Kpax Demo – Basic Operations

- Download Kpax from: http://kpax.loria.fr/download-3.2-beta/
- Example pairs of structures: http://hex.loria.fr/emmsb/kpax_examples/
- Aligning two structures
- Viewing the results in Hex and VMD
- Performing flexible structural alignments
- Building and searching a structural database
- Performing multiple structural alignments
- Viewing multiple alignments in Hex/VMD
- ...
- Ask me!
- Disclaimer: Kpax is not "commercial" software!

Practical Activities – 1

Downloading the data

- Download the API-A sequence from: http://hex.loria.fr/emmsb/t40.tgz
  - t40_c.fasta (API-A)
- Download the CATH database from: http://hex.loria.fr/emmsb/cath/
  - CathDomainPdb.S35.v3_4_0.tgz (260 Mb of compressed PDB files)
  - CathDomainList.gz (1.3 Mb file of CATH codes)
  - build_cath.sh (shell script to build a Kpax database)

Building a Kpax database

- Unzip the two zip files (use gunzip)
- Edit the script to have the correct path to the data (CATH_ROOT=???)
- Run the script to build that database (takes a few minutes)
- Run kpax with -help option to show all the parameters and options; try:
  - kpax -db=cath -list

Practical Activities – 2

Searching a database and visualising the results

- Try searching the database with t40_c.pdb as the query
- Go to the results folder (kpax_results/t40_c) and look at the results files
- Use Hex or VMD to visualise the results (.mac for Hex and .tcl for VMD)
- Do you agree with the superpositions?

Making a MSA for homology modeling

- Run kpax to make a multiple structure alignment from the seed sequence
- The command for this is of the form:
  - kpax -db=cath -model -top=24 t40_c.fasta
- cd to the results folder (kpax_results/2qn4A00) and examine the contents

Making a homology model (optional)

- Run Modeler (the actual command may differ on your machine):
  - /opt/modeller/bin/mod9.13 t40_c_modeller.py
- Use Kpax/Hex to compare the model and real structure (t40_c.pdb)