

Supplementary Information for (New Journal of Chemistry):

**Self-assembly of manganese(I) based thiolato bridged dinuclear
metallacycles: synthesis, characterization, cytotoxicity evaluation
and CO-releasing studies**

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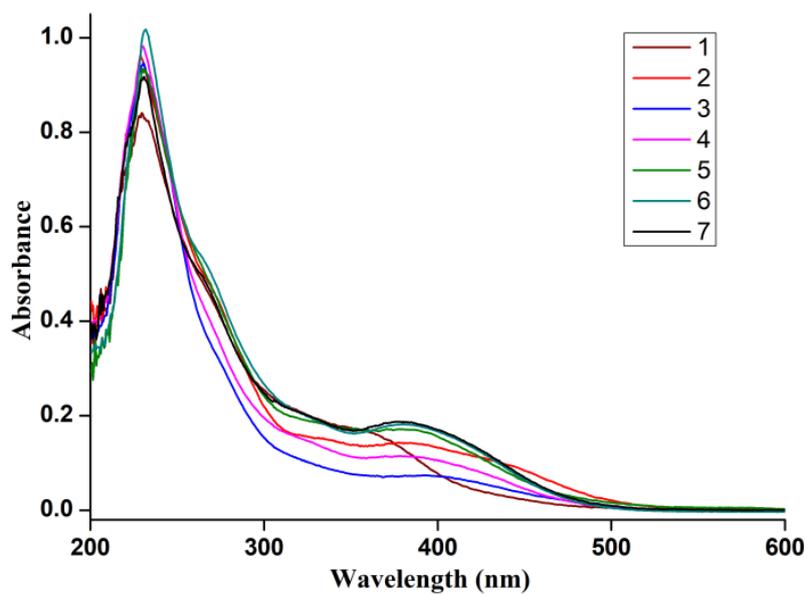


Fig. S1 Overlay plot of UV-Vis spectra of compounds 1–7 in CH₂Cl₂ solvent.

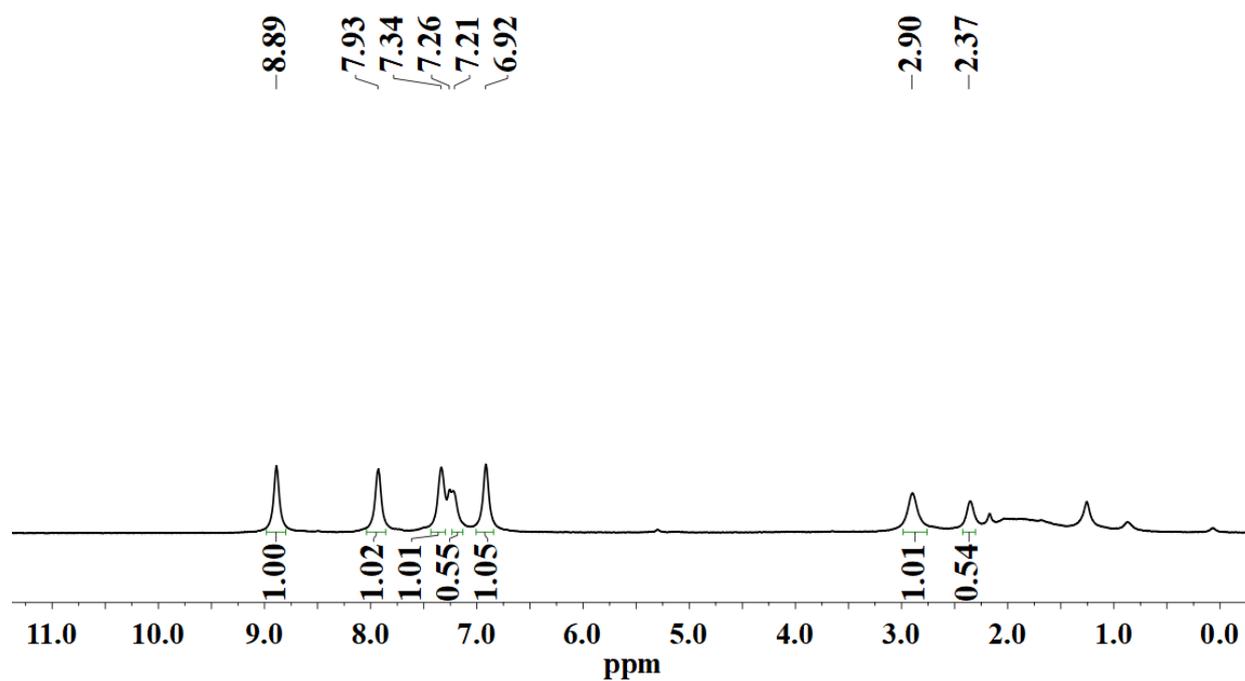


Fig. S2 ¹H NMR spectrum of compound 1 in CDCl₃.

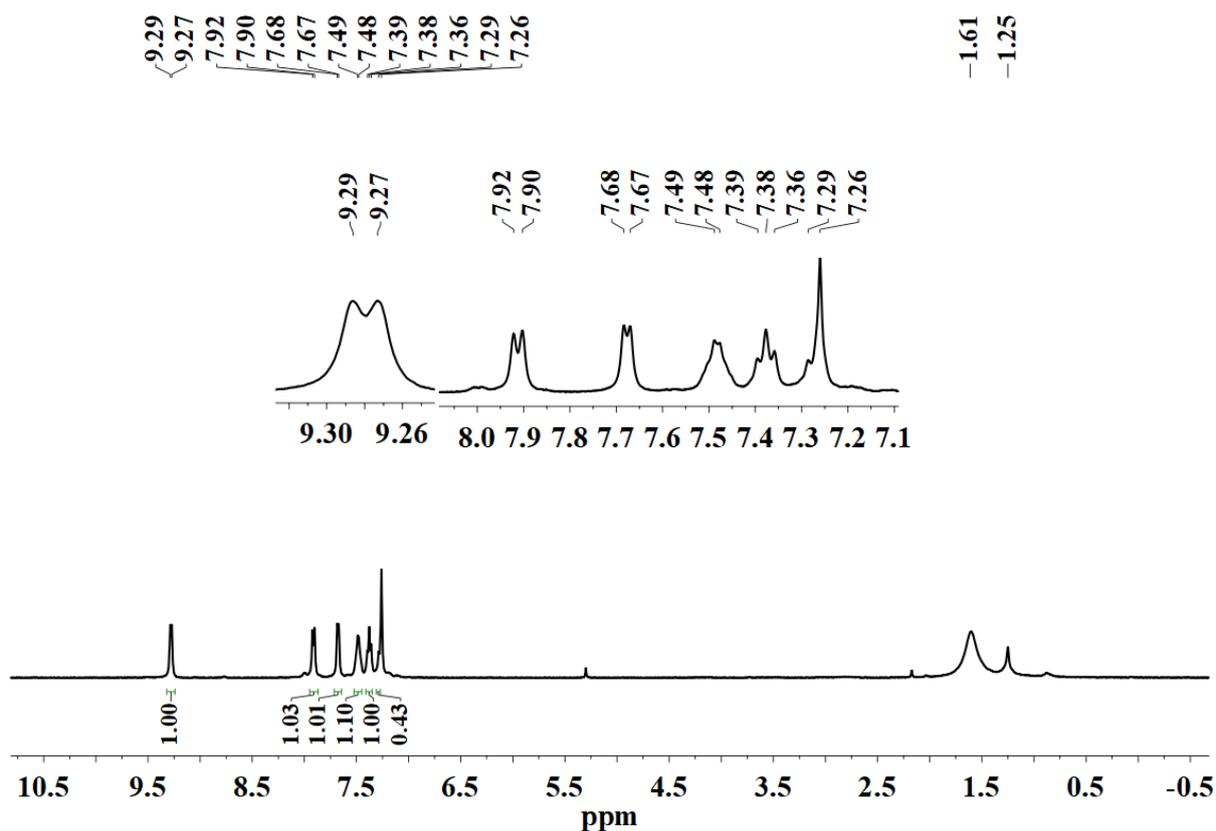


Fig. S3 ^1H NMR spectrum of compound **2** in CDCl_3 .

