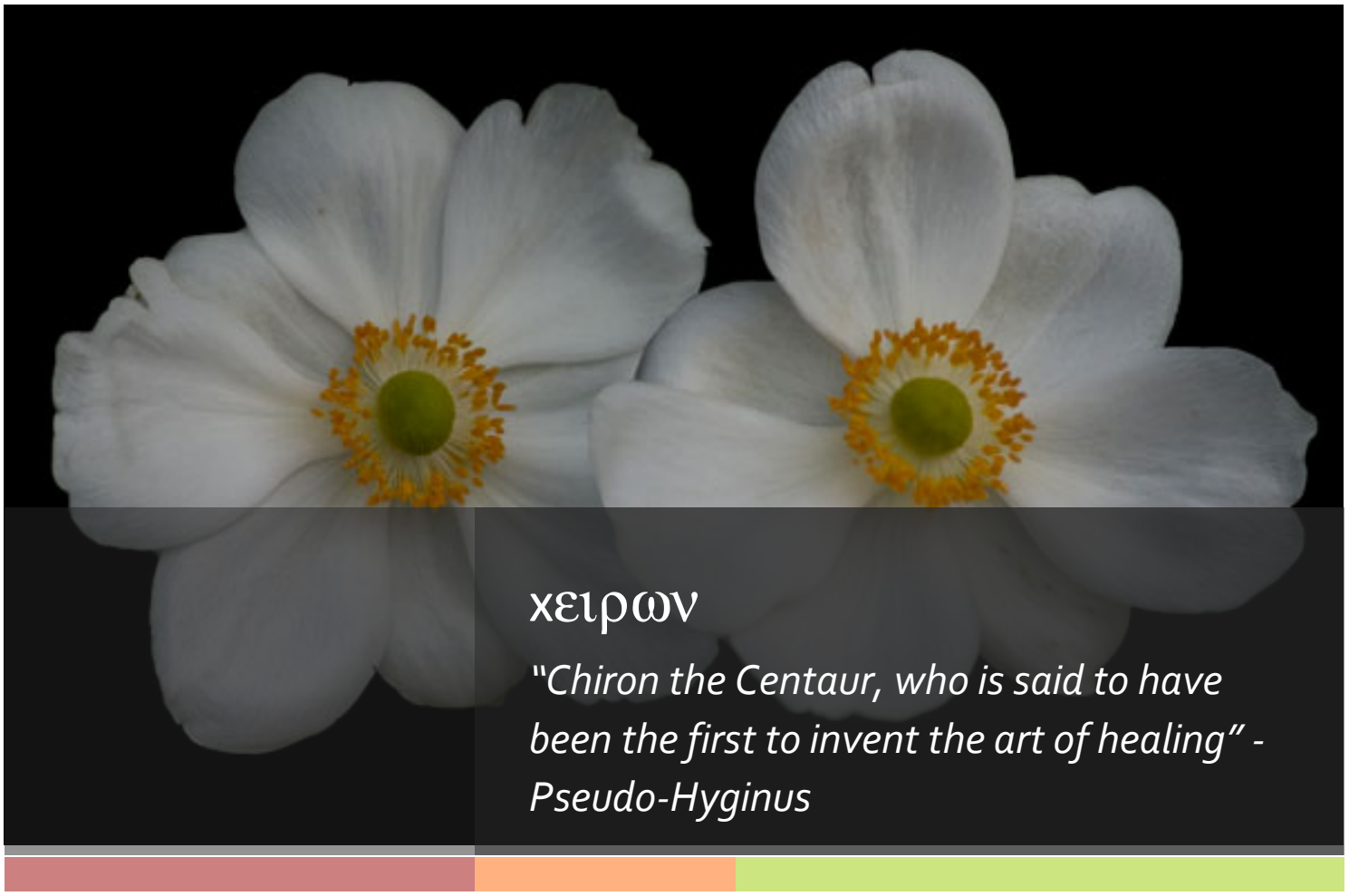
Molecules in Action, LLC

MiA Suite

V 1.0



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"Chiron the Centaur, who is said to have been the first to invent the art of healing" - Pseudo-Hyginus

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:

Ramachandran, S., Kota, P., Ding, F. and Dokholyan, N. V., Proteins: Structure, Function and Bioinformatics, 79: 261-270 (2011)

F. Ding, D. Tsao, H. Nie, and N. V. Dokholyan, "Ab initio folding of proteins with all-atom discrete molecular dynamics." *Structure*, 16:1010-1018 (2008)

D. Shirvanyants, F. Ding, D. Tsao, S. Ramachandran, and N. V. Dokholyan, "DMD: an efficient and versatile simulation method for fine protein characterization." *Journal of Physical Chemistry*, in press (2012)

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.

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