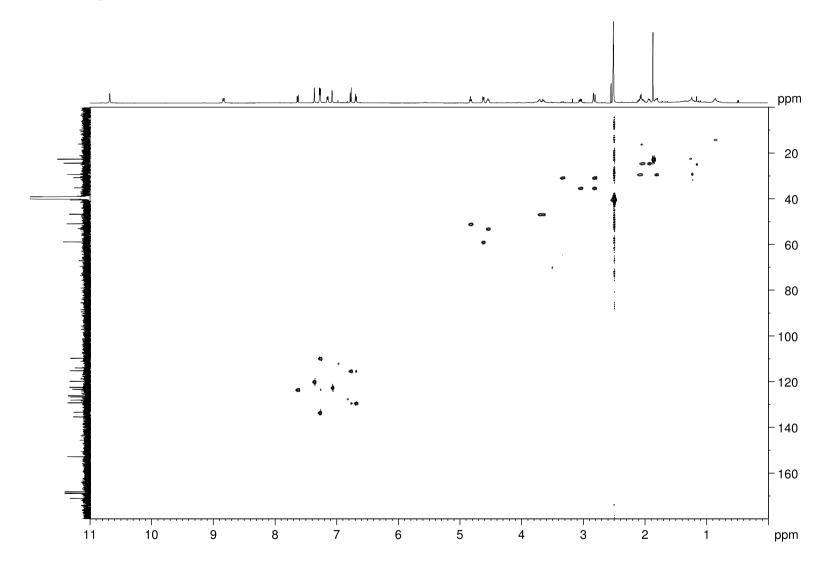


Figure S6. HMBC spectrum of **1** (500 MHz, DMSO-*d*₆).

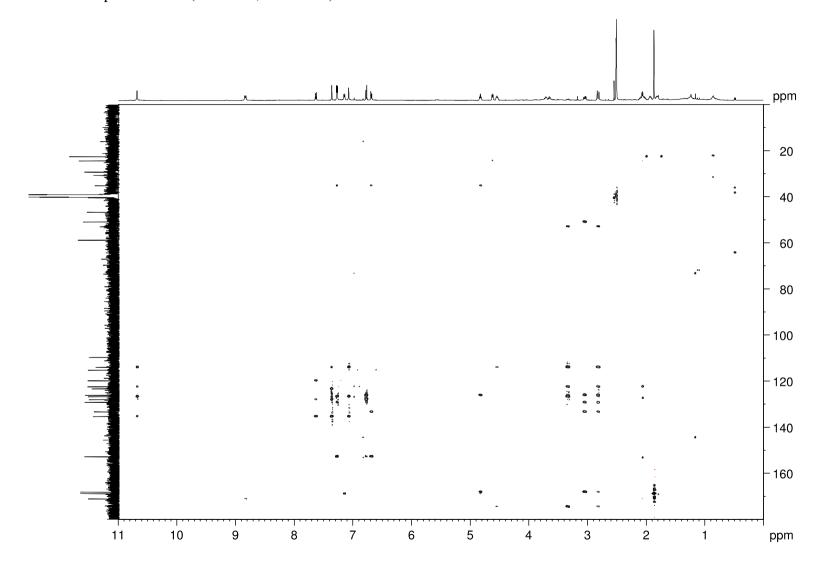
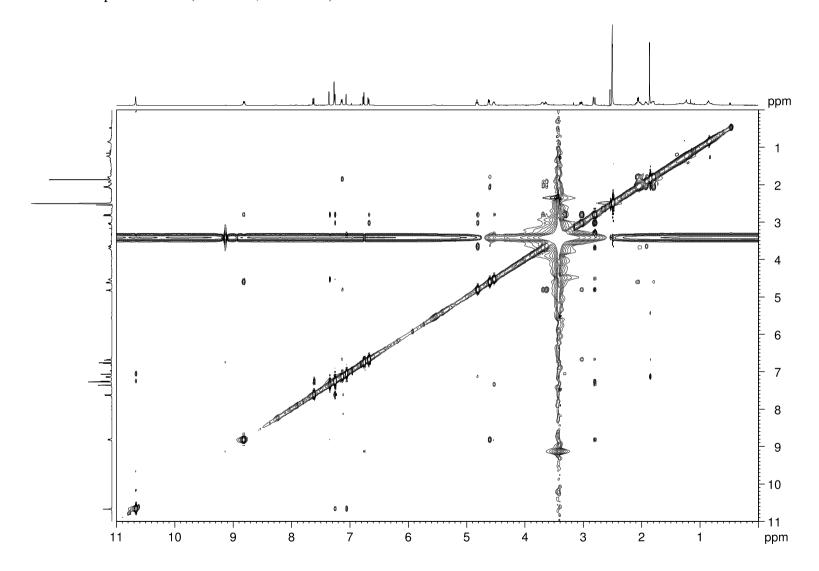


Figure S7. ROESY spectrum of 1 (500 MHz, DMSO-*d*₆).