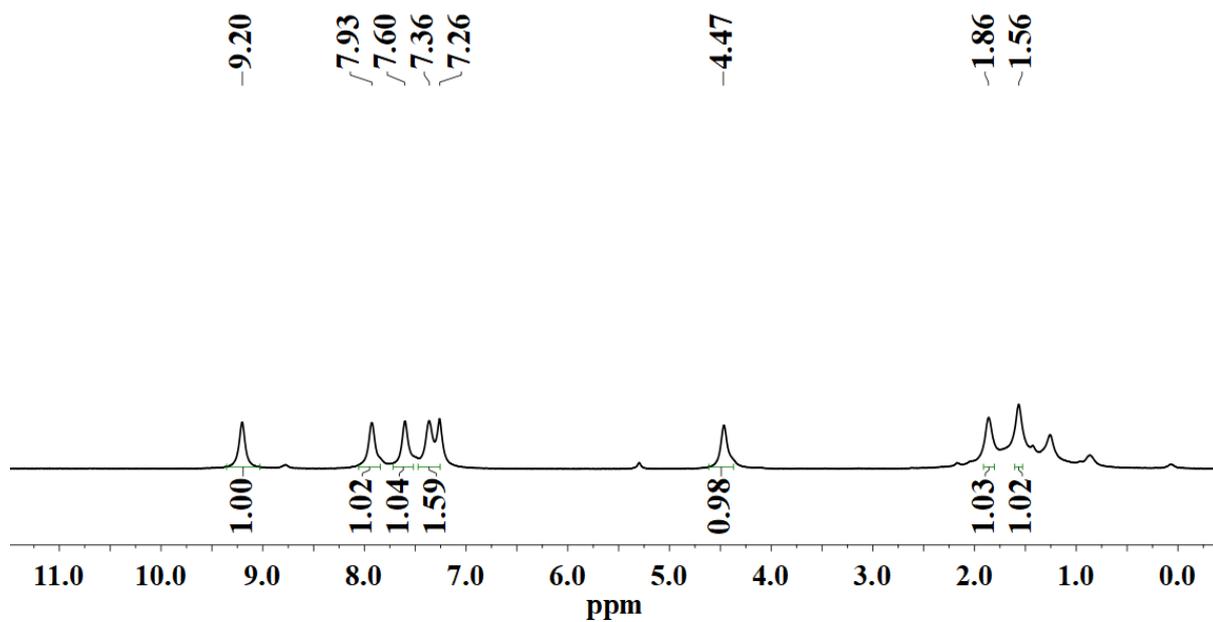


Fig. S4 ^1H NMR spectrum of compound **5** in CDCl_3 .

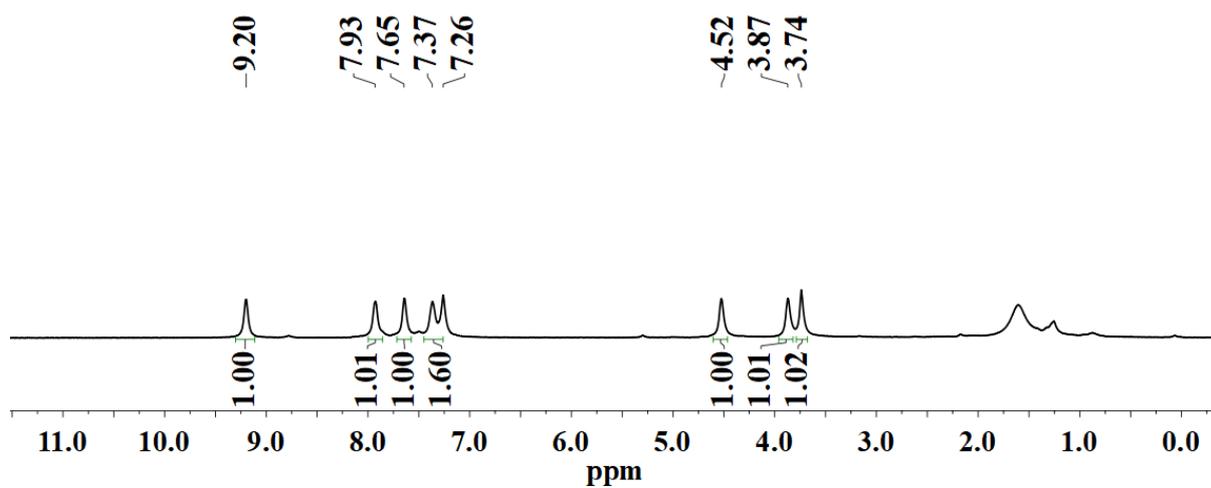


Fig. S5 ^1H NMR spectrum of compound **7** in CDCl_3 .

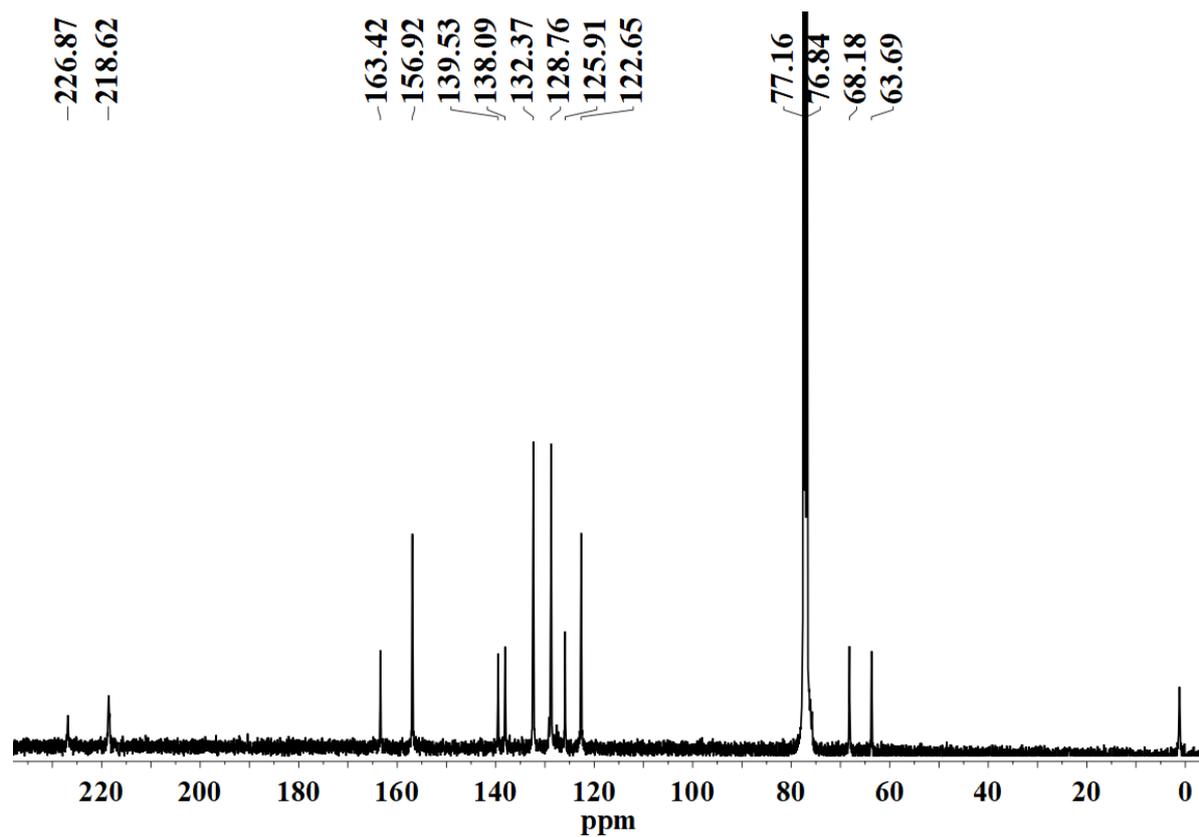


Fig. S6 ^{13}C NMR spectrum of compound **6** in CDCl_3 .

