

Self-Optimizing Process Control: Fluorescent Carbon Nanoparticle Synthesis

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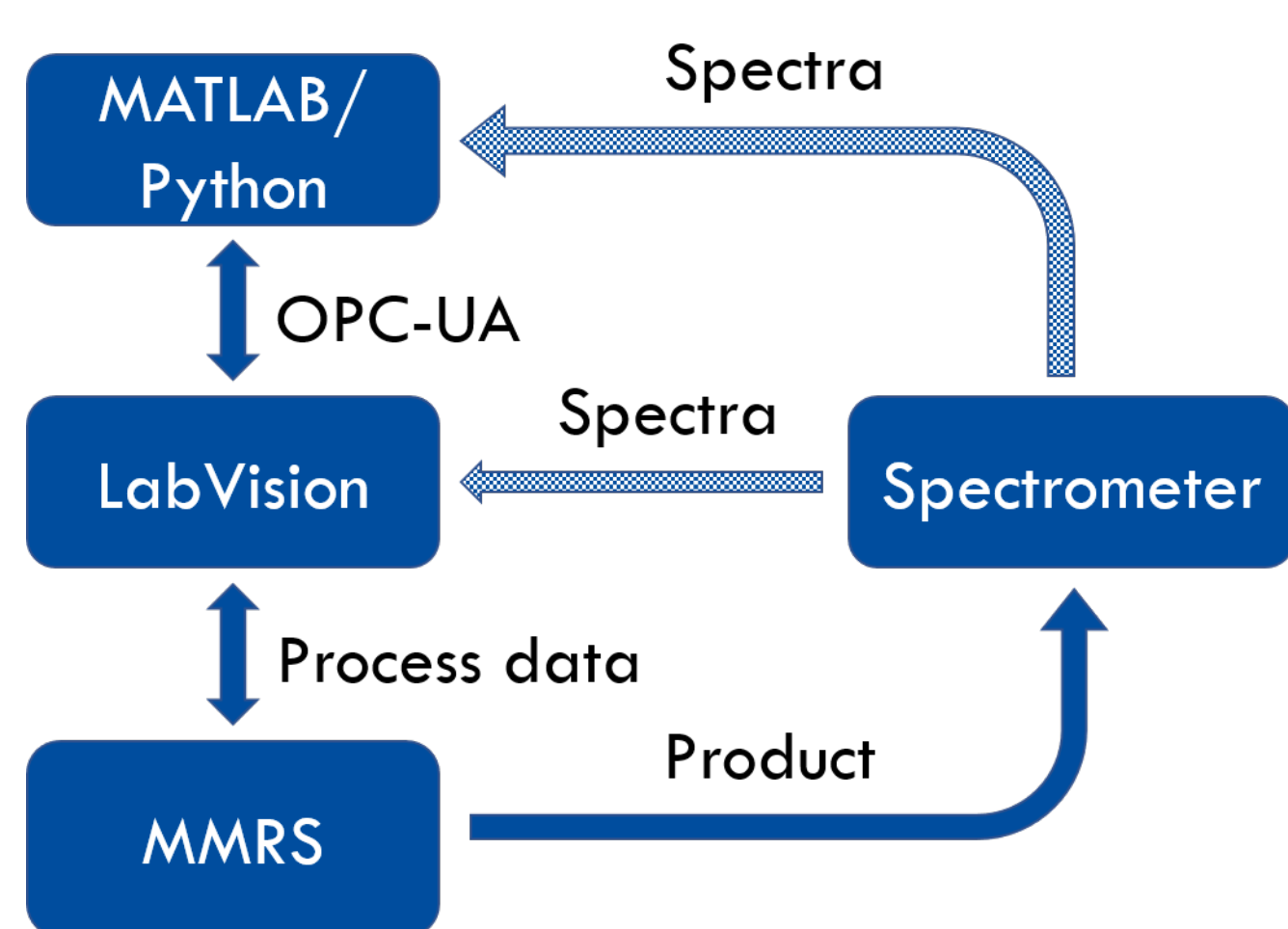


INTRODUCTION

Self-optimizing process control is a trend in today chemistry. The task of used algorithms is to find the optimum operating point to automatically achieve the desired extremum. This poster shows the implementation of two algorithms (SNOBFIT & BO) to automatically maximize the fluorescence intensity of carbon dots in flow.