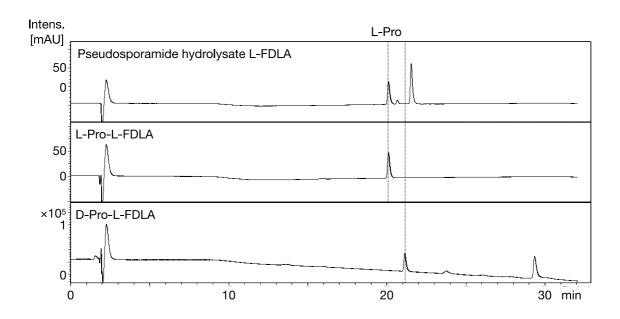


Figure S8. HPLC chromatogram of hydrolysate from **1** and comparison to standard amino acids, derivatized with Marfey's reagent (FDLA).

Column: Cosmosil AR-II (Nacalai Tesque, 4.6×250 mm)

Solvent: MeCN-0.1% HCO₂H

Gradient MeCN (%): 0-30 min: 15-80%, 30-35 min: 80%

Flow rate: 1.0 mL/min Absorbance: 340 nm

Figure S9. 1 H NMR spectrum of **5a** (500 MHz, DMSO- d_6).

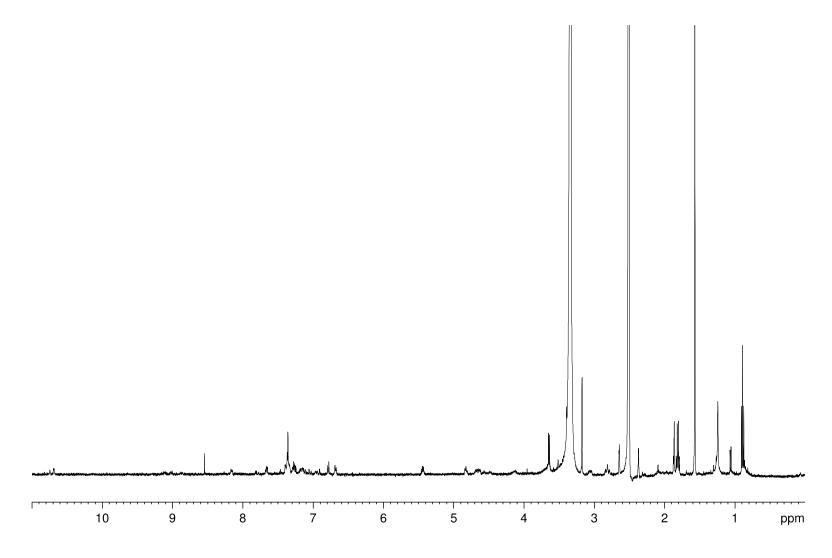


Figure S10. 1 H- 1 H COSY spectrum of **5a** (500 MHz, DMSO- d_6).

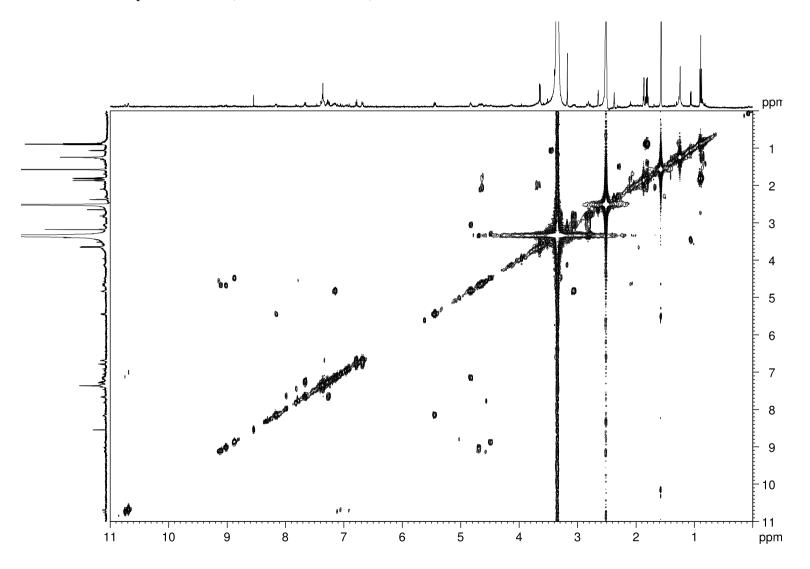


Figure S11. ¹H NMR spectrum of **5b** (500 MHz, DMSO-*d*₆).

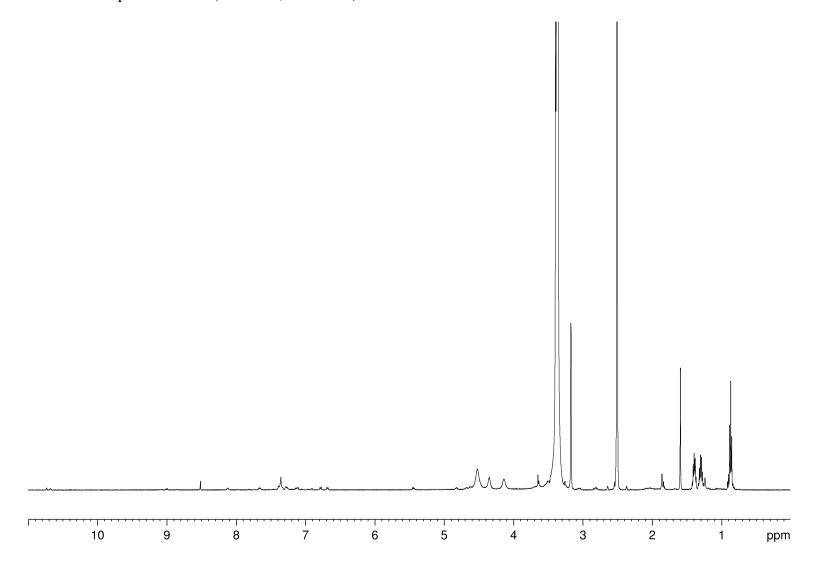


Figure S12. ¹H-¹H COSY spectrum of **5b** (500 MHz, DMSO-*d*₆).

