ProDy

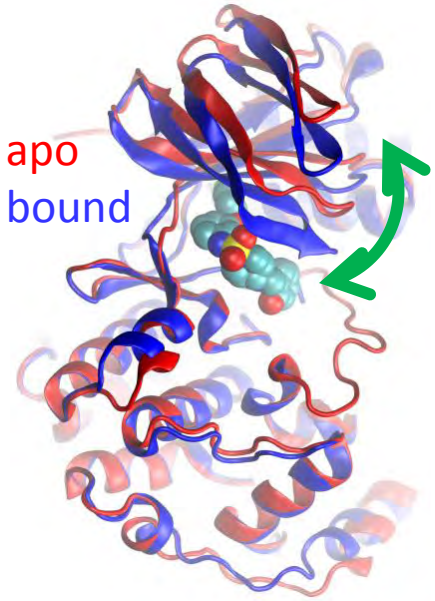
Ahmet Bakan

ProDy

Protein Dynamics & Sequence Analysis

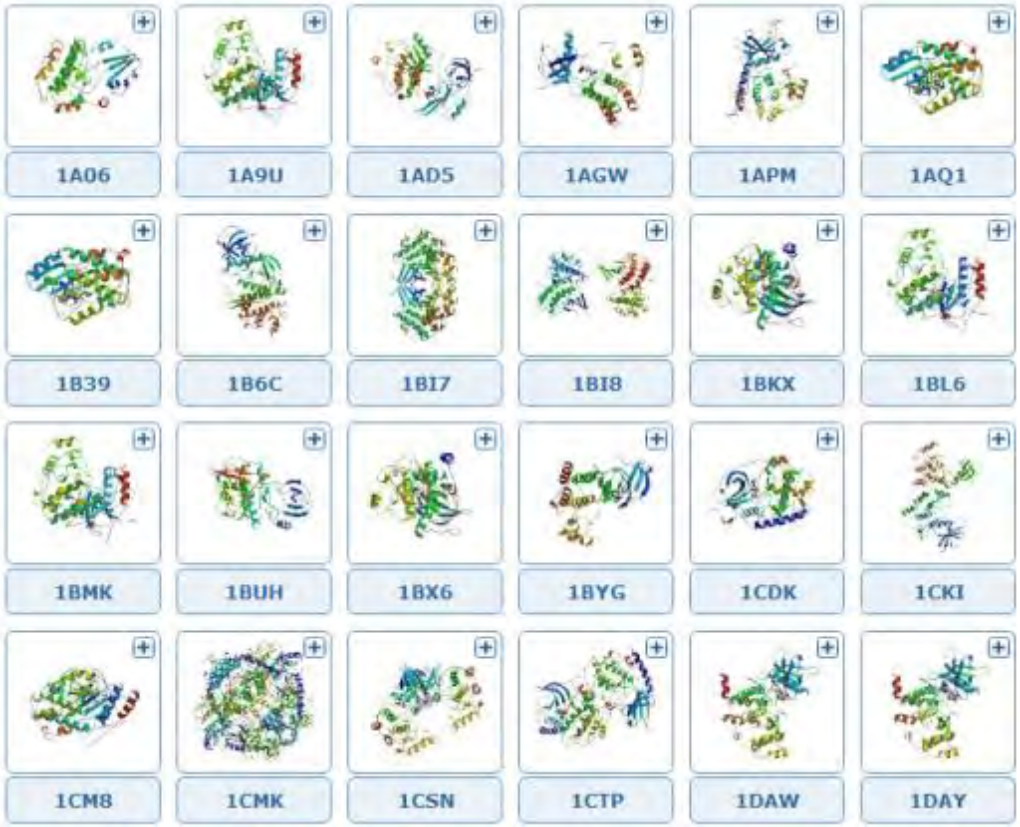
Structure Analysis

Analyzing a **pair of structures**



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

Analyzing a **hundreds of structures**

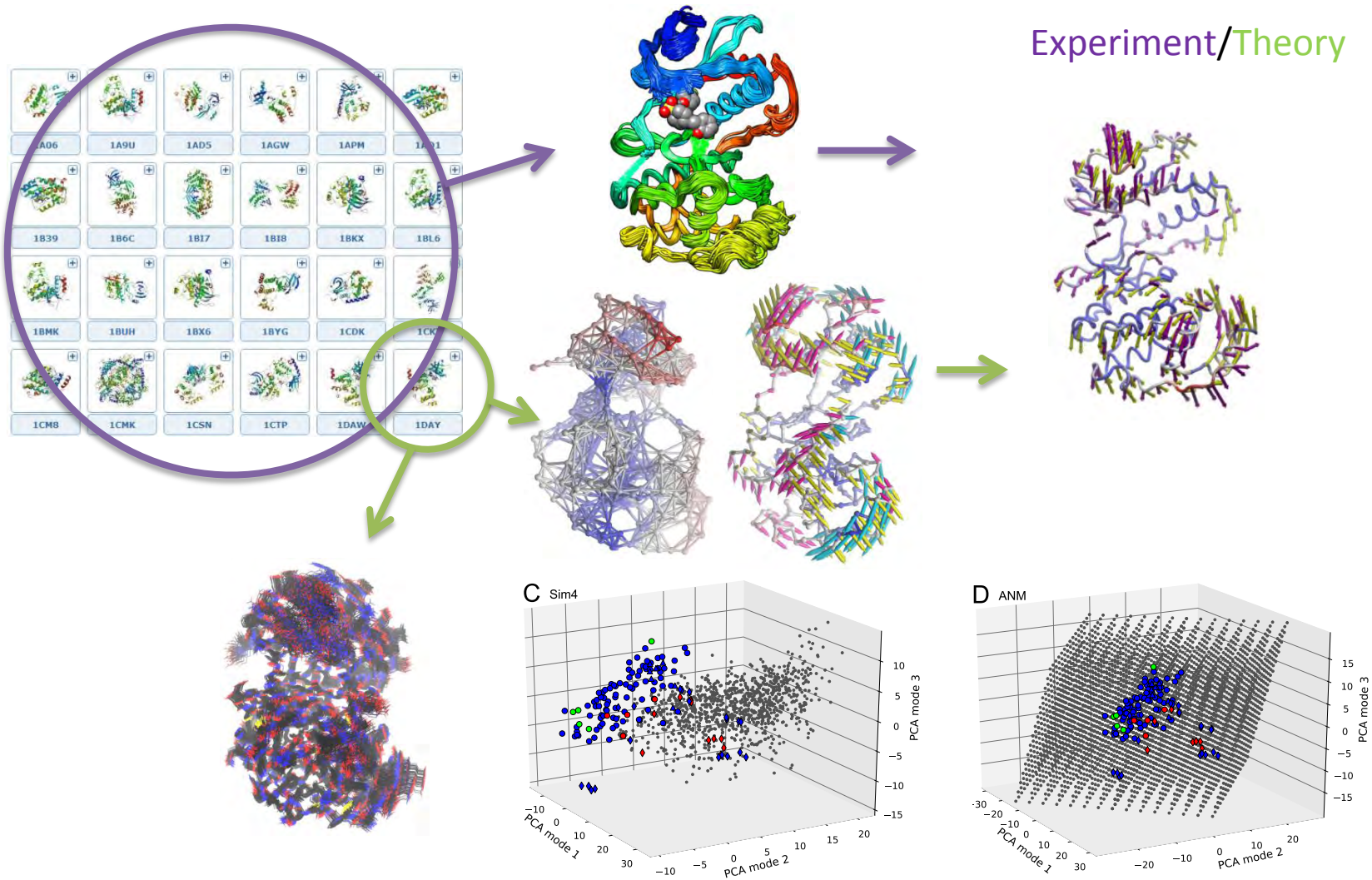


there is ***ProDy*** for that

ProDy

Protein Dynamics & Sequence Analysis

Experiment & Theory



Bakan A, Bahar I **2011** *Pacific Symposium on Biocomputing* 16:181-192

ProDy

Protein Dynamics & Sequence Analysis

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

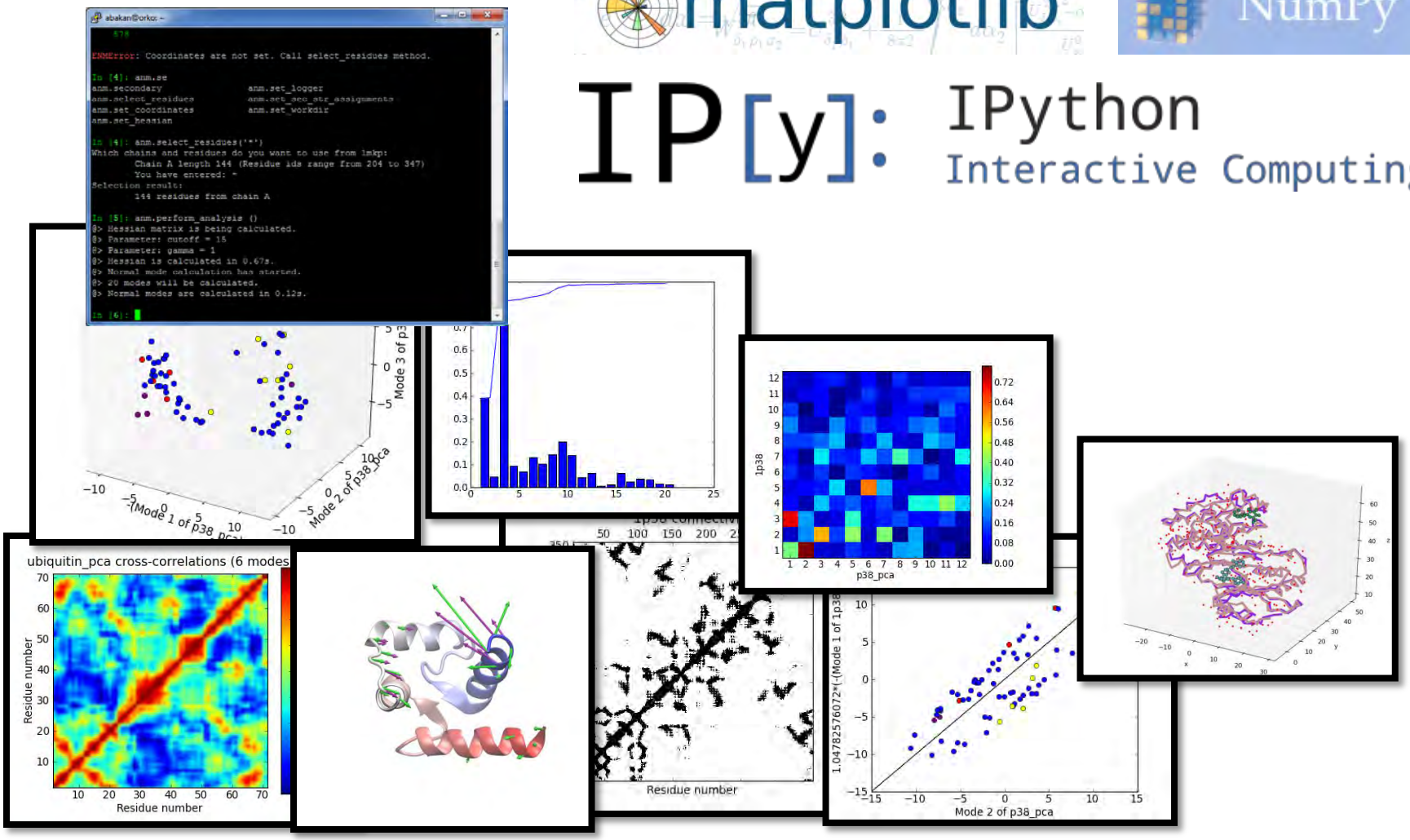
Interactive Usage

matplotlib

NumPy

IP[y]: IPython

