Supplementary Materials: Topsensterols A–C, Cytotoxic Polyhydroxylated Sterol Derivatives from a Marine Sponge *Topsentia* sp.

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List of Supplementary Materials

Figure S1. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 1 Figure S2. ¹³C NMR and DEPT (100 MHz, CD₃OD) spectra of compound 1 Figure S3. HSQC (CD₃OD) spectrum of compound 1 Figure S4. ¹H–¹H COSY (CD₃OD) spectrum of compound 1 Figure S5. HMBC (CD₃OD) spectrum of compound 1 Figure S6. NOESY (CD₃OD) spectrum of compound 1 Figure S7. Partial NOESY (CD₃OD) spectrum of compound 1 Figure S8. ESIMS spectrum of compound 1 Figure S9. HRESIMS spectrum of compound 1 Figure S10. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 2 Figure S11. ¹³C NMR and DEPT (100 MHz, CD₃OD) spectra of compound 2 Figure S12. HSQC (CD₃OD) spectrum of compound 2 Figure S13. 1H-1H COSY (CD3OD) spectrum of compound 2 Figure S14. HMBC (CD₃OD) spectrum of compound 2 Figure S15. NOESY (CD₃OD) spectrum of compound 2 Figure S16. HRESIMS spectrum of compound 2 Figure S17. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 3 Figure S18. ¹³C NMR and DEPT (100 MHz, CD₃OD) spectra of compound 3 Figure S19. HSQC (CD₃OD) spectrum of compound 3 Figure S20. ¹H–¹H COSY (CD₃OD) spectrum of compound 3 Figure S21. HMBC (CD₃OD) spectrum of compound 3 Figure S22. HRESIMS spectrum of compound 3



Figure S2. ¹³C NMR and DEPT (100 MHz, CD₃OD) spectra of compound 1.



Figure S4. ¹H–¹H COSY (CD₃OD) spectrum of compound 1.











Figure S7. Partial NOESY (CD₃OD) spectrum of compound 1.



Figure S8. ESIMS spectrum of compound 1.

Elemental Composition Report Page 1 Single Mass Analysis Tolerance = 10.0 PPM / DBE: min = -1.5, max = 50.0 Isotope cluster parameters: Separation = 1.0 Abundance = 1.0% Monoisotopic Mass, Odd and Even Electron Ions 19 formula(e) evaluated with 1 results within limits (all results (up to 1000) for each mass) SY-22A 20110518-SY-22A 57 (2 031) AM (Cen,8, 80 00, Ht,5000.0,0.00,1.00); Sm (Md, 3.00) TOF MS ES+ 2.04e3 556.2771 100 585.3340 % 545.3392 563,3600 557,2831 564.3784 575.3492 577.3521 580.4007 501.3399 509.3396 546.3625 586.3540 513.3406 525.3156 527.3514 531.3460 543.3386 599.3322 m/z 0 510.0 530.0 540.0 520.0 550.0 560.0 570.0 580.0 590.0 Minimum: Maximum: -1.5 10.0 200.0

Mass Calc. Mass mDa PPM DBE Score Formula

563.3600 563.3584 1.6 2.9 7.5 1 C32 H51 08





Figure S10. ¹H NMR (400 MHz, CD₃OD) spectrum of compound 2.



Figure S11. ¹³C NMR and DEPT (100 MHz, CD₃OD) spectra of compound 2.



Figure S12. HSQC (CD₃OD) spectrum of compound 2.



Figure S13. ¹H–¹H COSY (CD₃OD) spectrum of compound 2.



Figure S14. HMBC (CD₃OD) spectrum of compound 2.











Figure S18. ¹³C NMR and DEPT (100 MHz, CD₃OD) spectra of compound 3.







Figure S20. ¹H–¹H COSY (CD₃OD) spectrum of compound 3.







Figure S22. HRESIMS spectrum of compound 3.