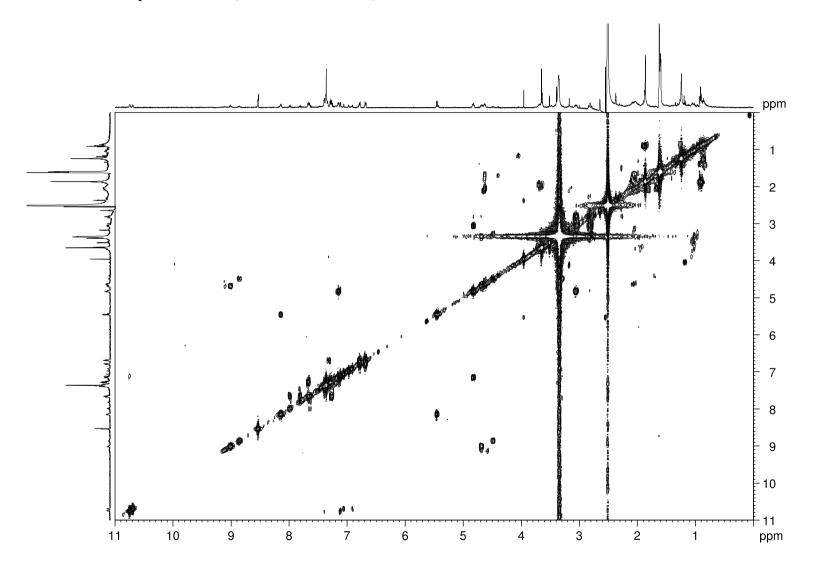


Figure S13. ¹H NMR spectrum of pseudosporamicin A (2) (500 MHz, CDCl₃).

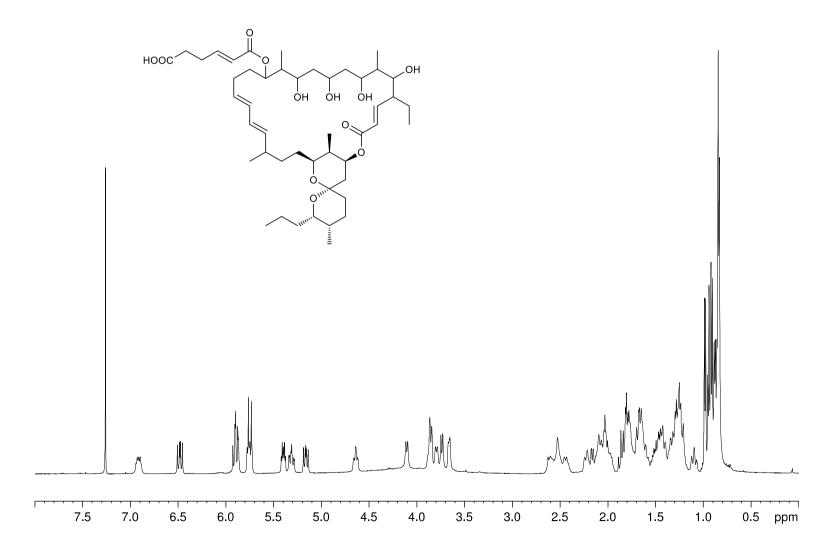


Figure S14. ¹³C NMR spectrum of 2 (125 MHz, CDCl₃).

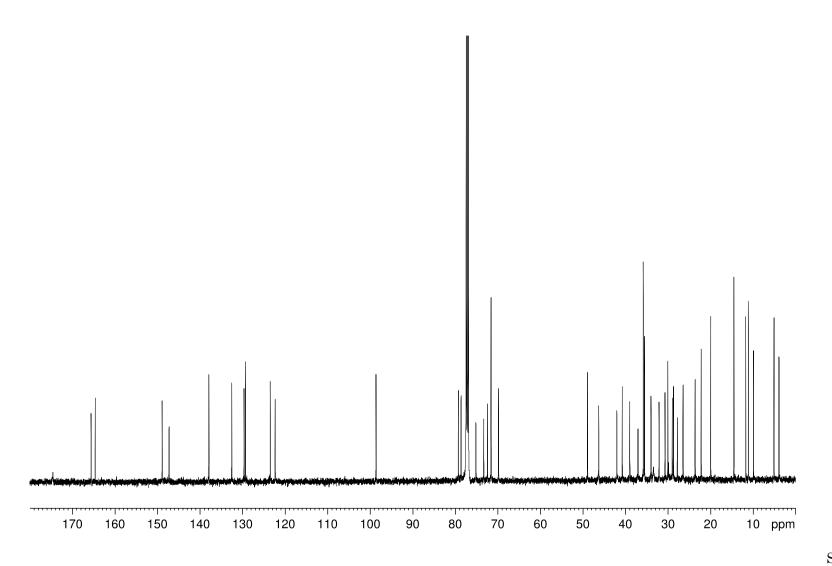


Figure S15. ¹H-¹H COSY spectrum of **2** (500 MHz, CDCl₃).

