Electronic Supplementary Material (ESI) for Molecular BioSystems.

Supplementary Data:

Insights on molecular interactions of Thymoquinone with Histone deacetylase: Evaluation of therapeutic intervention potential against breast cancer

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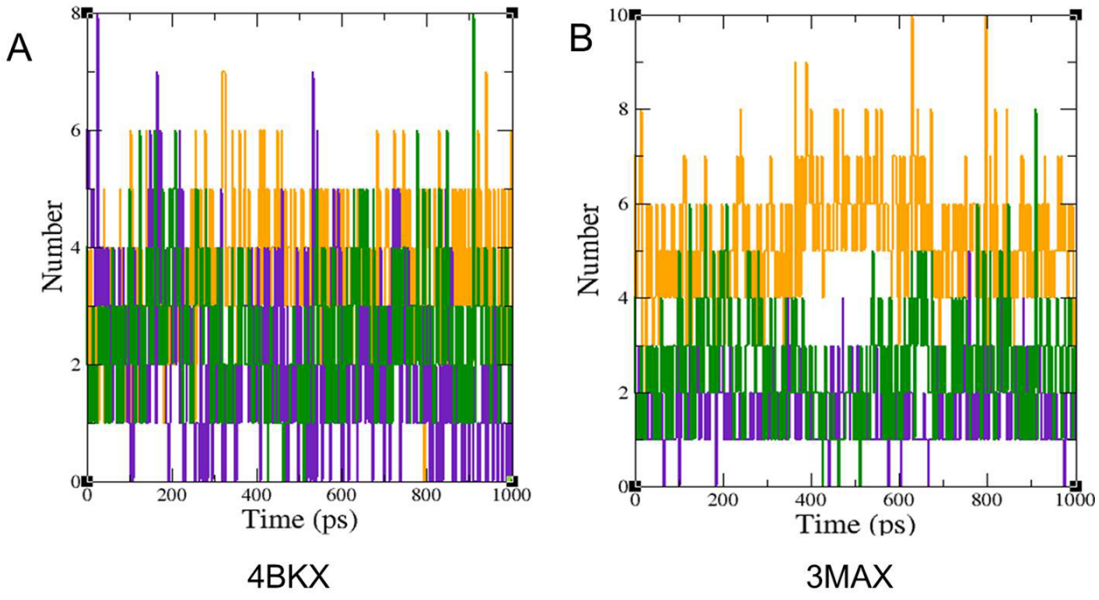

Figure S1: Depiction of intermolecular hydrogen bond in Å between TSA (orange), SFN (violet), TQ (green) with active site amino acid residues of (A) 4BKX and (B) 3MAX. On an average the number of hydrogen bond formed by TQ is similar to that of SFN.

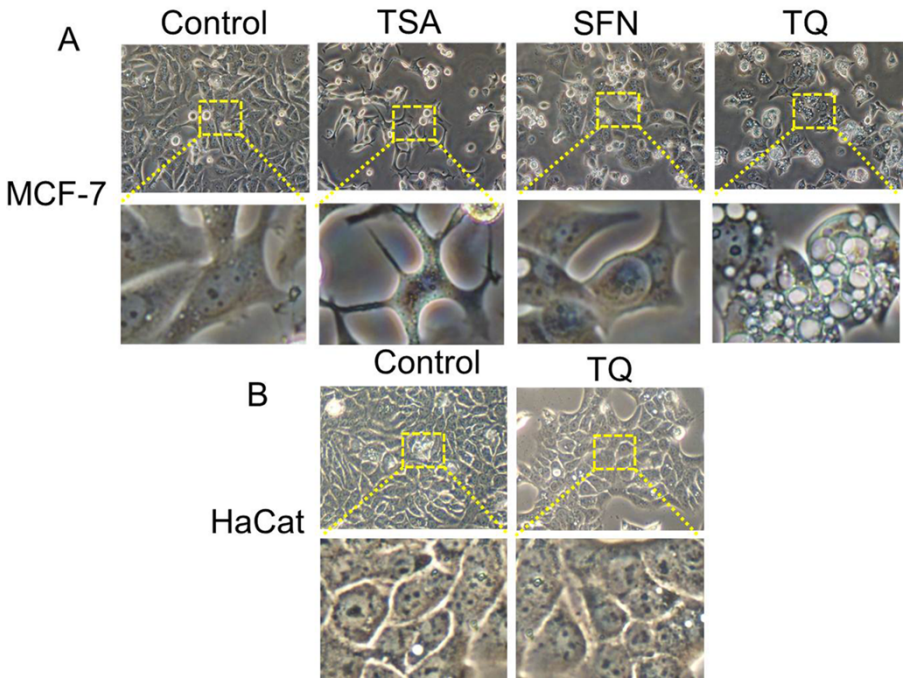

Figure S2: Representative images of phenotypic alterations of MCF-7 breast cancer cells in response to TSA, SFN and TQ treatment observed by phase-contrast light microscopy. TQ elicits no change in the morphology of normal skin cells, HaCat, while leading to cytoplasmic vacuolization in MCF-7 cells.

