

1. 2D QSAR analysis

Table 1S: Experimental and estimated activity of training and test set compounds **1-17**

Cpds.	pIC50_MCF-7	\$PRED_MCF7	pIC50_RPE-1	\$PRED_RPE-1	pIC50_HCT-116	\$PRED_HCT-116
Training set						
1	4.483	4.482	4.379	4.413	4.215	4.185
2	4.728	4.725	4.59	4.586	4.213	4.24
4	4.564	4.571	4.453	4.462	4.257	4.207
5	4.699	4.697	4.62	4.574	4.22	4.269
7	4.532	4.53	4.526	4.526	4.214	4.223
8	4.506	4.562	4.461	4.49	4.154	4.224
10	4.519	4.519	4.472	4.416	4.131	4.163
11	4.561	4.562	4.48	4.526	4.233	4.158
13	4.631	4.632	4.521	4.495	4.194	4.207
14	4.807	4.809	4.548	4.595	4.339	4.285
15	4.619	4.616	4.622	4.599	4.038	4.078
16	4.631	4.631	4.428	4.413	4.408	4.425
17	4.659	4.661	4.466	4.456	4.314	4.311
Test set						
3	4.622	4.562	4.444	4.49	4.358	4.344
6	4.504	4.505	4.425	4.435	4.226	4.215
9	4.458	4.457	4.408	4.418	4.167	4.18
12	4.666	4.666	4.572	4.551	4.202	4.239
Doxorubicin	4.706	6.132	4.646	4.759	4.194	4.655

Table 2S : the Z-score of the target products 1-17

	\$Z\$-SCORE_mcf7	\$Z\$-SCORE_hct116	\$Z\$-SCORE_RPE-1
1	0.01697637	1.1130153	0.83677042
2	0.17487699	0.13405564	0.76464283
3	2.9849298	1.4903405	0.3782531
4	0.3379592	0.27857989	1.4105554
5	0.077910095	1.4892653	1.3610055
6	0.030910673	0.32741761	0.31407404
7	0.069427371	0.007662103	0.25124091
8	2.8025138	0.0125	0.2135
9	0.053574778	0.3254143	0.3659147
10	0.043049004	1.8405719	0.91687667
11	0.082863122	1.5014175	2.118978
12	0.047065146	0.68167078	1.045627
13	0.082238495	0.86612308	0.34462792
14	0.099830285	1.5083652	1.5342196
15	0.20771068	0.73322046	1.1331122
16	0.013874196	0.4984839	0.4962976
17	0.072850548	0.30882126	0.086494915
Doxorubicin			

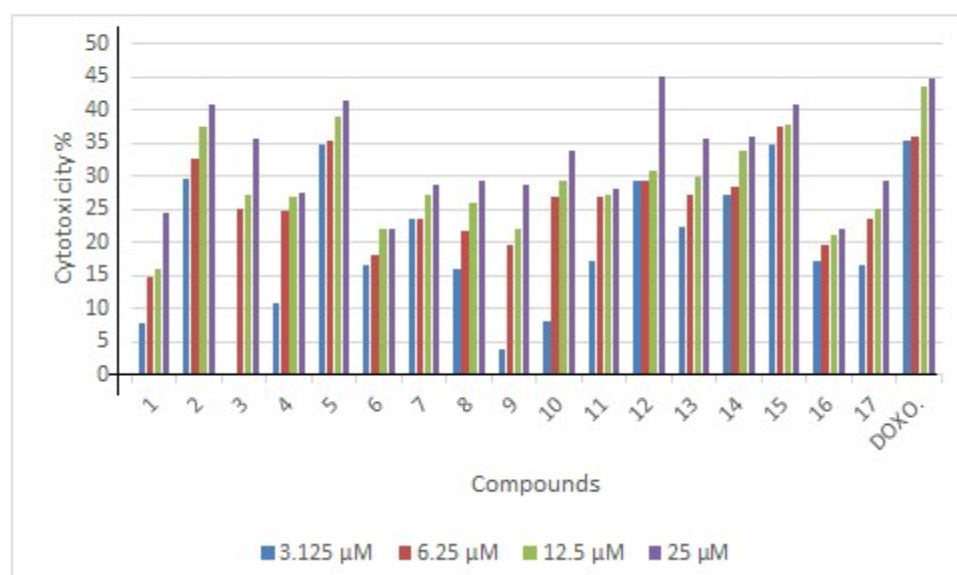


Fig. S1 Dose-dependent cytotoxic activities of 1-17 against HCT-116 cancer cells as depicted by the MTT assay.