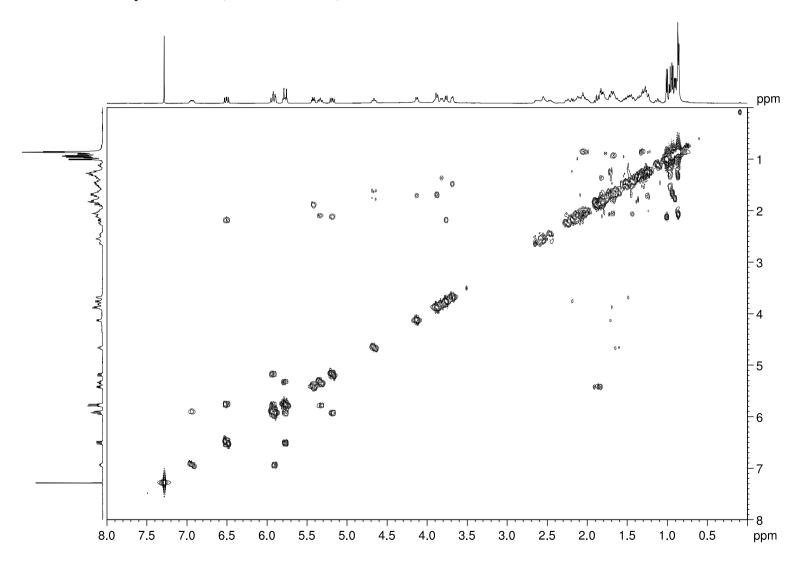


Figure S16. HSQC spectrum of **2** (500 MHz, CDCl₃).

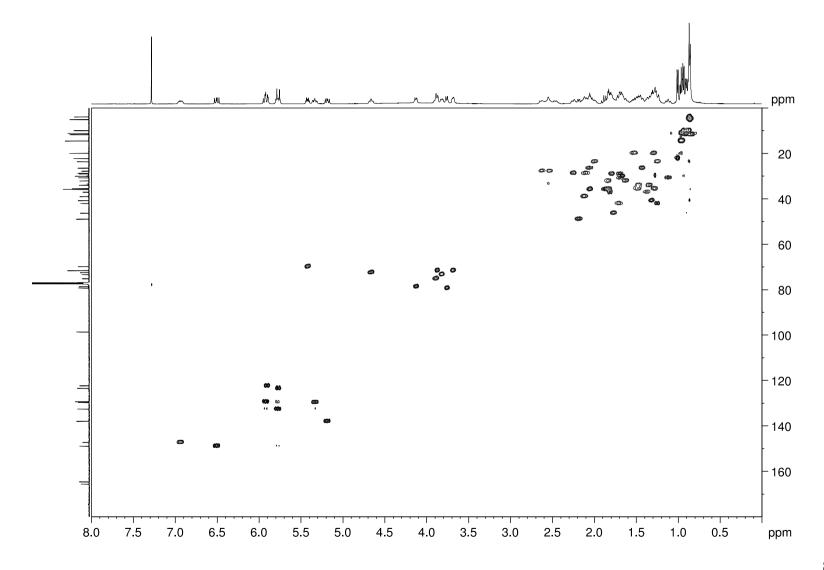


Figure S17. HMBC spectrum of 2 (500 MHz, CDCl₃).

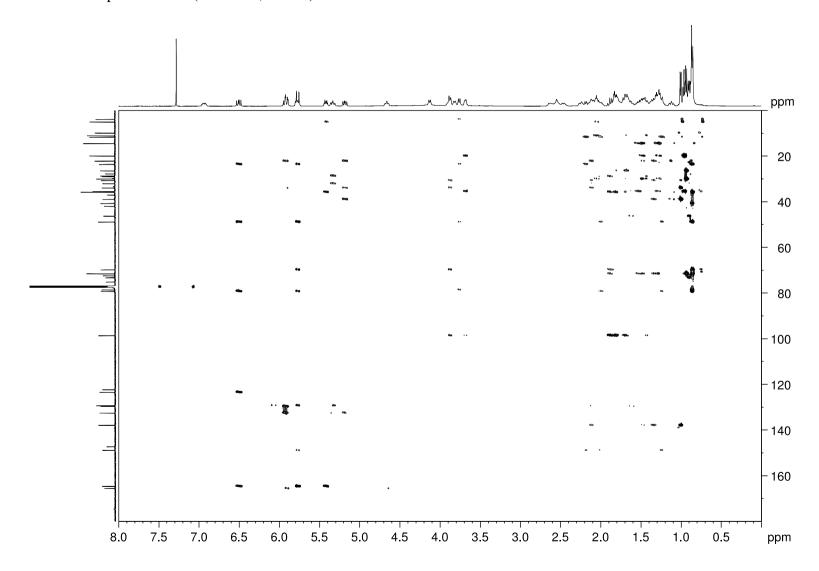


Figure S18. NOESY spectrum of 2 (500 MHz, CDCl₃).

