

# *In vitro* anticancer screening and preliminary mechanistic study of A-ring substituted anthraquinone derivatives

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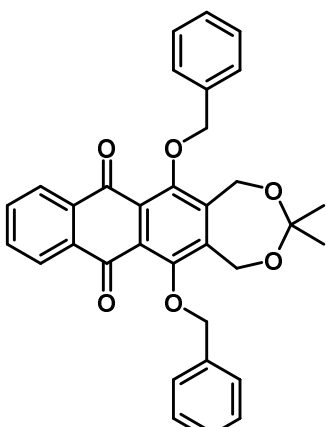
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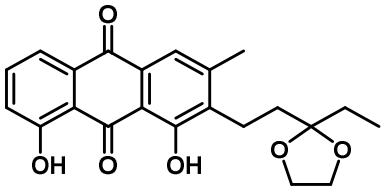
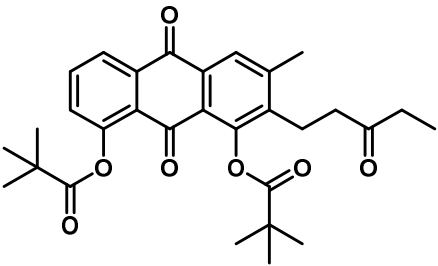
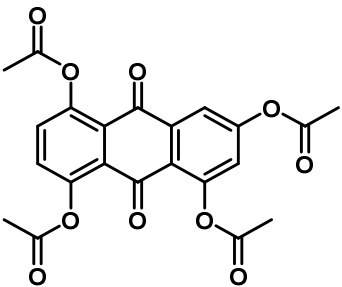
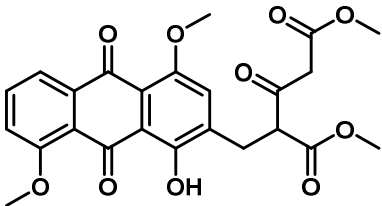
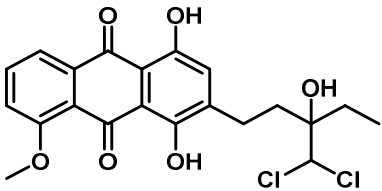
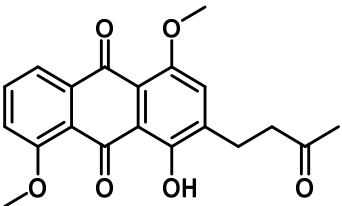
## Supporting Information

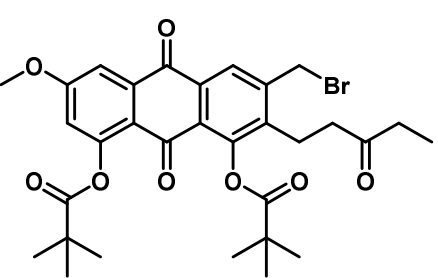
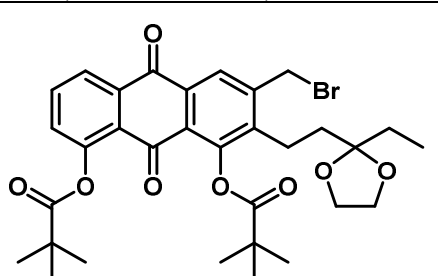
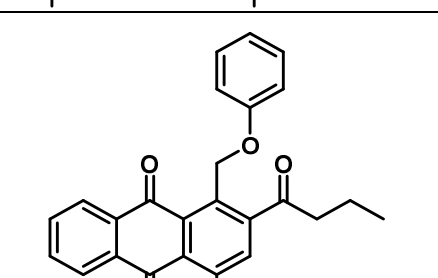
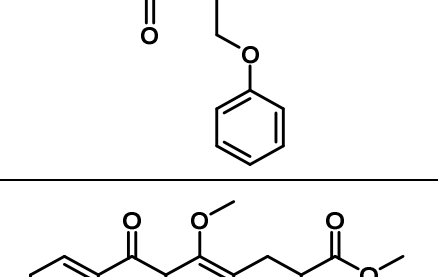
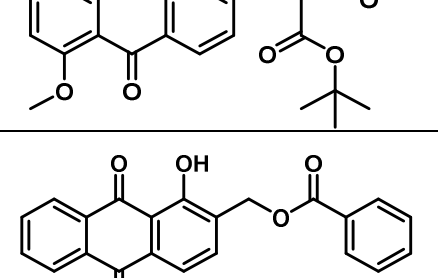
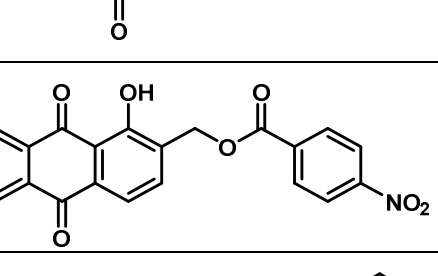
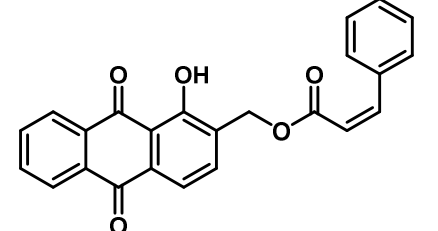
### 1. Structures and IC<sub>50</sub> values of anthraquinone derivatives

