## **Supplementary Information**

## Ptxplatin: An multifunctional Pt(IV) antitumor prodrug

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Fig. S1. HR-MS spectrum of compound 1.







**Fig. S3**. Structural characterization of PTX, **3** and **4**. <sup>1</sup>H NMR spectra of (a) PTX in CDCl<sub>3</sub>, (b) compound **3** in CDCl<sub>3</sub>, (c) PTX in DMSO- $d_6$ , (d) compound **4** in DMSO- $d_6$ .



Fig. S4. <sup>13</sup>C NMR spectrum of compound 3 in CDCl<sub>3</sub>



Fig. S5. HR-MS spectrum of compound 3.



Fig. S6. HPLC characterization of compound 3.



Fig. S7. <sup>13</sup>C NMR spectrum of compound 4 in DMSO- $d_6$ .



Fig. S8. HR-MS spectrum of compound 4.



Fig. S9. HPLC characterization of compound 4.



Fig. S10. <sup>1</sup>H-NMR spectrum of compound 5 in DMSO- $d_6$ .



Fig. S11. <sup>13</sup>C-NMR spectrum of compound 5 in DMSO- $d_6$ .



Fig. S12. HR-MS spectrum (positive mode) of compound 5.



Fig. S14. <sup>1</sup>H-NMR spectrum of compound 6 in DMSO- $d_6$ .



Fig. S15. <sup>13</sup>C-NMR spectrum of compound 6 in DMSO- $d_6$ .



Fig. S16. HR-MS spectrum (positive mode) of compound 6.



Fig. S18. <sup>1</sup>H-NMR spectrum of compound 7 in DMSO- $d_6$ .



Fig. S19. <sup>13</sup>C-NMR spectrum of compound 7 in DMSO- $d_6$ .



Fig. S20. HR-MS spectrum (positive mode) of compound 7.



Fig. S22. <sup>1</sup>H-NMR spectrum of compound 8 in DMSO- $d_6$ .



Fig. S23. <sup>13</sup>C-NMR spectrum of compound 8 in DMSO- $d_6$ .



Fig. S24. HR-MS spectrum (positive mode) of compound 8.



Fig. S26. <sup>1</sup>H-NMR spectrum of compound 9 in DMSO-*d*<sub>6</sub>.



Fig. S27. <sup>13</sup>C-NMR spectrum of compound 9 in DMSO- $d_6$ .



S28. HR-MS spectrum (positive mode) of compound 9.







Fig. S32. HR-MS spectrum (positive mode) of compound 10.



Fig. S34. <sup>1</sup>H-NMR spectrum of compound 11 in DMSO-*d*<sub>6</sub>.



Fig. S35. <sup>13</sup>C-NMR spectrum of compound 11 in DMSO- $d_6$ .



Fig. S36. HR-MS spectrum (positive mode) of compound 11. S21



Fig. S37. HPLC characterization of compound 11.







Fig. S40. HR-MS spectrum (positive mode) of compound 12.



Fig. S42. Western blotting analysis of MMP-2 in MCF-7 cells after treatment with various compounds (5  $\mu$ M) for 24 h, Mixture stands for a combination of CDDP (5  $\mu$ M) and PTX (5  $\mu$ M).



Fig. S43. Cellular accumulation of the indicated compounds at 10  $\mu$ M for 9 h treatment.



**Fig. S44** The results of HPLC and HR-MS analysis for MCF-7 cells extract after treated with **5** for 4 h, using untreated cells extract as controls.