Supplementary Information

Taurospongins B and C, new acetylenic fatty acid derivatives possessing a taurine amide residue from a marine sponge of the family Spongiidae

Takaaki Kubota,^{*a*} Haruna Suzuki,^{*a*} Azusa Takahashi-Nakaguchi,^{*b*} Jane Fromont,^{*c*} Tohru Gonoi^{*b*} and Jun'ichi Kobayashi^{**a*}

^a Graduate School of Pharmaceutical Sciences, Hokkaido University, Sapporo 060-0812, Japan

^b Mycology Research Center, Chiba University, Chiba 260-0856, Japan

^c Western Australian Museum, Locked Bag 49, Welshpool DC, WA 6986, Australia

Table of Contents:

Figure S1. ¹H NMR spectrum of taurospongin B (1) in CD₃OD (600 MHz). Figure S2. ¹³C NMR spectrum of taurospongin B (1) in CD₃OD (150 MHz). **Figure S3.** ¹H-¹H COSY spectrum of taurospongin B (1) in CD₃OD (600 MHz). Figure S4. TOCSY spectrum of taurospongin B (1) in CD₃OD (600 MHz). Figure S5. HMQC spectrum of taurospongin B (1) in CD₃OD (600 MHz). Figure S6. HMBC spectrum of taurospongin B (1) in CD₃OD (600 MHz). Figure S7. ¹H NMR spectrum of taurospongin C (2) in CD₃OD (600 MHz). Figure S8. ¹³C NMR Spectrum of taurospongin C (2) in CD₃OD (150 MHz). **Figure S9.** ¹H NMR spectrum of **4** in CDCl₃ (600 MHz). **Figure S10.** ¹H NMR spectrum of **7** in CDCl₃ (500 MHz). Figure S11. ¹³C NMR spectrum of 7 in CDCl₃ (100 MHz). **Figure S12.** ¹H NMR spectrum of **12** in CDCl₃ (400 MHz). Figure S13. ¹³C NMR spectrum of 12 in CDCl₃ (150 MHz). Figure S14. ¹H NMR spectrum of 11a in CDCl₃ (400 MHz). Figure S15. 13 C NMR spectrum of 11a in CDCl₃ (100 MHz). Figure S16. ¹H NMR spectrum of 11b in CDCl₃ (400 MHz). **Figure S17.** ¹³C NMR spectrum of **11b** in $CDCl_3$ (100 MHz). Figure S18. ¹H NMR spectrum of 13a in CDCl₃ (400 MHz). Figure S19. ¹³C NMR spectrum of 13a in CDCl₂ (100 MHz). Figure S20. ¹H NMR spectrum of 13b in CDCl₃ (400 MHz). Figure S21. 13 C NMR spectrum of 13b in CDCl₃ (100 MHz). Figure S22. ¹H NMR spectrum of 14a in CDCl₃ (400 MHz).

- Figure S23. ¹³C NMR spectrum of 14a in CDCl₃ (100 MHz).
- **Figure S24.** ¹H NMR spectrum of **14b** in CDCl₃ (400 MHz).
- **Figure S25.** ¹³C NMR spectrum of **14b** in CDCl₃ (100 MHz).
- **Figure S26.** ¹H NMR spectrum of **15a** in CDCl₃ (400 MHz).
- **Figure S27.** ¹³C NMR spectrum of **15a** in $CDCl_3$ (100 MHz).
- **Figure S28.** ¹H NMR spectrum of **15b** in CDCl₃ (400 MHz).
- **Figure S29.** ¹³C NMR spectrum of **15b** in $CDCl_3$ (100 MHz).
- **Figure S30.** ¹H NMR spectrum of **6a** in CD₃OD (600 MHz).
- Figure S31. ¹³C NMR spectrum of 6a in CD₃OD (100 MHz).
- **Figure S32.** ¹H NMR spectrum of **6b** in CD₃OD (600 MHz).
- **Figure S33.** ¹³C NMR spectrum of **6b** in CD_3OD (100 MHz).
- Figure S34. ¹H NMR spectra of 4, 6a, and 6b in CD₃OD (600 MHz).



Figure S1. ¹H NMR spectrum of taurospongin B (1) in CD₃OD (600 MHz).



Figure S2. ¹³C NMR spectrum of taurospongin B (1) in CD₃OD (150 MHz).

Figure S3. ¹H-¹H COSY spectrum of taurospongin B (1) in CD₃OD (600 MHz).



Figure S4. TOCSY spectrum of taurospongin B (1) in CD₃OD (600 MHz).











Figure S7. ¹H NMR spectrum of taurospongin C (2) in CD_3OD (600 MHz).





Figure S8. ¹³C NMR Spectrum of taurospongin C (2) in CD₃OD (150 MHz).

Figure S9. ¹H NMR spectrum of **4** in CD_3OD (600 MHz).



Figure S10. ¹H NMR spectrum of 7 in CDCl₃ (500 MHz).



Figure S11. ¹³C NMR spectrum of 7 in $CDCl_3$ (100 MHz).









Figure S13. ¹³C NMR spectrum of 12 in CDCl₃ (150 MHz).

Figure S14. ¹H NMR spectrum of 11a in CDCl₃ (400 MHz).







Figure S16. ¹H NMR spectrum of 11b in CDCl₃ (400 MHz).



Figure S17. ¹³C NMR spectrum of 11b in $CDCl_3$ (100 MHz).







Figure S19. ¹³C NMR spectrum of 13a in CDCl₃ (100 MHz).







Figure S21. ¹³C NMR spectrum of 13b in CDCl₃ (100 MHz).



Figure S22. ¹H NMR spectrum of 14a in CDCl₃ (400 MHz).







Figure S24. ¹H NMR spectrum of 14b in $CDCl_3$ (400 MHz).



Figure S25. ¹³C NMR spectrum of 14b in $CDCl_3$ (100 MHz).



Figure S26. ¹H NMR spectrum of 15a in CDCl₃ (400 MHz).



Figure S27. ¹³C NMR spectrum of 15a in CDCl₃ (100 MHz).



Figure S28. ¹H NMR spectrum of 15b in CDCl₃ (400 MHz).



Figure S29. ¹³C NMR spectrum of 15b in CDCl₃ (100 MHz).



Figure S30. ¹H NMR spectrum of 6a in CD₃OD (600 MHz).



Figure S31. ¹³C NMR spectrum of 6a in CD₃OD (100 MHz).



Figure S32. ¹H NMR spectrum of 6b in CD₃OD (600 MHz).





Figure S33. ¹³C NMR spectrum of 6b in CD₃OD (100 MHz).

Figure S34. ¹H NMR spectra of 4, 6a, and 6b in CD₃OD (600 MHz).

