## Supplementary information

## Multi-spectroscopic and molecular modelling studies on the interaction of esculetin with calf thymus DNA

Tarique Sarwar, Mohammed Amir Husain, Sayeed Ur Rehman, Hassan Mubarak Ishqi and Mohammad Tabish\*

Department of Biochemistry, Faculty of Life Sciences, A.M. University, Aligarh, U.P. 202002, India

\*Corresponding author: Email: tabish.bcmlab@gmail.com; Tel: +91-9634780818

**Table S1.** Relative binding energy at different poses obtained from Hex 6.3 molecular docking programme.

S.No.	Energy (kcal/mol)
1	-3.60
2	-2.97
3	-2.92
4	-2.89
5	-2.85
6	-2.83

## Figures



**Fig. S1.** Different docked structures of esculetin with DNA dodecamer duplex sequence d(CGCGAATTCGCG)<sub>2</sub> (PDB ID: 1BNA) at different relative binding energies. (A) -3.60 kcal/mol (B) -2.89 kcal/mol (C) -2.85 kcal/mol (D) -2.83 kcal/mol