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April 21, 2009

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Primary contributors: Ivelin Georgiev, Ryan Lilien, and Bruce Donald

Contact Info:
Bruce R. Donald
Duke University
Department of Computer Science
Levine Science Research Center (LSRC)
Durham, NC 27708-0129
USA
e-mail: www.cs.duke.edu/brd/

<signature of Bruce Donald>, 12 Apr, 2009
Bruce Donald, Professor of Computer Science

2 Citation Requirements

The citation requirements for the various different modules of our software are:

- For a general citation, please use:

C. Chen, I. Georgiev, A. C. Anderson, and B. R. Donald. Computational structure-based redesign of enzyme activity. *PNAS USA*, 106(10):3764–3769, 2009.

- MinDEE:

I. Georgiev, R. Lilien, and B. R. Donald. The minimized dead-end elimination criterion and its application to protein redesign in a hybrid scoring and search algorithm for computing partition functions over molecular ensembles. *J Comput Chem*, 29(10):1527–42, 2008.

- BD:

I. Georgiev and B. R. Donald. Dead-end elimination with backbone flexibility. *Bioinformatics*, 23(13):i185–94, 2007. Proc. International Conference on Intelligent Systems for Molecular Biology (ISMB), Vienna, Austria (2007).

- BRDEE:

I. Georgiev, D. Keedy, J. S. Richardson, D. C. Richardson, and B. R. Donald. Algorithm for backrub motions in protein design. *Bioinformatics*, 24(13):i196–204, 2008. Proc. International Conference on Intelligent Systems for Molecular Biology (ISMB), Toronto, Canada (2008).

- DACS:

I. Georgiev, R. Lilien, and B. R. Donald. Improved pruning algorithms and divide-and-conquer strategies for dead-end elimination, with application to protein design. *Bioinformatics*, 22(14):e174–183, 2006. Proc. International Conference on Intelligent Systems for Molecular Biology (ISMB), Fortaleza, Brazil (2006).

- K^* (current implementation):

I. Georgiev, R. Lilien, and B. R. Donald. The minimized dead-end elimination criterion and its application to protein redesign in a hybrid scoring and search algorithm for computing partition functions over molecular ensembles. *J Comput Chem*, 29(10):1527–42, 2008.

To cite the general idea of K^* , you can also cite:

R. Lilien, B. Stevens, A. Anderson, and B. R. Donald. A novel ensemble-based scoring and search algorithm for protein redesign, and its application to modify the substrate specificity of the Gramicidin Synthetase A phenylalanine adenylation enzyme. *J Comp Biol*, 12(6–7):740–761, 2005.

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