

Protein structures
in a common
reference frame

Ligand poses in a
common reference
frame.

Complex structures
ready for docking
and easy to analyze
or visually inspect.

Aligned Coordinates Within Protein Families

Interested in getting a jump start on your structure based discovery project?

When you start a structure based drug-discovery project, you commonly find many structures for the same protein or related proteins. Do you:

- Wish that the PDB structures can all be referenced to a single reference frame?
- Wish that their ligands could be cross referenced to the other structures?
- Wish that you could easily see each monomeric unit in the X-ray structure superimposed?
- Wish that you had common sets of grouped water molecules?

Accelrys' Contract Research Group is currently offering 3-D coordinate alignments for any protein family of interest to you. You identify the protein class of interest and we will work with the 3-D structures specific to your project.

We will deliver to you a set of aligned 3-D coordinates: proteins, ligands, complexes. You choose what you want and we will customize your deliverable.

Tell us what you want; all discussions will be under a mutual NDA, and strict confidentiality will be assured.

The key advantages to this service are:

- The results serve as a desirable starting point for all structure based discovery efforts.
- Systems with a large amount of published data can be referenced in one single reference frame.
- Any proprietary data available can also be oriented in the same reference frame

Overview of Workflow

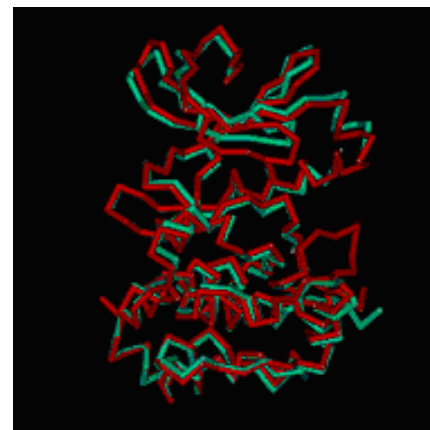
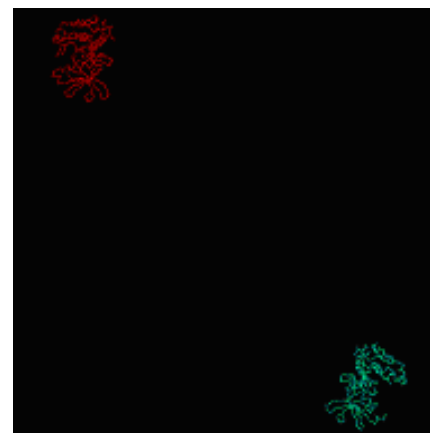


Fig 1. (top) Unaligned proteins. (Bottom) Aligned 3-D protein coordinates.

A Contract Research Services representative is available to provide a project proposal and more details about the service. Please contact your Accelrys account manager.