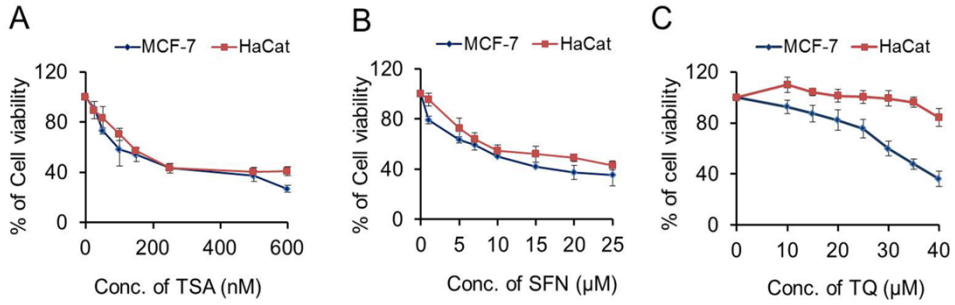

Figure S3: Effect of (A) TSA (B) SFN and (C) TQ on viability and growth of MCF-7 breast cancer cells and normal skin keratinocytes, HaCat. Both cell lines were treated with drugs shown at the dosages indicated for 24 h. Cytotoxicity of drugs were then determined by MTT assay. Data are represented as the mean±SD of three different observations. The IC_{50} of TSA, SFN and TQ was determined to be 180 nM, 10 μM and 34 μM, respectively for MCF-7 cells. Data are expressed as mean ± S.D., n=3.

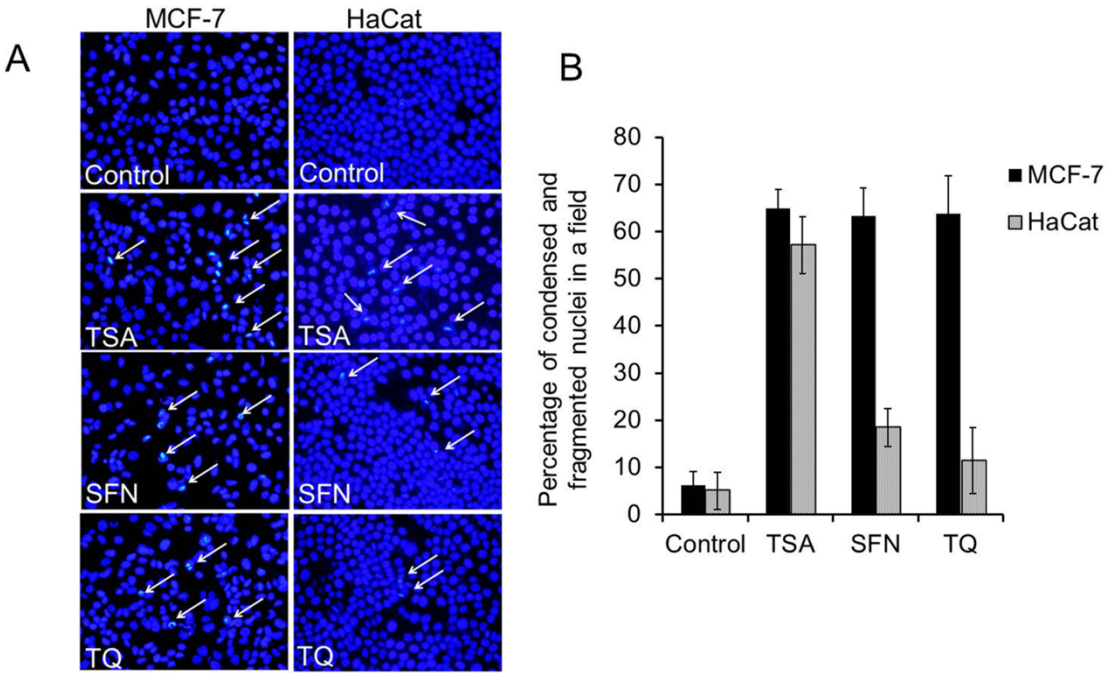

Figure S4: (A) Representative images of Hoechst 33342 stained nuclei (arrow) of MCF7 and HaCat cells after treatment with TSA, SFN and TQ for 24 h. (B) Percentage of condensed nuclei of MCF7 and HaCat cells are represented graphically (n=3, mean±S.D.). $p < 0.05$. Scale Bar = 20 μm.

