Supporting Information

Mo (VI) based Coordination Polymer as antiproliferative agent against cancer cells

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EXPERIMENTAL SECTION.

Single Crystal X-ray Diffraction. For single crystal X-ray diffraction studies, a suitably sized crystal was mounted on a capillary. A BRUKER AXS SMART-APEX three-circle diffractometer with a CCD area detector (Kα = 0.71073 Å, monochromator: graphite) was used for data collection.[1] Frames were collected at T = 293 or 100 K by ω, φ, and 2θ-rotation at 10 s per frame with SAINT.[2] The measured intensities were reduced to F2 and corrected for absorption with SADABS. Structure solution, refinement, and data output were carried out with the SHELXTL program.[3] Non-hydrogen atoms were refined anisotropically. C−H hydrogen atoms were placed in geometrically calculated positions by using a riding model. O−H hydrogen atoms were localized by difference Fourier maps and refined in subsequent refinement cycles. Images were created with the Diamond program.[4] Hydrogen bonding interactions in the crystal lattice were calculated with SHELXTL and Diamond.

Cell cytotoxicity assay. The L929 cell line was used to evaluate the biocompatibility while the other three cancer cell lines (A549, MCF-7 and HepG2) were used to determine the cytotoxicity effect of the synthesized compound by the conventional MTT [3-(4, 5-dimetheylthiazol-2)-2,5 diphenyl tetrazolium bromide] assay. To do so, $1x10^4$ cells/mL were seeded in each well of a 96-well tissue culture plate. After incubation for 24 h at 37°C under 5% CO2, cells were treated with varying concentration of the compound (0.1-25 µmol/L) for a period of 24 and 48 h respectively. For this the 1mmol/L stock solution of the CP **1** was once prepared in PBS (pH = 7.4) and then stored at 4ºC until use. Working solutions were made fresh according to the experiments.

Post-appropriate incubation period, 5 mg/mL of MTT solution in PBS was added to each well and cells were further incubated for 4 hours at 37°C. Following solubilization of the formazan crystals formed using DMSO, the optical density of each well was determined

using a microplate reader (BIO-RAD) at 595 nm. The untreated cells were set as controls. The relative inhibition rate (%) was calculated as [100-(At/Ac)x100]; where At is the absorbance of test samples and Ac is the absorbance of control. For each of the cell line used, all experiments were done in triplicates. GraphPad Prism 6 was used to investigate the statistical significance of the data obtained. The P value <0.05 denotes the data to be statistically significant as determined by two-way ANOVA analysis keeping a 95% confidence interval.

Table S1. Bond valence calculations for $[Mo_2(\mu_2\text{-}O)O_4(2\text{-}pyc)_2(H_2O)]$ (**1**).

			Bond length	**Bond valence**
Ot	O7	Mo1	1.706	1.722
	O8	Mo1	1.695	1.774
	O5	Mo2	1.699	1.754
	O6	Mo2	1.698	1.759
	O00B	Mo2	2.325	0.323
μ_2-O	O9	Mo1	1.884	1.064
		Mo2	1.893	1.039
				2.103

Table S2. H-Bonding interactions in $[Mo_2(\mu_2\text{-}O)O_4(2\text{-}pyc)_2(H_2O)]$ (**1**).

$[Mo_2(\mu_2\text{-}O)O_4(2\text{-}pyc)_2(H_2O)]$ (1)	Distance (Å)
C3 – H3…..O4	2.61
C3 – H3…..O5	2.23
C4 – H4…..O7	2.02
C4 – H4…..O8	2.78
C4 – H4…..O9	2.55
C6 – H6…..O5	2.41
C10 – H10…..Ow	2.91
C11 – H11…..O6	2.15
C11 – H11…..O8	2.44
C12 – H12…..O7	2.91

