Coda

We hope these short tutorials have given you a broad set of basic abilities in protein structure prediction and design. PyRosetta's power is in its flexibility. You are now able to interactively combine folding, docking, and design operations and to use fold trees, move maps, and movers to tailor each operation to operate on the portion of the protein that is appropriate for the particular biological problem at hand.

There are many more features available in Rosetta and PyRosetta that you may find useful. Several particular useful features that are beyond the scope of this manual but currently implemented in PyRosetta include:

- *Ligands* composed of non-protein atoms or heteroatoms
- Nucleic acids, DNA and RNA
- Post-translationally modified and non-canonical amino acids

Each of these can be loaded into poses, measured, scored, manipulated, designed or designed around, and docked. Ligands and modified amino acids require manipulation of the params files in the PyRosetta database. Example params files are provided in Appendix B. Fuller details can be found in the PyRosetta User's Manual available on http://www.pyrosetta.org.

PyRosetta is being continually expanded, particularly with the expansion of the underlying Rosetta code. Please watch the website for future updates.