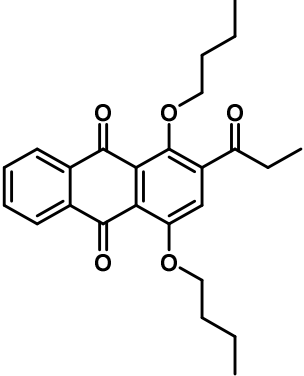
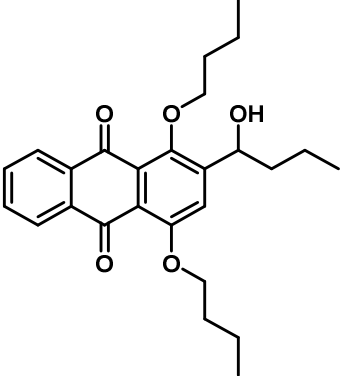
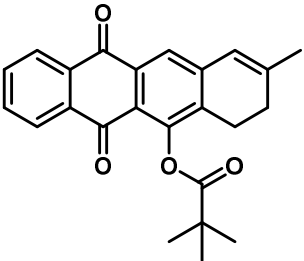
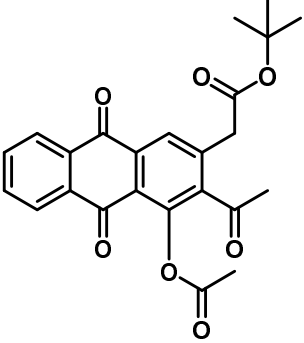
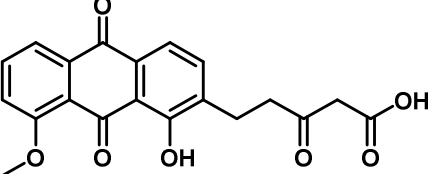
**Table S1:** Structures and IC<sub>50</sub> values (μM) of anthraquinones tested, determined by MTT and CV assay against HT-29, HeLa and HepG2 cell lines (48 h of treatment)

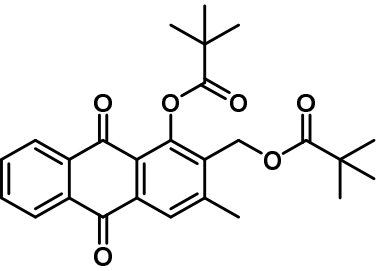
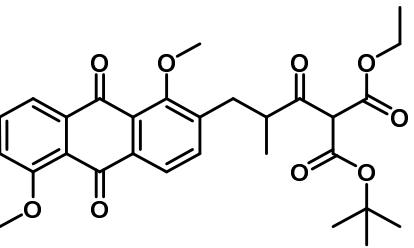
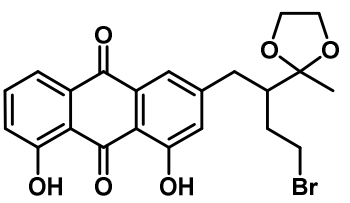
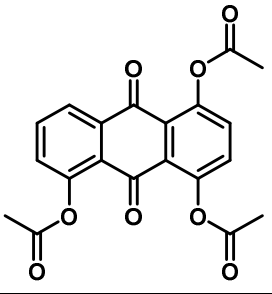
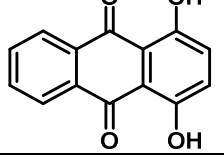
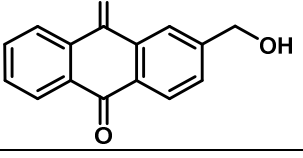
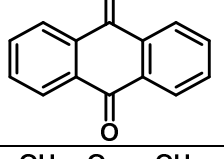
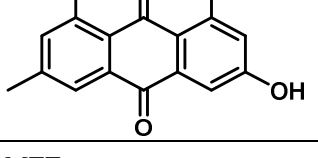
Compound no.	Structure	PC3		HT-29		HeLa		HepG2	
		IC <sub>50</sub> [μM]							
		CV	MTT	CV	MTT	CV	MTT	CV	MTT
1		7.46±1.37	7.30±0.53	7.78±0.23	13.93±0.26	7.80±0.27	11.94±1.57	5.65±0.89	7.38±0.66



8						
9						
10						
11						
12						
13						

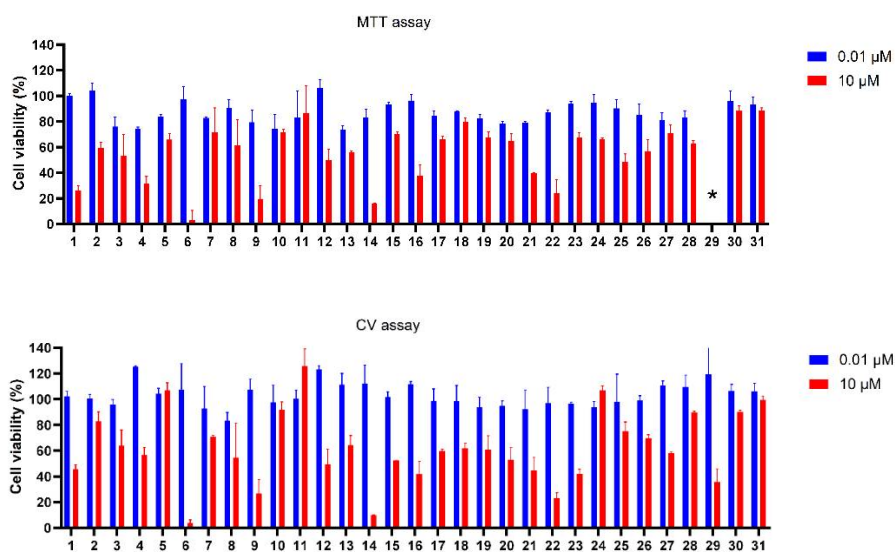
12.36±0.95	24.19±2.51	10.20±0.89	20.07±0.11	25.26±3.26	14.94±1.76	9.90±1.98
11.65±0.79	12.03±0.82	6.82±0.36	5.98±0.37	10.57±0.33	15.06±0.73	6.08±1.82
8.42±0.08	14.16±0.31	44.92±3.26	35.19±2.24	9.58±0.73	14.26±1.42	9.63±1.23
6.18±0.56	11.23±0.68	14.66±0.02	29.23±2.29	8.35±1.32	22.49±1.21	7.84±1.75
18.78±1.74	28.23±1.78	>100	30.56±0.40	21.37±1.87	37.32±1.68	16.72±1.41
9.29±1.53	31.19±1.64	>100	13.37±0.59	4.72±0.33	40.35±1.57	2.52±0.67
8.52±0.47	14.71±1.33	24.62±2.18	29.00±4.58	18.79±1.76	27.28±2.96	12.97±0.41
8.94±1.52	15.18±1.15	19.82±1.03	30.99±2.58	13.94±1.44	31.71±1.22	10.15±1.73
						

					17.79±0.35
					9.32±0.92
					95.23±5.37
					41.31±3.37
					>100
					>100
					30.00±2.28
					26.29±1.73
21					
22					
23					
24					
25					

