



## **Supplementary Material**

## New $9\alpha$ -Hydroxy- $5\alpha$ , $6\alpha$ -epoxyhydroxysterols from the Vietnamese Marine Sponge *Ircinia echinata*

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## **Content:**

**Figure S1.** <sup>1</sup>H NMR spectrum (600 MHz) of  $5\alpha$ , $6\alpha$ -Epoxycholesta-7,22(*E*)-dien-3 $\beta$ , $9\alpha$ -diol (1) in CD<sub>3</sub>OD.

Figure S2. DEPT spectrum (150.9 MHz) of 1 in CD<sub>3</sub>OD.

Figure S3. COSY spectrum (600 MHz) of 1 in CD<sub>3</sub>OD.

Figure S4. HSQC spectrum (600 MHz) of 1 in CD<sub>3</sub>OD.

Figure S5. HMBC spectrum (600 MHz) of 1 in CD<sub>3</sub>OD.

Figure S6. NOESY spectrum (600 MHz) of 1 in CD<sub>3</sub>OD.

Figure S7. HR-ESI mass spectrum of 1.

**Figure S8.** <sup>1</sup>H NMR spectrum (600 MHz) of  $5\alpha$ , $6\alpha$ -Epoxycholesta-7,24(28)-dien-3 $\beta$ , $9\alpha$ -diol (2) in CD<sub>3</sub>OD.

Figure S9. DEPT spectrum (150.9 MHz) of 2 in CD<sub>3</sub>OD

Figure S10. COSY spectrum (600 MHz) of 2 in CD<sub>3</sub>OD.

Figure S11. HSQC spectrum (600 MHz) of 2 in CD<sub>3</sub>OD.

Figure S12. HMBC spectrum (600 MHz) of 2 in CD<sub>3</sub>OD.

Figure S13. NOESY spectrum (600 MHz) of 2 in CD<sub>3</sub>OD.

Figure S14. HR-ESI mass spectrum of 2.

**Figure S15.** <sup>1</sup>H NMR spectrum (600 MHz) of (24*R*)-5 $\alpha$ ,6 $\alpha$ -Epoxy-24-ethyl-cholesta-7-en-3 $\beta$ ,9 $\alpha$ -diol (3) in CD<sub>3</sub>OD.

Figure S16. DEPT spectrum (150.9 MHz) of 3 in CD<sub>3</sub>OD.

Figure S17. COSY spectrum (600 MHz) of 3 in CD<sub>3</sub>OD.

Figure S18. HSQC spectrum (600 MHz) of 3 in CD<sub>3</sub>OD.

Figure S19. HMBC spectrum (600 MHz) of 3 in CD<sub>3</sub>OD.

Figure S20. NOESY spectrum (600 MHz) of 3 in CD<sub>3</sub>OD.

Figure S21. HR-ESI mass spectrum of 3.

**Figure S22.** <sup>1</sup>H NMR spectrum (600 MHz) of  $5\alpha$ , $6\alpha$  -Epoxycholesta-7-en- $3\beta$ , $9\alpha$ -diol (4) in CD<sub>3</sub>OD.

Figure S23. DEPT spectrum (150.9 MHz) of 4 in CD<sub>3</sub>OD.

Figure S24. COSY spectrum (600 MHz) of 4 in CD<sub>3</sub>OD.

Figure S25. HSQC spectrum (600 MHz) of 4 in CD<sub>3</sub>OD.

Figure S26. HMBC spectrum (600 MHz) of 4 in CD<sub>3</sub>OD.

Figure S27. NOESY spectrum (600 MHz) of 4 in CD<sub>3</sub>OD.

Figure S28. HR-ESI mass spectrum of 4.

**Figure S29.** <sup>1</sup>H NMR spectrum (600 MHz) of (24*S*)- $5\alpha$ , $6\alpha$ -Epoxyergosta-7,22-dien- $3\beta$ , $9\alpha$ -diol (5) in CD<sub>3</sub>OD.

Figure S30. DEPT spectrum (150.9 MHz) of 5 in CD<sub>3</sub>OD.

Figure S31. COSY spectrum (600 MHz) of 5 in CD<sub>3</sub>OD.

Figure S32. HSQC spectrum (600 MHz) of 5 in CD<sub>3</sub>OD.

Figure S33. HMBC spectrum (600 MHz) of 5 in CD<sub>3</sub>OD.