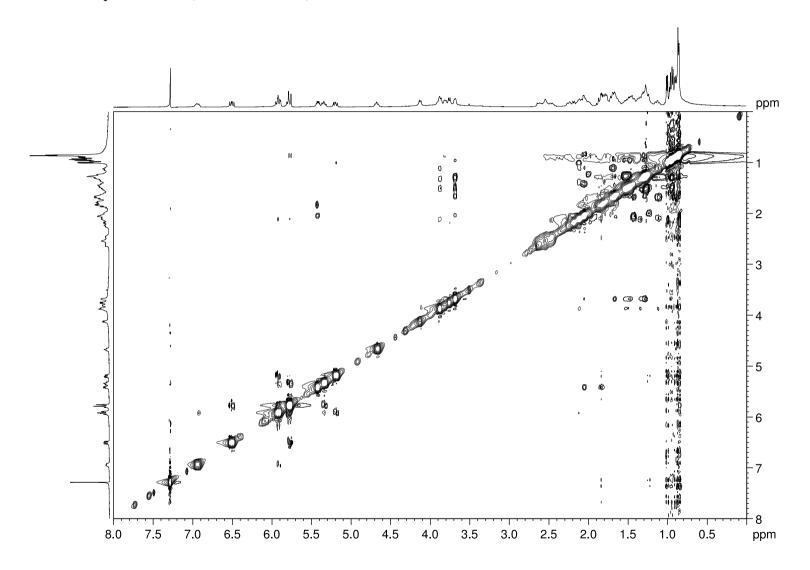


Figure S19. ¹H NMR spectrum of pseudosporamicin B (**3**) (500 MHz, CDCl₃).

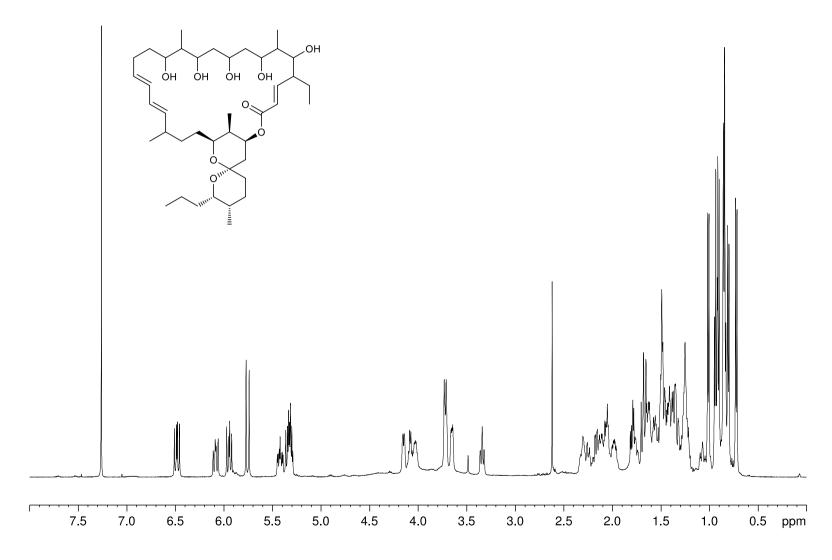


Figure S20. ¹³C NMR spectrum of 3 (125 MHz, CDCl₃).

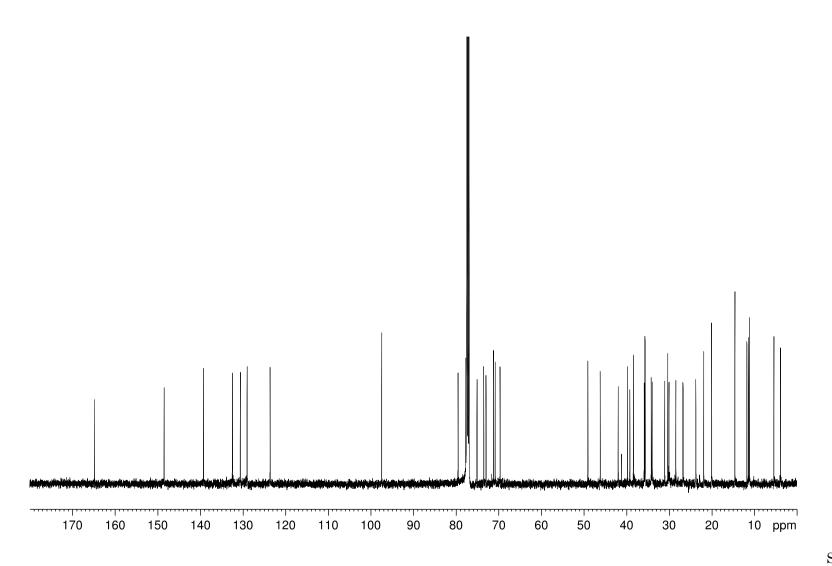


Figure S21. ¹H-¹H COSY spectrum of **3** (500 MHz, CDCl₃).