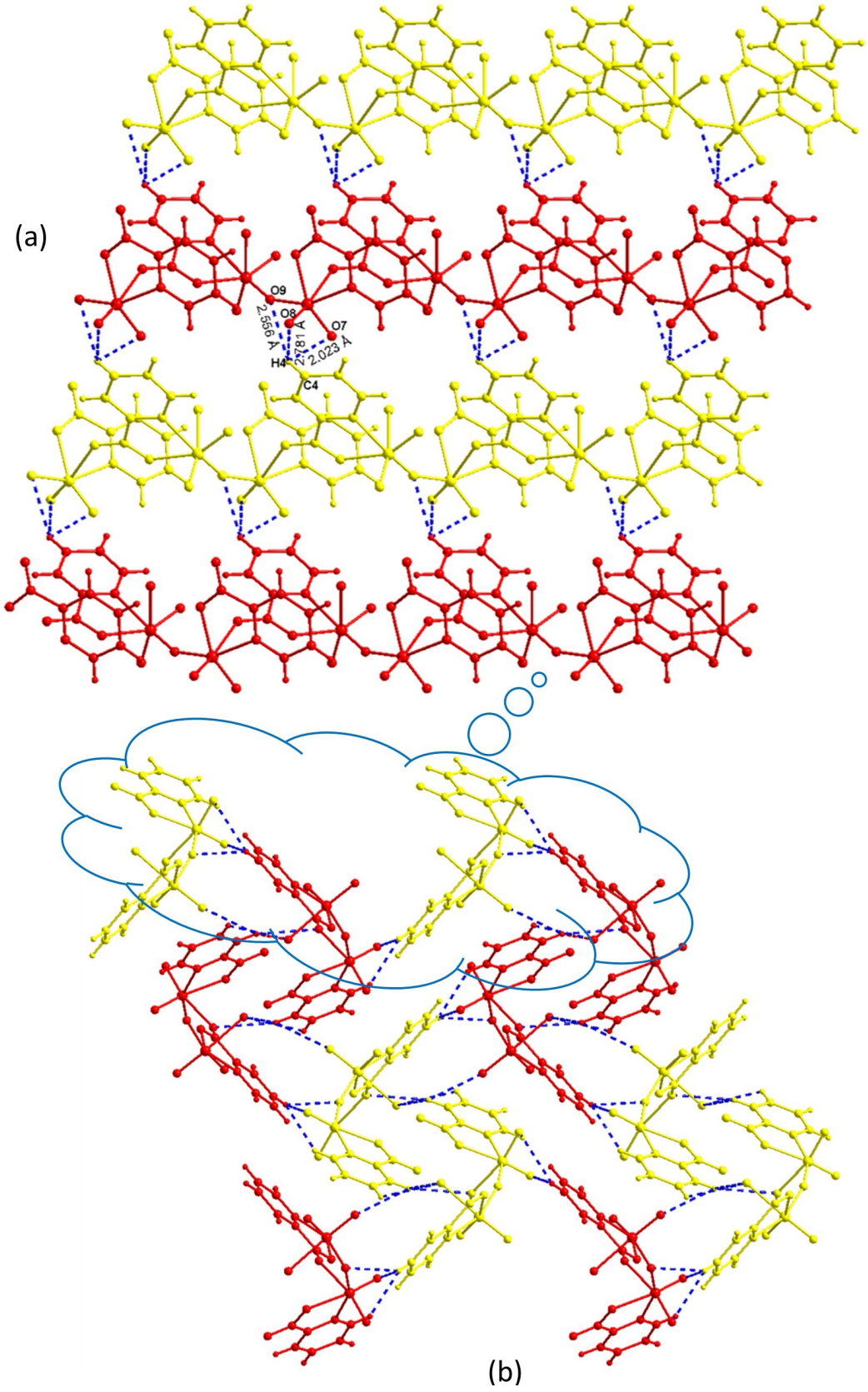

Figure S1. 3D framework structure of $[Mo_2(\mu_2\text{-}O)O_4(2\text{-}pyc)_2(H_2O)]$ (**1**) (b), hydrogen bonding interaction between two adjacent chains (a).