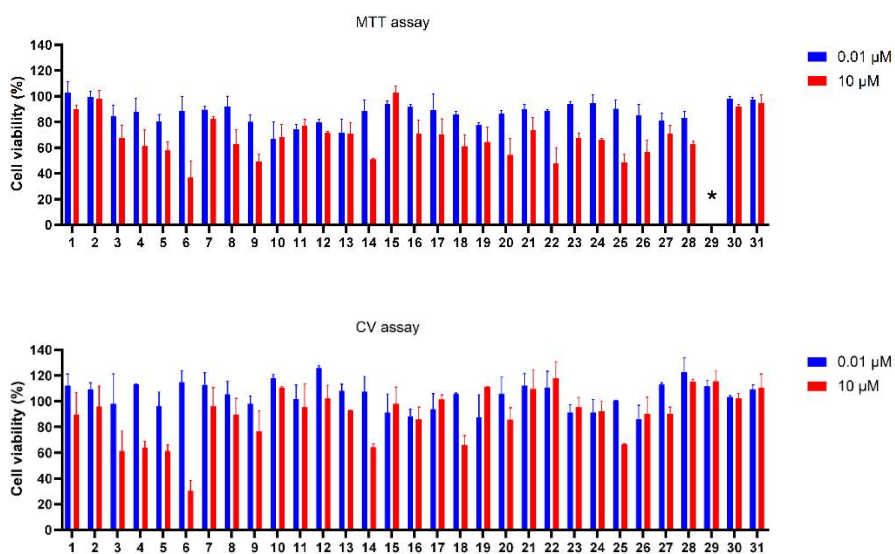
26		23.48±1.19	9.54±1.03	>100	30.75±3.40	3.81±0.57	38.29±2.99	62.52±2.21	>100	23.50±1.22
27		45.84±3.23	27.78±1.93	5.48±0.21	6.31±0.35	*	13.34±0.22	53.32±4.10	>100	20.63±2.92
28		16.50±1.86	22.51±1.78	60.34±1.72	12.12±1.45	*	20.64±1.11	10.65±0.60	83.13±1.32	5.95±0.96
29		*	24.09±2.16	94.11±1.59	27.49±1.79	32.22±1.69	41.45±3.82	54.86±4.74	>100	41.70±1.62
30		>100	15.64±1.39	80.71±4.19	10.50±1.86	*	21.24±0.67	39.13±2.83	>100	43.76±1.64
31		>100	28.12±1.81	38.77±3.82	22.05±2.95	10.89±1.87	>100	>100	>100	30.07±2.66
32		>100	27.12±1.88	67.18±3.55	20.00±2.51	13.05±1.21	30.56±0.43	13.75±1.72	80.72±1.68	7.36±0.62
33		22.01±1.34	27.78±1.93	5.48±0.21	6.31±0.35	*	13.34±0.22	53.32±4.10	>100	20.63±2.92

\*Interfering with MTT assay

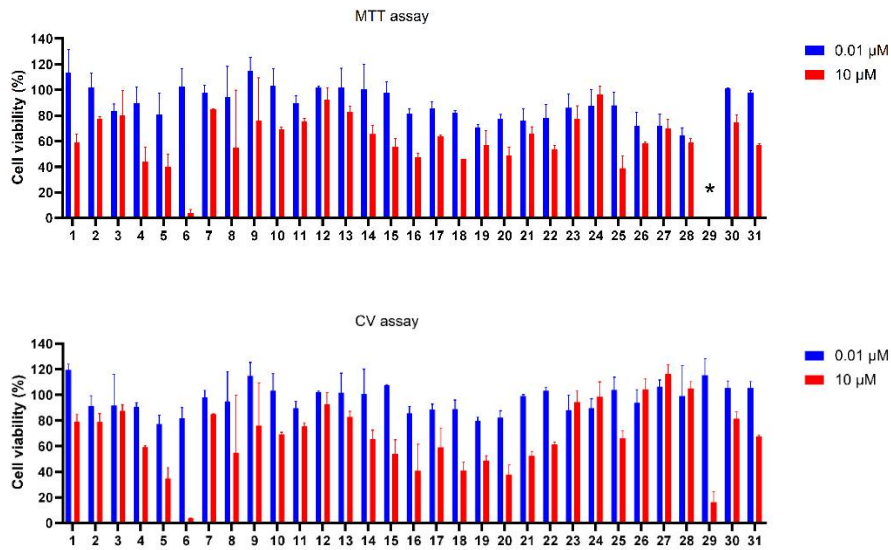
## 2. Fast screening results



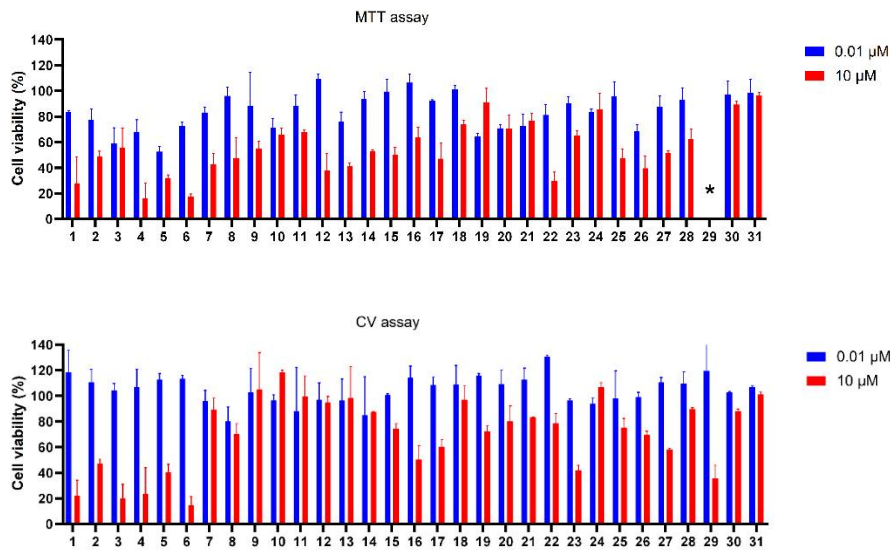
**Figure S1:** PC3 cell viability after 48 h treatment with anthraquinone derivatives  
(\*Interfering with MTT assay)



