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January 15, 2015

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<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*, 523:87-107, 2013.

- 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*, 8.4:e1002477, 2012.

- 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*, 81(1):18–39, 2013.

- COMETS:

M. A. Hallen and B. R. Donald. COMETS (Constrained Optimization of Multistate Energies by Tree Search): A provable and efficient algorithm to optimize binding affinity and specificity with respect to sequence. *Research In Computational Molecular Biology (RECOMB)* proceedings, in press, 2015.

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If you develop a new program, and you want it to be of the greatest possible use to the public, the best way to achieve this is to make it free software which everyone can redistribute and change under these terms.

To do so, attach the following notices to the program. It is safest

to attach them to the start of each source file to most effectively state the exclusion of warranty; and each file should have at least the "copyright" line and a pointer to where the full notice is found.

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

This program is free software: you can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

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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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Defining a subclass of a class defined by the Library is deemed a mode
of using an interface provided by the Library.

A "Combined Work" is a work produced by combining or linking an
Application with the Library. The particular version of the Library
with which the Combined Work was made is also called the "Linked
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based on the Application, and not on the Linked Version.

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Application, but excluding the System Libraries of the Combined Work.

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You may place library facilities that are a work based on the Library side by side in a single library together with other library facilities that are not Applications and are not covered by this License, and convey such a combined library under terms of your choice, if you do both of the following:

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