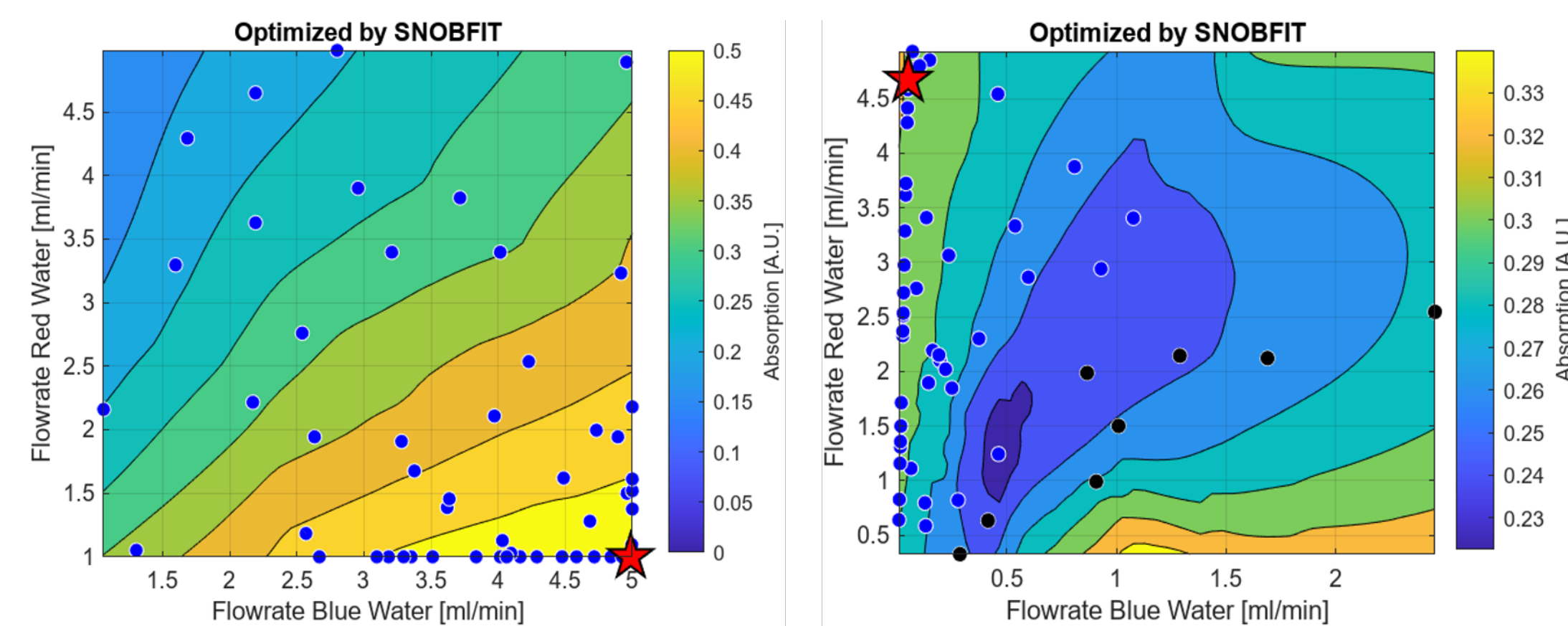
MATERIALS & METHODS

- » Citric Acid and Urea
- » Ehrfeld Modular Micro-reactor System (MMRS)
- » Synthesis of CQDs
- » Inline spectrometer fluorescence measurement
- » Automation: LabVision® (HiTec Zang)
- » Algorithms: Matlab & Python