**Figure S2:** HT-29 cell viability after 48 h treatment with anthraquinone derivatives  
(\*Interfering with MTT assay)



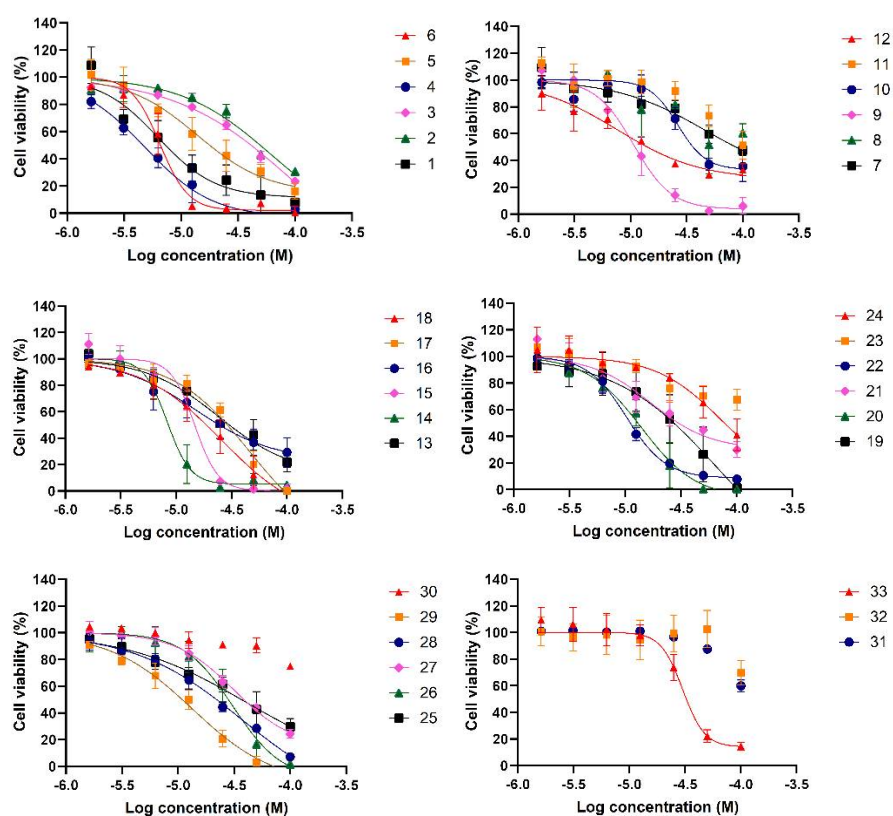
**Figure S3:** HeLa cell viability after 48 h treatment with anthraquinone derivatives  
(\*Interfering with MTT assay)



**Figure S4:** HepG2 cell viability after 48 h treatment with anthraquinone derivatives  
(\*Interfering with MTT assay)



### 3. IC<sub>50</sub> determination



**Figure S5:** Dose-dependent response of PC3 cells treated with anthraquinone derivatives determined by MTT assay (48 h)