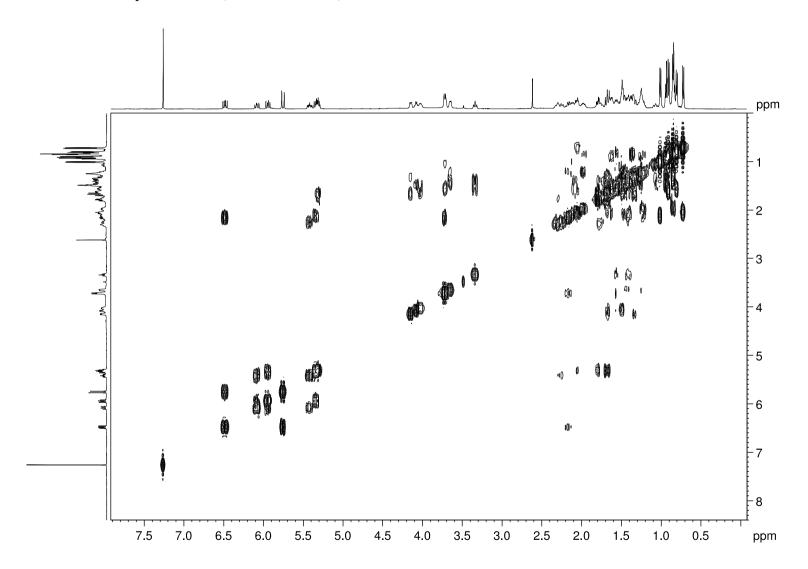


Figure S22. HSQC spectrum of 3 (500 MHz, CDCl₃).

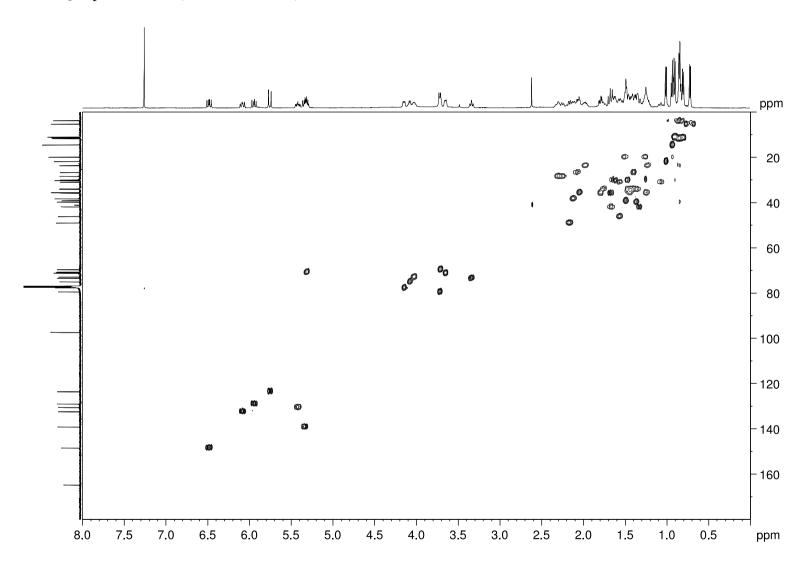


Figure S23. HMBC spectrum of 3 (500 MHz, CDCl₃).

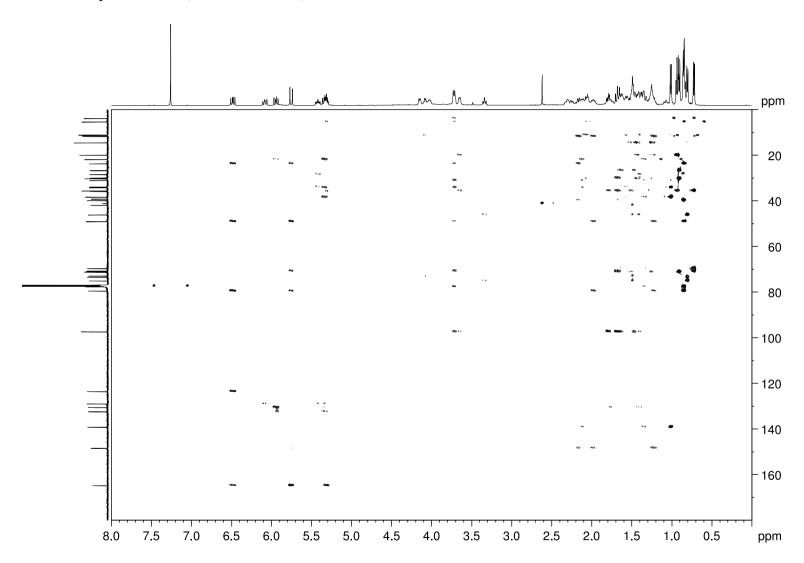


Figure S24. NOESY spectrum of 3 (500 MHz, CDCl₃).

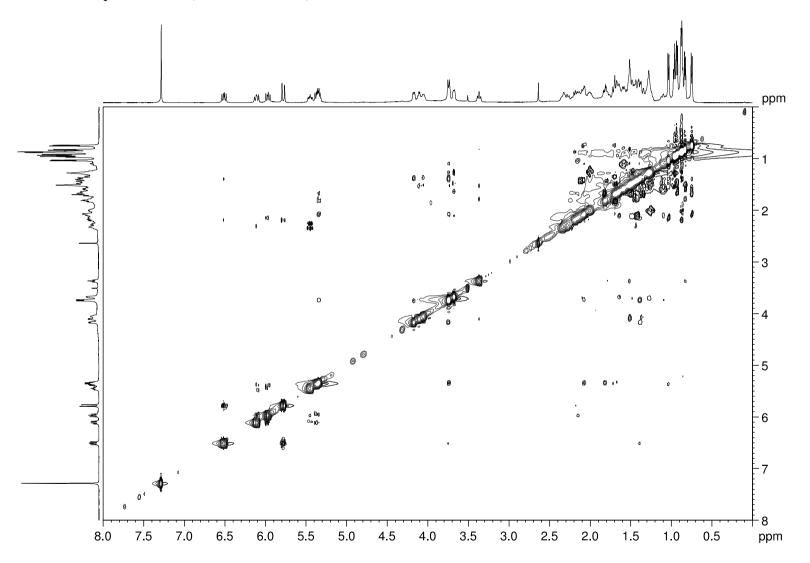


Figure S25. ¹H NMR spectrum of pseudosporamicin C (**4**) (500 MHz, CDCl₃).

