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Topological decoding of biomolecular fold complexity

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CURRICULUM VITAE

Barbara Scalvini was born on the 19th of March 1992, in Chiari, Italy. After focusing on languages and humanities as a high school major, she decided to deepen her interest in science, with a Bachelor's and Master's degree in Physics (2011 - 2018), at the University of Milano Bicocca, Milan. Next to her studies, she tutored high school students in their first experiences in the Physics lab, in the context of the LabEx programme. In 2017, she took the opportunity to carry out her master thesis abroad, supported by an Erasmus+ (traineeship) scholarship. She thus worked on smart adaptive optics devices for microscopy, at the Delft Center for Systems and Control (DCSC, TU Delft), under the supervision of Michel Varhaegen. This very positive experience, together with the desire to learn more about biological systems, led her to the decision of continuing her studies in the Netherlands, in the field of Biophysics. In the summer of 2018, she got a PhD position at Leiden University (LACDR), under the supervision of Alireza Mashaghi. The project, whose outcome is summarized in this thesis, involved a combination of in-silico and single-molecule experimental methods to study the effects and predictive power of bio-polymer topology over biological function and interaction. In this context, she received extensive training in force spectroscopy experiments with optical tweezers, delivered by the Sander Tans lab, located in AMOLF (Amsterdam), and LUMICKS B.V. (The Netherlands). Alongside her research work, she expressed her interest in science communication by participating in the FameLab competition, where young scientists pitch their projects to a wider audience. Next to her PhD work, she maintained a passion for language, which led her to attend several courses in her spare time, from foreign languages to computational linguistics training. This side passion led her to start a project bridging topological methods and natural language processing, and, ultimately, to the decision of using the modelling skills acquired in her PhD to language, as a next step in her scientific career. As of January 2023, she is employed as Assistant Professor at the University of the Faroe Islands (Fróðskaparsetur Føroya), where she is working on natural language processing methods for low resource languages.

LIST OF PUBLICATIONS

- [1] Barbara Scalvini, Vahid Sheikhassani, Jaie Woodard, Jana Aupič, Remus T. Dame, Roman Jerala, Alireza Mashaghi, Topology of Folded Molecular Chains: From Single Biomolecules to Engineered Origami, *Trends in Chemistry*, 2(7), 609-622, 2020 (Chapter 1).
- [2] Barbara Scalvini, Vahid Sheikhassani, Alireza Mashaghi, Topological principles of protein folding, *Phys. Chem. Chem. Phys.*, 23(37), 21316-21328, 2021 (Chapter 2).
- [3] Barbara Scalvini, Helmut Schiessel, Anatoly Golovnev, Alireza Mashaghi, Circuit topology analysis of cellular genome reveals signature motifs, conformational heterogeneity, and scaling, *iScience*, 25(3), 103866, 2022 (Chapter 5).
- [4] Vahid Sheikhassani*, Barbara Scalvini*, Julian Ng, Laurens W. H. J. Heling, Yosri Ayache, Tom M. J. Evers, Eva Estébanez-Perpiñá, Iain J. McEwan, Alireza Mashaghi, Topological dynamics of an intrinsically disordered N-terminal domain of the human androgen receptor, *Protein Science*, 31(6), 1-17, 2022 (Chapter 3).
*VS and BS contributed equally to this study.
- [5] Maziar Heidari, Duane Moes, Otto Schullian, Barbara Scalvini, Alireza Mashaghi, A topology framework for macromolecular complexes and condensates, *Nano Research*, 15(11), 9809- 9817, 2022.
- [6] Duane Moes, Elnaz Banijamali, Vahid Sheikhassani, Barbara Scalvini, Jaie Woodard, Alireza Mashaghi, ProteinCT: An implementation of the protein circuit topology framework, *MethodsX*, 9, 101861, 2022.
- [7] Barbara Scalvini, Vahid Sheikhassani, Nadine van de Brug, Laurens W.H.J. Heling, Jeremy D. Schmit, Alireza Mashaghi, Circuit topology approach for the comparative analysis of intrinsically disordered proteins, *J. Chem. Inf. Model.*, 63(8), 2586–2602, 2023 (Chapter 3).
- [8] Barbara Scalvini, Laurens W.H.J. Heling, Vahid Sheikhassani, Vanda Sunderlikova, Sander J. Tans, Alireza Mashaghi, Cytosolic interactome protects against protein unfolding in a single molecule experiment. Submitted (Chapter 4).
- [9] Barbara Scalvini, Alireza Mashaghi, The circuit topology of semantic similarity highlights statistical differences in the communication style of true and fake news. Submitted (Chapter 6).