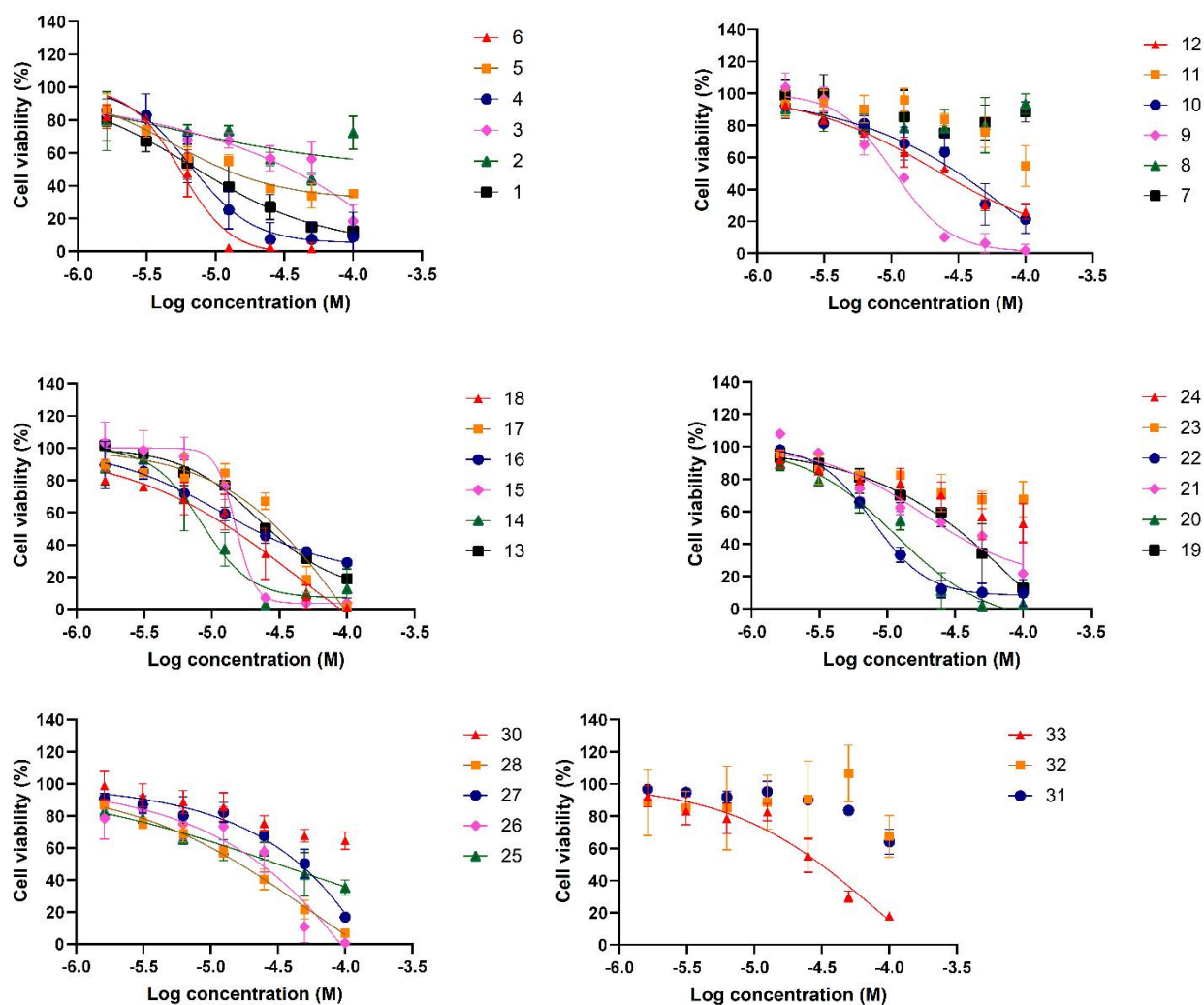
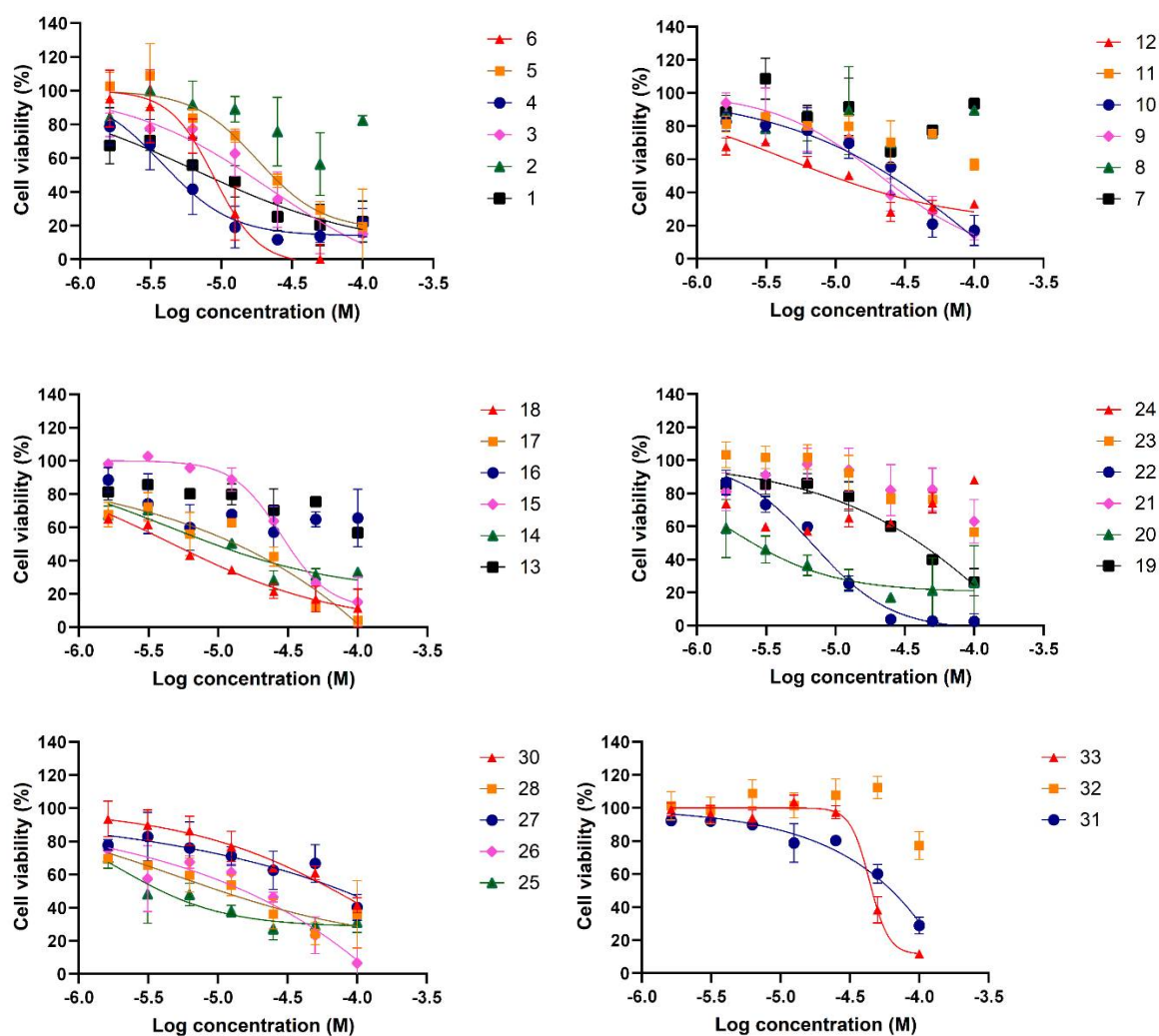


Figure S6: Dose-dependent response of PC3 cells treated with anthraquinone derivatives determined by CV assay (48 h)



**Figure S7:** Dose-dependent response of HT-29 cells treated with anthraquinone derivatives determined by MTT assay (48 h)

