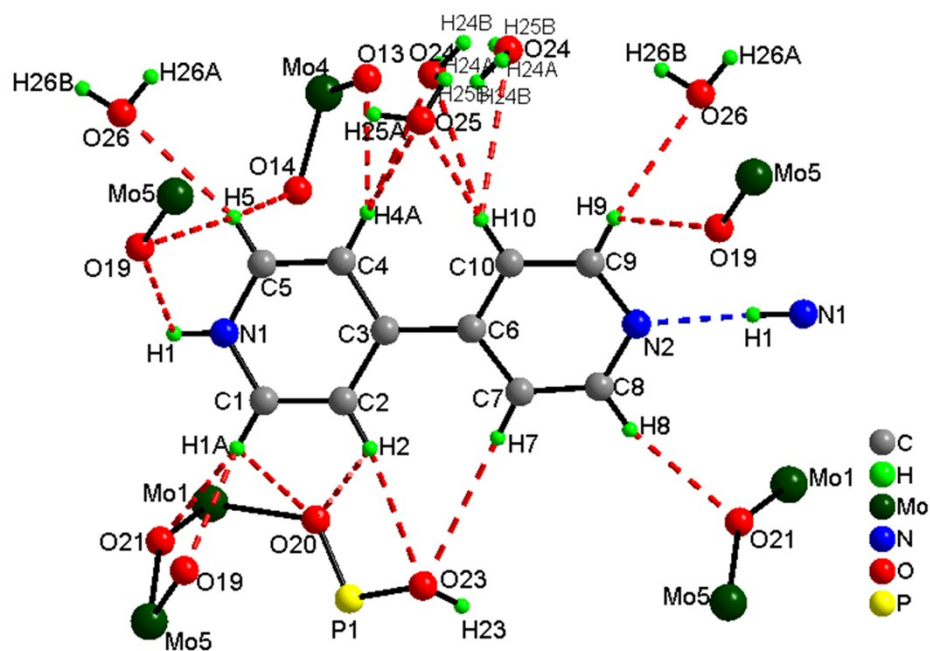


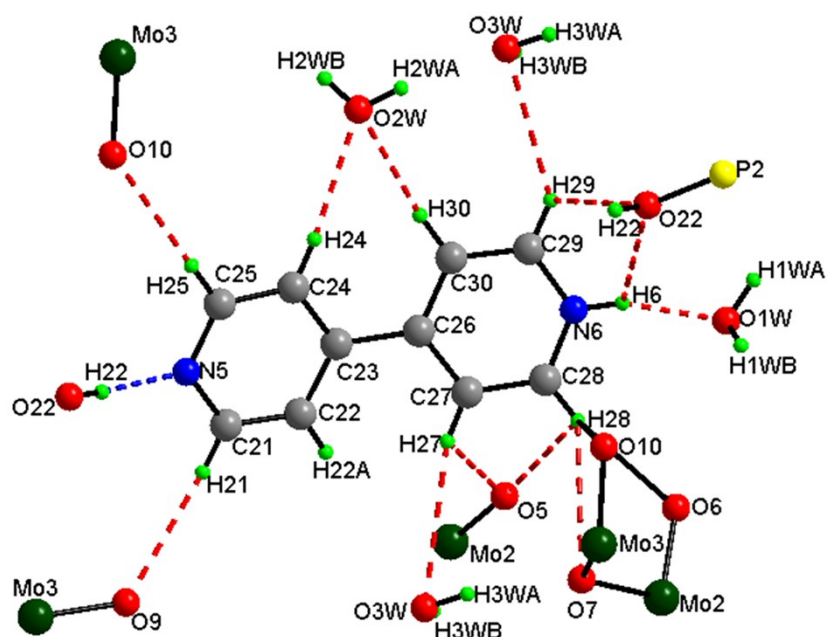
Effective inhibitory activity against MCF-7, A549 and HepG2 cancer cells by phosphomolybdate based hybrid solid

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Supplementary Information



(a)



(b)

Figure S1. H-bonding environment around protonated 4,4'-bpy moieties in $[[4,4'$ - $H_2bpy]\{4,4'$ - $Hbpy\}_2\{H_2P_2Mo_5O_{23}\} \cdot 5H_2O$ (**1**).

