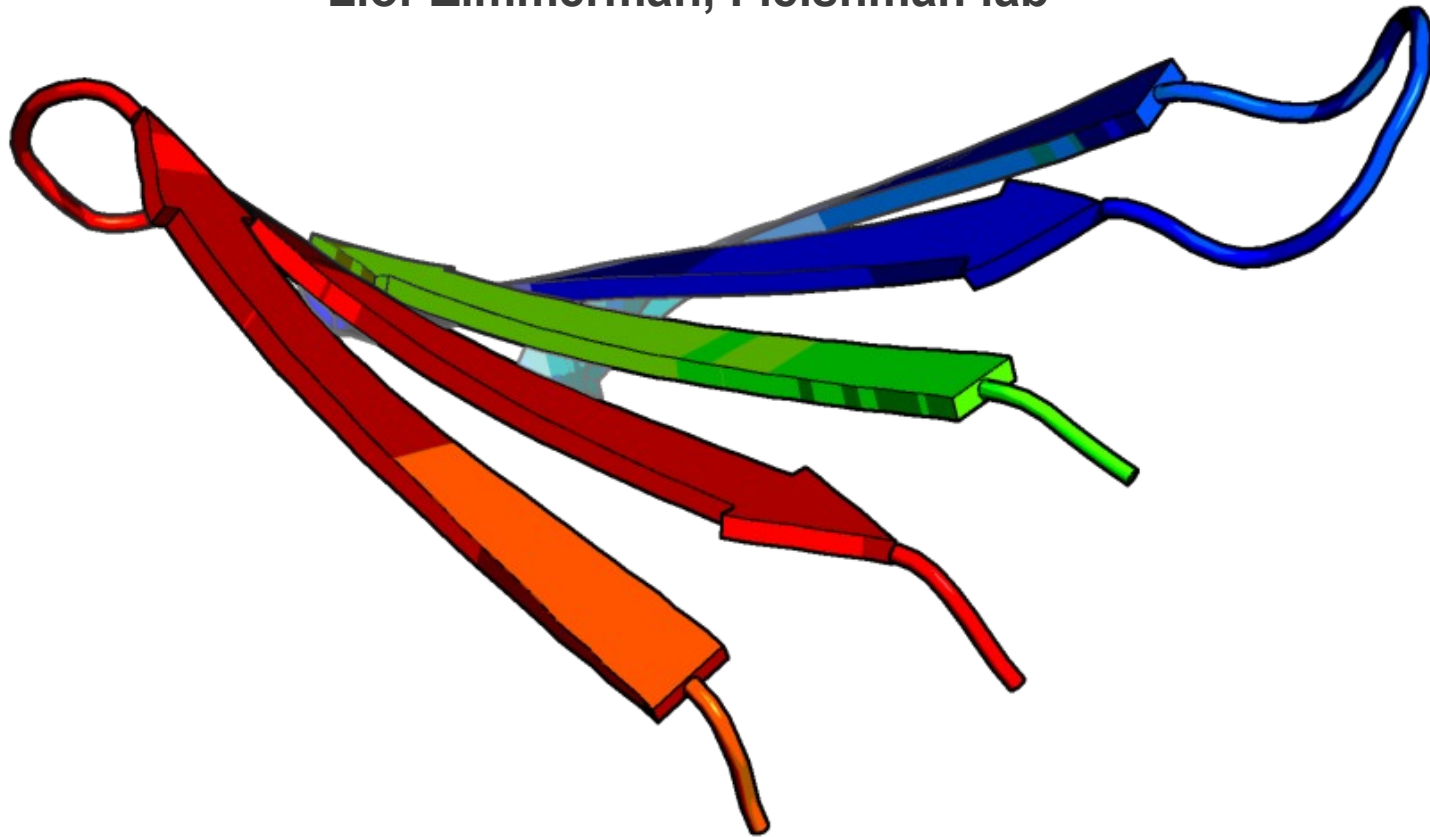


Rosetta Diagrams

Lior Zimmerman, Fleishman lab

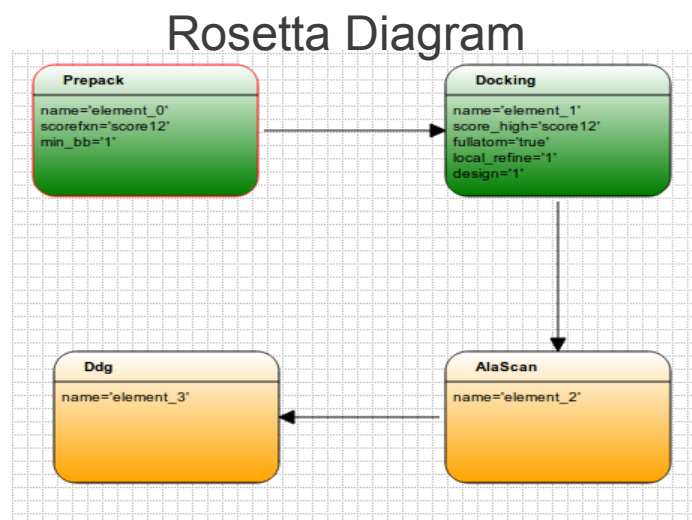


Rapid prototyping of Rosetta protocols

With style

What is Rosetta Diagrams?