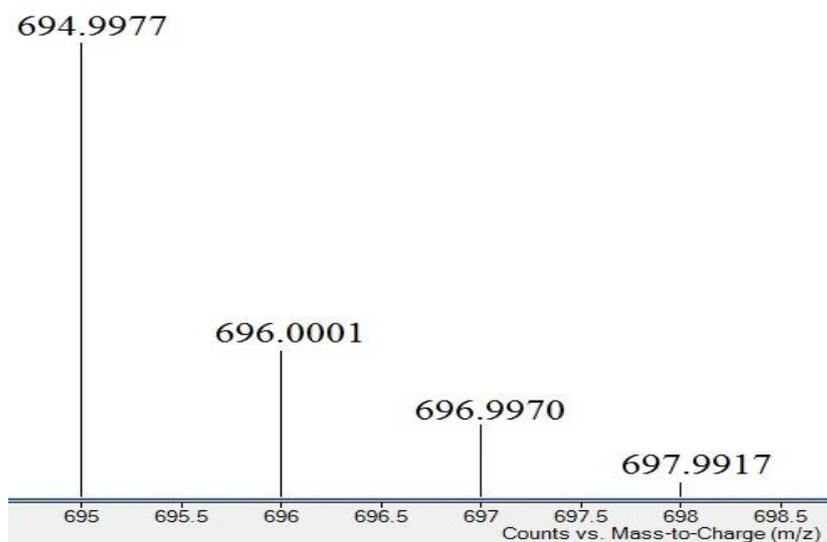
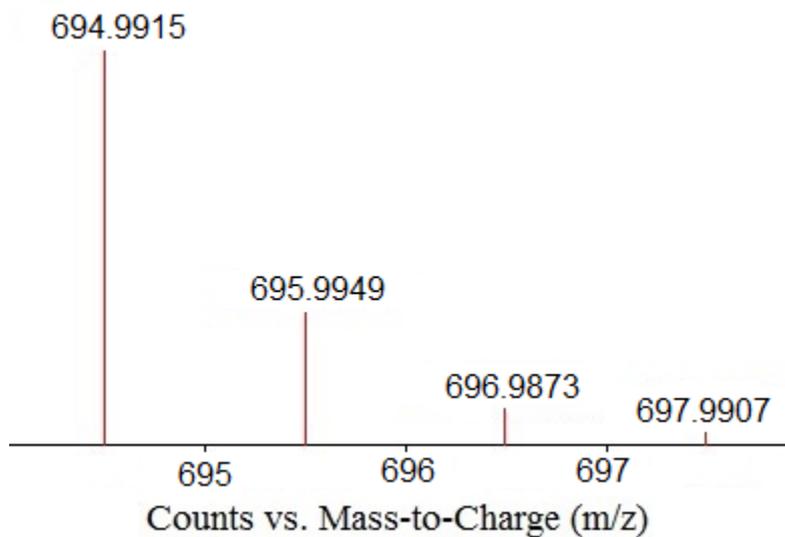


Fig. S7 ESI-MS experimental (bottom) and theoretical (top) isotopic distribution patterns of $[\{(\text{CO})_3\text{Mn}(\mu\text{-SC}_6\text{H}_5)_2\text{Mn}(\text{CO})_3\}(\mu\text{-bpp})]$ (**1**): $[\text{M}+\text{H}]^+$.

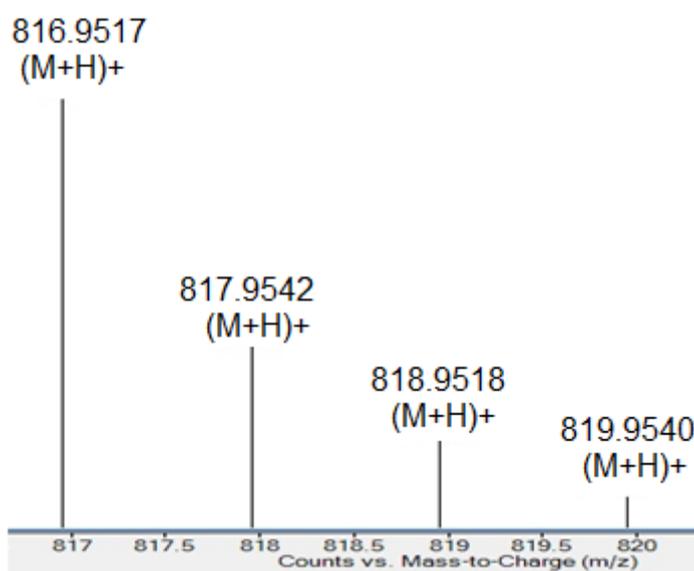
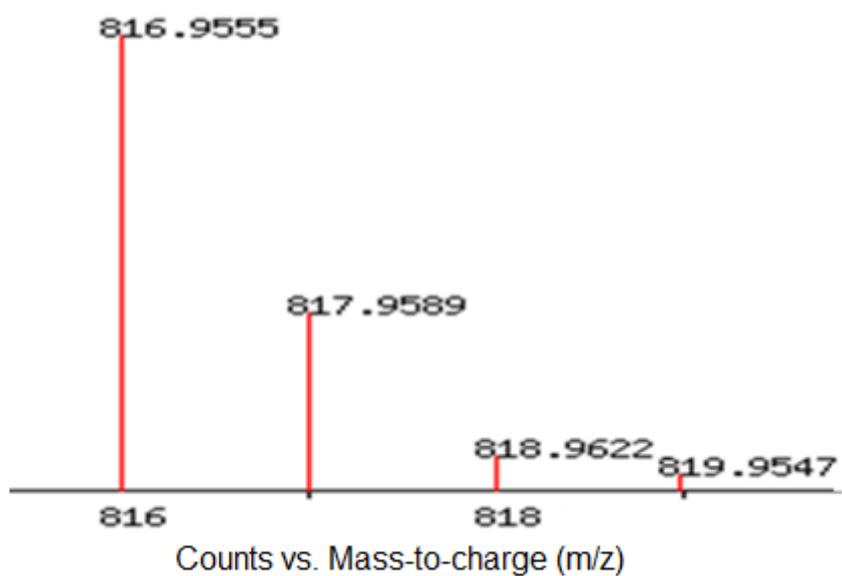


Fig. S8 ESI-MS experimental (bottom) and theoretical (top) isotopic distribution patterns of $[(\text{CO})_3\text{Mn}(\mu\text{-SC}_6\text{H}_5)_2\text{Mn}(\text{CO})_3](\mu\text{-pdi})$ (**2**): $[\text{M}+\text{H}]^+$.

