

# KINARI-Web Case Study: 1HRC

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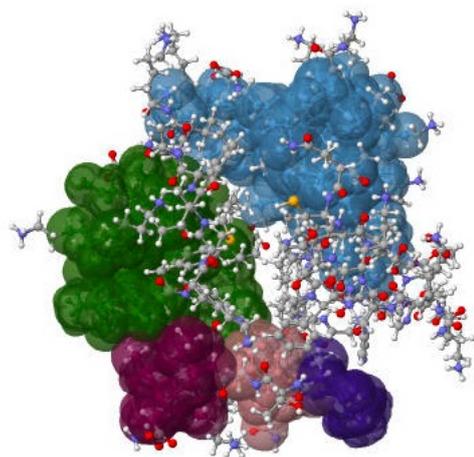
We demonstrate the use of KINARI-Web on 1HRC [1]. We performed rigidity analysis of the X-ray crystal structure of horse heart cytochrome *c*, a 105 residue heme protein found loosely associated with the inner membrane of mitochondria. The rigidity of this protein was previously investigated by Thorpe and collaborators [3, 2]. We invoked the quick-start analysis option of KINARI-Web with PDB code 1HRC. The curating of the PDB file (the ligand was automatically removed) and the rigidity analysis using default options were performed in less than 5 seconds.

Using the visualizer tool, it is easy to explore the calculated rigid regions of a protein. Fig. 1 (a) shows the ball-and-stick model rendition of 1HRC that is generated by the *Jmol* applet within the KINARI-Web visualizer. The 5 rigid bodies that are composed of at least 20 atoms are displayed with randomly-colored surfaces. The different visualizer features can be used to customize the parts of the protein and the set of rigid clusters displayed. Fig. 1(b) shows the same protein, but the cartoon display option is selected, and only a subset of the clusters are highlighted.

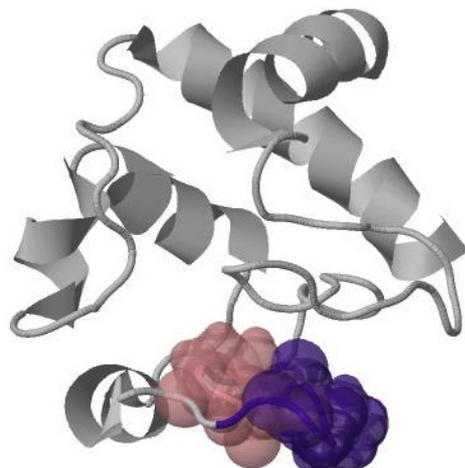
The pink and purple clusters share a rotatable bond that acts as a hinge. The two clusters can be displayed in isolation (Fig. 1 (c)), or with the hinge axis and hydrogen bonds (green) and hydrophobic interactions (blue) Fig. 1 (d). The hydrogen bonds and hydrophobic interactions hold the two clusters rigidly together, but do not cross-brace between the clusters. Visualizing the hinge up-close gives insight into the range of motion that the bond might exhibit.

## References

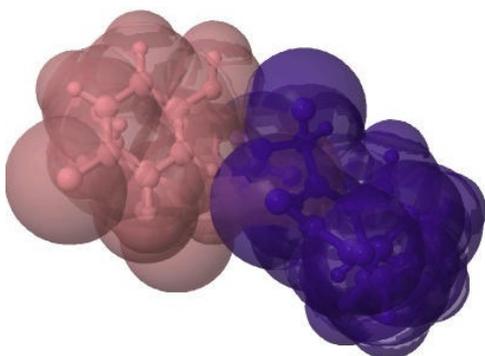
- [1] KINARI-Web server for rigidity analysis of proteins. <http://kinari.linkage.cs.umass.edu>, 2011.
- [2] A. J. Rader, B. M. Hesperheide, L. A. Kuhn, and M. F. Thorpe. Protein unfolding: rigidity lost. *PNAS USA.*, 99:3540–3545, Mar 2002. [PubMed Central:PMC122559] [DOI:10.1073/pnas.062492699] [PubMed:11891336].
- [3] M. F. Thorpe, B. M. Hesperheide, Y. Yang, and L. A. Kuhn. Flexibility and critical hydrogen bonds in cytochrome *c*. *Pac Symp Biocomput*, pages 191–202, 2000. [PubMed:10902168].



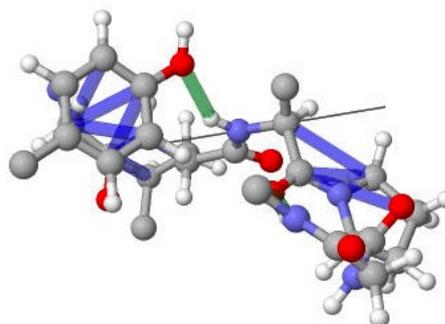
(a) Rigidity results w/ default options



(b) Viewing specific clusters



(c) Viewing hinge regions



(d) Hinge between 2 bodies

Figure 1: The visualizer can be used to display different rigidity features of 1HRC. The quick-start option uses default curation and modeling options, and displays the largest rigid clusters as highlighted surfaces (a) in a bar-and-stick model. Many other visualization options are available. The same protein can be viewed as a cartoon (b), two bodies that connect at a mechanical hinge can be shown (c), while hydrogen bonds and hydrophobic interactions can be displayed in the vicinity of a mechanical hinge region.