Rigidity and Flexibility of Nucleic Acid Protein Complexes

Emily Flynn ‘14, Sharon Pamela Santana ‘14, and Ileana Streinu

Four College Biomathematics Consortium (4CBC) Project

Computer Science Department, Smith College, Northampton, MA 01063

Introduction

Nucleic acid protein complexes play essential roles in many biological processes, including transcription, translation, replication, and recombination. KINARI-Web [1] is a freely available server for protein rigidity analysis developed by Dr. Ileana Streinu’s Linkage Lab at Smith College (kinari.cs.umass.edu). Rigidity analysis is a fast, graph-based computational method for decomposing a macromolecule into a series of rigid clusters, which provide insight into how the molecule might move. Previously, KINARI could only analyze the protein portion of these complexes. Here we present an extension to KINARI to analyze nucleic acids.

Methods

Modifications for Nucleic Acids Extension
Before performing rigidity analysis, interactions between atoms in the structure are calculated. To analyze nucleic acids, the structures of DNA and RNA nucleotides were added to the methods for finding covalent and double covalent bonds. KINARI-Web uses HBPlus [2] to place hydrogen bonds. In order to use this software for analyzing nucleic acids, a pre-processing step was added to change the nomenclature of DNA and RNA residues to a format recognized by HBPlus.

Data Set of Nucleic Acid Protein Complexes
A data set of 40 high-resolution complexes was collected from the Protein Data Bank (PDB) [3]. Each structure was run through KINARI three times: analyzing 1) the nucleic acid portion, 2) the protein portion, and 3) the entire complex. We developed a visual classification method for dividing the structures into categories based on how the nucleic acid affected the rigidity of the structure.

<table>
<thead>
<tr>
<th>Category</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>Clusters combined to form one large cluster</td>
</tr>
<tr>
<td>B</td>
<td>Clusters mostly combined</td>
</tr>
<tr>
<td>C</td>
<td>Some clusters combined</td>
</tr>
<tr>
<td>D</td>
<td>Clusters remained separate</td>
</tr>
</tbody>
</table>

Discussion

The data set of 40 complexes was separated based on the classification scheme shown in Table 1. The results show that for 10 complexes, the rigidity changed greatly (category A), while for 8 complexes, the rigidity changed but to a lesser extent (category B). 15 complexes had only small changes in rigidity (category C) and 7 had no change in rigidity (category D).

![Figure 3. Structure 3EYI shows no change in rigidity upon addition of nucleic acids (category D).](image)

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References