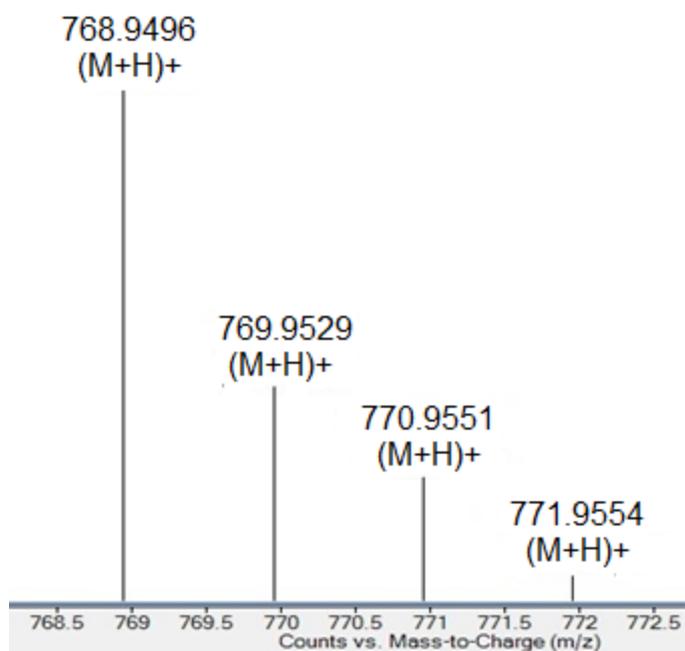
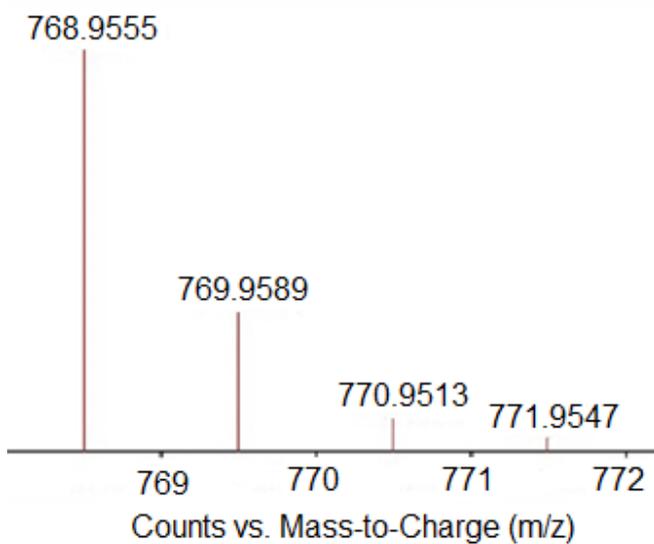


Fig. S9 ESI-MS experimental (bottom) and theoretical (top) isotopic distribution patterns of $[(\text{CO})_3\text{Mn}(\mu\text{-SC}_6\text{H}_5)_2\text{Mn}(\text{CO})_3](\mu\text{-edp})$ (**3**): $[\text{M}+\text{H}]^+$.

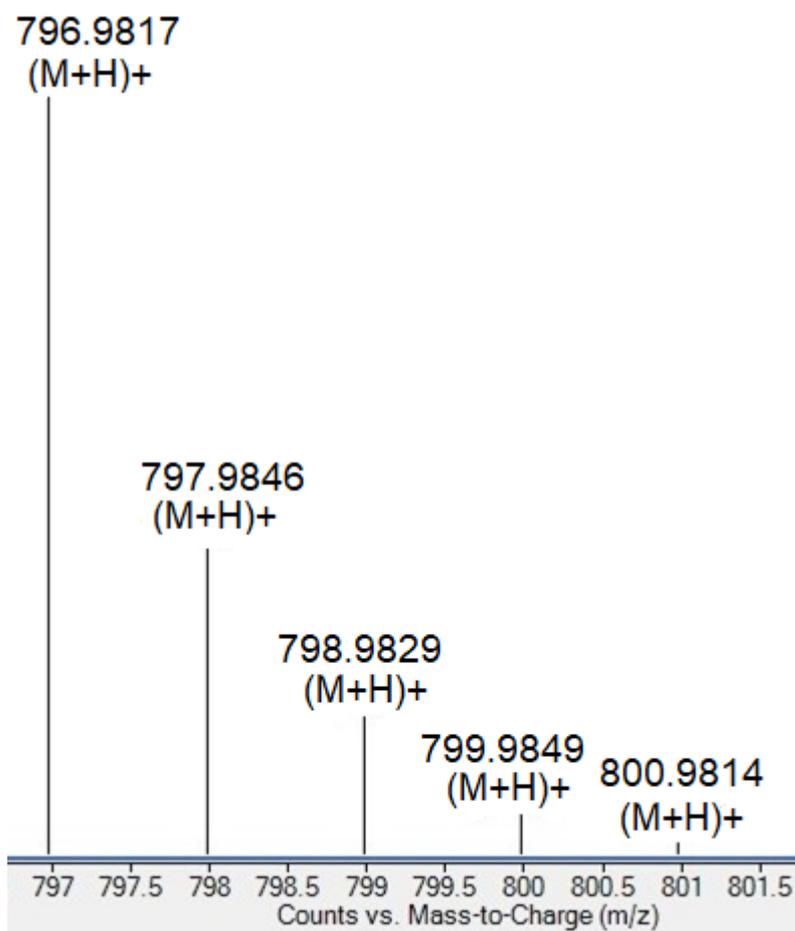
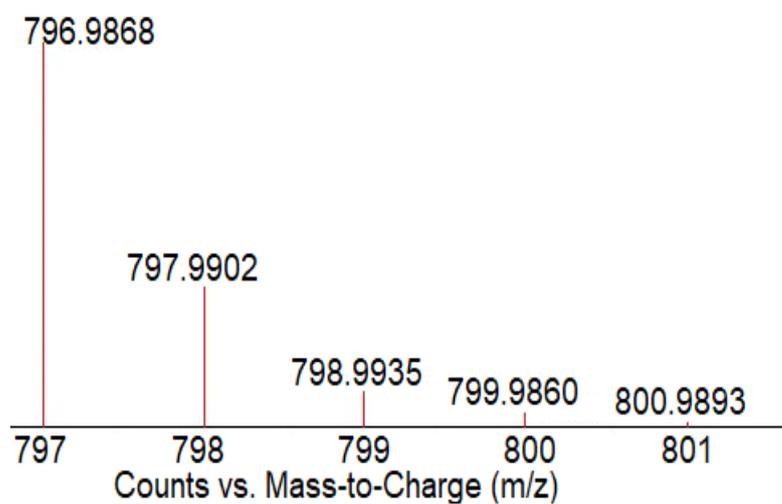


Fig. S10 ESI-MS experimental (bottom) and theoretical (top) isotopic distribution patterns of $[(\text{CO})_3\text{Mn}(\mu\text{-SC}_6\text{H}_5)_2\text{Mn}(\text{CO})_3](\mu\text{-bdp})$ (**4**): $[\text{M}+\text{H}]^+$.