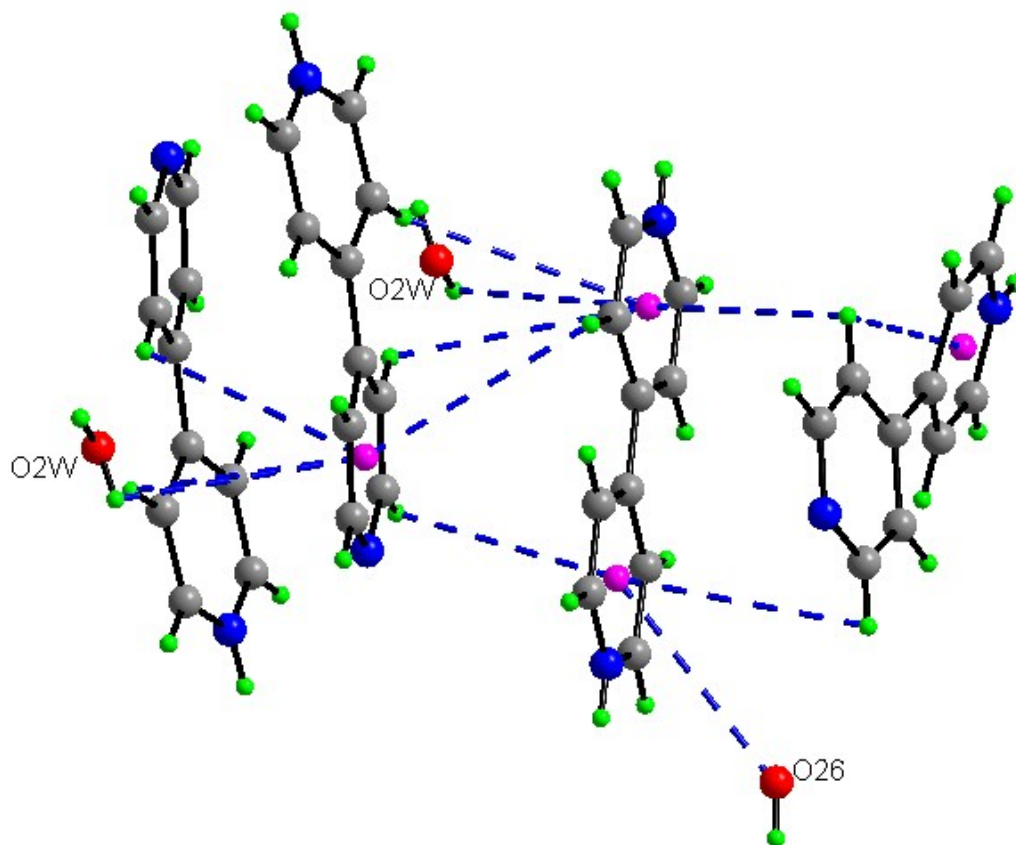


Figure S2. C-H... π and O-H... π interactions among protonated 4,4'-*bpy* molecules and lattice water in $[\{4,4'\text{-H}_2\text{bpy}\}\{4,4'\text{-Hbpy}\}_2\{\text{H}_2\text{P}_2\text{Mo}_5\text{O}_{23}\}]\cdot 5\text{H}_2\text{O}$ (**1**).