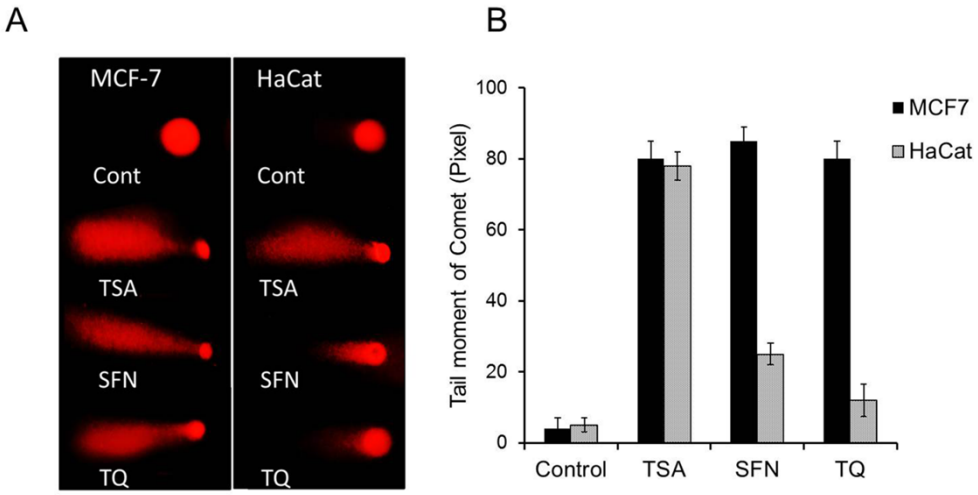

Figure S5: (A) Representative images of Comets formed in MCF7 and HaCat cells after treatment with TSA, SFN and TQ for 24 h. (B) Tail moments of comets in untreated and treated MCF7 and HaCat cells are represented graphically. Data are expressed as mean ± S.D., n=3.

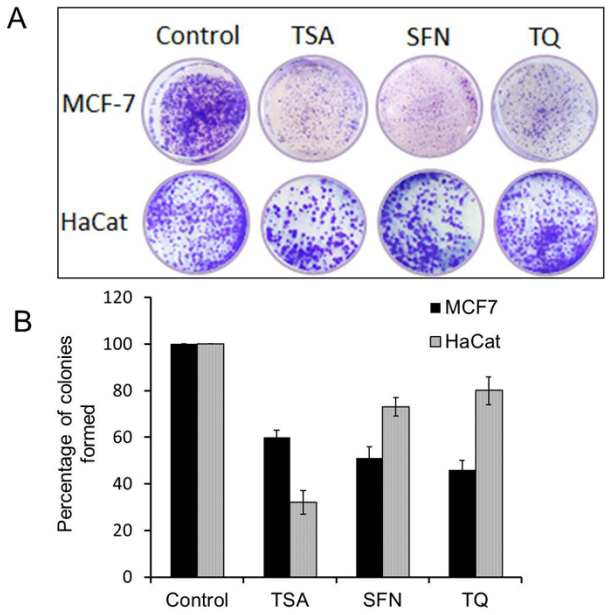

Figure S6: (A) TQ supresses MCF-7 breast cancer cell migration. MCF7 and HaCat cells were exposed to TSA, SFN and TQ treatment at their respective IC_{50}. The monolayer cultures were scratched and the wound areas were photographed at the indicated time points. The denuded areas were calculated and compared with the initial open areas. Scale Bar = 4 µm. (B) Graphical representation of percentage of migrated cells in wound area in untreated and treated MCF-7 and HaCat cells. Shown are mean ± S.D., n=3.

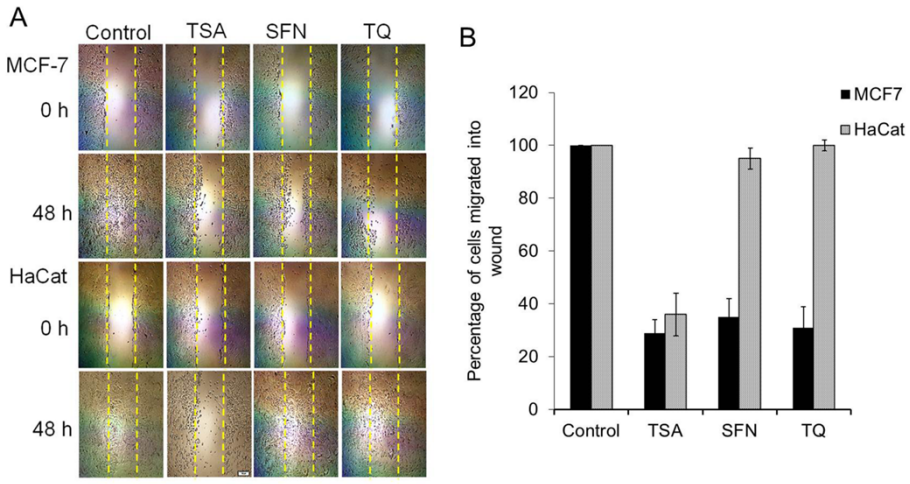

Figure S7: (A) Representative images of colonies formed in MCF7 and HaCat cells treated with TSA, SFN and TQ at their respective IC_{50}. The colonies were counted by colony counter. (B) Graphical representation of percentage of colonies formed in untreated and treated MCF-7 and HaCat cells. Data are expressed as mean ± S.D., n=3.