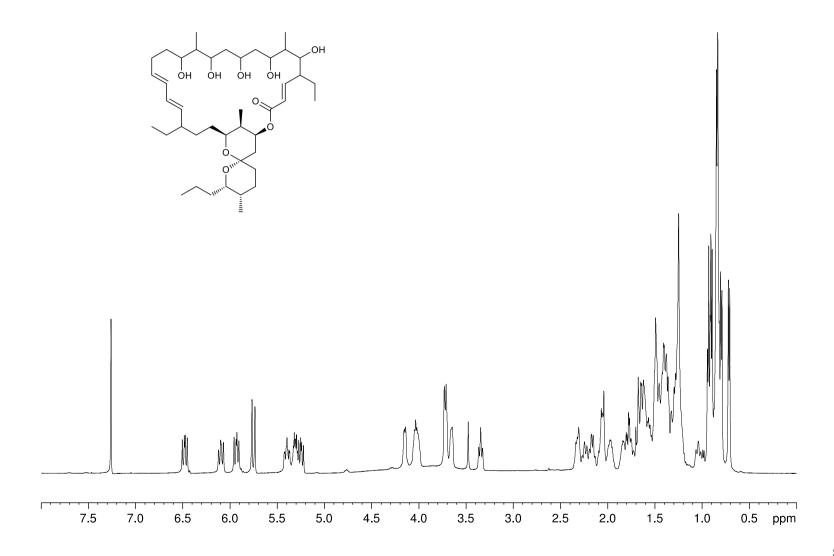


Figure S26. ¹³C NMR spectrum of 4 (125 MHz, CDCl₃).

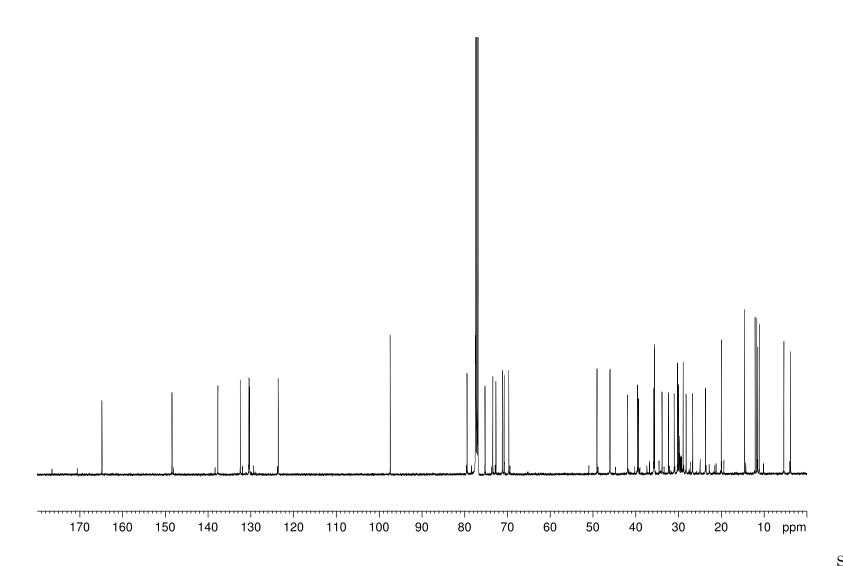


Figure S27. ¹H-¹H COSY spectrum of **4** (500 MHz, CDCl₃).

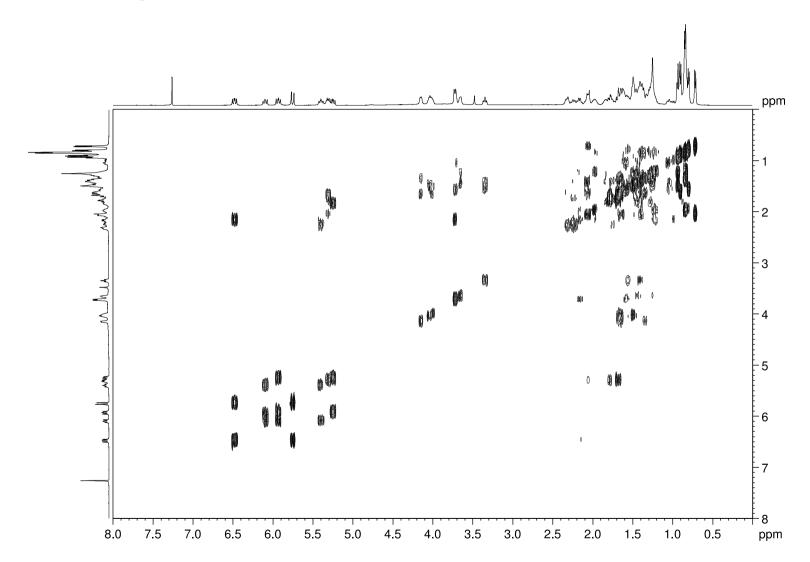


Figure S28. HSQC spectrum of 4 (500 MHz, CDCl₃).

