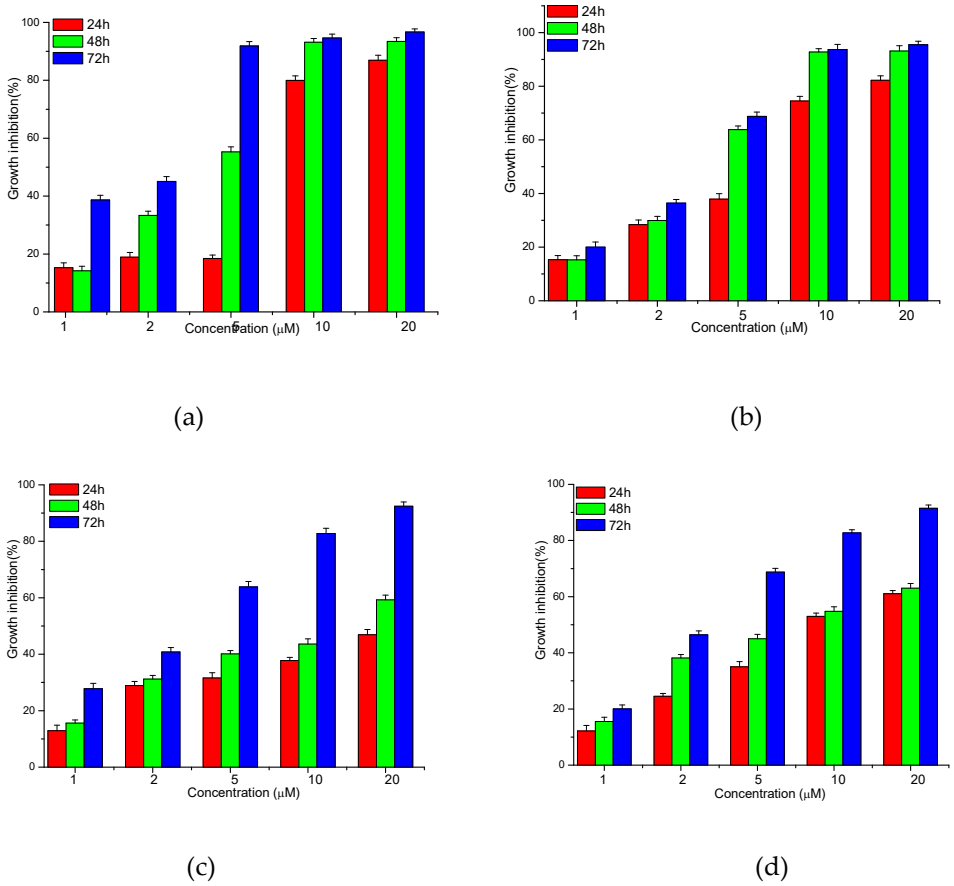

Figure S1. Time-dependent growth inhibition of **7c** and **7d** on H22 and S180 cell lines. Cells were cultured for 24–72h at concentrations of 1–20 μM. (a)**7c**, H22; (b)**7c**, S180; (c) **7d**, H22; (d) **7d**, S180.

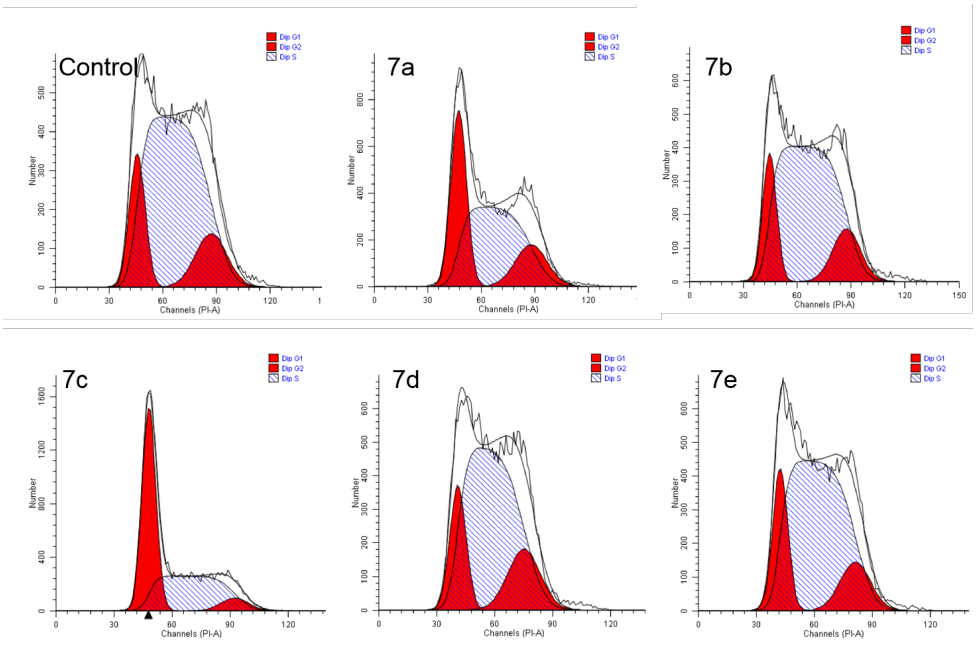

Figure S2. Cell cycle inhibition in H22 cell line by treating with compounds **7a**–**7e** for 48 h.

Table S1. Cell cycle analysis by flow cytometry of H22 cells treated with compounds **7a–7e** for.48 h.

Sample	Distribution (%)		
	G1	S	G2/M
Control	15.32	72.42	12.26
7a	32.02	52.83	15.15
7b	15.44	71.86	12.70
7c	51.22	42.48	6.30
7d	16.10	68.24	15.66
7e	17.21	71.04	11.75

Table S2. Docking statistics of synthesized compounds **7a–7e** against DNA-Top I.

Compound	Glide Score	Glide Energy	H-bonding Ligand/ Receptor	π-π Interaction
CPT	-8.704	-88.330	N of quinoline group/ H of ARG364; H of hydroxyl group / O of ASP533	CPT/TGP11 and DT10 of DNA
7a	-9.614	-98.615	O of carbonyl group / H of TYR426; H of ammonium group / O of GLU356	Aromatic group of compound/TGP11 of DNA
7b	-9.999	-108.058	O of carbonyl group / H of MET428; H of ammonium group / O of LEU356	Aromatic group of compound/TGP11 of DNA
7c	-8.793	-104.546	O of carbonyl group / H of TYR426; Cl of mustard nitrogen / H of DC111	Aromatic group of compound/TGP11 and DT10 of DNA
7d	-8.920	-110.507	O of carbonyl group / H of ASN352; Cl of mustard nitrogen / H of DC111	Aromatic group of compound/TGP11 and DT10 of DNA
7e	-9.565	-93.638	O of carbonyl group / H of ASN352; H of ammonium group / O of GLU356	Aromatic group of compound/TGP11 of DNA