Interactive Computing



Python & *ProDy* Demo

- 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

ProDy

Protein Dynamics & Sequence Analysis

What's next?

ProDy

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

Tutorial | Manual

Normal Mode Wizard

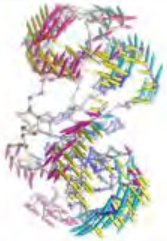
Learn how to depict normal modes and generate animations of protein dynamics along them with NMWiz.

Go to Tutorial

Evol Tutorial

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

Go to Tutorial



Elastic Network Models

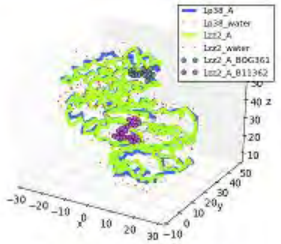
Learn how to perform normal mode analysis and developing customized force constant functions.

Go to Tutorial

Ensemble Analysis

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

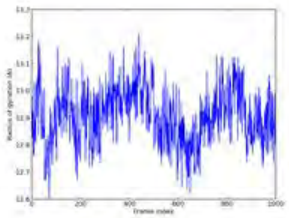
Go to Tutorial



Structure Analysis

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

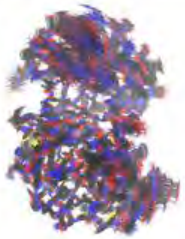
Go to Tutorial



Trajectory Analysis

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

Go to Tutorial



Conformational Sampling

Learn how to generate alternate protein conformations along ANM modes and to refine them using NAMD.

Go to Tutorial

Online Documentation

- Prefer the online HTML documentation
  - Frequently revised and improved
  - Easy to copy and past code into a Python shell

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

```
showProtein(p38);
```

  - Show code in a page for copying