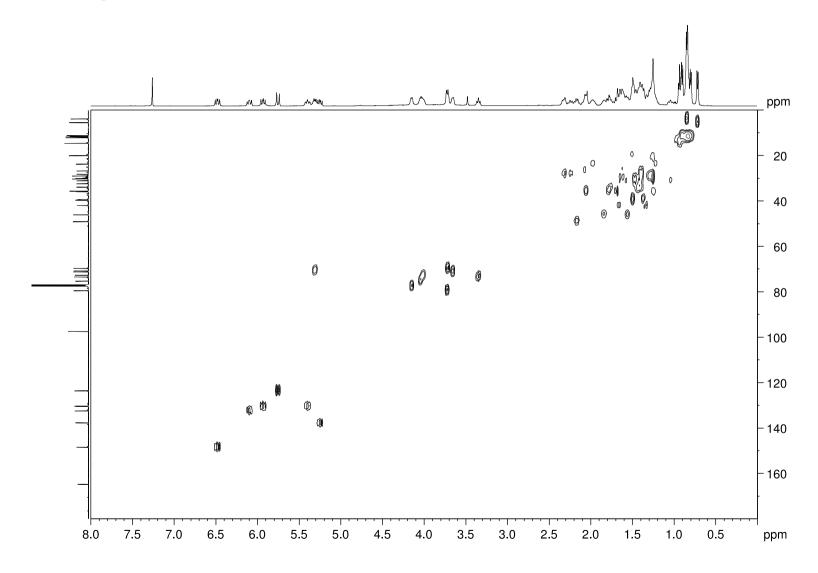


Figure S29. HMBC spectrum of 4 (500 MHz, CDCl₃).

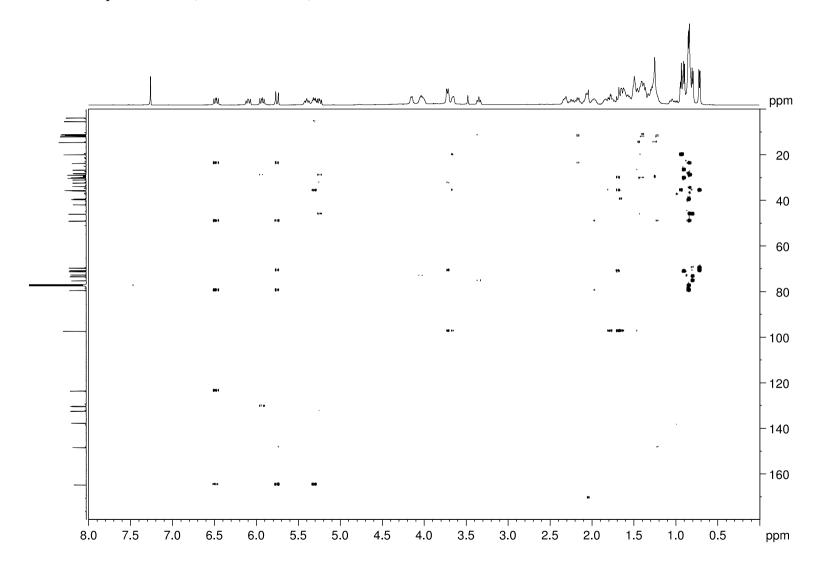


Figure S30. NOESY spectrum of 4 (500 MHz, CDCl₃).

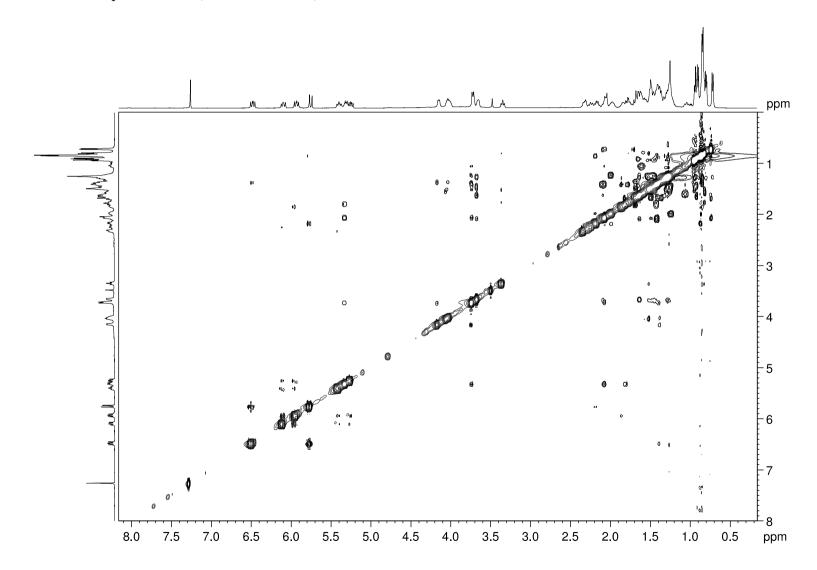


Figure S31. COSY, key HMBC and NOESY correlations of 3 and 4.