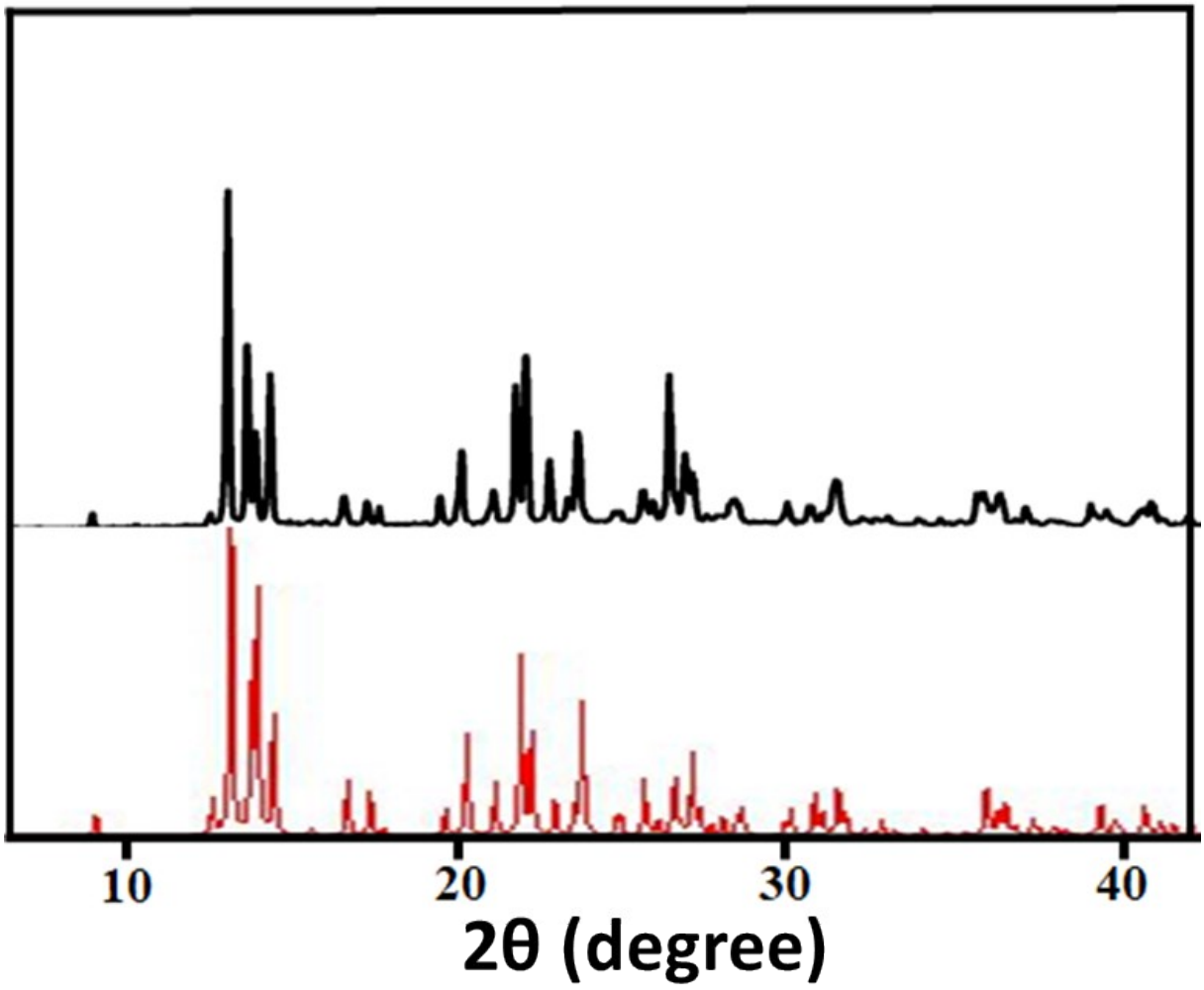

Figure S2. Simulated (red) and experimental (black) XRD patterns of $[Mo_2(\mu_2\text{-}O)O_4(2\text{-}pyc)_2(H_2O)]$ **(1)**.

