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December 7, 2012

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Contact Info:
Bruce 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>, Mar 1, 2012
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.

P. Gainza, K. E. Roberts, I. Georgiev, R. H. Lilien, D. A. Keedy, C. Chen, F. Reza, A. C. Anderson, D. C. Richardson, J. S. Richardson, and B. R. Donald. OSPREY: Protein design with ensembles, flexibility, and provable algorithms. *Methods in Enzymology*, in press, 2012.

- 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

K.E. Roberts, P.R. Kushing, P. Boisguerin, DR Madden, and B.R. Donald. Computational Design of a PDZ Domain Peptide Inhibitor that Rescues CFTR Activity. *PLoS Computational Biology*, 2012. In press.

- 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.

- DEEPer:

M. A. Hallen, D. A. Keedy, and B. R. Donald. Dead-End elimination with perturbations (DEEPer): A provable protein design algorithm with continuous sidechain and backbone flexibility. *Proteins*, in press, 2012.

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```
<one line to give the program's name and a brief idea of what it does.>
Copyright (C) <year> <name of author>
```

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Also add information on how to contact you by electronic and paper mail.

If the program does terminal interaction, make it output a short notice like this when it starts in an interactive mode:

```
<program> Copyright (C) <year> <name of author>
This program comes with ABSOLUTELY NO WARRANTY; for details type 'show w'.
This is free software, and you are welcome to redistribute it
under certain conditions; type 'show c' for details.
```

The hypothetical commands 'show w' and 'show c' should show the appropriate parts of the General Public License. Of course, your program's commands might be different; for a GUI interface, you would use an "about box".

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Version 3, 29 June 2007

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