IMPLEMENTATION OF A NEW METODOLOGY FOR THE 2D REPRESENTATION AND VISUALIZATION OF 3D INTERFACES IN PROTEIN-DNA COMPLEXES

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ABSTRACT

Modelling DNA protein complex in a 3D graphic representation has showed technical problems distinguishing the protein-DNA interfaces. This is because these interfaces are produced between the observed bodies, making harder to visualize them.

Considering this problem, novel computer software has been developed, which is capable of generating 2D interface visualization as an alternative solution to the Nucplot software.

The software, named “iDNA” was developed using the classic software design methodology with an “object oriented” programming, specifying precise requirements for the development of a bioinformatic tool using C#.

The “iDNA” design considers as a reference point the DNA structure, locating the interaction based in the atoms positions in the nucleotides and not by marking the interactions based in the protein like Nucplot does. The proposed model takes as a template the DNA structure due to its “conformational stability or rubustness”. This allows the observation of data in a more constant way and also a more efficient comparison between two or more interfaces.
The application of this software in the observation of the interfaces allows to clearly distinguish the interactions between the protein and the DNA, showing the improvement of observing the protein-DNA using a 2D projection instead of a complex 3D representation.

![Diagram showing 3D to 2D projection of protein-DNA interface](image)

The conclusion is that a 2D observation facilitates the visualization of the characteristics in a protein-DNA interface through the diagram provided by “iDNA”. The observation is more efficient than other 2D models like Nucplot.