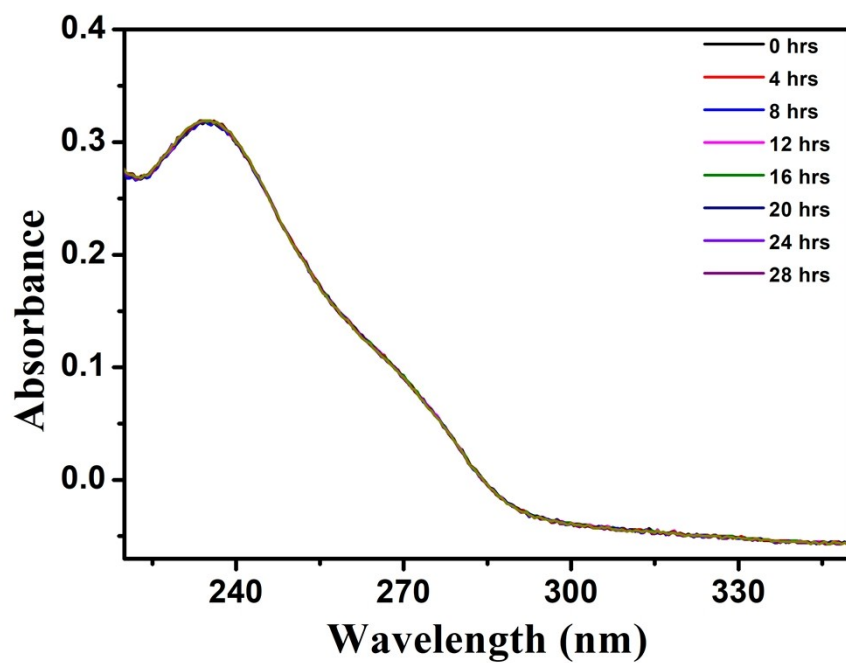


Figure S3. UV-vis spectra of $[[4,4'\text{-H}_2\text{bpy}]\{4,4'\text{-Hbpy}\}_2\{\text{H}_2\text{P}_2\text{Mo}_5\text{O}_{23}\}]\cdot 5\text{H}_2\text{O}$ (**1**) in PBS buffer (pH 7.4) solution at different time intervals.

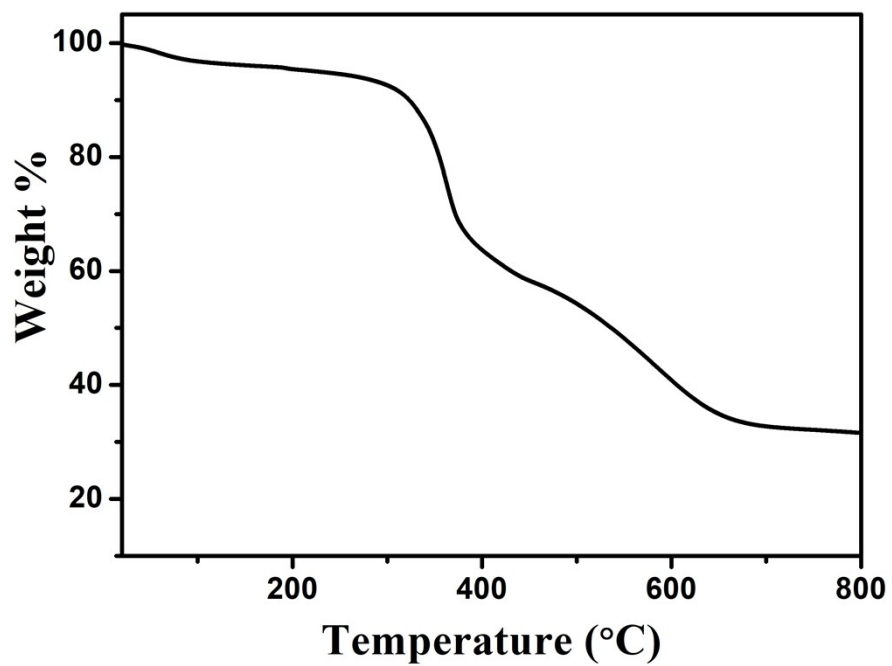


Figure S4. TGA curve of $[[4,4'\text{-H}_2\text{bpy}]\{4,4'\text{-Hbpy}\}_2\{\text{H}_2\text{P}_2\text{Mo}_5\text{O}_{23}\}]\cdot 5\text{H}_2\text{O}$ (**1**).