Rosetta diagrams is a visual layer on top of RosettaScripts
It allows you to create Rosetta protocols by drawing them as diagrams



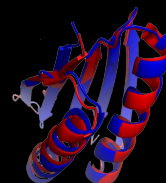
Translate



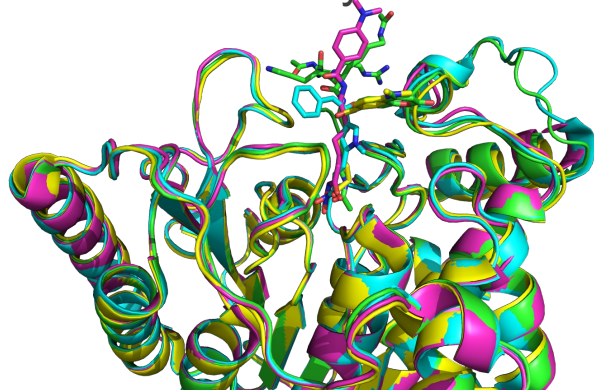
```
<ROSETTASCRIP>  
...  
</ROSETTASCRIP>
```



Rosetta



Decoys



[(not) Live Demo]

RosettaDiagrams + PyRosetta?

- Enabling users to test their protocols on the fly
- Watch the protocol flow live on pymol
 - Note: will use in the future HTML5 molecular viewer such as **jolecule**
- Used **Tornado** (A python web framework, similar to nodejs) together with PyRosetta

Two possible development paths

Option 1: An integrated development environment for rapid prototyping

Rosetta Diagrams
Create protein modeling protocols for Rosetta, with style.

[Try the alpha version](#) [User's manual](#) [Sign in with Google](#)

Easily create complex protocols
Rosetta Diagrams allows you to create complex Rosetta protocols by drawing them as diagrams

Export to Rosetta Scripts
Export the diagram to Rosetta Scripts and run it on any machine that has Rosetta installed.

Completely open source
Follow us on **GitHub**

Log in to a personalized workspace area

Mockup of a Personalized workspace

Saved protocols

- **Protocol 1**
- Protocol 2
- Protocol 3
- Protocol 4
- ...

Analysis

Structures

Diagram

- **Analysis:**
 - Basic plotting capabilities
 - Score file manipulations
 - More?
- **Structures**
 - Viewing decoys using an html5 plugin (jolecule)
- **Diagram**
 - The diagram editor, running protocols straight from the diagram on a local/remote cluster

Two possible development paths (cont.)

Option 2: Make Rosetta Diagrams more friendly to novices, remains **mainly client side**

- Enforce types of attributes in the Properties section. (real/boolean/score Functions, etc)
- Possible values
- **Requires a substantial rewrite of the RosettaScripts internals**

Properties

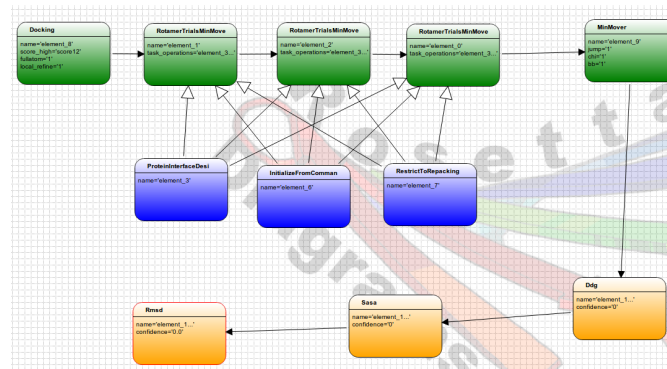
Add Attribute

Name	Value	Delete
name	element_6	X
score_low		X
score_high		X



Improve wiki/documentation integration

RosettaScripts → Diagram



```
<?xml version="1.0"?>
<ROSETTASCRIPTS>
  <SCOREFXNS></SCOREFXNS>
  <TASKOPERATIONS>
    <ProteinInterfaceDesign name="element_3" />
    <InitializeFromCommandLine name="element_6" />
    <RestrictTolerancing name="element_7" />
  </TASKOPERATIONS>
  <FILTERS>
    <Ddg name="element_10" confidence="0" />
    <Sasa name="element_11" confidence="0" />
    <Rmsd name="element_12" confidence="0.0" />
  </FILTERS>
  <MOVES>
    <RotamerTrialsMinMove name="element_0" task_operations="element_3,element_6,element_7" />
    <RotamerTrialsMinMove name="element_1" task_operations="element_3,element_6,element_7" />
    <RotamerTrialsMinMove name="element_2" task_operations="element_3,element_6,element_7" />
    <MinMove name="element_5" jump="1" chi="1" bb="1" />
  </MOVES>
  <APPLY_TO_POSE></APPLY_TO_POSE>
  <PROTOCOLS>
    <Add mover_name="element_0" />
    <Add mover_name="element_1" />
    <Add mover_name="element_2" />
    <Add mover_name="element_5" />
    <Add filter_name="element_10" />
    <Add filter_name="element_11" />
    <Add filter_name="element_12" />
  </PROTOCOLS>
</ROSETTASCRIPTS>
```

Current Limitations

- Saving diagrams (in future – server? LocalStorage?)
- Undoing changes
- Missing attributes
- More...

Thanks!



<http://www.RosettaDiagrams.org>