

A Post-doctoral position in development of Computational Protein Design methods available at LISBP-INSA, CNRS, INRA Toulouse, France

The Biosystems and Process Engineering Laboratory (LISBP), located on the grounds of the INSA-Toulouse (France) is seeking for a postdoctoral researcher to work at the intersection of Computational Structural Biology and Discrete Optimization, on models and algorithms for Computational Protein Design. The laboratory is affiliated to the French National Centre for Scientific Research (CNRS, UMR INSA-CNRS 5504) and the French National Institute for Agricultural Research (INRA, UMR INSA-INRA 792).

The work will take place in an interdisciplinary project, funded by the 'Initiative d'excellence de l'Université de Toulouse' and associating computational structural biologists of LISBP with computer scientists specialized in discrete optimization from the INRA MIAT lab, in Toulouse. Together, they have recently shown that cutting-edge combinatorial optimization techniques from Artificial Intelligence, namely "Cost Function Network" (CFN) could push Computational Protein Design well beyond the limits of usual methods [1-6]. Capitalizing on prior work with the aim of further exploring the potential of CFN-based approaches to meet the Computational Protein Design challenges, the work will mainly involve the development of novel computational enzyme design methods capable of handling more complex protein design models, incorporating local and global backbone flexibility with positive and negative design targets.

We are looking for a highly motivated scientist who has an excellent research background and expertise in computational structural biology (especially in 3D protein structure modeling and simulation) and excellent programming skills in efficient compiled languages (ideally C++). Background in search algorithms and combinatorial optimizations methods would be extremely beneficial.

The perspective researcher will have the opportunity to work in a diverse and rich multidisciplinary environment, surrounded by both computational and experimental experts in the field of enzyme engineering. Applicants should enjoy teamwork and have very good communication skills. Good English skills are required and notions of French would be a plus.

The position is available from March 1st, 2016 and for duration of one year (from six to nine additional months could be possible upon funding).

Applicants should send as soon as possible CV, summary of previous research and contact addresses of references to: Sophie Barbe, Research Scientist INRA: sophie.barbe@insa-toulouse.fr

- [1] Traoré S, Roberts K, Allouche D, Donald B-R, André I, Schiex T, Barbe S. Fast search algorithms for Computational Protein Design. *Journal of Computational Chemistry* 2015 (in press).
- [2] Traoré S, Allouche D, André I, de Givry S, Katsirelos G, Schiex T, Barbe S. A new framework for computational protein design through Cost function optimization. *Bioinformatics*, 2013. 29:2129-36.
- [3] Simoncini D, Allouche D., de Givry S, Delmas C, Barbe S, Schiex T. Guaranteed Discrete Energy Optimization on Large Protein Design Problems. *Journal of Chemical Theory and Computation* 2015 11 (12), 5980-5989.
- [4] Traoré S, Allouche D, André I, de Givry S, Katsirelos G, Barbe S, Schiex T. Computational Protein Design as a Cost Function Network Optimization Problem. CP2012 Proceedings. 18th International Conference on Principles and Practice of Constraint Programming, Québec, Canada, Oct, 8-12, 2012–Proceeding.
- [5] Allouche D, Davies J, de Givry S, Katsirelos G, Schiex T, Traoré S, André I, Barbe S, Prestwich S, O'Sullivan B. Computational Protein Design as an Optimization Problem. *Artificial Intelligence Journal*, 2014. 212:59-79.
- [6] Viricel C, Simoncini D, Allouche D, de Givry S, Barbe S, Schiex T. 2015. Approximate Counting with Deterministic guarantees for Affinity Computation. In, proceedings of the international conference on Modelling, Computation and Optimization in Information Systems and Management Sciences, MCO 2015, Metz, France: Advances in Intelligent Systems and Computing - Springer.

Laboratory address :

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