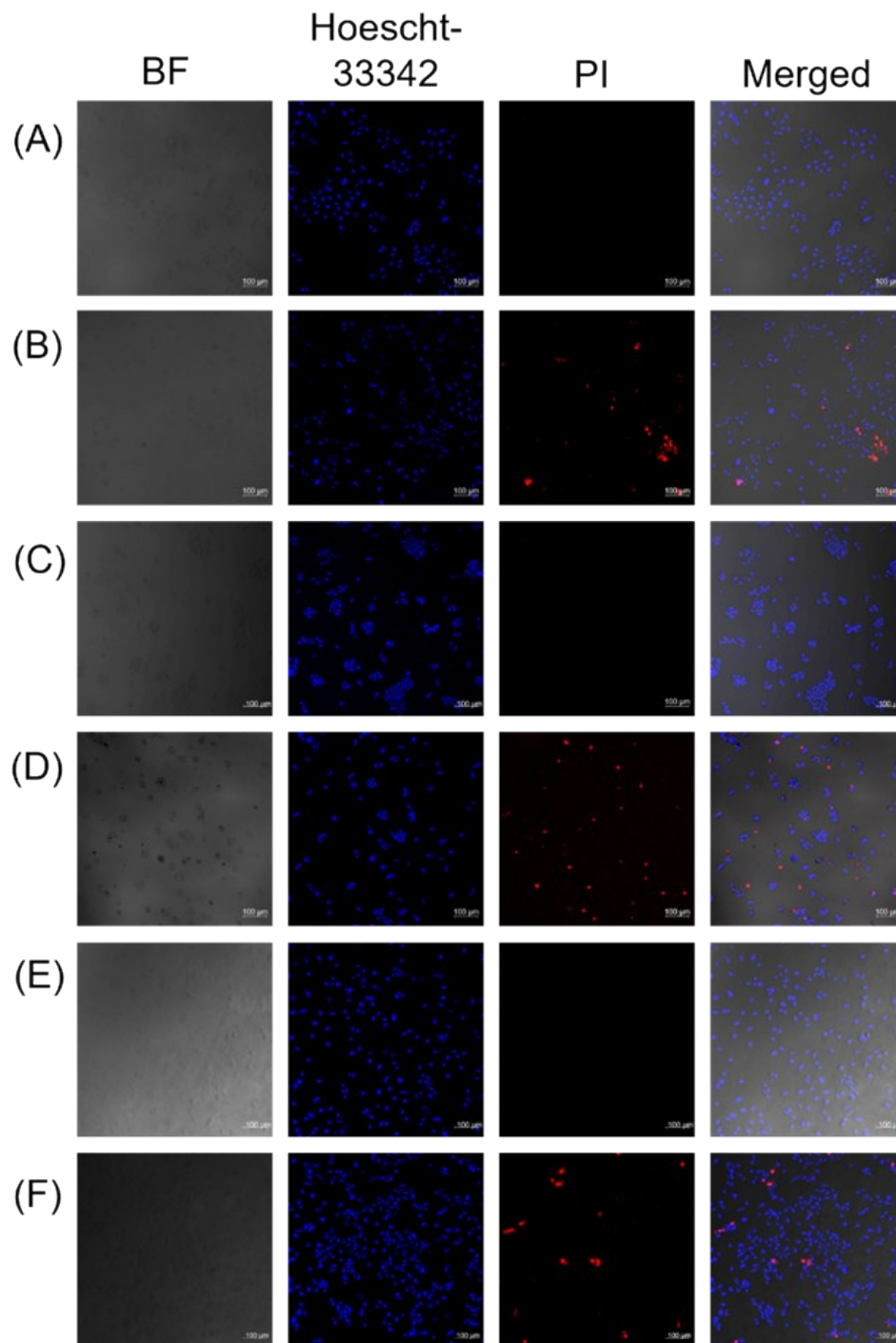


Figure S5. Propidium iodide exclusion assay for A549 (A and B), HepG2 (C and D) and MCF7 (E and F) cells after treatment with the synthesized compound for 24 h (B, D and F) with respect to the controls (A, C and E). The nuclei are stained blue using Hoescht-33342, the cells excluding PI are stained red and BF represents brightfield images of cells (Scale bar = 100 μ m).