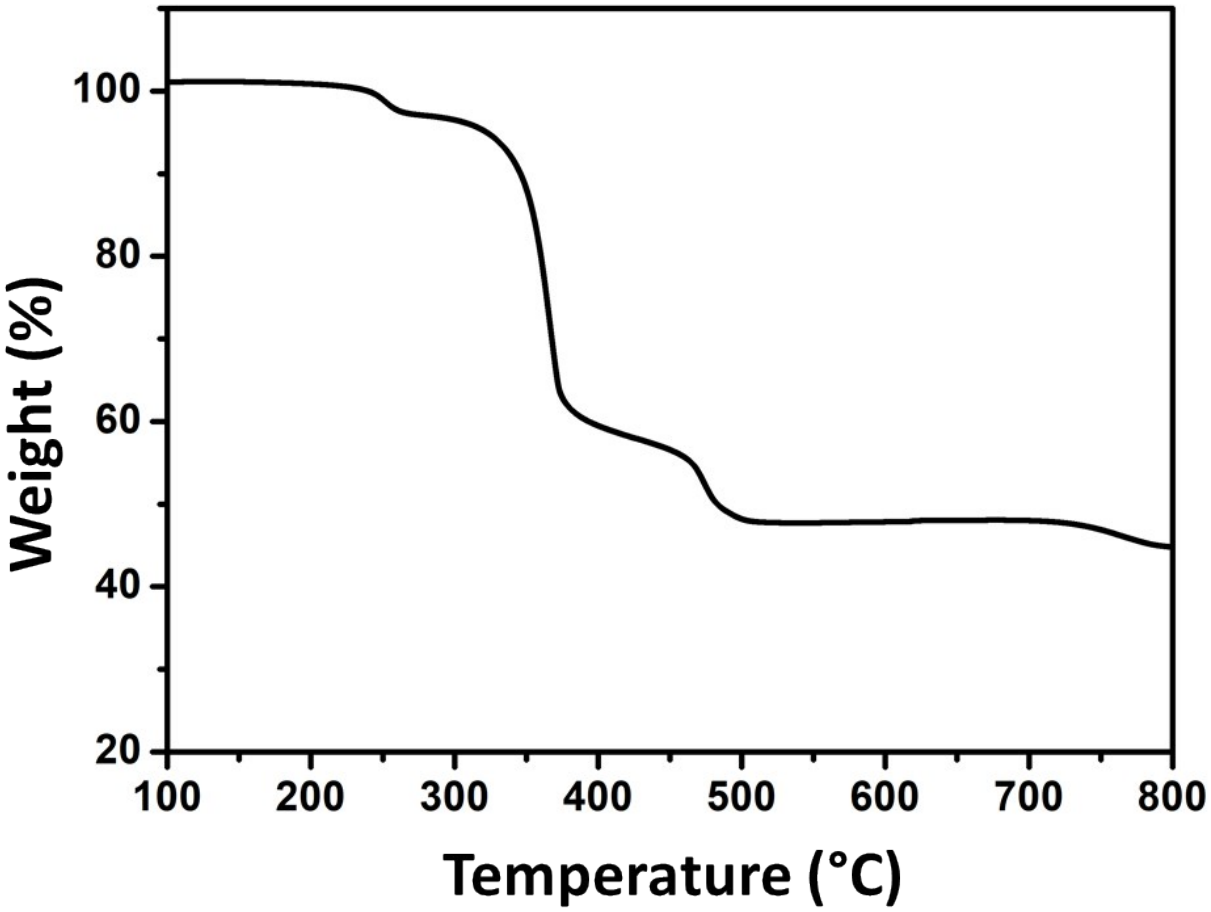

Figure S3. TGA curve of $[Mo_2(\mu_2\text{-}O)O_4(2\text{-}pyc)_2(H_2O)]$ (**1**).

