

# Improvements in *ProMode* (a Database of Normal Mode Analyses of Proteins)

Hiroshi Wako<sup>1</sup>

wako@waseda.jp

Masaki Kato<sup>2</sup>

kato@tsurumi.yokohama-cu.ac.jp

Shigeru Endo<sup>3</sup>

endo@sci.kitasato-u.ac.jp

<sup>1</sup> School of Social Sciences, Waseda University, 1-6-1 Nishi-Waseda, Shinjuku-ku, Tokyo 169-8050, Japan

<sup>2</sup> Department of Science of Biological Supramolecular Systems, Graduate School of Integrated Science, Yokohama City University, 1-7-29 Suehiro-cho, Tsurumi-ku, Yokohama 230-0045, Japan

<sup>3</sup> Department of Physics, School of Science, Kitasato University, 1-15-1 Kitasato, Sagami-hara 228-8555, Japan

**Keywords:** normal mode analysis, dynamic domain, database, computer simulation, molecular graphics

## 1 Introduction

*ProMode* (<http://promode.socs.waseda.ac.jp/>) is a database collecting the results from normal mode analyses (NMA) of various protein molecules [3]. Although NMA is based on the harmonic approximation, it has been shown by many studies that the results from NMA are not only reasonable qualitatively in most cases, but also can provide a proper description of the functionally important motions of the protein. The collection of the NMA results for various proteins is useful for comparative and statistical studies of the dynamic structures of proteins.

For further details of the method of NMA and the contents of *ProMode*, see the reference 3.

## 2 Improvements in *ProMode*

(1) In *ProMode*, we have collected more than 1,000 proteins, which have relatively low sequence similarity (< 50%) to each other and the sizes of which are less than 200 amino acid residues. We will collect data as many as possible in the future. Since a comparative study among homologous proteins is interesting, we are planning to perform NMA for proteins belonging to the same family. The calculations for larger-sized proteins are also planned.

(2) One of the distinctive features of *ProMode* is the animations of vibrating protein molecules which can be seen with a free plug-in, Chime (MDL Information Systems, Inc.). Figure 1 shows a screenshot of *ProMode*. A protein is displayed in the two windows: 3D animation in the left and 3D static images (the energy-minimum conformation and the two fluctuated ones superimposed on it) in the right. The mouse events for translation, rotation, and zoom on the one window affect the other simultaneously. The dynamic domains defined by DynDom are distinguished by different colors in both windows. The axes of screw motions between the domains also defined by DynDom are shown in the right window.

Since the input data file for the animation has no information about amino acid residues in Chime (which contains only atom types and their coordinates), while the static image contains such information, a user cannot manipulate the molecule displayed in the animation window. To overcome this inconvenience, we developed the manipulation dialog (superimposed in the upper left in Fig. 1) which can be used for selecting residues and/or atoms and then changing color and atomic representation to highlight them in the animation window by referring the information contained in the static-image window.

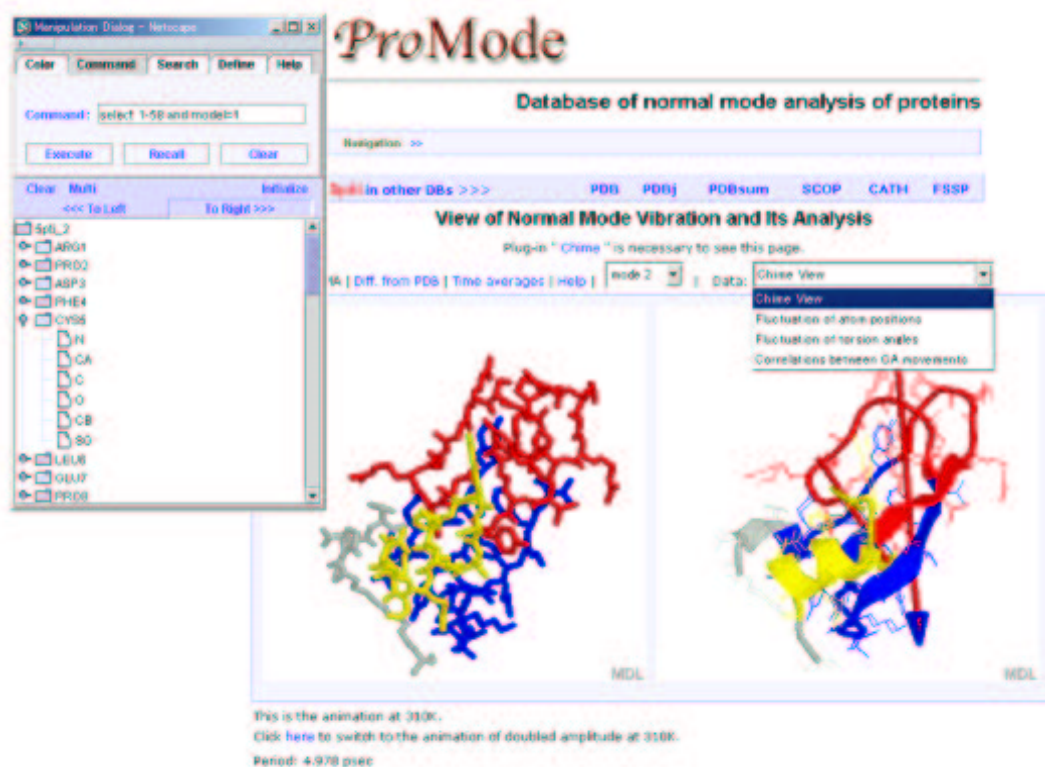


Figure 1: Screenshot of *ProMode*.

### 3 Discussion

Recently, a couple of databases for NMA of proteins were developed [1, 2]. They used a simplified molecular model and a simplified energy potential function (e.g., an elastic proteins model in which atoms representative of residues are connected with harmonic springs). In *ProMode*, however, a full-atom molecular model is used together with the program FEDER/2 [4]. This makes it possible to provide realistic molecular motions in full-atom details. We hope that researchers, especially who are not familiar to the simulation of protein dynamics and have seen only static images of protein structures, will get access to *ProMode*.

This work was financially supported by BIRD-JST (Institute for Bioinformatics Research and Development of Japan Science and Technology Corporation), and is running as a subgroup of one of the BIRD project PDBj (supervised by H. Nakamura, Osaka University; URL is <http://www.pdbj.org/>).

### References

- [1] Chacon, P., Tama, F., and Wrighers, W., Mega-dalton biomolecular captured from electron microscopy reconstructions, *J. Mol. Biol.*, 326:485–492, 2003.
- [2] Echols, N., Milburn, D., and Gerstein, M., MolNovDB: analysis and visualization of conformational change and structural flexibility, *Nucleic Acid Res.*, 31:478–482, 2003.
- [3] Wako, H. and Endo, S., *ProMode*: a database of normal mode analysis of proteins, *Genome Informatics*, 13:519–520, 2003.
- [4] Wako, H., Endo, S., Nagayama, K., and Go, N., FEDER/2: program for static and dynamic conformational energy analysis of macro-molecules in dihedral angle space, *Comp. Phys. Comm.*, 91:233–251, 1995.