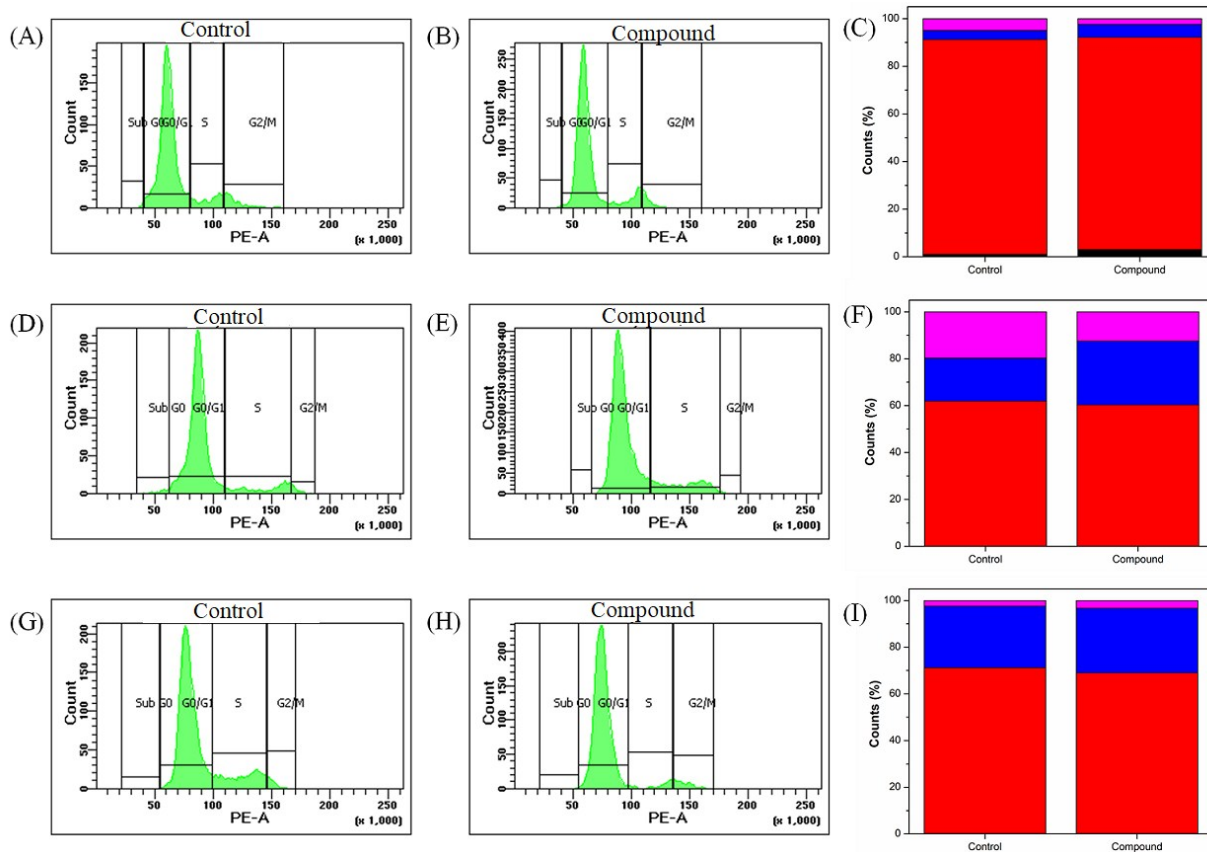


Figure S6. Cell cycle analysis of A549 (A-C), HepG2 (D-F) and MCF-7 (G-I) on treatment with the synthesized Compound. Sub-G0 phase is represented in black, G0/G1 phase is represented in red, S phase is represented in blue and G2/M phase is represented in magenta (C, F and I).

