### **Supplementary Material**

## Design, Synthesis and Anticancer Evaluation of Novel Indole Derivatives of Ursolic Acid as Potential Topoisomerase II Inhibitors

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### Figure S1~Figure S42. <sup>1</sup>H and <sup>13</sup>C NMR spectra of compounds



### 4a-f, 5a-f, 6a-f and 7a-c.

Figure S1. <sup>1</sup>H-NMR spectrum of compound 4a (600 MHz, CDCl<sub>3</sub>).



Figure S2. <sup>13</sup>C-NMR spectrum of compound 4a (150 MHz, CDCl<sub>3</sub>).



Figure S3. <sup>1</sup>H-NMR spectrum of compound 4b (600 MHz, CDCl<sub>3</sub>).



Figure S4. <sup>13</sup>C-NMR spectrum of compound 4b (150 MHz, CDCl<sub>3</sub>).

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Figure S5. 1H-NMR spectrum of compound 4c (600 MHz, CDCl<sub>3</sub>).



Figure S6. <sup>13</sup>C-NMR spectrum of compound 4c (150 MHz, CDCl<sub>3</sub>).

### -7.8510 -7.8510 7.11501 7.11501 7.11501 7.11501 7.11503 7.1



Figure S7. <sup>1</sup>H-NMR spectrum of compound 4d (600 MHz, CDCl<sub>3</sub>).





Figure S9. 1H-NMR spectrum of compound 4e (600 MHz, CDCl<sub>3</sub>).



Figure S10. <sup>13</sup>C-NMR spectrum of compound 4e (150 MHz, CDCl<sub>3</sub>).

### -7.9734 0.8722 9001 5.9178 5.525



Figure S11. <sup>1</sup>H-NMR spectrum of compound 4f (600 MHz, CDCl<sub>3</sub>).



Figure S12. <sup>13</sup>C-NMR spectrum of compound 4f (150 MHz, CDCl<sub>3</sub>).



Figure S13. <sup>1</sup>H-NMR spectrum of compound 5a (600 MHz, CDCl<sub>3</sub>).



Figure S14. <sup>13</sup>C-NMR spectrum of compound 5a (150 MHz, CDCl<sub>3</sub>).



Figure S15. <sup>1</sup>H-NMR spectrum of compound 5b (600 MHz, CDCl<sub>3</sub>).



Figure S16. <sup>13</sup>C-NMR spectrum of compound 5b (150 MHz, CDCl<sub>3</sub>).

### 7,8531 (7,12) (2



Figure S17. <sup>1</sup>H-NMR spectrum of compound 5c (600 MHz, CDCl<sub>3</sub>).



Figure S18. <sup>13</sup>C-NMR spectrum of compound 5c (150 MHz, CDCl<sub>3</sub>).

### -7.8163 0.9248 0.8742 0.0029 1045 0239 9381 9207 8284 7740 6267 5006 4318 747.



Figure S19. <sup>1</sup>H-NMR spectrum of compound 5d (600 MHz, CDCl<sub>3</sub>).



Figure S21. <sup>1</sup>H-NMR spectrum of compound 5e (600 MHz, CDCl<sub>3</sub>).





Figure S23. <sup>1</sup>H-NMR spectrum of compound 5f (600 MHz, CDCl<sub>3</sub>).



Figure S24. <sup>13</sup>C-NMR spectrum of compound 5f (150 MHz, CDCl<sub>3</sub>).

### 7,8553 7,75288 6,6326 6,6326 6,6326 6,6326 6,6326 6,6326 6,6326 6,6326 6,6326 6,6326 6,6326 6,6326 6,6326 6,6326 6,6326 6,6326 7,1788 6,6326 7,2526 7,356 6,6325 7,356 6,6325 7,356 6,6325 7,356 6,6325 7,356 7,367 7,366 7,2759 7,367 7,475 7,275 7,475 7,2759 7,



Figure S25. <sup>1</sup>H-NMR spectrum of compound 6a (600 MHz, CDCl<sub>3</sub>).



![](_page_13_Figure_1.jpeg)

Figure S27. <sup>1</sup>H-NMR spectrum of compound 6b (600 MHz, CDCl<sub>3</sub>).

![](_page_14_Figure_0.jpeg)

Figure S28. <sup>13</sup>C-NMR spectrum of compound 6b (150 MHz, CDCl<sub>3</sub>).

# $-7.8824 \\ -7.8824 \\ 7.13737 \\ 7.13737 \\ 7.13737 \\ 7.13737 \\ 7.13737 \\ 7.13737 \\ 7.13737 \\ 6.9208 \\ 6.9208 \\ 6.9208 \\ 6.9208 \\ 6.9208 \\ 6.9208 \\ 6.9208 \\ 6.9208 \\ 6.9208 \\ 6.9208 \\ 6.9208 \\ 6.0008 \\ 6.9208 \\ 6.0008 \\ 6$

![](_page_14_Figure_3.jpeg)

Figure S29. <sup>1</sup>H-NMR spectrum of compound 6c (600 MHz, CDCl<sub>3</sub>).

![](_page_15_Figure_0.jpeg)

Figure S31. <sup>1</sup>H-NMR spectrum of compound 6d (600 MHz, CDCl<sub>3</sub>).

![](_page_16_Figure_0.jpeg)

Figure S32. <sup>13</sup>C-NMR spectrum of compound 6d (150 MHz, CDCl<sub>3</sub>).

## $\begin{array}{c} -7.9279\\ -7.19276\\ -7.172805\\ -7.1748\\ -7.1748\\ -7.1748\\ -7.1748\\ -5.9821\\ -5.9821\\ -5.9821\\ -5.9823\\ -5.1256\\ -5.1256\\ -2.1279\\ -2.1276\\ -2.2305\\ -2$

![](_page_16_Figure_3.jpeg)

Figure S33. <sup>1</sup>H-NMR spectrum of compound 6e (600 MHz, CDCl<sub>3</sub>).

![](_page_17_Figure_0.jpeg)

Figure S34. <sup>13</sup>C-NMR spectrum of compound 6e (600 MHz, CDCl<sub>3</sub>).

### 0.9158 0.8745 -0.0008 -7.8833 6957

![](_page_17_Figure_3.jpeg)

Figure S35. 1H-NMR spectrum of compound 6f (600 MHz, CDCl3).

![](_page_18_Figure_0.jpeg)

Figure S37. <sup>1</sup>H-NMR spectrum of compound 7a (600 MHz, CDCl<sub>3</sub>).

![](_page_19_Figure_0.jpeg)

Figure S38. <sup>13</sup>C-NMR spectrum of compound 7a (150 MHz, CDCl<sub>3</sub>).

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![](_page_19_Figure_3.jpeg)

Figure S39. <sup>1</sup>H-NMR spectrum of compound 7b (600 MHz, CDCl<sub>3</sub>).

![](_page_20_Figure_0.jpeg)

Figure S40. <sup>13</sup>C-NMR spectrum of compound 7b (150 MHz, CDCl<sub>3</sub>).

![](_page_20_Figure_2.jpeg)

Figure S41. <sup>1</sup>H-NMR spectrum of compound 7c (600 MHz, CDCl<sub>3</sub>).

![](_page_21_Figure_0.jpeg)

Figure S42. <sup>13</sup>C-NMR spectrum of compound 7c (150 MHz, CDCl<sub>3</sub>).