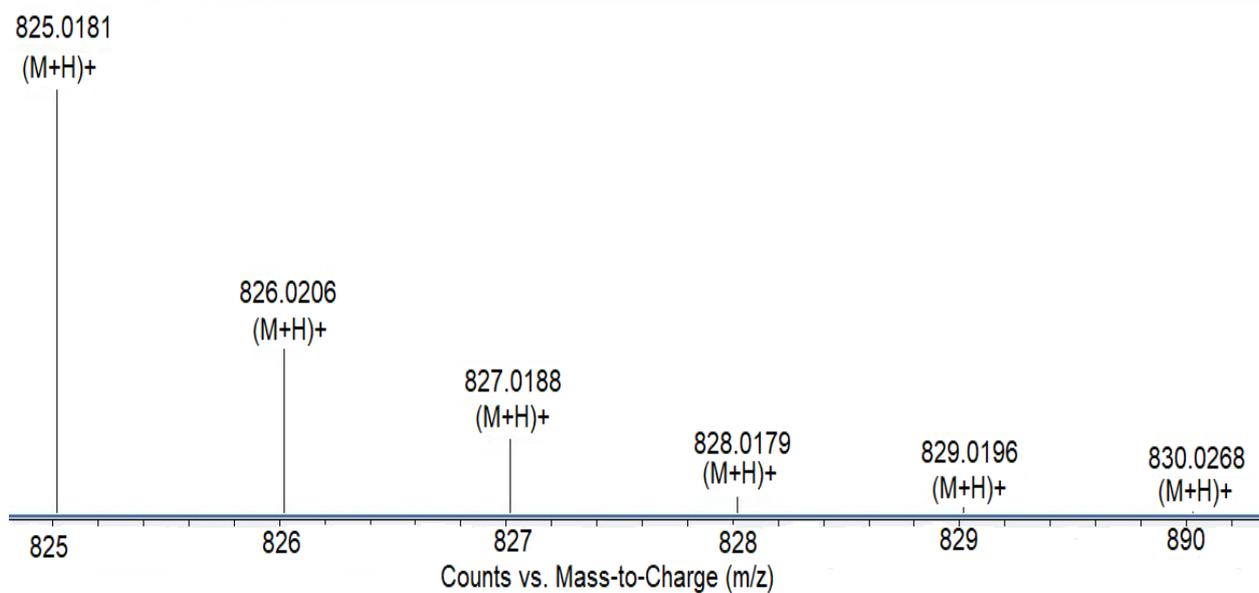
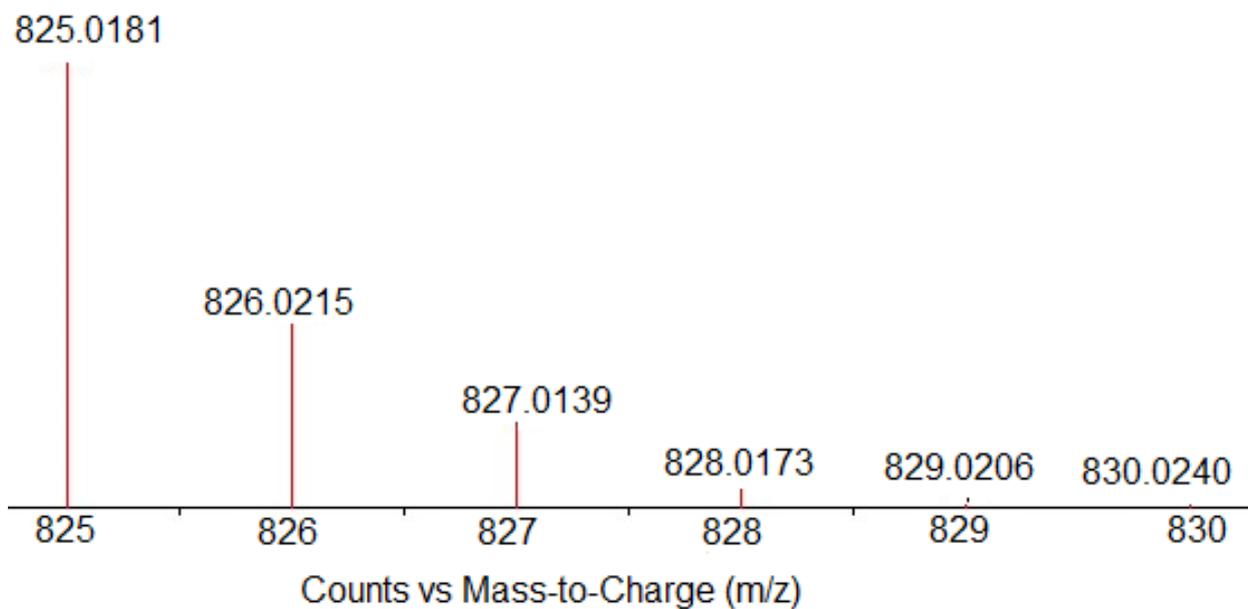


Fig. S11 ESI-MS experimental (bottom) and theoretical (top) isotopic distribution patterns of $[\{(\text{CO})_3\text{Mn}(\mu\text{-SC}_6\text{H}_5)_2\text{Mn}(\text{CO})_3\}(\mu\text{-hdp})]$ (**5**): $[\text{M}+\text{H}]^+$.

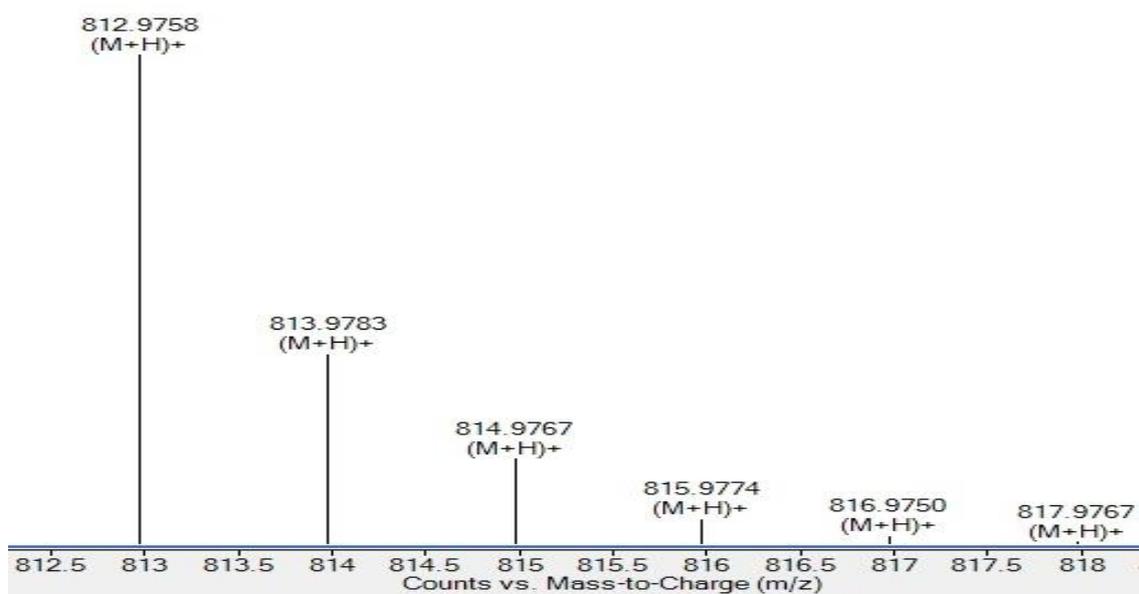
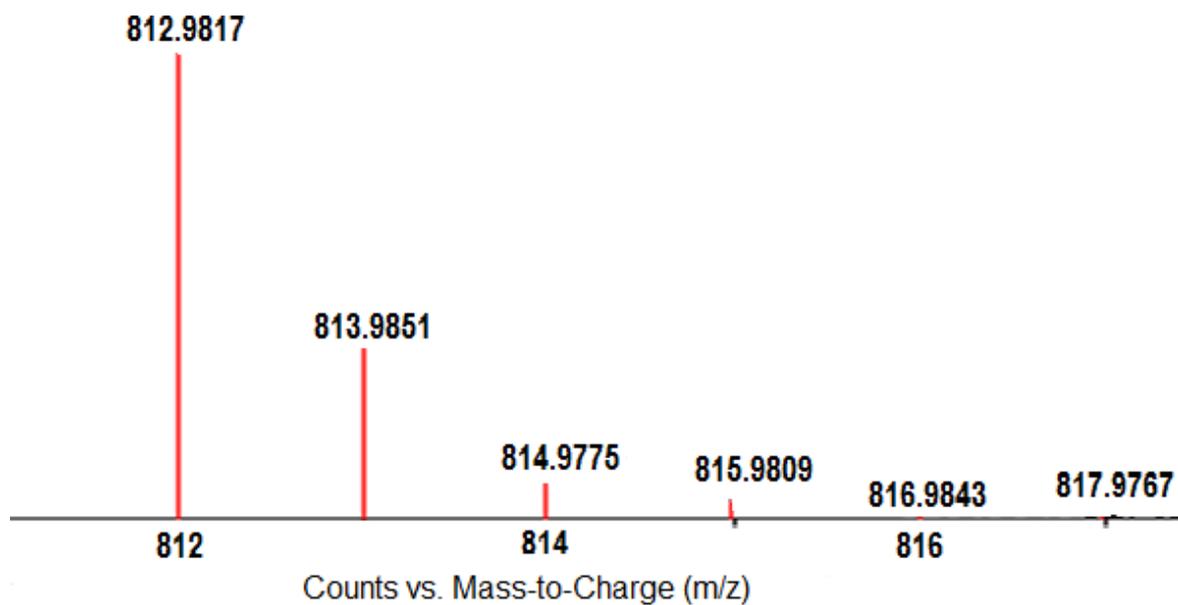


Fig. S12 ESI-MS experimental (bottom) and theoretical (top) isotopic distribution patterns of $[(\text{CO})_3\text{Mn}(\mu\text{-SC}_6\text{H}_5)_2\text{Mn}(\text{CO})_3](\mu\text{-pcadgd})$ (**6**): $[\text{M}+\text{H}]^+$.

