Cologne Evolution Colloquium

CRC 1310 Predictability in Evolution

Barbara Bravi

École polytechnique fédérale de Lausanne

Coevolution based inference of allosteric architectures

We analyze maximum entropy approaches to infer the functional design of elastic materials exhibiting allostery, i.e. the property of highly specific responses to ligand binding at a distant active site. To guide and inform protocols of *de novo* drug design, it is fundamental to understand what architectures underlie such a transmission of information and whether their features can be predicted from sequence data alone.

We consider the functional designs of *in silico* evolved allosteric architectures which propagate efficiently energy (including shear, hinge, twist) or strain (resulting in a less-constrained trumpet-shaped region between the allosteric and the active site).

We benchmark existing maximum-entropy inference methods on these computationally evolved functional architectures. We show that such approaches, similarly to a sector analysis, capture key aspects of the allosteric designs and provide quantitative predictions on the pattern of mutational effects; we provide an interpretation of the inferred couplings in terms of propagation of the elastic response.

In collaboration with:
Carolina Brito, Riccardo Ravasio, Matthieu Wyart

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University of Cologne
Institute for Biological Physics
Zülpicher Str. 77
Seminar Room Theoretical Physics, Old Building

Hosted by Michael Lässig