ProDy

Protein Dynamics & Sequence Analysis

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Analyzing a **pair of structures**

is easy using VMD, Chimera, PyMol, or etc.

Analyzing a **hundreds of structures**

there is **ProDy** for that
What is ProDy?

ProDy is an **Application Programming Interface** (API) or a toolkit designed for

- analysis of **large** and **heterogeneous** structural datasets,
- normal mode analysis of **elastic network models**,
- **essential dynamics analysis** of trajectories,

and, **application development**
ProDy
Protein Dynamics & Sequence Analysis

Interactive Usage

Interactive Computing

matplotlib
NumPy

IP[y]: IPython
• **Python**
  – numbers, strings, lists, dictionaries, slicing, indexing
  – files, loops, exception control

• **NumPy**
  – Arrays and efficiency

• **Matplotlib**
  – Plotting, showing an image

• **ProDy**
  – Parsers
  – AtomGroups
     • Iterations, hierarchical view, slicing, indexing
  – Plotting functions
     • Show protein
  – Ensemble Analysis
What's next?

ProDy
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ProDy
Learn how to use ProDy from the introductory ProDy tutorial or from the comprehensive API reference manual.

Normal Mode Wizard
Learn how to depict normal modes and generate animations of protein dynamics along them with NMWiz.

Evol Tutorial
Learn how to identify conserved and coevolved residues and characterizing their dynamical properties.

Elastic Network Models
Learn how to perform normal mode analysis and developing customized force constant functions.

Ensemble Analysis
Learn how to analyze large and heterogeneous ensembles of protein structures to infer dynamical properties.

Structure Analysis
Learn how to compare and align structures, identify ligand contacts, and extract ligands from PDB files.

Trajectory Analysis
Learn how to analyze simulation trajectories, in particular handling large trajectory files that don't fit in memory.

Conformational Sampling
Learn how to generate alternate protein conformations along ANM modes and to refine them using NAMD.
• Prefer the online HTML documentation
  – Frequently revised and improved
  – Easy to copy and paste code into a Python shell

```python
In [15]: showProtein(p38);
```

– Show code in a page for copying

![Code Snippets](image)