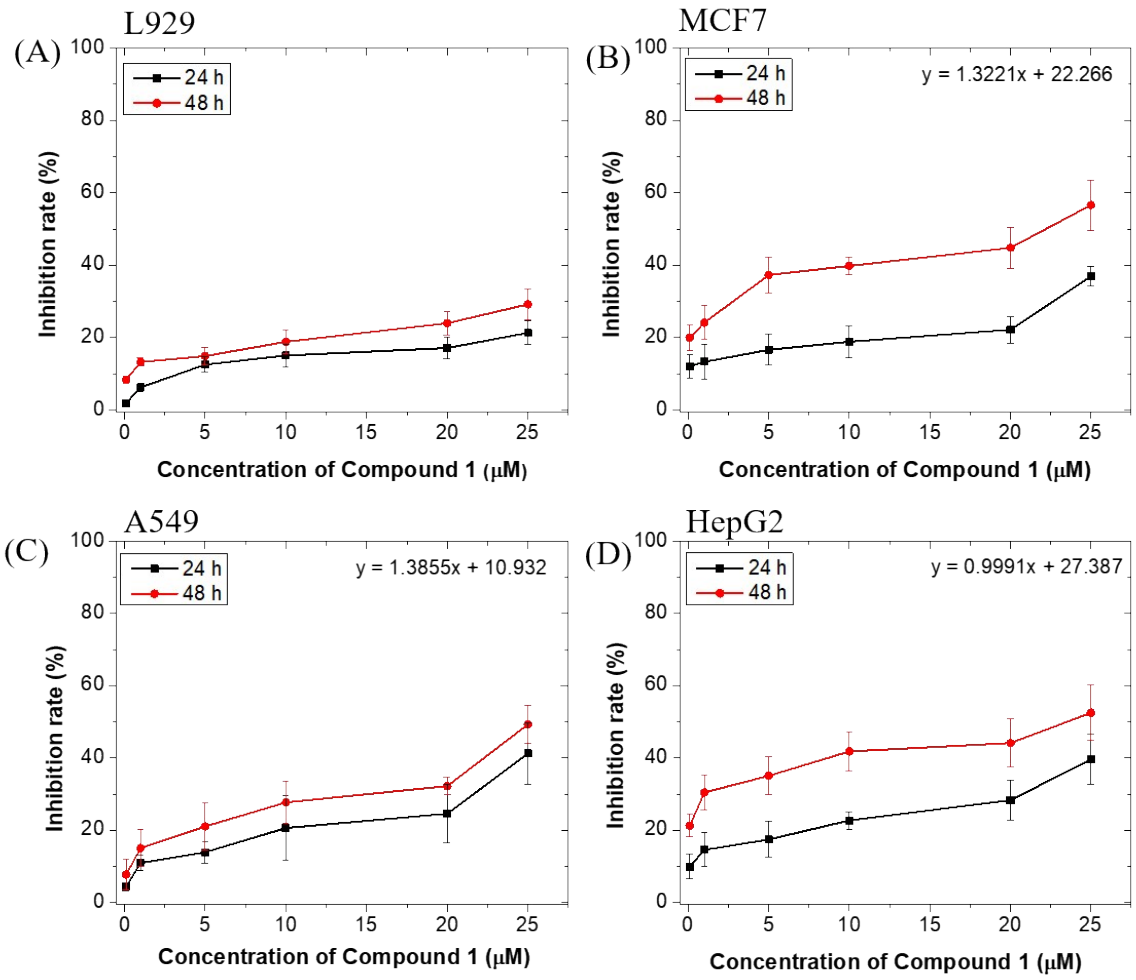

Figure S4. In vitro cytotoxicity assay of the synthesized $[Mo_2(\mu_2\text{-}O)O_4(2\text{-}pyc)_2(H_2O)]$ (1) on (A) L929 (B) MCF-7, (C) A549 and (D) HepG2 cells for 24 h and 48 h. All experiments were performed in triplicates. The equations in graphs (B-D) represents the trendline equation for 48 h used to calculate the IC50 value for the CP for each respective cancer cell line.

