

Analysis of Complementarity of Protein-DNA Interactions Using the Electrostatic Potential and the Molecular Surface Geometry

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1 Introduction

Protein-DNA interactions play a crucial role in the translation of genomic information to the biological consequences. Because specific recognition of DNA sequences by proteins is extremely complicated, it is hard to predict how those proteins interact with DNA. Under this circumstance, we carried out the analyses for the interfaces of protein-DNA complexes, using physicochemical properties of protein molecular surfaces, e.g. the electrostatic potentials and the shapes of molecular surface.

2 Method

Molecular surfaces were generated by Connolly's algorithm [1], which had a set of triangle meshes with normal vectors to the surfaces at the vertices. The electrostatic potential at each vertex was calculated by solving the Poisson-Boltzmann equations numerically for a precise continuum model [3], and the shape of protein surface was represented by the geometry curvatures calculated around each vertex. Those calculations were performed separately for the protein and DNA in a protein-DNA complex. Then, we identified such a pair of vertexes, one from protein and the other from DNA, whose distance was within a certain threshold (1Å was used in this analysis). Figure 1 shows these calculation methods.

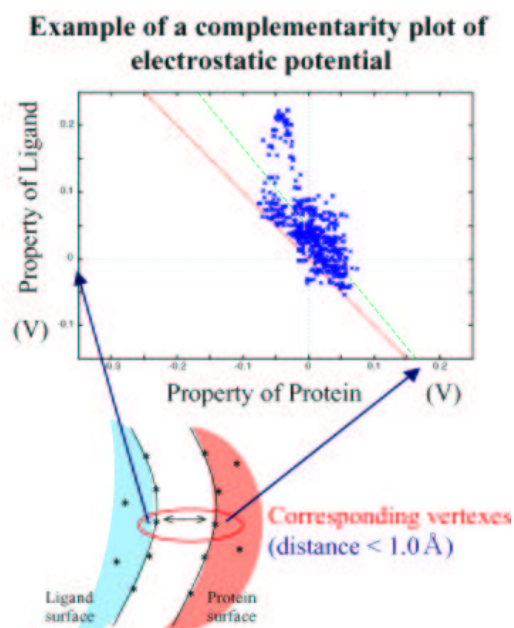


Figure 1: Calculation methods.

3 Results

We applied this method to the well-determined 101 protein-DNA complexes to draw a map of protein-DNA complementarity (Figure 2), and investigated what kinds of interactions contribute to the complementarity map.

The map showed a preferred tendency of the complementarity pattern in protein-DNA interactions, but it was not a simple pattern like that a vertex with the positive potential would always complement a vertex with the negative potential. The complementarity patterns which were formed by the protein-DNA non-specific interactions show almost the same features of the complementarity map in a large number of protein-DNA complexes. In contrast, the complementarity patterns which were formed by the protein-DNA specific interactions show the unique features in the protein-DNA specific interactions, respectively.

Furthermore, we provide the new functions, which could evaluate whether a certain protein binds to DNA or not by analyzing the protein and the DNA surfaces. Using these functions, we evaluated the potentials of the DNA binding for the proteins with a helix-turn-helix motif.

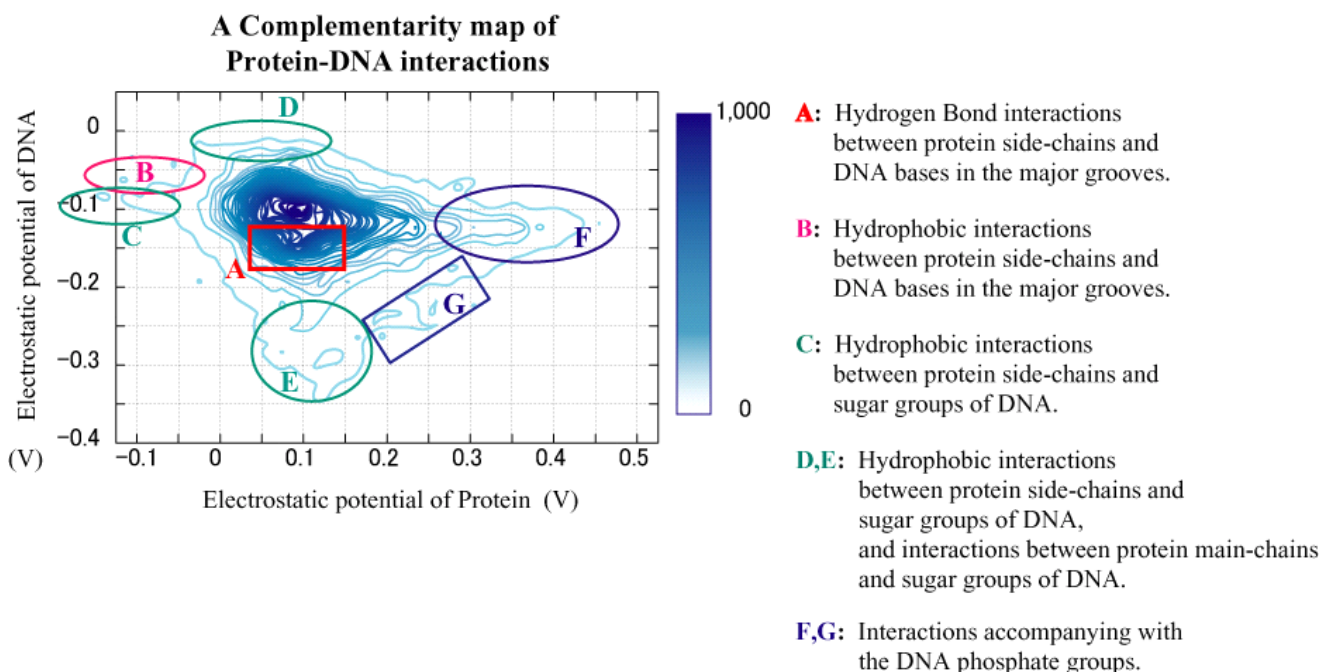


Figure 2: Complementarity map.

References

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