Insights on Binding and Selectivity of Surfen Towards Different DNA Topologies

Laxmi Kashyap[a], Kritika Varshney[a], Manoj Munde[a]*

[1] School of Physical Sciences, Jawaharlal Nehru University, New Delhi-110067, India

*Corresponding Author
*Manoj Munde;
Email: mundemanoj@gmail.com

Table S1: Interaction between surfen and various DNAs used in this study

Duplex DNA

Donor	**Acceptor**	**D-H..A distance (Å)**
-NH_2 group of the amino-quinoline compound	T19 (Oxygen atom of the carbonyl functional group attached to the C2 carbon of the thymine pyrimidine ring)	2.060
-NH group of the amino-quinoline compound	T8 (Oxygen atom of the carbonyl functional group attached to the C2 carbon of the thymine pyrimidine ring of chain A)	1.938
-NH group of the amino-quinoline compound	T8 (Oxygen atom of the carbonyl functional group attached to the C2 carbon of the thymine pyrimidine ring of chain A)	2.232
an -NH_2 group of the amino-quinoline compound	C9 (Chain A oxygen atom double-bonded to the C2 carbon of the cytosine ring.) of chain A interacts with the -NH_2 group of the amino-quinoline ring.	1.921

AP Q-DNA

Donor	**Acceptor**	**D-H..A distance (Å)**
-NH group of the amino-quinoline compound	OP2, a non-bridging oxygen atom in the phosphate group connected to G16	1.836
-NH group of the amino-quinoline compound	OP2, a non-bridging oxygen atom in the phosphate group connected to G16	2.124
an -NH_2 group of the amino-quinoline compound	OP2, a non-bridging oxygen atom in the phosphate group connected to T17	2.161
G20-Nitrogen atom in the	Oxygen atom at 2nd position	3.452

exocyclic amino group (–NH_2) attached to the C2 carbon of guanine	of Surfen	

HB Q-DNA

Donor	**Acceptor**	**D-H..A distance (Å)**
-NH_2 group of the amino-quinoline compound	oxygen atom bonded to the 3' carbon of the sugar ring in the DNA backbone at G11	2.202
G11 (nitrogen atom in the exocyclic amino group (–NH_2) attached to the C2 carbon of guanine)	-NH group of the amino-quinoline compound	2.182

Table S2: Time-resolved fluorescence decay parameters of surfen measured with and without DNA.

Complex	**T1(ns)**	**T2(ns)**	**T3(ns)**	**Average life time(τa)(ns)**	**χ2**
Surfen	**1.34023**	**0.528643**	**0.233114**	**1.459455**	**1.13357**
Surfen-GQ(AP)	**2.03146**	**0.693939**	**0.458109**	**2.195054**	**1.050276**
Surfen-GQ(H)	**1.77727**	**0.780467**	**0.327037**	**1.968442**	**1.031221**
Surfen-Duplex DNA	**4.1457**	**0.680807**	**0.537048**	**4.235**	**1.23653**

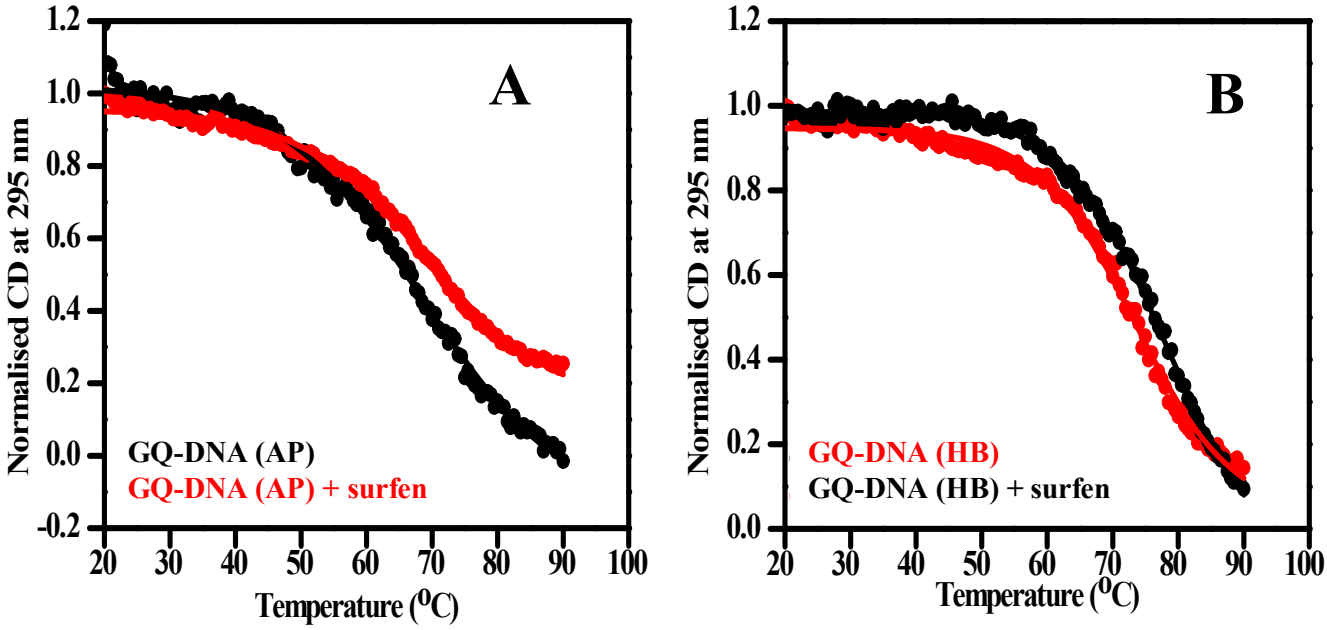

Fig S1: CD melting profiles of GQ-DNA (1 μM) at 295 nm in the absence and presence of surfen (1.5 μM) for (A) AP GQ-DNA and (B) HB GQ-DNA.