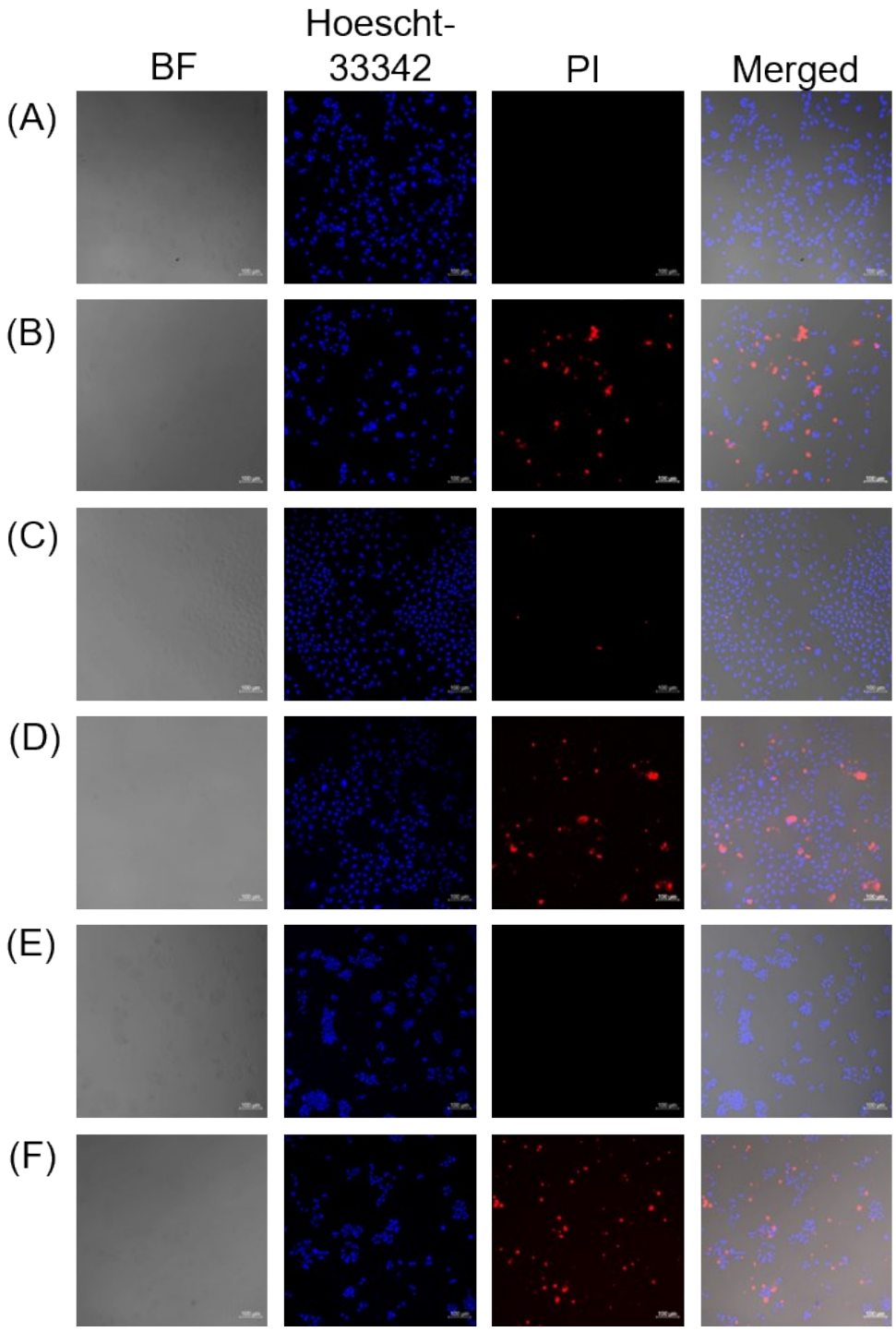

Figure S5. Propidium iodide exclusion assay for MCF-7 (A-B), A549 (C-D) and HepG2 (E-F) cancer cells after treatment with the synthesized CP **1** for 48 h. Controls are represented in A, C and E while cells treated with the compound are represented by B, D and F for the respective cell lines. The nuclei are stained blue using Hoescht-33342 and the cells excluding PI are stained red (Scale bar = 100 μm).

