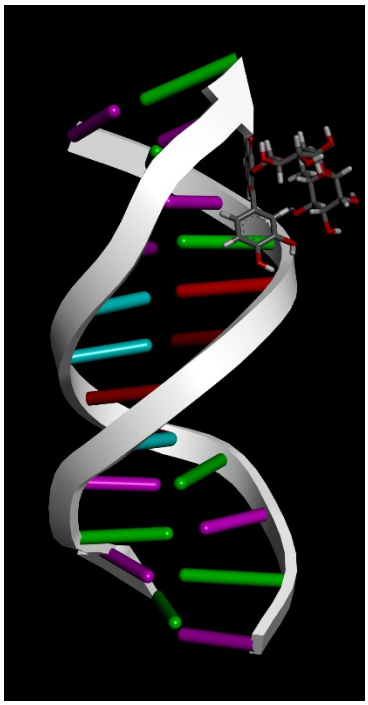
Electronic Supplementary Material (ESI) for Toxicology Research.

Material and method

Another molecular docking program *i.e.* Hex 8.0 was also employed for further validation of *in silico* results. The PBD structure of DNA d(CGCGAATTCGCG)$_2$ was downloaded from protein data bank (http://www.rcsb.org./pdb). The SDF file of rutin downloaded from pubchem [CID: 5280805] was converted to PDB using Avogadro software. The parameters used in this study were: FFT mode –3D, correlation type – shape only, grid dimension –0.6, ligand range –180, receptor range –180, twist range –360, distance range –40.

Result and discussion

The structure of rutin was made flexible to obtain most thermodynamically stable conformation and best fit orientation. Supplementary Fig S1 is the best fit of docking result which shows that rutin interacts in the minor groove of DNA. The binding energy was found to be -7.01 kcal/mole. Rutin was found to interact with dG22, dG23, dG24, dC3, dG4 and dA5 of DNA with hydrophobic bonds. The docking result by Hex 8.0 further validate the groove binding mode between rutin and DNA.



Supplementary Fig S1. Molecular docked structure of rutin complexed with DNA. Dodecamer duplex sequence (CGCGAATTCGCG)$_2$ (PDB ID: 1BNA) was used in the docking studies.