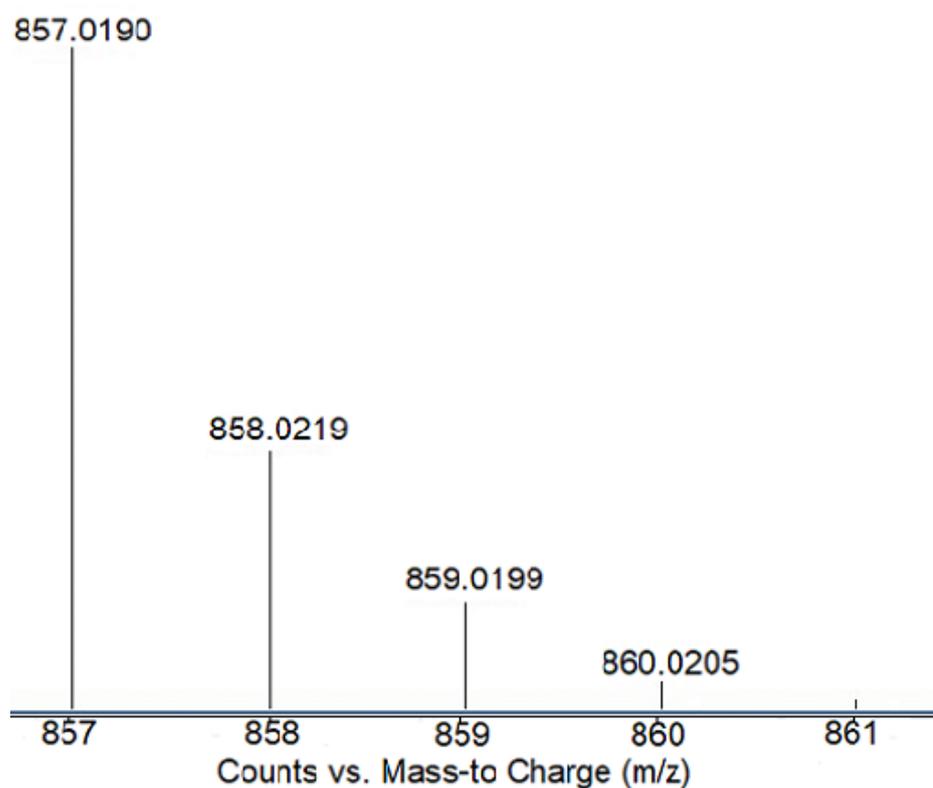
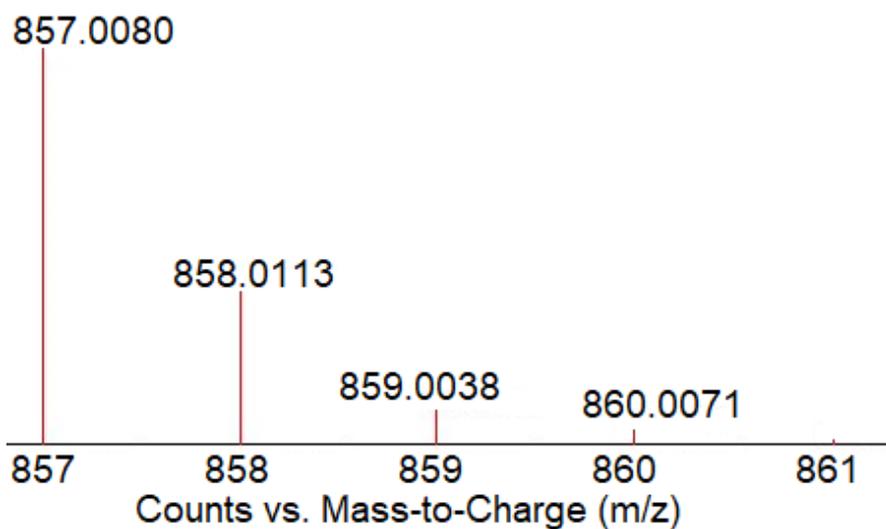


Fig. S13 ESI-MS experimental (bottom) and theoretical (top) isotopic distribution patterns of $[(\text{CO})_3\text{Mn}(\mu\text{-SC}_6\text{H}_5)_2\text{Mn}(\text{CO})_3](\mu\text{-pcatgd})$ (**7**): $[\text{M}+\text{H}]^+$.

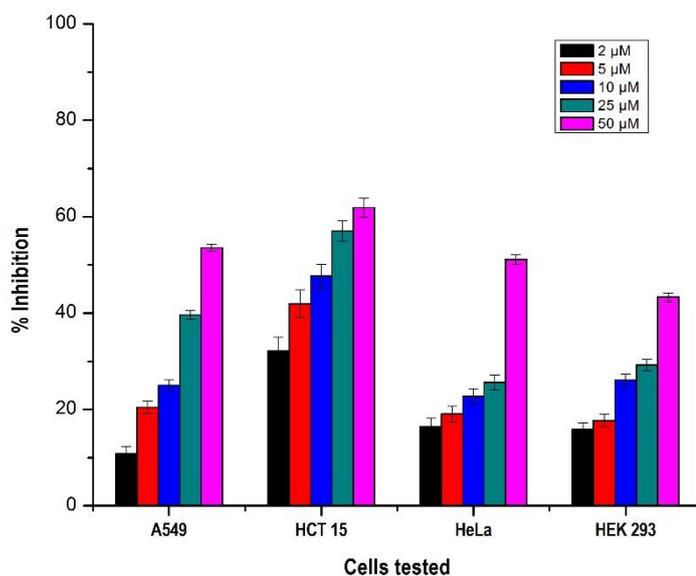


Fig. S14 Cytotoxic activities of different concentrations (2, 5, 10, 25, and 50 μ M) of compound **1** in lung (A549), colon (HCT-15), and cervical (HeLa) cancer cells and normal human embryonic kidney (HEK 293) cells upon 48 h of treatment.

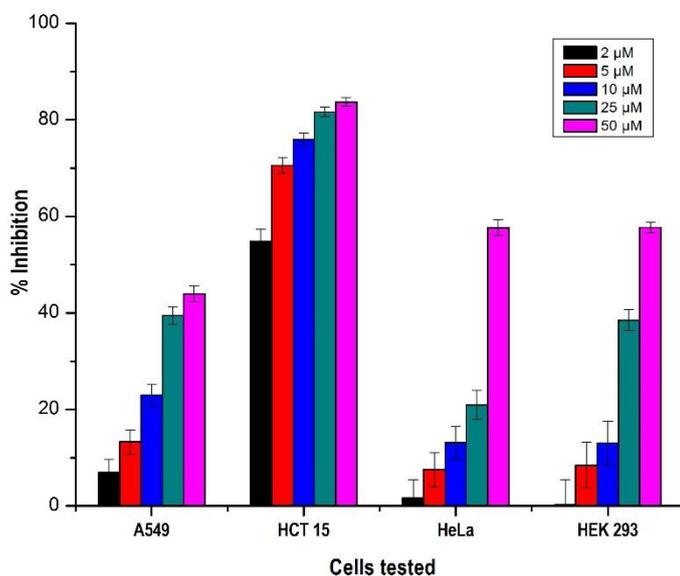


Fig. S15 Cytotoxic activities of different concentrations (2, 5, 10, 25, and 50 μ M) of compound **2** in lung (A549), colon (HCT-15), and cervical (HeLa) cancer cells and normal human embryonic kidney (HEK 293) cells upon 48 h of treatment.