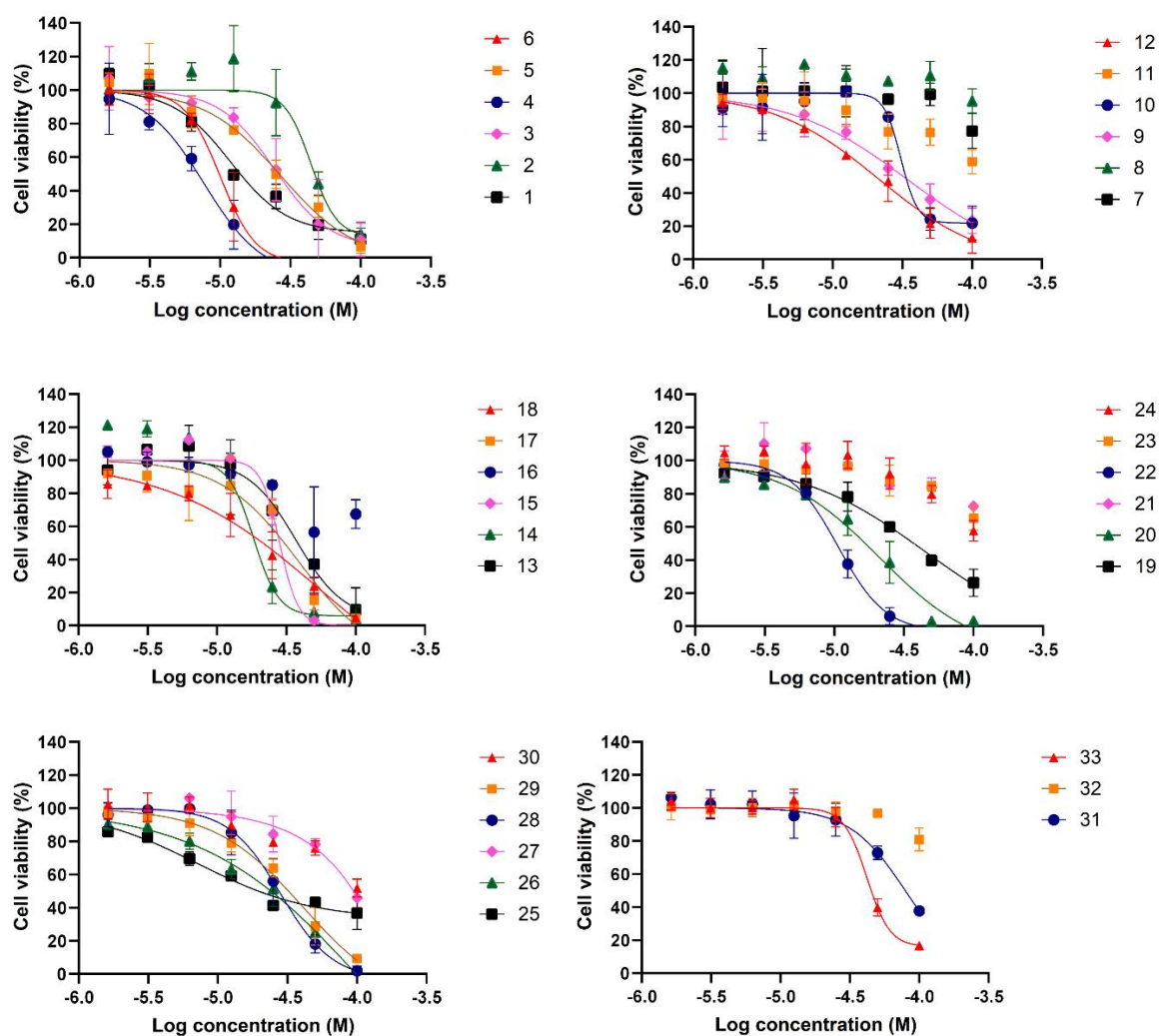
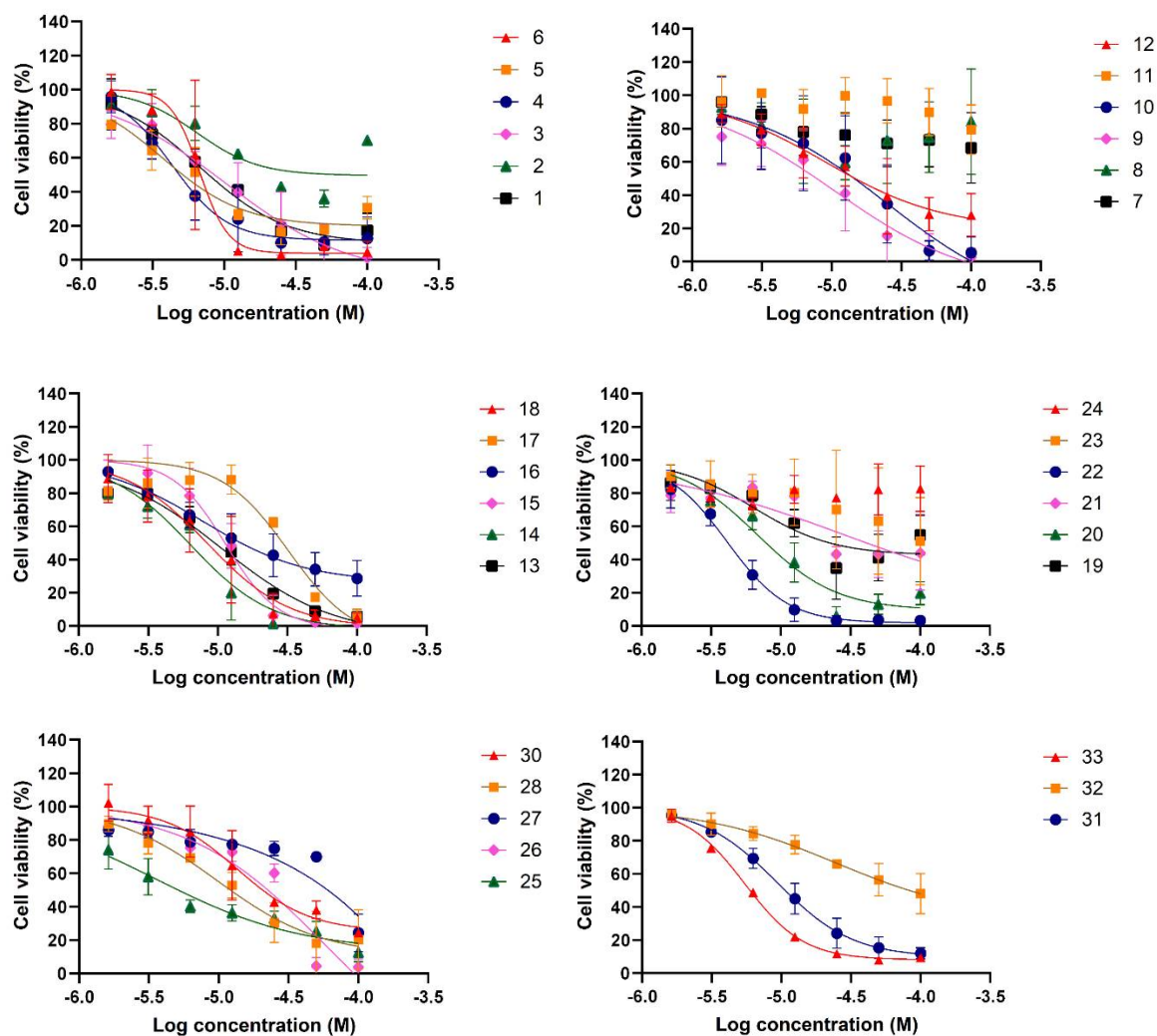
