Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information:

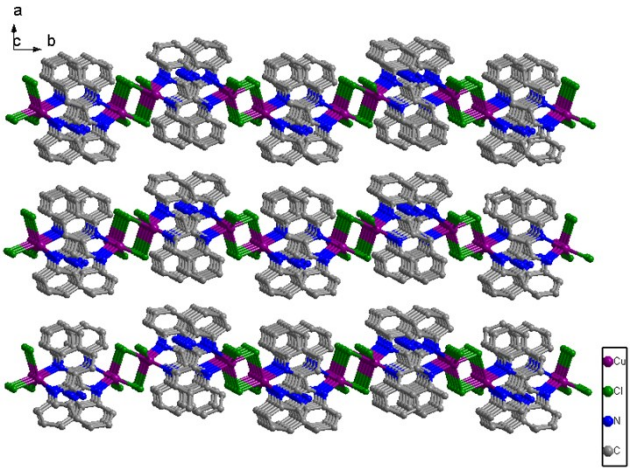

Figure S1 The 3D supramolecular structure of compound **1** stabilized by hydrogen bonds and π–π interactions (all hydrogen atoms are omitted for clarity).

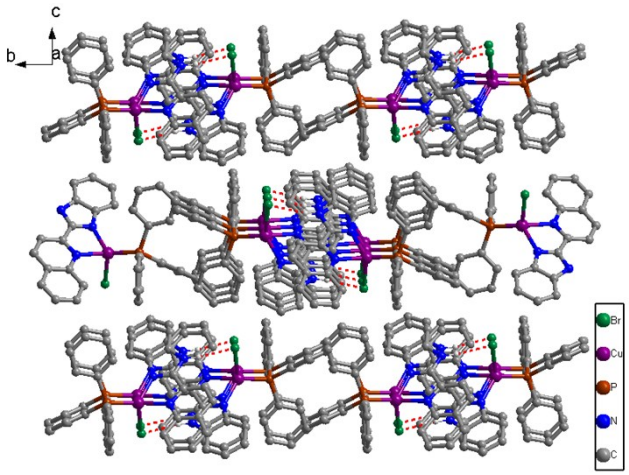

Figure S2 The 3D supramolecular structure of compound **2** stabilized by hydrogen bonds and π–π interactions.

Table S1 HCT116 cells were treated with **1** and **2** at 37 °C for 12 h. Cellular uptake data of Cu in 10^6 tumor cells obtained from three independent measurements for each experiment.

Complex	Cu content (ng)
Control	17.19 ± 0.13
Complex **1**	89.73 ± 0.23
Complex **2**	57.33 ± 0.92

Table S2 HCT116 cells were treated with **1** and **2** at 37 °C for 12 h. Copper content in nucleus, mitochondria and cytoplasm of 10^6 cells were obtained from three independent measurements for each experiment.

	Cu content (ng)		
Complex	Cu in nucleus	Cu in mitochondria	Cu in cytoplasm
Control	8.47 ± 0.14	8.04 ± 0.18	2.18 ± 0.10
Complex **1**	47.60 ± 0.40	12.67 ± 0.20	39.08 ± 0.17
Complex **2**	22.13 ± 0.22	16.43 ± 0.10	26.65 ± 0.13

Table S3 Inhibitory effects of NAC plus **2** on cell viability in HCT116 cells. Cells were treated with NAC (10 mM) for 1 h and then incubated with **2** (5 and 10 μM) for 24 h, and cell viability was obtained by the MTT assay.

Compounds	Cell viability(% of control)
NAC (10 mM)	98.41 ± 1.40
NAC (10 mM) + Complex **2** (5 μM)	80.49 ± 3.42
NAC (10 mM) + Complex **2** (10 μM)	23.83 ± 1.44
Complex **2** (5 μM)	62.94 ± 3.95
Complex **2** (10 μM)	14.63 ± 3.55