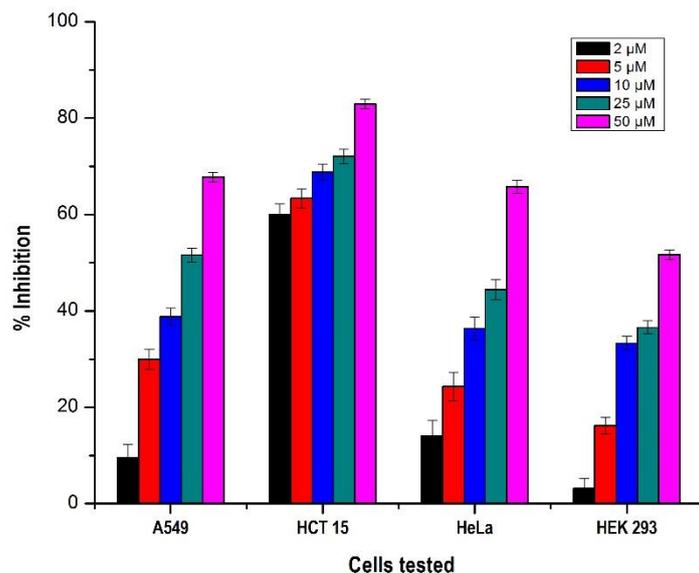


Fig. S16 Cytotoxic activities of different concentrations (2, 5, 10, 25, and 50 μ M) of compound **4** in lung (A549), colon (HCT-15), and cervical (HeLa) cancer cells and normal human embryonic kidney (HEK 293) cells upon 48 h of treatment.

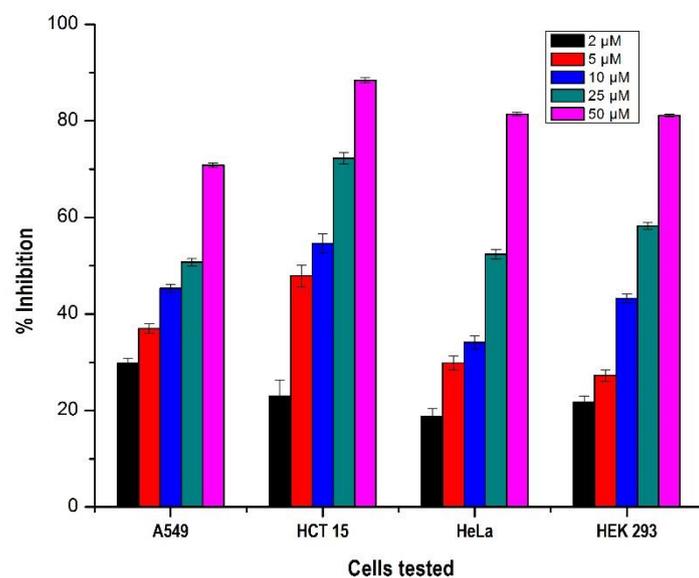


Fig. S17 Cytotoxic activities of different concentrations (2, 5, 10, 25, and 50 μ M) of compound **5** in lung (A549), colon (HCT-15), and cervical (HeLa) cancer cells and normal human embryonic kidney (HEK 293) cells upon 48 h of treatment.

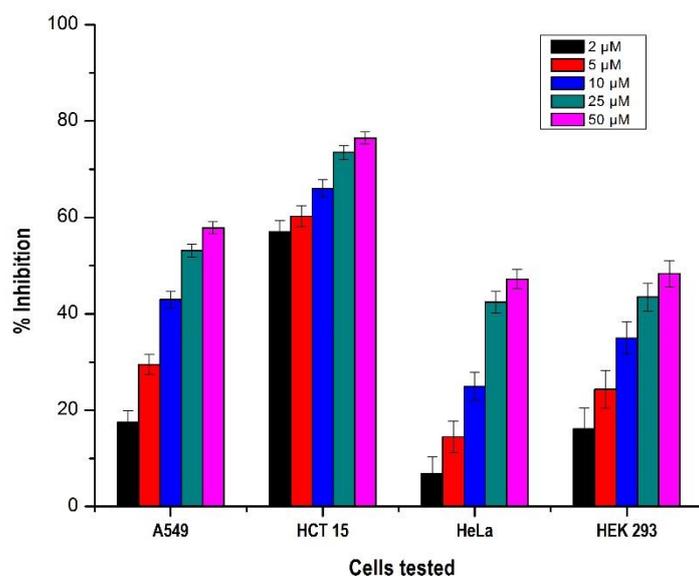


Fig. S18 Cytotoxic activities of different concentrations (2, 5, 10, 25, and 50 μM) of compound **6** in lung (A549), colon (HCT-15), and cervical (HeLa) cancer cells and normal human embryonic kidney (HEK 293) cells upon 48 h of treatment.

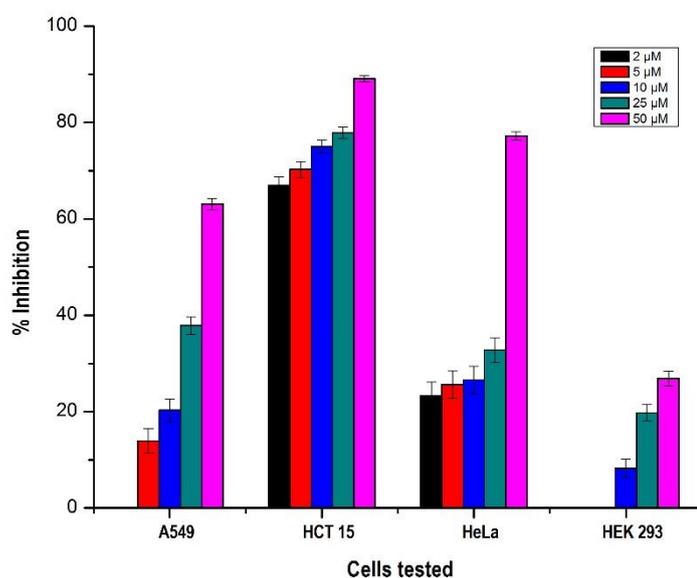


Fig. S19 Cytotoxic activities of different concentrations (2, 5, 10, 25, and 50 μM) of compound **7** in lung (A549), colon (HCT-15), and cervical (HeLa) cancer cells and normal human embryonic kidney (HEK 293) cells upon 48 h of treatment.

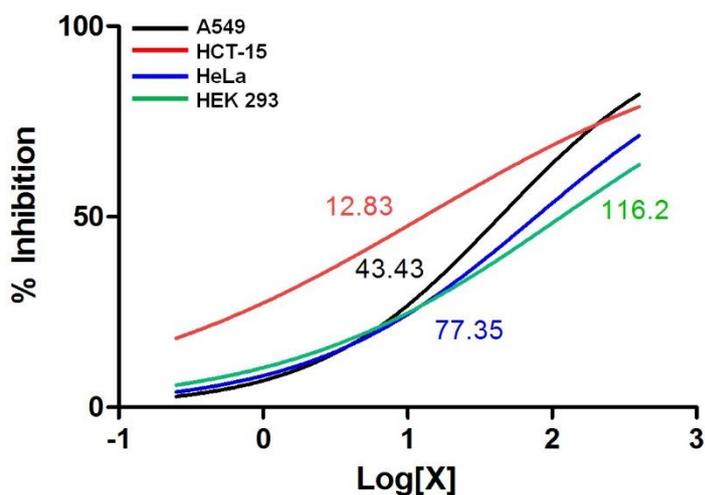


Fig. S20 Dose response curves showing sigmoidal model fit with the deduced IC₅₀ values of compound 1 for lung (A549), colon (HCT-15), cervical (HeLa) and human embryonic kidney (HEK 293) cells.