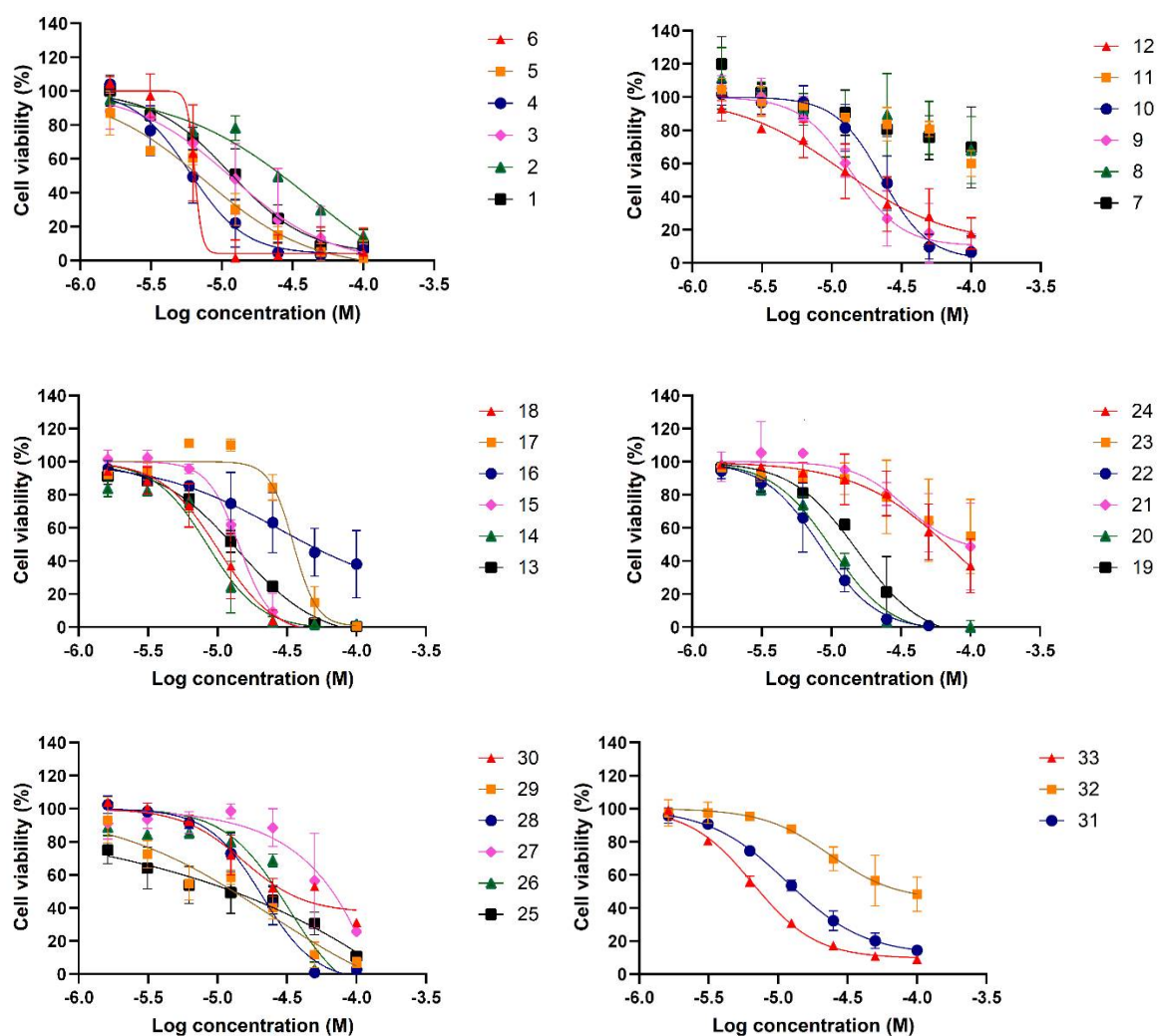


