Electronic Supplementary Material (ESI) for Food & Function.

Supplementary Material

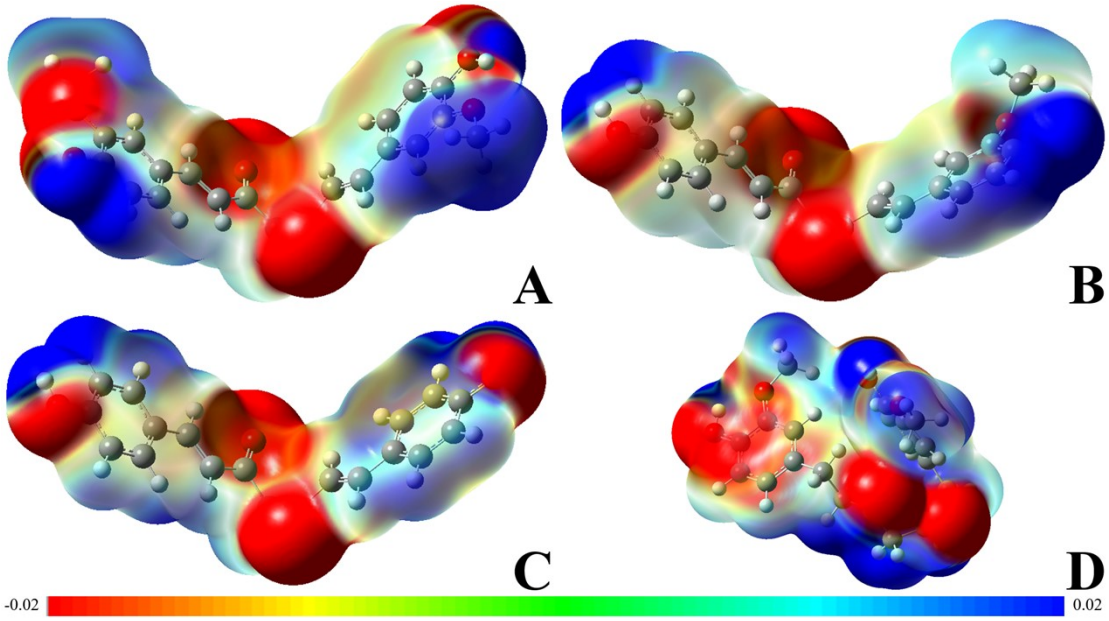

Fig. S1. Molecular electrostatic potential surfaces (MEPS) of curcumin (A), demethoxycurcumin (B), bisdemethoxycurcumin (C), and tetrahydrocurcumin (D). The electronegative and electropositive MEPS are shown in red and blue respectively.

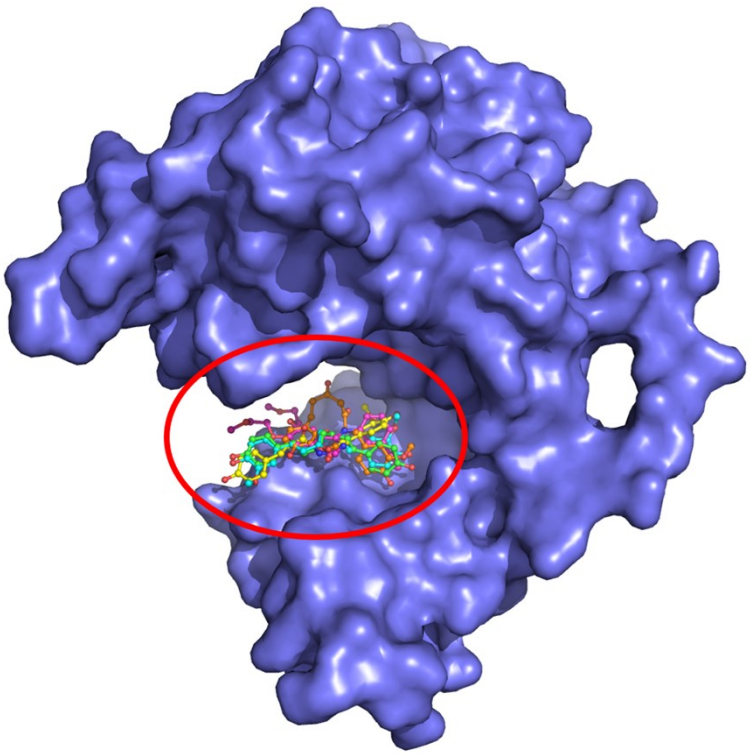

Fig. S2. The docked ligands curcumin (cyan), demethoxycurcumin (yellow), bisdemethoxycurcumin (green), and tetrahydrocurcumin (orange) as well as the co-crystal ligand erlotinib (magenta) in the hydrophobic cavity of EGFR.

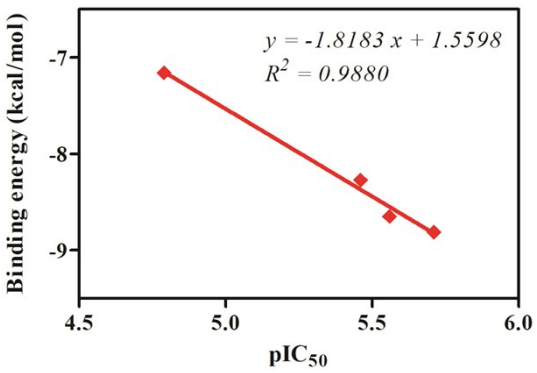

Fig. S3. Correlation of the calculated binding energies with the experimental pIC_{50} values.