MiA Suite is a protein structural modeling software consisting of two modules, Chiron and Loop.

Chiron, named after the Thessalian god of healing, is a protein structure refinement module. Chiron performs rapid refinement of protein structures using discrete molecular dynamics with an all-atom representation for each residue in the protein. Chiron can be used to resolve even severe clashes that cause traditional MD to fail. Additionally, Chiron causes minimal perturbation (less than 1 Å Cα RMSD in a benchmark set of structures with severe clashes).

Loop module utilizes programs that automate loop-building during protein structural modeling. More details are available in the following references:


Unique capabilities of Chiron deliver rapid, efficient protein structure refinement with minimum perturbations:

- Soft-core potentials enable refinement of structures with overlapping atoms, which cause other programs to fail.
- High heat-exchange coefficient ensures minimal perturbation of the protein structure during refinement.

The unique capabilities make Chiron especially advantageous:

- Chiron can minimize structures with severe clashes, where other methods fail.
- In benchmark tests, Chiron is able to resolve clashes from the homology models within 1 Å of the initial model and yet not drift away from the native structure.
- Chiron is the first program to use an energetic measure for steric clashes, which is a more realistic way to evaluate quality of a protein structure.

Loop module exploits the unparalleled sampling efficiency of DMD and the accuracy of the all-atom Medusa force field to deliver physically realistic structural models for protein loops that are essential for design of biologics such as antibodies and immunogens.