University of Zurich[UZH]

Department of Chemistry

Research project / Master project: Pick the right molecule – machine learning and molecular sorting for intensity based single-molecule studies

The following project is conducted at the laboratory of Roland K.O. Sigel at the Department of Chemistry, University of Zurich, and will be supervised by Dr. Richard Börner.

Abstract

Novel video microscopy techniques allow the detection of thousands of single-(bio)-molecules at the same time[1]. Despite careful sample preparation and purification, single-molecule methods suffer from sample contamination and sample degradation, both leading to the detection of artificial single-molecule trajectories. Such trajectories compromise the experimental results and need to be removed before further analyzing the experimental data. The removal of such traces is a time-consuming step, as it demands the inspection of individual trajectories on a user-based trace-by trace procedure. First advances have been made to accelerate this procedure in the field of fluorescence spectroscopy by introducing pre-selection criteria like the anti-correlation in the state transition characteristics. However, these pre-selection criteria still oversee many trajectories which would be dismissed in a user-based selection. To overcome this issue, we will use machine learning capabilities to select single-molecule trajectories based on simulated and experimentally achieved and pre-selected training data sets[2].

[1] R. Börner, D. Kowerko et al., Coord. Chem. Rev. 2016, 327-328, 123-142.
[2] R. Börner, D. Kowerko, M. Ritter et al. PONE 2019, 13(4), e0195277.

The project

We recently developed the Matlab-based software package MASH-FRET. We provide both code (https://github.com/RNA-FRETools/MASH-FRET) and documentation (https://rna-fretools.github.io/MASH-FRET/) on github. In this project, you will develop a pre-selection algorithm with machine learning capabilities for the purpose of molecular sorting of single-molecule fluorescence trajectories. You will implement your approach in our MASH-FRET software package. You will simulate SMV test data sets to train the machine learning algorithm and you will evaluate your approach with the help of the ground truth of these test data sets.

We offer

You will work in an interdisciplinary team of (bio)physicists and (bio)computer scientist. You will learn the principles of fluorescence spectroscopy (single-molecule FRET in particular) and video microscopy (TIRF microscopy). You will learn how to implement and use machine learning in Matlab. Finally, you will learn how to evaluate your developed algorithms with the help of test data sets with known ground truth[3].

[3] M. CAS. Hadzic, D. Kowerko et al. J. Phys. Chem. B 2018, 18, 29045-29055.

We expect

We are looking for a motivated student. The candidate should have a liking for (bio)informatics and data analysis, previous programming experience in Matlab or Python is an asset but not required. The starting date will be mutually agreed upon.

Application / Contact Details

Please send a short motivation letter (not more than half a page) and your CV (two pages max.) to Dr. Richard Börner (richard.boerner@chem.uzh.ch).