SUPPLEMENTARY MATERIALS

New Discorhabdins from the Antarctic Deep-Sea Sponge Latrunculia biformis

Fengjie Li¹, Christian Peifer², Dorte Janussen³, and Deniz Tasdemir^{1,4*}

- ¹ GEOMAR Centre for Marine Biotechnology (GEOMAR-Biotech), Research Unit Marine Natural Products Chemistry, GEOMAR Helmholtz Centre for Ocean Research Kiel, Am Kiel-Kanal 44, 24106, Kiel, Germany; fli@geomar.de
- ² Pharmaceutical Chemistry, Kiel University, Gutenbergstraße 76, 24118 Kiel, Germany; cpeifer@pharmazie.unikiel.de
- ³ Senckenberg Research Institute and Natural History Museum, Senckenberganlage 25, D-60325 Frankfurt, Germany; dorte.janussen@senckenberg.de
- ⁴ Faculty of Mathematics and Natural Sciences, Kiel University, Christian-Albrechts-Platz 4, 24118 Kiel, Germany;
- * Correspondence: dtasdemir@geomar.de; Tel.: +49-431-600-4430

Figure No

- Figure S1. ¹H NMR spectrum of compound 1 (TFA salt, 600 MHz, CD₃OD).
- Figure S2. ¹³C NMR spectrum of compound 1 (TFA salt, 150 MHz, CD₃OD).
- Figure S3. HSQC spectrum of compound 1 (TFA salt, 600 MHz, CD₃OD).
- Figure S4. HMBC spectrum of compound 1 (TFA salt, 600 MHz, CD₃OD).
- Figure S5. COSY spectrum of compound 1 (TFA salt, 600 MHz, CD₃OD).
- Figure S6. NOESY spectrum of compound 1 (TFA salt, 600 MHz, CD₃OD).
- Figure S7. HR-ESIMS spectrum of compound 1.
- Figure S8. Experimental ECD spectra (raw) of compounds 1, 4, 5, and 6 (TFA salt) in CH₃OH.
- Figure S9. ¹H NMR spectrum of compound 2 (TFA salt, 600 MHz, DMSO-d6).
- Figure S10. HSQC spectrum of compound 2 (TFA salt, 600 MHz, DMSO-d6).
- Figure S11. HMBC spectrum of compound 2 (TFA salt, 600 MHz, DMSO-d6).
- Figure S12. COSY spectrum of compound 2 (TFA salt, 600 MHz, DMSO-d6).
- Figure S13. NOESY spectrum of compound 2 (TFA salt, 600 MHz, DMSO-d6).
- Figure S14. HR-ESIMS spectrum of compound 2.
- Figure S15. ¹H NMR spectrum of compound 3 (TFA salt, 600 MHz, CD₃OD).
- Figure S16. HSQC spectrum of compound 3 (TFA salt, 600 MHz, CD₃OD).
- Figure S17. HMBC spectrum of compound 3 (TFA salt, 600 MHz, CD₃OD).
- Figure S18. COSY spectrum of compound 3 (TFA salt, 600 MHz, CD₃OD).
- Figure S19. NOESY spectrum of compound 3 (TFA salt, 600 MHz, CD₃OD).
- Figure S20. ¹H NMR spectrum of compound 3 (TFA salt, 600 MHz, Acetone-d₆).
- Figure S21. HR-ESIMS spectrum of compound 3.
- Figure S22. ¹H NMR spectrum of compound 4 (TFA salt, 600 MHz, CD₃OD).
- Figure S23. HSQC spectrum of compound 4 (TFA salt, 600 MHz, CD₃OD).
- Figure S24. HMBC spectrum of compound 4 (TFA salt, 600 MHz, CD₃OD).

Figure S25. COSY spectrum of compound 4 (TFA salt, 600 MHz, CD₃OD).

Figure S26. NOESY spectrum of compound 4 (TFA salt, 600 MHz, CD₃OD).

Figure S27. HR-ESIMS spectrum of compound 4.

Figure S28. ¹H NMR spectrum of compound 5 (TFA salt, 600 MHz, CD₃OD).

Figure S29. ¹³C NMR spectrum of compound 5 (TFA salt, 150 MHz, CD₃OD).

Figure S30. HSQC spectrum of compound 5 (TFA salt, 600 MHz, CD₃OD).

Figure S31. HMBC spectrum of compound 5 (TFA salt, 600 MHz, CD₃OD).

Figure S32. COSY spectrum of compound 5 (TFA salt, 600 MHz, CD₃OD).

Figure S33. NOESY spectrum of compound 5 (TFA salt, 600 MHz, CD₃OD).

Figure S34. HR-ESIMS spectrum of compound 5.

Figure S35. ¹H NMR spectrum of compound 6 (TFA salt, 600 MHz, CD₃OD).

Figure S36. ¹³C NMR spectrum of compound 6 (TFA salt, 150 MHz, CD₃OD).