CD melting studies assess the thermal stability of different types of DNA, both with and without ligands, by comparing their melting temperatures (Tm), which represent the midpoint of the melting transition at specific wavelengths. Using Figure 7 (A, B) to illustrate the change in ellipticity at 295 nm, we investigated the melting of Surfen-quadruplex complexes in potassium ion (hybrid topology) and sodium ion (antiparallel topology). The melting temperature of GQ-DNA (AP) and GQ-DNA (HB), respectively, is 65°C and 67°C when the ligand is not present. GQ-DNA's melting temperature increases by 3°C when hybrid GQ DNA is present and by 2°C when antiparallel GQ DNA is present

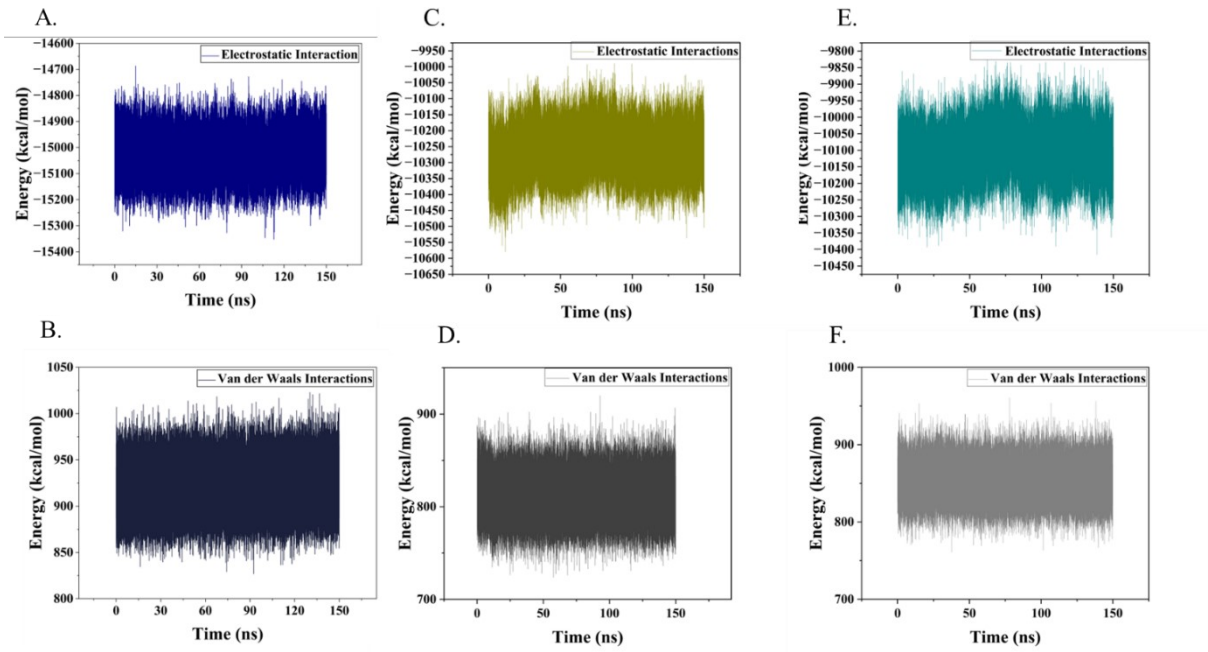

Fig S2. The contribution of surfen binding (A) electrostatic and (B) Van der Waals interactions with dsDNA; (C) electrostatic and (D) Van der Waals interactions with AP GQ-DNA; (E) electrostatic and (F) Van der Waals interactions with HB GQ-DNA.

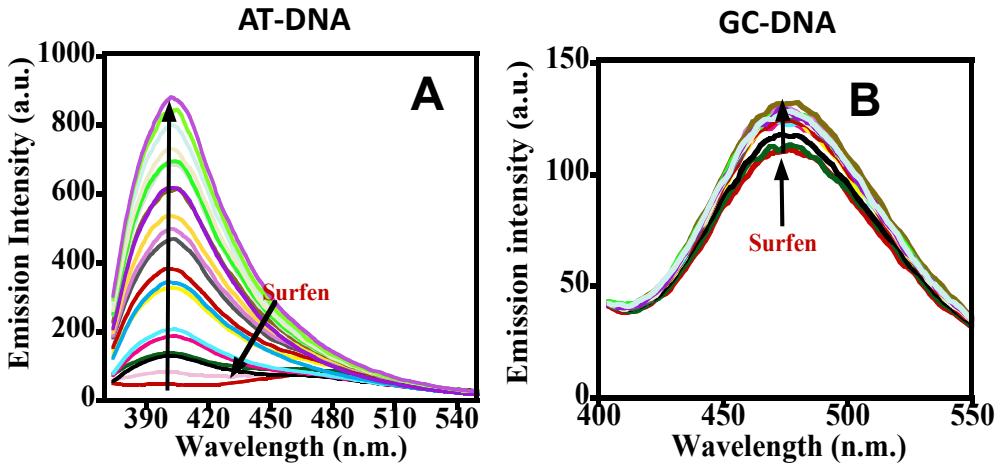

Fig S3: Binding of surfen using fluorescence with (A) AT-DNA and (B) GC-DNA. The concentration of surfen was used as 1μM and DNA was titrated from 0.01 to 1 μM pe DNA strand concentration. Surfen binds very strongly with AT-DNA compared to GC-DNA.