

OSPREY 3: Open-Source Protein Redesign for You, Refactored, with Powerful New Features

Donald Lab

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1 Abstract

2 Introduction

For over a decade, the OSPREY software package [?, ?] has offered the protein design community a unique combination of continuous flexibility modeling, ensemble modeling, and algorithms with provable guarantees. Having begun as a software release for the K^* algorithm, which approximates binding constants using ensemble modeling, it now boasts a wide array of algorithms found in no other software. OSPREY has been used in many designs that were empirically successful, *in vitro* and *in vivo* as well as in non-human primates. However, as we added more and more algorithms into OSPREY, the code became somewhat complicated and messy. Thus, we have now refactored it, to facilitate the adding of new features both by ourselves and by any others. We have also introduced a convenient Python interface and GPU support, allowing designs to be completed much more quickly and easily than in previous version of OSPREY. We thus believe OSPREY 3 will be a very useful tool for both developers and users of provably accurate protein design algorithms.

3 New features

References

- [1] Pablo Gainza, Kyle E. Roberts, Ivelin Georgiev, Ryan H. Lilien, Daniel A. Keedy, Cheng-Yu Chen, Faisal Reza, Amy C. Anderson, David C. Richardson, Jane S. Richardson, and Bruce R. Donald. OSPREY: Protein design with ensembles, flexibility, and provable algorithms. *Methods in Enzymology*, 523:87–107, 2013.

- [2] Ivelin Georgiev, Kyle E. Roberts, Pablo Gainza, Mark A. Hallen, and Bruce R. Donald. OSPREY (Open Source Protein Redesign for You) user manual. Available online: www.cs.duke.edu/donaldlab/software.php. Updated, 2015. 94 pages., 2009.