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(G*) (POS-61) Drug design of small molecules implementing a deep learning model.

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Antimicrobial resistance is a major global health threat, and it is on the rise. Roughly, 0.7 million people are dying of infections that in the past would have been cured by antibiotics. New techniques and approaches are therefore urgently needed. We are in a position to create new antibiotics and design new rules to combat Antimicrobial Resistance (AMR) by implementing deep learning, a technique that has already shown promise in the general area of small-molecule drug design. Deep learning is an artificial intelligence technique in which many layers of computational "neurons"are trained to solve a problem or recognize the underlying structure of the data. In particular, generative deep learning can create new data points "by analogy", by generalizing from large quantities of provided data.

We aim to identify potent small-molecule compounds and predict the properties of the fragments comprising them to find desirable traits in our molecules. We will implement a semi-supervised algorithm to learn from partially labelled data sets as we will be working largely with unlabelled data sets. The application of semi-supervised deep learning coupled with Fragment-Based Drug Design (FBDD) will enable us to combat AMR by identifying and optimizing desirable molecules. FBDD originated as an experimental approach in the pharmaceutical industry for reducing attrition and providing leads for previously intractable biological targets. FBDD identifies ˜150 Da (low-molecular-weight ligands) that bind to biologically significant macromolecules and uses them as seeds for novel drug development. We propose to develop a similar approach computationally to identify novel building blocks, predict their properties, and use them to create a combinatorial search space. Using the semi-supervised deep learning infrastructure, we have built, we will study "design pathways" , by projecting existing expert trajectories for designing new drugs into the search space learned by the generator.

The overarching goal of the project is to develop novel antibiotic hybrids (antibiotic hybrids are synthetic constructs of two molecules that are covalently linked) and new design rules for bypassing AMR and the creation of powerful antibiotics.

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