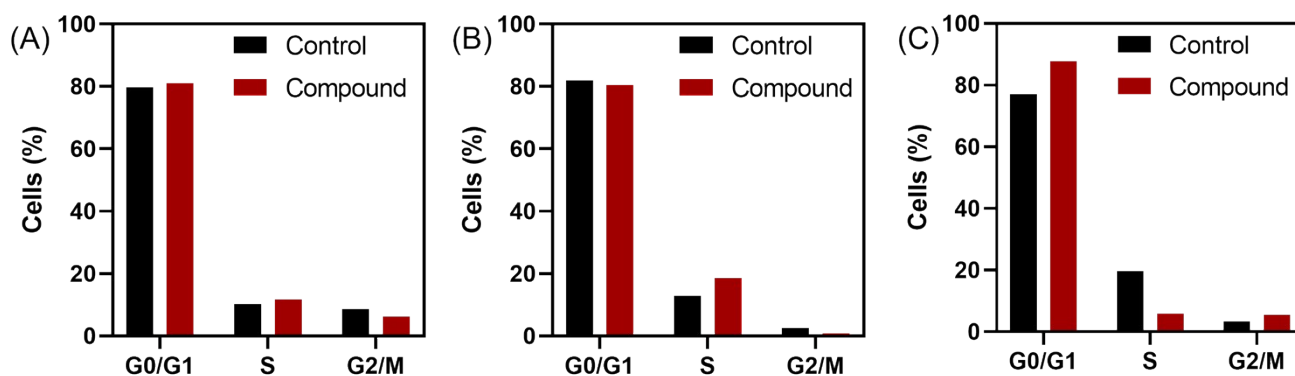


Figure S7. Percentage of cells arrested in different phases of cell cycle after treatment with Compound 1 for (A) A549, (B) HepG2 and (C) MCF-7 cancer cells.

Table S1. H-bonding interactions for $[\{4,4'-H_2bpy\}\{4,4'-Hbpy\}_2\{H_2P_2Mo_5O_{23}\}]\cdot 5H_2O$ (**1**)

Bond (H...A)	Distance (Å)	Bond (H...A)	Distance (Å)	Bond (H...A)	Distance (Å)
N1 – H1.....O19	2.741	C10 – H10.....O25	2.242	C24 – H24.....O _{2W}	2.399
N1 – H1.....N2	2.002	C11 – H11.....O14	2.258	C27 – H27.....O _{3W}	2.931
N3 – H3.....O17	2.776	C11 – H11.....O2	2.529	C29 – H29.....O _{3W}	2.884
N3– H3.....O14	2.677	C12 – H12.....O1	2.675	C30 – H30.....O _{2W}	2.406
N3– H3.....O15	1.901	C12 – H12.....O2	2.458	O1w–H1WA.....O1	1.994
N3– H3.....O26	2.751	C21 – H21.....O1	2.528	O1w–H1WB.....O1	2.894
N4– H4.....O6	2.864	C14 – H14.....O11	2.299	O2w–H2WB.....O9	2.127
N4– H4.....O20	2.714	C15 – H15.....O18	2.696	O3w–H3WB.....O6	2.174
N4– H4.....O2	3.053	C15 – H15.....O17	3.055	O4w–H4WB.....O10	2.011
N4– H4.....O3	1.828	C15 – H15.....O25	2.308	C30–H30...π	3.823
N5.....H22–O22	1.764	C15 – H15.....O24	2.836	C24–H24...π	3.777
N6– H6.....O22	2.983	C17 – H17.....O1	2.348	C24–H24...π	3.826
C1– H1A.....O20	2.770	C18 – H18.....O6	2.629	C7–H7...π	3.677
C1 – H1A.....O21	2.728	C19 – H19.....O14	2.750	C7–H7...π	3.773
C1 – H1A.....O19	2.420	C19 – H19.....O2	2.450	C9–H9...π	3.904
C2 – H2.....O23	2.754	C20 – H20.....O9	3.043	O26.... π	3.956
C2 – H2.....O20	2.866	C20 – H20.....O11	2.539	C25–H25...π	3.729
C4 – H4A.....O13	2.725	C20 – H20.....O14	2.467	O2w–H2WA..... π	3.777
C4 – H4A.....O24	2.863	C21 – H21.....O9	2.659	O2w–H2WB..... π	3.624
C4 – H4A.....O25	2.835	C22 – H22.....O17	2.789		
C5 – H5.....O26	2.607	H24B.....O13	2.186		
C5 – H5.....O19	2.721	H24A.....O13	2.197		
C5 – H5.....O14	2.952	C25 – H25.....O10	2.508		