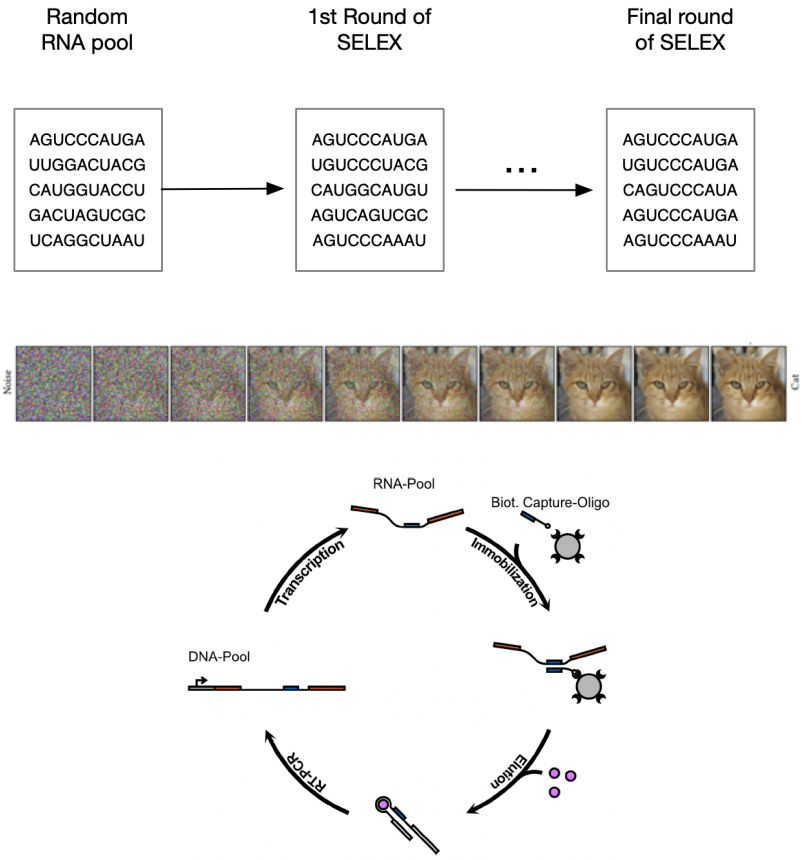
TECHNISCHE UNIVERSITÄT DARMSTADT

Thesis (B.Sc. / M.Sc.)
Virtual Evolution: Developing a SELEX Simulator with Diffusion

Background: Systematic Evolution of Ligands by Exponential Enrichment (SELEX) is a powerful method for discovering novel ligands with high affinity and specificity for target molecules. However, the experimental process is time-consuming, resource-intensive, and involves numerous parameters that can significantly impact the outcome. This thesis aims to develop an in-silico SELEX simulator using diffusion models, which are a class of generative models that learn to denoise data by iteratively refining a signal through a series of noise-removal steps. By leveraging the power of diffusion models, we can streamline ligand discovery and optimize experimental conditions.



Schematic representation of the SELEX process for aptamer selection. Starting from a random RNA library, iterative rounds of selection, binding, and amplification are performed to enrich for high-affinity aptamers against a specific target molecule. Image from [1].

Department 18
Electrical Engineering and Information Technology
Self-Organizing Systems Lab

Prof. Dr. Heinz Koeppl
Head of lab

Philipp Froehlich
Sebastian Wirth
Project supervisor

S3|06 206
Merckstrasse 25
64283 Darmstadt

philipp.froehlich@tu-darmstadt.de
sebastian.wirth@tu-darmstadt.de
https://www.bcs.tu-darmstadt.de

July 18, 2024

TECHNISCHE UNIVERSITÄT DARMSTADT

Objective: Join our interdisciplinary team and advance ligand discovery through in-silico SELEX simulation. We offer exciting thesis opportunities in the following areas:

- **Simulator Development:** Implement a diffusion-based generative model to simulate the SELEX process with state-of-the-art methods.
- **Virtual Screening:** Utilize the simulator to identify promising ligand candidates for experimental validation, optimizing the selection process.

Prerequisites:

- Background in medical engeneering, electrical engeneering, computer science, (computational) biology, mathematics, pysics, or related fields.
- Familiarity with Python and machine learning frameworks (e.g., TensorFlow, PyTorch).
- Knowledge in biology is not mandatory, we will give an introduction to the background.

The Self-Organizing-Systems Lab merges practical biological applications of machine learning with a pronounced emphasis on strong theoretical foundations. Within our interdisciplinary team, we actively work towards publications, offering students an opportunity to engage with cutting-edge research.

Fur further information, please contact Philipp Froehlich and Sebastian Wirth.

[1] Kramat, J., Kraus, L., Gunawan, V. J., Smyej, E., Froehlich, P., Weber, T. E., Spiehl, D., Koeppl, H., Blaeser, A., & Suess, B. (2024). Sensing Levofloxacin with an RNA Aptamer as a Bioreceptor. Biosensors, 14(1), 56. https://doi.org/10.3390/bios14010056