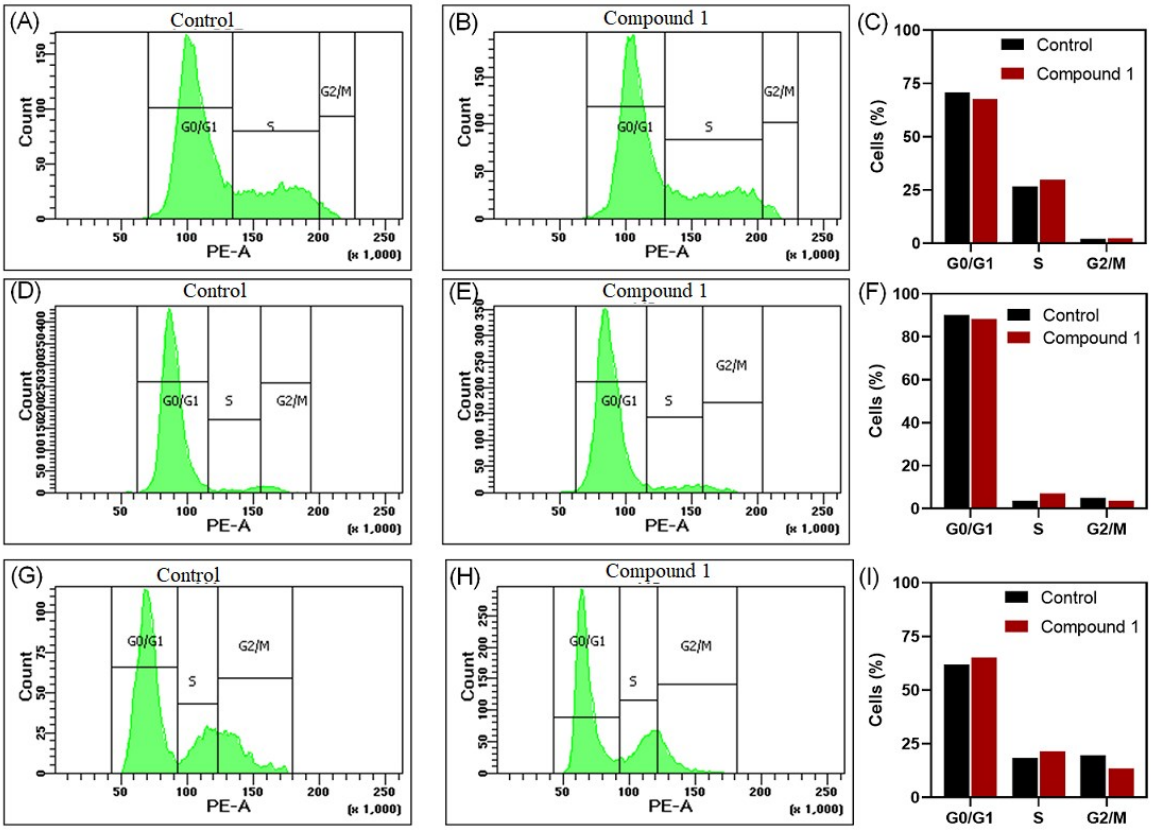

Figure S6. Cell cycle analysis of Compound 1 on MCF-7 (A-C), A549 (D-F) and HepG2 (G-I). (C,F, I) represents percentage of cells arrested in different phases of cell cycle after treatment with Compound 1 for (C) MCF7, (F) A549 and (I) HepG2.

References:

(1) Bruker Analytical X-ray Systems, SMART: Bruker Molecular Analysis Research Tool, Version 5.618; Bruker AXS: Madison, WI, 2000.

(2) Bruker Analytical X-ray Systems, SAINT-NT, Version 6.04; Bruker AXS: Madison, WI, 2001.

(3) Bruker Analytical X-ray Systems, SHELXTL-NT, Version 6.10; Bruker AXS: Madison WI 2000**.**

(4) Klaus, B. DIAMOND, version 1.2c; University of Bonn: Germany, **1999**.