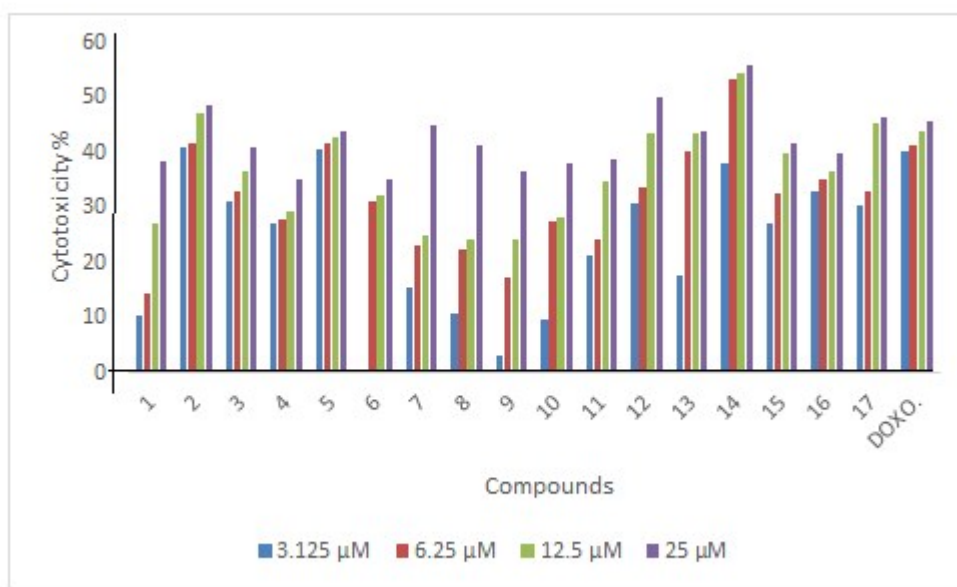


Fig. S2 Dose-dependent cytotoxic activities of 1–17 against MCF-7 cancer cells as depicted by the MTT assay.

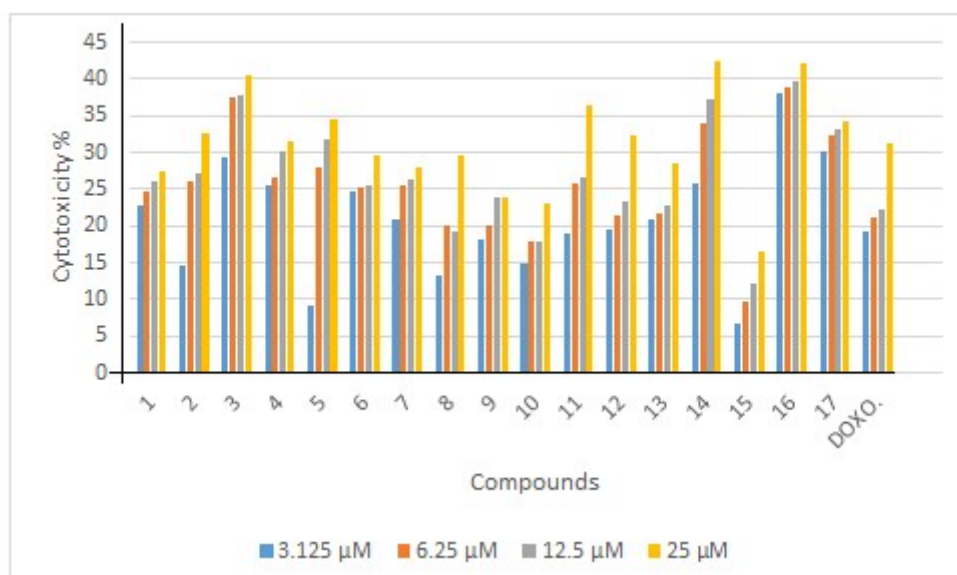


Fig. S3 Dose-dependent cytotoxic activities of 1–17 against RPE-1 normal cells as depicted by the MTT assay.