Figure S37. HSQC spectrum of compound 6 (TFA salt, 600 MHz, CD₃OD).

Figure S38. HMBC spectrum of compound 6 (TFA salt, 600 MHz, CD₃OD).

Figure S39. COSY spectrum of compound 6 (TFA salt, 600 MHz, CD₃OD).

Figure S40. NOESY spectrum of compound 6 (TFA salt, 600 MHz, CD₃OD).

Figure S41. HR-ESIMS spectrum of compound 6.



Figure S1. ¹H NMR spectrum of compound 1 (TFA salt, 600 MHz, CD₃OD).

Figure S2. ¹³C NMR spectrum of compound 1 (TFA salt, 150 MHz, CD₃OD).





Figure S3. HSQC spectrum of compound 1 (TFA salt, 600 MHz, CD₃OD).

Figure S4. HMBC spectrum of compound 1 (TFA salt, 600 MHz, CD₃OD).





Figure S5. COSY spectrum of compound 1 (TFA salt, 600 MHz, CD₃OD).

Figure S6. NOESY spectrum of compound 1 (TFA salt, 600 MHz, CD₃OD).



Figure S7. HR-ESIMS spectrum of compound 1.



Figure S8. Experimental ECD spectra (raw) of compounds 1, 4, 5, and 6 (TFA salt) in CH₃OH.





Figure S9. ¹H NMR spectrum of compound 2 (TFA salt, 600 MHz, DMSO-d6).

Figure S10. HSQC spectrum of compound 2 (TFA salt, 600 MHz, DMSO-d6).





Figure S11. HMBC spectrum of compound 2 (TFA salt, 600 MHz, DMSO-d6).

Figure S12. COSY spectrum of compound 2 (TFA salt, 600 MHz, DMSO-d6).





Figure S13. NOESY spectrum of compound 2 (TFA salt, 600 MHz, DMSO-d6).

Figure S14. HR-ESIMS spectrum of compound 2.





Figure S15. ¹H NMR spectrum of compound 3 (TFA salt, 600 MHz, CD₃OD).

Figure S16. HSQC spectrum of compound 3 (TFA salt, 600 MHz, CD₃OD).





Figure S17. HMBC spectrum of compound 3 (TFA salt, 600 MHz, CD₃OD).

Figure S18. COSY spectrum of compound 3 (TFA salt, 600 MHz, CD₃OD).





Figure S19. NOESY spectrum of compound 3 (TFA salt, 600 MHz, CD₃OD).

Figure S20. ¹H NMR spectrum of compound 3 (TFA salt, 600 MHz, Acetone- *d*₆).



8.4 8.2 8.0 7.8 7.6 7.4 7.2 7.0 6.8 6.6 6.4 6.2 6.0 5.8 5.6 5.4 5.2 5.0 4.8 4.6 4.4 4.2 4.0 3.8 3.6 3.4 3.2 3.0 2.8 2.6 2.4 2. fl (ppm)

Figure S21. HR-ESIMS spectrum of compound 3.





Figure S22. ¹H NMR spectrum of compound 4 (TFA salt, 600 MHz, CD₃OD).

Figure S23. HSQC spectrum of compound 4 (TFA salt, 600 MHz, CD₃OD).





Figure S24. HMBC spectrum of compound 4 (TFA salt, 600 MHz, CD₃OD).

Figure S25. COSY spectrum of compound 4 (TFA salt, 600 MHz, CD₃OD).





Figure S26. NOESY spectrum of compound 4 (TFA salt, 600 MHz, CD₃OD).

Figure S27. HR-ESIMS spectrum of compound 4.





Figure S28. ¹H NMR spectrum of compound 5 (TFA salt, 600 MHz, CD₃OD).

Figure S29. ¹³C NMR spectrum of compound 5 (TFA salt, 150 MHz, CD₃OD).





Figure S30. HSQC spectrum of compound 5 (TFA salt, 600 MHz, CD₃OD).

Figure S31. HMBC spectrum of compound 5 (TFA salt, 600 MHz, CD₃OD).





Figure S32. COSY spectrum of compound 5 (TFA salt, 600 MHz, CD₃OD).

Figure S33. NOESY spectrum of compound 5 (TFA salt, 600 MHz, CD₃OD).



Figure S34. HR-ESIMS spectrum of compound 5.





Figure S35. ¹H NMR spectrum of compound 6 (TFA salt, 600 MHz, CD₃OD).

Figure S36. ¹³C NMR spectrum of compound 6 (TFA salt, 150 MHz, CD₃OD).





Figure S37. HSQC spectrum of compound 6 (TFA salt, 600 MHz, CD₃OD).

Figure S38. HMBC spectrum of compound 6 (TFA salt, 600 MHz, CD₃OD).





Figure S39. COSY spectrum of compound 6 (TFA salt, 600 MHz, CD₃OD).

Figure S40. NOESY spectrum of compound 6 (TFA salt, 600 MHz, CD₃OD).



Figure S41. HR-ESIMS spectrum of compound 6.

