Supplementary Materials: An Unusual Diterpene–Enhygromic Acid and Deoxyenhygrolides from a Marine Myxobacterium, *Enhygromyxa* sp.

Tomohiko Tomura, Shiori Nagashima, Satoshi Yamazaki, Takashi Iizuka, Ryosuke Fudou and Makoto Ojika

Contents

Spectral data and conformational analysis of enhygromic acid (1)

Figure S1: ¹H NMR spectrum of **1** (600 MHz, DMSO-*d*₆), Figure S2: ¹³C NMR spectrum of **1** (150 MHz, DMSO-*d*₆), Figure S3: DQF-COSY of **1** (600 MHz, DMSO-*d*₆), Figure S4: HSQC spectrum of **1** (600 MHz, DMSO-*d*₆), Figure S5: HMBC spectrum of **1** (600 MHz, DMSO-*d*₆), Figure S6: NOESY of **1** (600 MHz, DMSO-*d*₆), Figure S7: UV spectrum of **1**, Figure S8: IR spectrum of **1**, Figure S9: ESI-TOF-MS (+) spectrum of **1**, Figure S10: Local minimum energy (orange line) and dihedral angle C2–C3–C4–C5 (blue dotted line) against the input dihedral angle in **1**

Spectral data of deoxyenhygrolide A (2)

Figure S11: ¹H NMR spectrum of **2** (400 MHz, C₆D₆), Figure S12: ¹³C NMR spectrum of **2** (100 MHz, C₆D₆), Figure S13: DQF-COSY of **2** (400 MHz, C₆D₆), Figure S14: HSQC spectrum of **2** (400 MHz, C₆D₆), Figure S15: HMBC spectrum of **2** (400 MHz, C₆D₆), Figure S16: NOESY of **2** (400 MHz, C₆D₆), Figure S17: UV spectrum of **2**, Figure S18: IR spectrum of **2**, Figure S19: ESI-TOF-MS spectrum of **2**

Spectral data of deoxyenhygrolide B (3)

Figure S20: ¹H NMR spectrum of **3** (400 MHz, C₆D₆), Figure S21: ¹³C NMR spectrum of **3** (100 MHz, C₆D₆), Figure S22: DQF-COSY of **3** (400 MHz, C₆D₆), Figure S23: HSQC spectrum of **3** (400 MHz, C₆D₆), Figure S24: HMBC spectrum of **3** (400 MHz, C₆D₆), Figure S25: NOESY of **3** (400 MHz, C₆D₆), Figure S26: UV spectrum of **3**, Figure S27: IR spectrum of **3**, Figure S28: ESI-TOF-MS spectrum of **3**.



Figure S1. ¹H NMR spectrum of 1 (600 MHz, DMSO-*d*₆).



Figure S2. ¹³C NMR spectrum of 1 (150 MHz, DMSO-*d*₆).









Figure S4. HSQC spectrum of 1 (600 MHz, DMSO-d₆).







Figure S6. NOESY of **1** (600 MHz, DMSO-*d*₆).



Figure S7. UV spectrum of 1.



Figure S9. ESI-TOF-MS (+) spectrum of 1.



Figure S10. Local minimum energy (orange line) and dihedral angle C2–C3–C4–C5 (blue dotted line) against the input dihedral angle in **1**. Only two energy minimized conformers **A** and **B** were obtained.



Figure S11. ¹H NMR spectrum of 2 (400 MHz, C₆D₆).





Figure S13. DQF-COSY of 2 (400 MHz, C6D6).





0 200

400





Figure S17. UV spectrum of 2.



Figure S18. IR spectrum of 2.



Figure S19. ESI-TOF-MS spectrum of 2.



Figure S21. ¹³C NMR spectrum of 3 (100 MHz, C₆D₆).







Figure S24. HMBC spectrum of 3 (400 MHz, C₆D₆).



Figure S25. NOESY of 3 (400 MHz, C₆D₆).



Figure S27. IR spectrum of 3.





Figure S28. ESI-TOF-MS spectrum of 3.