Jana Aupič

Education:

October 2015 to July 2020
Doctoral Programme in Chemical Sciences
Faculty of Chemistry and Chemical Technology, University of Ljubljana
Doctoral thesis title: De novo design of coiled-coil protein switch

October 2013 to September 2015
University Study Programme Chemistry-2nd Cycle
Faculty of Chemistry and Chemical Technology, University of Ljubljana
Master's thesis title: Analytical theory for a five-site water model

October 2010 to September 2013
University Study Programme Chemistry-1st Cycle
Faculty of Chemistry and Chemical Technology, University of Ljubljana
Bachelor's thesis title: Adsorption of organic compounds on graphene

Research experience:

March 2021 to present
CNR-IOM, Trieste, Italy
Postdoctoral researcher; Advisor: Dr. Alessandra Magistrato
Project title: Exploiting copper transport routes for anticancer theranostic applications (AIRC fellowship Giovanni Fraviga)

- Exploring hCtr1 Cu(I) intake mechanism via multi-scale computer simulations.

September 2015 to February 2021
National Institute of Chemistry, Slovenia
Graduate student, Postdoctoral researcher; Advisor: Prof. Dr. Roman Jerala

- Design of polypeptide polyhedra from coiled-coil forming segments. Design of Zn(II)-responsive coiled-coil dimers.
- Designing and modeling coiled-coil based protein cages.
- Studying folding pathway of designed protein cages using molecular dynamics and stopped-flow FRET measurements.

October 2013 to September 2015
Faculty of Chemistry and Chemical Technology, University of Ljubljana
Master's Student; Advisor: Assoc. Prof. Dr. Tomaž Urbič

- Studied structural and thermodynamic properties of rigid polyelectrolytes using Monte Carlo simulations and Ornstein-Zernike equation.
- Proposed a new five point water model and assessed its structural and thermodynamic properties via Monte Carlo simulations and Wertheim's integral equation theory.

Publications:

AUPIČ, Jana, LAPENTA, Fabio, JANOŠ, Pavel, and MAGISTRATO, Alessandra. "Intrinsically disordered ectodomain modulates ion permeation through a metal transporter." *Proceedings of the National Academy of Sciences* 119.48 (2022)

BORIŠEK, Jure; AUPIČ, Jana, and MAGISTRATO, Alessandra. "Establishing the catalytic and regulatory mechanism of RNA-based machineries." *Wiley Interdisciplinary Reviews: Computational Molecular Science* (2022)

AUPIČ, Jana, LAPENTA, Fabio, STRMŠEK, Žiga, MERLJAK, Estera, PLAPER, Tjaša, and JERALA, Roman. "Metal ion–regulated assembly of designed modular protein cages." *Science advances* 8.24 (2022)

JANOŠ, Pavel, AUPIČ, Jana, RUTHSTEIN, Sharon, and MAGISTRATO, Alessandra. "The conformational plasticity of the selectivity filter methionines controls the in-cell Cu (I) uptake through the CTR1 transporter." *QRB Discovery* 3 (2022)

WALKE, Gulshan, AUPIČ, Jana, et al. "Dynamical interplay between the human high-affinity copper transporter hCtr1 and its cognate metal ion." *Biophysical Journal* 121.7 (2022)

PLAPER, Tjaša, AUPIČ, Jana, DEKLEVA, Petra, LAPENTA, Fabio, MANČEK KEBER, Mateja, JERALA, Roman, and BENČINA, Mojca. "Coiled-coil heterodimers with increased stability for cellular regulation and sensing SARS-CoV-2 spike protein-mediated cell fusion." *Scientific reports* 11.1 (2021)

LAINŠČEK, Duško, et al. "A Nanoscaffolded Spike-RBD Vaccine Provides Protection against SARS-CoV-2 with Minimal Anti-Scaffold Response." *Vaccines* 9.5 (2021)

MAJERLE, Andreja, HADŽI, San, AUPIČ, Jana, SATLER, Tadej, LAPENTA, Fabio, STRMŠEK, Žiga, LAH, Jurij, LORIS, Remy, and JERALA, Roman. "A nanobody toolbox targeting dimeric coiled-coil modules for functionalization of designed protein origami structures." *Proceedings of the National Academy of Sciences* 118.17 (2021)

AUPIČ, Jana, STRMŠEK, Žiga, LAPENTA, Fabio, PAHOVNIK, David, PISANSKI, Tomaž, DROBNAK, Igor, LJUBETIČ, Ajasja, and JERALA, Roman. "Designed folding pathway of modular coiled-coil-based proteins." *Nature Communications* 12.1 (2021)

LAPENTA, Fabio, AUPIČ, Jana, VEZZOLI, Marco, STRMŠEK, Žiga, DA VELA, Stefano, SVEGRUN, Dmitri, and JERALA, Roman. "Self-assembly of polyhedral protein cages from pre-organised coiled-coil modules." *Nature Communications* 12.1 (2021)

BOŽIČ ABRAM, Sabina, GRADIŠAR, Helena, AUPIČ, Jana, ROUND, Adam R., and JERALA, Roman. "Triangular in Vivo Self-Assembling Coiled-Coil Protein Origami." *ACS Chemical Biology* (2021)

VRANCKEN, Jeroen P.M., et al. "Molecular assemblies built with the artificial protein Pizza." *Journal of Structural Biology: X* 4 (2020)

SCALVINI, Barbara, et al. "Topology of folded molecular chains: from single biomolecules to engineered origamis." *Trends in chemistry* 2.7 (2020)

LEBAR, Tina, LAINŠČEK, Duško, MERLJAK, Estera, AUPIČ, Jana, and JERALA, Roman. "A tunable orthogonal coiled-coil interaction toolbox for engineering mammalian cells." *Nature Chemical Biology* 16.5 (2020)

AUPIČ, Jana, LAPENTA, Fabio, and JERALA, Roman. "SwitCCh: Metal-Site Design for Controlling the Assembly of a Coiled-Coil Homodimer." *ChemBioChem* 19.23 (2018)

LAPENTA, Fabio, AUPIČ, Jana, STRMŠEK, Žiga, and JERALA, Roman. "Coiled coil protein origami: from modular design principles towards biotechnological applications." *Chemical Society Reviews* 47.10 (2018)

LJUBETIČ, Ajasja, et al. "Design of coiled-coil protein-origami cages that self-assemble in vitro and in vivo." *Nature biotechnology* 35.11 (2017)

PRSLJA, Paulina, AUPIC, Jana, and URBIC, Tomaz. "Thermodynamics and structure of a two-dimensional asymmetric electrolyte by integral equation theory." *Molecular Physics* 115.13 (2017)

AUPIČ, Jana, LAPENTA, Fabio, STRMŠEK, Žiga, and JERALA, Roman. "Towards designing new nano-scale protein architectures." *Essays in Biochemistry* 60.4 (2016)

BOŽIČ ABRAM, Sabina, AUPIČ, Jana, DRAŽIĆ, Goran, GRADIŠAR, Helena, and JERALA, Roman. "Coiled-coil forming peptides for the induction of silver nanoparticles." *Biochemical and Biophysical Research Communications* 472.3 (2016)

AUPIC, Jana, and URBIC, Tomaz. "A structural study of a two-dimensional electrolyte by Monte Carlo simulations." *The Journal of chemical physics* 142.1 (2015)

AUPIC, Jana, and URBIC, Tomaz. "Thermodynamics and structure of a two-dimensional electrolyte by integral equation theory." *The Journal of chemical physics* 140.18 (2014)

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