Figure S34. NOESY spectrum (600 MHz) of 5 in CD<sub>3</sub>OD.

Figure S35. HR-ESI mass spectrum of 5.

**Figure S36.** <sup>1</sup>H NMR spectrum (600 MHz) of (24*R*)-5 $\alpha$ ,6 $\alpha$ -Epoxy-24-methyl-cholesta-7-en-3 $\beta$ ,9 $\alpha$ -diol (6) in CD<sub>3</sub>OD.

Figure S37. DEPT spectrum (150.9 MHz) of 6 in CD<sub>3</sub>OD.

Figure S38. COSY spectrum (600 MHz) of 6 in CD<sub>3</sub>OD.

Figure S39. HSQC spectrum (600 MHz) of 6 in CD<sub>3</sub>OD.

Figure S40. HMBC spectrum (600 MHz) of 6 in CD<sub>3</sub>OD.

Figure S41. NOESY spectrum (600 MHz) of 6 in CD<sub>3</sub>OD.

Figure S42. HR-ESI mass spectrum of 6.

**Figure S43.** Growth inhibition of curves of the active compounds **3** and **4** against three human cancer cell lines.



**Figure S1.** <sup>1</sup>H NMR spectrum (600 MHz) of  $5\alpha,6\alpha$ -Epoxycholesta-7,22(*E*)-dien-3 $\beta$ ,9 $\alpha$ -diol (1)- in CD<sub>3</sub>OD.





Figure S3. COSY spectrum (600 MHz) of 1 in CD<sub>3</sub>OD.



Figure S4. HSQC spectrum (600 MHz) of 1 in CD<sub>3</sub>OD.



Figure S6. NOESY spectrum (600 MHz) of 1 in CD<sub>3</sub>OD.

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**Figure S8.** <sup>1</sup>H NMR spectrum (600 MHz) of  $5\alpha$ , $6\alpha$ -Epoxycholesta-7,24(28)-dien-3 $\beta$ , $9\alpha$ -diol (2) in CD<sub>3</sub>OD.





Figure S10. COSY spectrum (600 MHz) of 2 in CD<sub>3</sub>OD.



Figure S11. HSQC spectrum (600 MHz) of 2 in CD<sub>3</sub>OD.







Figure S13. NOESY spectrum (600 MHz) of 2 in CD<sub>3</sub>OD.





**Figure S15.** <sup>1</sup>H NMR spectrum (600 MHz) of (24*R*)- $5\alpha$ , $6\alpha$ -Epoxy-24-ethyl-cholesta-7-en- $3\beta$ , $9\alpha$ -diol (3) in CD<sub>3</sub>OD.



Figure S16. DEPT spectrum (150.9 MHz) of 3 in CD<sub>3</sub>OD.









Figure S20. NOESY spectrum (600 MHz) of 3 in CD<sub>3</sub>OD.



Figure S21. HR-ESI mass spectrum of 3.





Figure S23. DEPT spectrum (150.9 MHz) of 4 in CD<sub>3</sub>OD.











Figure S27. NOESY spectrum (600 MHz) of 4 in CD<sub>3</sub>OD.



Figure S28. HR-ESI mass spectrum of 4.



**Figure S29.** <sup>1</sup>H NMR spectrum (600 MHz) of (24*S*)- $5\alpha$ , $6\alpha$ -Epoxyergosta-7,22-dien- $3\beta$ , $9\alpha$ -diol (5) in CD<sub>3</sub>OD.





Figure S30. DEPT spectrum (150.9 MHz) of 5 in CD<sub>3</sub>OD.







Figure S33. HMBC spectrum (600 MHz) of 5 in CD<sub>3</sub>OD.



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Figure S35. HR-ESI mass spectrum of 5.



**Figure S36.** <sup>1</sup>H NMR spectrum (600 MHz) of (24*R*)-5 $\alpha$ , $6\alpha$ -Epoxy-24-methyl-cholesta-7-en-3 $\beta$ , $9\alpha$ -diol (6) in CD<sub>3</sub>OD.



Figure S37. DEPT spectrum (150.9 MHz) of 6 in CD<sub>3</sub>OD.



Figure S38. COSY spectrum (600 MHz) of 6 in CD<sub>3</sub>OD.











Figure S42. HR-ESI mass spectrum of 6.



Figure S43. Growth inhibition curves of the active compounds 3 and 4 against three human cancer cell lines.