Contribution ID: **9**   Type: **Talk**

Discovering highly potent antimicrobial peptides with deep generative model HydrAMP

Antimicrobial peptides emerge as compounds that can alleviate the global health hazard of antimicrobial resistance, prompting a need for novel computational approaches to peptide generation. Here, we propose HydrAMP, a conditional variational autoencoder that learns lower-dimensional, continuous representation of peptides and captures their antimicrobial properties. The model disentangles the learnt representation of a peptide from its antimicrobial conditions and leverages parameter-controlled creativity. HydrAMP is the first model that is directly optimized for diverse tasks, including unconstrained and analogue generation and outperforms other approaches in these tasks. An additional preselection procedure based on ranking of generated peptides and molecular dynamics simulations increases experimental validation rate. Wet-lab experiments on five bacterial strains confirm high activity of nine peptides generated as analogues of clinically relevant prototypes, as well as six analogues of an inactive peptide. HydrAMP enables generation of diverse and potent peptides, making a step towards resolving the antimicrobial resistance crisis.

Primary authors: SZYMCZAK, Paulina (Faculty of Mathematics, Informatics and Mechanics, University of Warsaw);   MOŻEJKO, Marcin (Faculty of Mathematics, Informatics and Mechanics, University of Warsaw)

Co-authors: GRZEGORZEK, Tomasz (Faculty of Mathematics, Informatics and Mechanics, University of Warsaw);   JURCZAK, Radosław (Faculty of Mathematics, Informatics and Mechanics, University of Warsaw);   BAUER, Marta (Department of Inorganic Chemistry, Faculty of Pharmacy, Medical University of Gdańsk);   NEUBAUER, Damian (Department of Inorganic Chemistry, Faculty of Pharmacy, Medical University of Gdańsk);   SIKORA, Karol (Department of Inorganic Chemistry, Faculty of Pharmacy, Medical University of Gdańsk);   MICHALSKI, Michał (The Centre of New Technologies, University of Warsaw);   SROKA, Jacek (Faculty of Mathematics, Informatics and Mechanics, University of Warsaw);   SETNY, Piotr (The Centre of New Technologies, University of Warsaw);   KAMYSZ, Wojciech (Department of Inorganic Chemistry, Faculty of Pharmacy, Medical University of Gdańsk);   SZCZUREK, Ewa (Faculty of Mathematics, Informatics and Mechanics, University of Warsaw)

Session Classification: Break + Posters session

Track Classification: Poster