DNA-DRUG INTERACTION ENERGY AND ΔTm PREDICTION

INPUT FILE FORMAT:

(a) The input file should be in the PDB format e.g

```
  A        B    C    D       E          F       G       H
ATOM       1   H5T  DC5      1       28.637  38.525  50.527
ATOM       2   O5*  DC5      1       29.242  39.039  49.972
ATOM       3   C5*  DC5      1       29.131  38.531  48.647
ATOM       4  1H5*  DC5      1       29.879  39.008  48.007
ATOM       5  2H5*  DC5      1       28.141  38.751  48.248
ATOM       6   C4*  DC5      1       29.342  37.012  48.636
ATOM       7   H4*  DC5      1       30.230  36.783  49.227
ATOM       8   O4*  DC5      1       28.229  36.319  49.183
ATOM       9   C1*  DC5      1       28.362  34.975  48.755
ATOM      10   H1*  DC5      1       29.175  34.496  49.315
ATOM      11   N1   DC5      1       27.102  34.199  48.947
ATOM      12   C6   DC5      1       25.884  34.727  48.592
```

- The spacing between columns is not important unless two columns merge at any place.
- Note that it is important that Column D represents the residue name, and columns F, G, H represent the x, y, z coordinates
- Any extra columns after column H are acceptable

(b) Please ensure that hydrogens are present (especially when starting with crystal structures)

(c) Ensure that the structure does not contain steric clashes-simple geometry optimization is recommended.

Try our Sample file!!!