

Data Management Plan

Products of research

The data to be collected in this research are kinetic assay measurements and computer models of protein-intermediate complexes. Because we are attempting to discern between the mechanistic possibilities, the data collected will be unique.

We anticipate at least 10 GB of kinetics and simulation data will be collected per enzyme over the course of the project.

We will also generate plasmids for each enzyme with mutations to putative catalytic amino acids.

Data format

Kinetics data will be in the format of Excel spreadsheets or R workbooks.

Simulations will be in YASARA Obj or RCSB PDB file format. Molecular dynamics simulations will be in YASARA .SIM and copied into .XTC format.

Access to data and data sharing practices and policies

Raw kinetic data will be available for download from the Open Science Framework component associated with the work.

Data will be stored on Open Science Framework and backed-up to local external hard disks.

Plasmids will be stored in the Department -80 °C and all plasmids will be deposited in Addgene. Sequencing data of the plasmid will be digitally stored and deposited with the Addgene company.

Policies and provision for re-use, re-distribution and products of derivatives

These data will be distributed in peer-reviewed publications; therefore, anyone is allowed to use these data at any time according to the copyright policies of the journal.

Archiving of data

Molecular modeling data and kinetic data will be saved onto a local computer and institutional server, which in turn backs up data to a non-local server.

Data will also be stored off-site on the Open Science Framework. The PI also pays for private data storage space as a redundant back-up to the institutional back-up. In this way, any data we generate will be saved in at least three locations.

Data will be stored for 20 years beyond the end of the project.