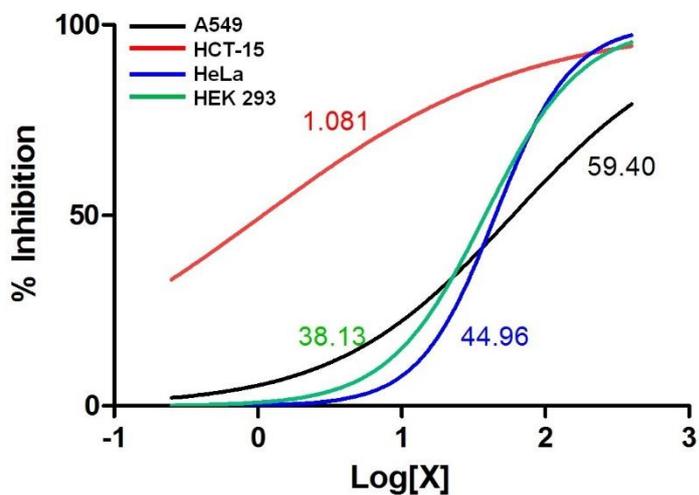


Fig. S21 Dose response curves showing sigmoidal model fit with the deduced IC₅₀ values of compound 2 for lung (A549), colon (HCT-15), cervical (HeLa) and human embryonic kidney (HEK 293) cells.

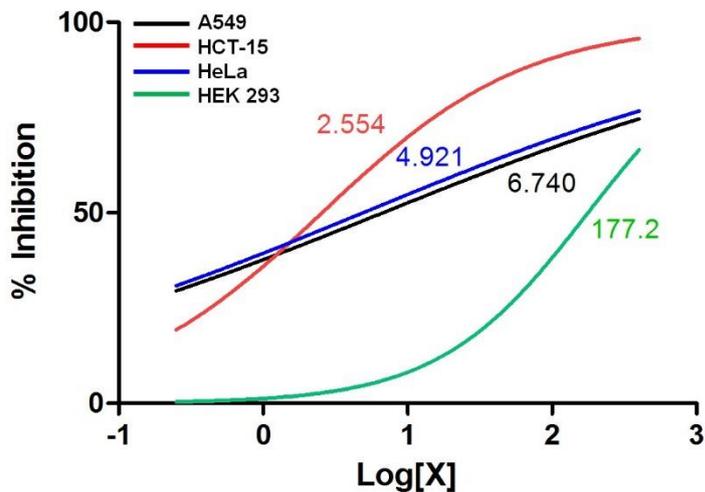


Fig. S22 Dose response curves showing sigmoidal model fit with the deduced IC₅₀ values of compound **3** for lung (A549), colon (HCT-15), cervical (HeLa) and human embryonic kidney (HEK 293) cells.

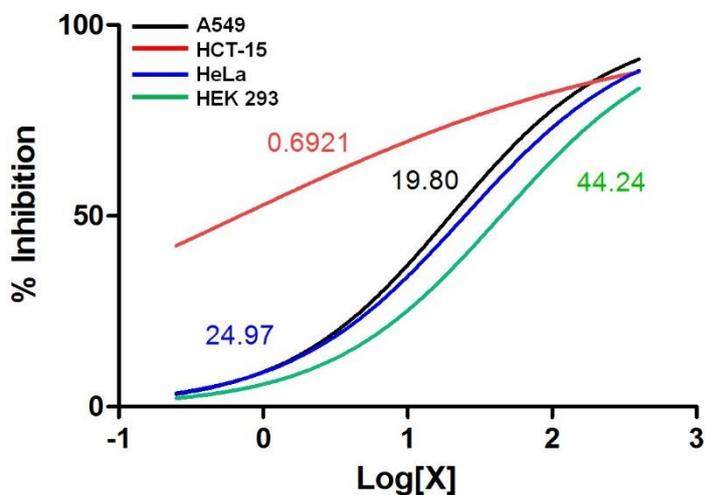


Fig. S23 Dose response curves showing sigmoidal model fit with the deduced IC₅₀ values of compound **4** for lung (A549), colon (HCT-15), cervical (HeLa) and human embryonic kidney (HEK 293) cells.

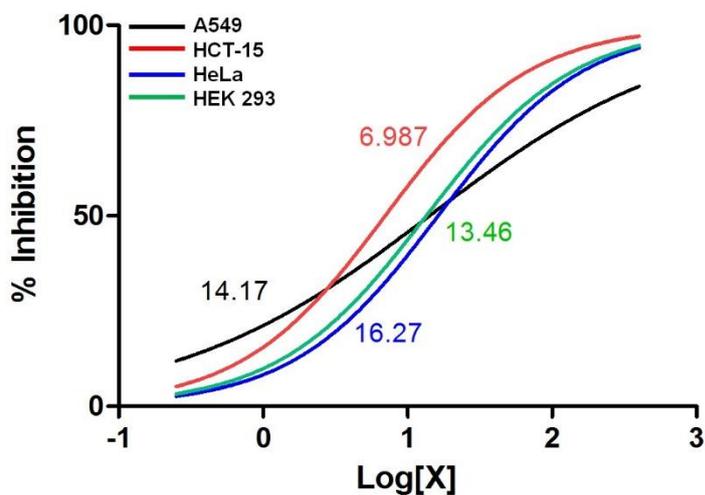


Fig. S24 Dose response curves showing sigmoidal model fit with the deduced IC₅₀ values of compound **5** for lung (A549), colon (HCT-15), cervical (HeLa) and human embryonic kidney (HEK 293) cells.

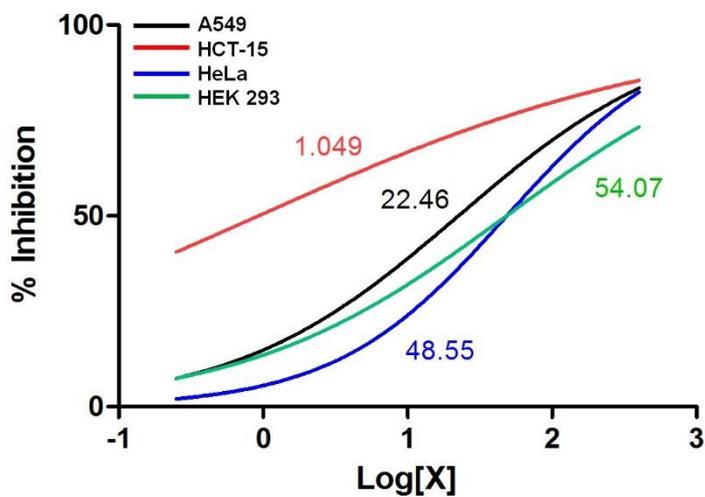


Fig. S25 Dose response curves showing sigmoidal model fit with the deduced IC₅₀ values of compound **6** for lung (A549), colon (HCT-15), cervical (HeLa) and human embryonic kidney (HEK 293) cells.

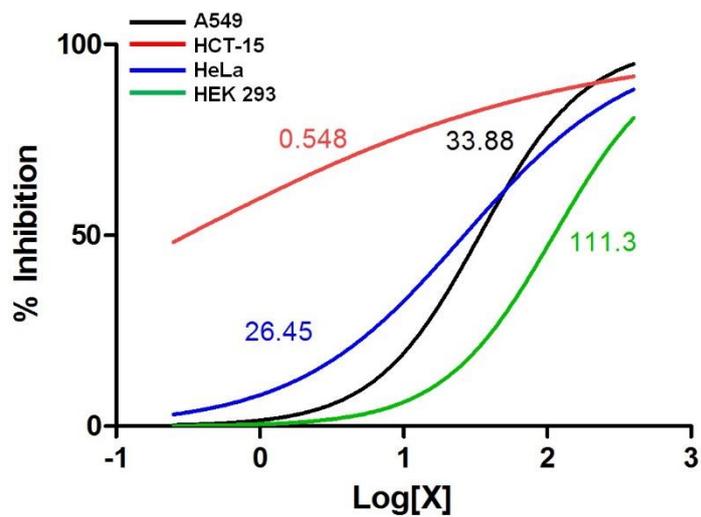


Fig. S26 Dose response curves showing sigmoidal model fit with the deduced IC₅₀ values of compound 7 for lung (A549), colon (HCT-15), cervical (HeLa) and human embryonic kidney (HEK 293) cells.