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February 20, 2012

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<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.

• iMinDEE:

P. Gainza, K.E. Roberts, and B.R. Donald. Protein Design using Continuous Rotamers *PLoS Computational Biology*, (1): e1002335. doi:10.1371/journal.pcbi.1002335, 2012.

• Protein:Protein Interactions:

K.E. Roberts, P.R. Kushing, P. Boisguerin, DR Madden, and B.R. Donald. Design of protein-protein interactions with a novel ensemble-based scoring algorithm. *Research in Computational Molecular Biology.*, volume 6577 of Lecture Notes in Computer Science. Heidelberg: Springer Berlin. pp. 361376. 2011

• 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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