Figure S8: Dose-dependent response of HT-29 cells treated with anthraquinone derivatives determined by CV assay (48 h)

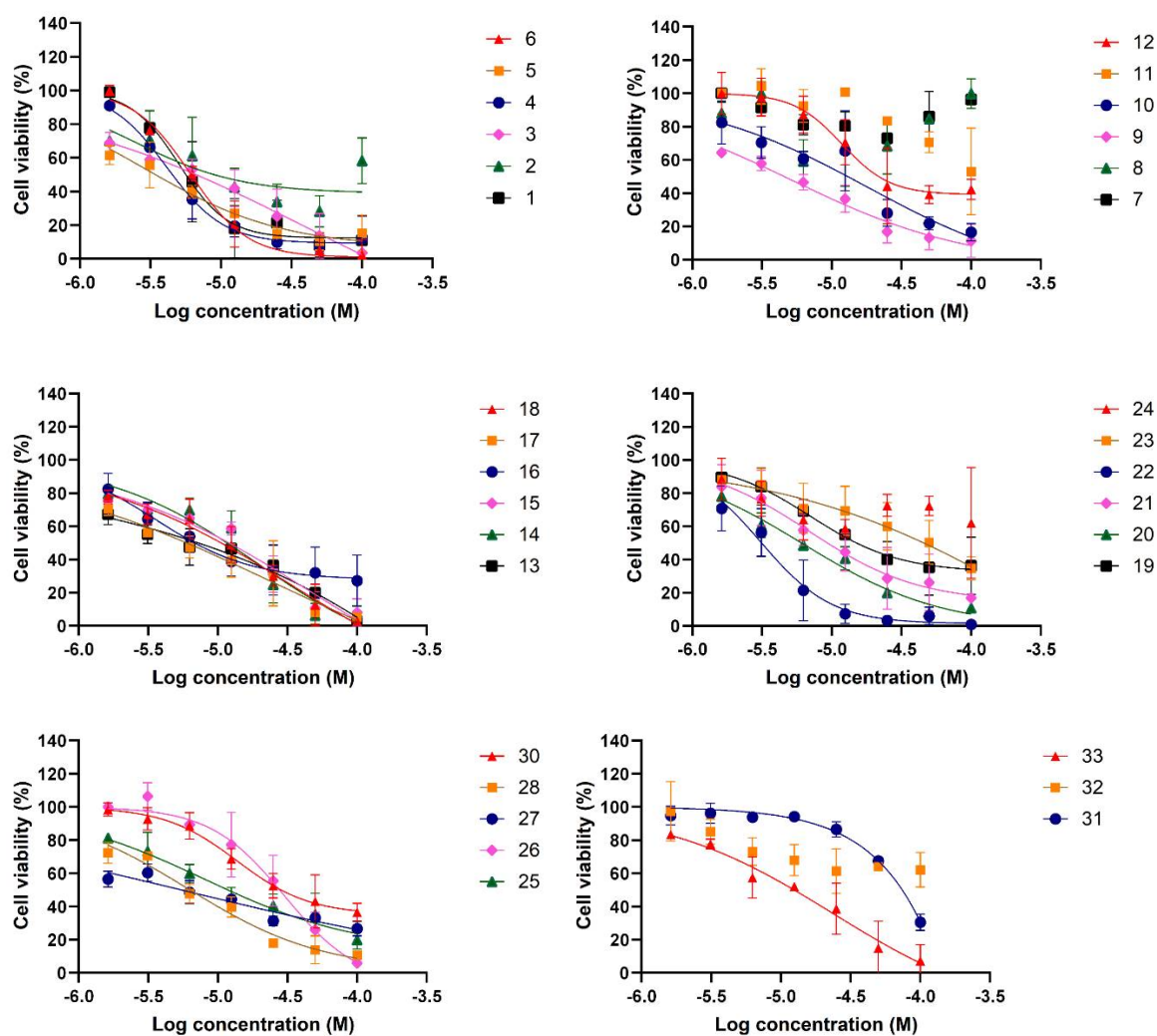


**Figure S9:** Dose-dependent response of HeLa cells treated with anthraquinone derivatives determined by MTT assay (48 h)



**Figure S10:** Dose-dependent response of HeLa cells treated with anthraquinone derivatives determined by CV assay (48 h)





**Figure S11:** Dose-dependent response of HepG2 cells treated with anthraquinone derivatives determined by MTT assay (48 h)

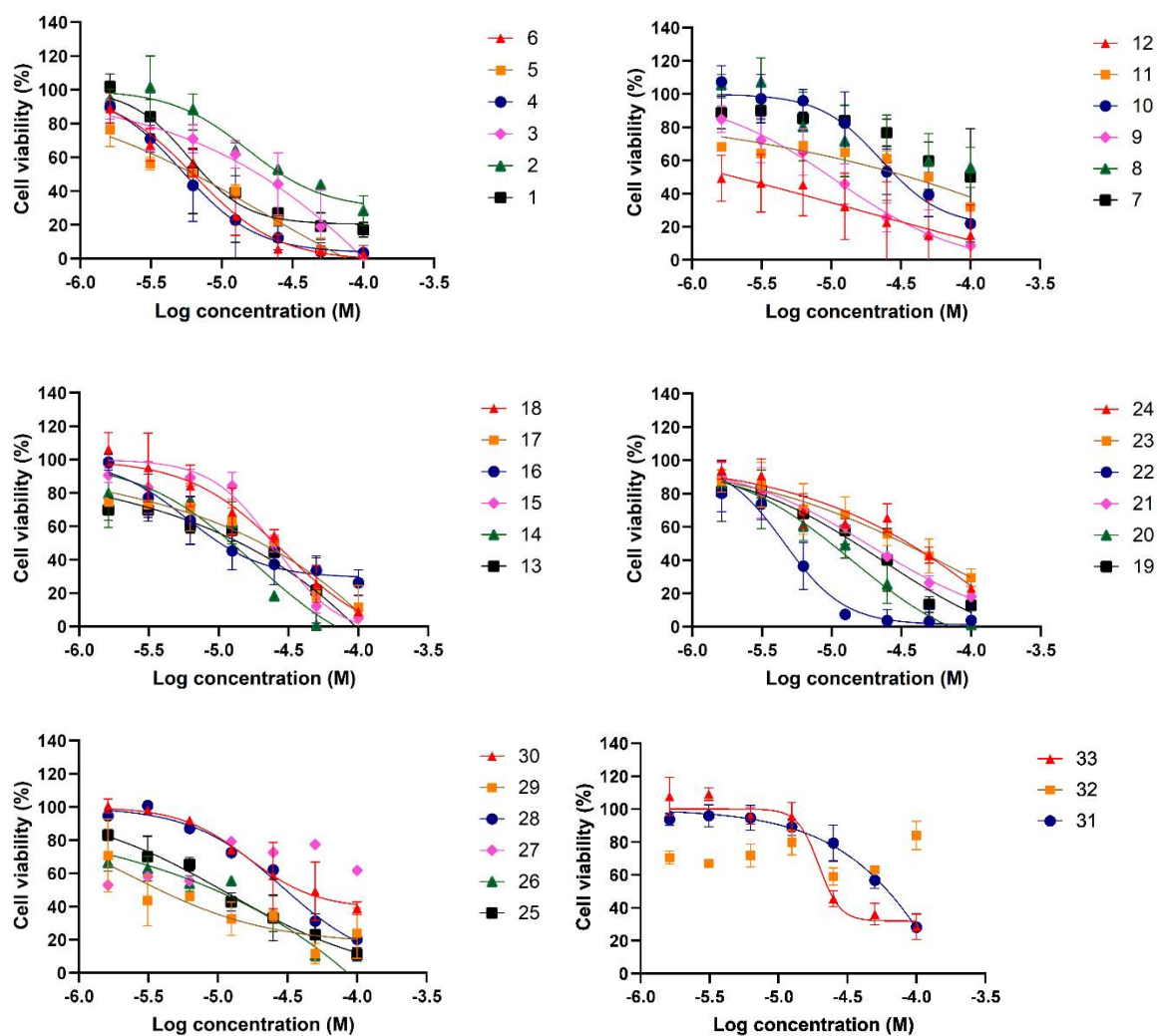


Figure S12: Dose-dependent response of HepG2 cells treated with anthraquinone derivatives determined by CV assay (48 h)