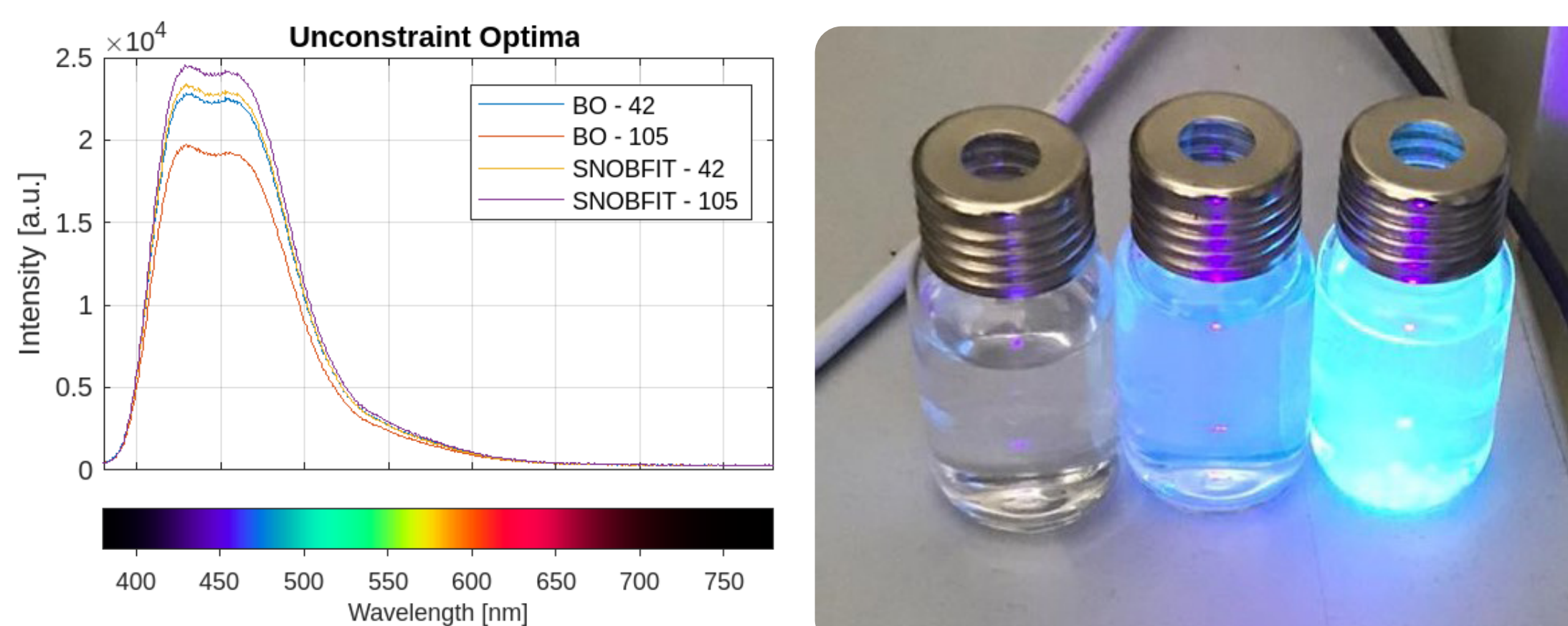
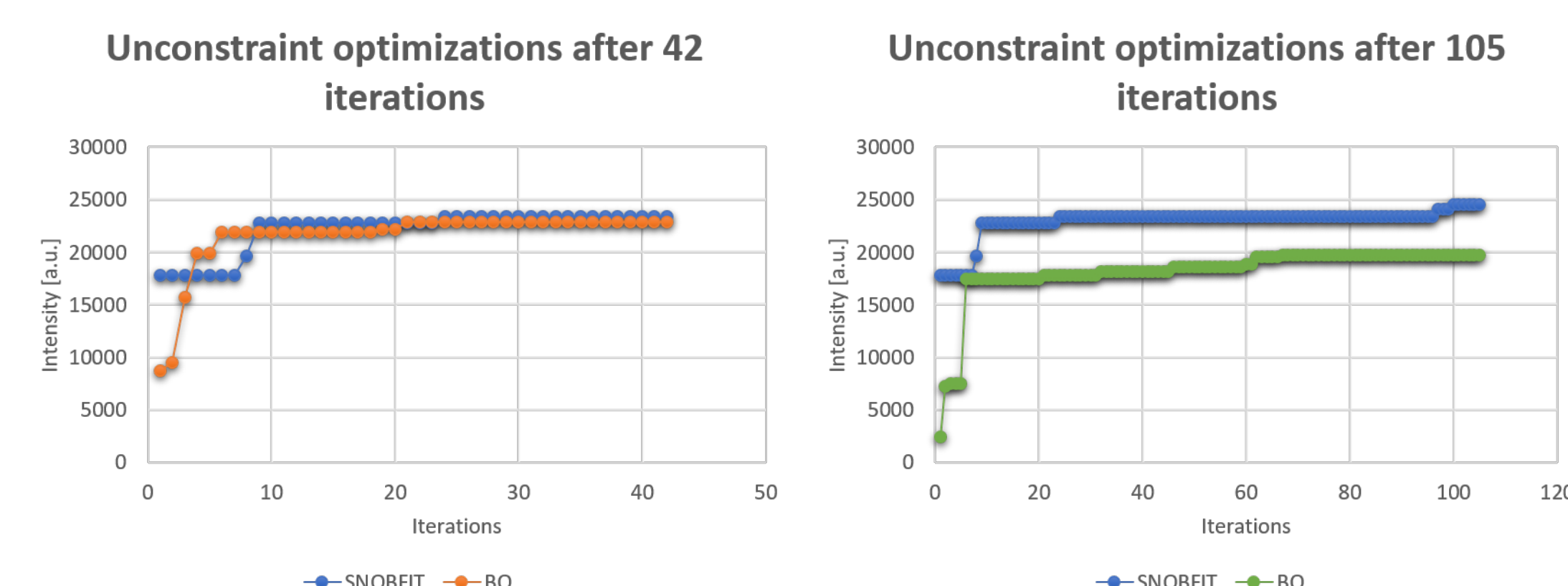
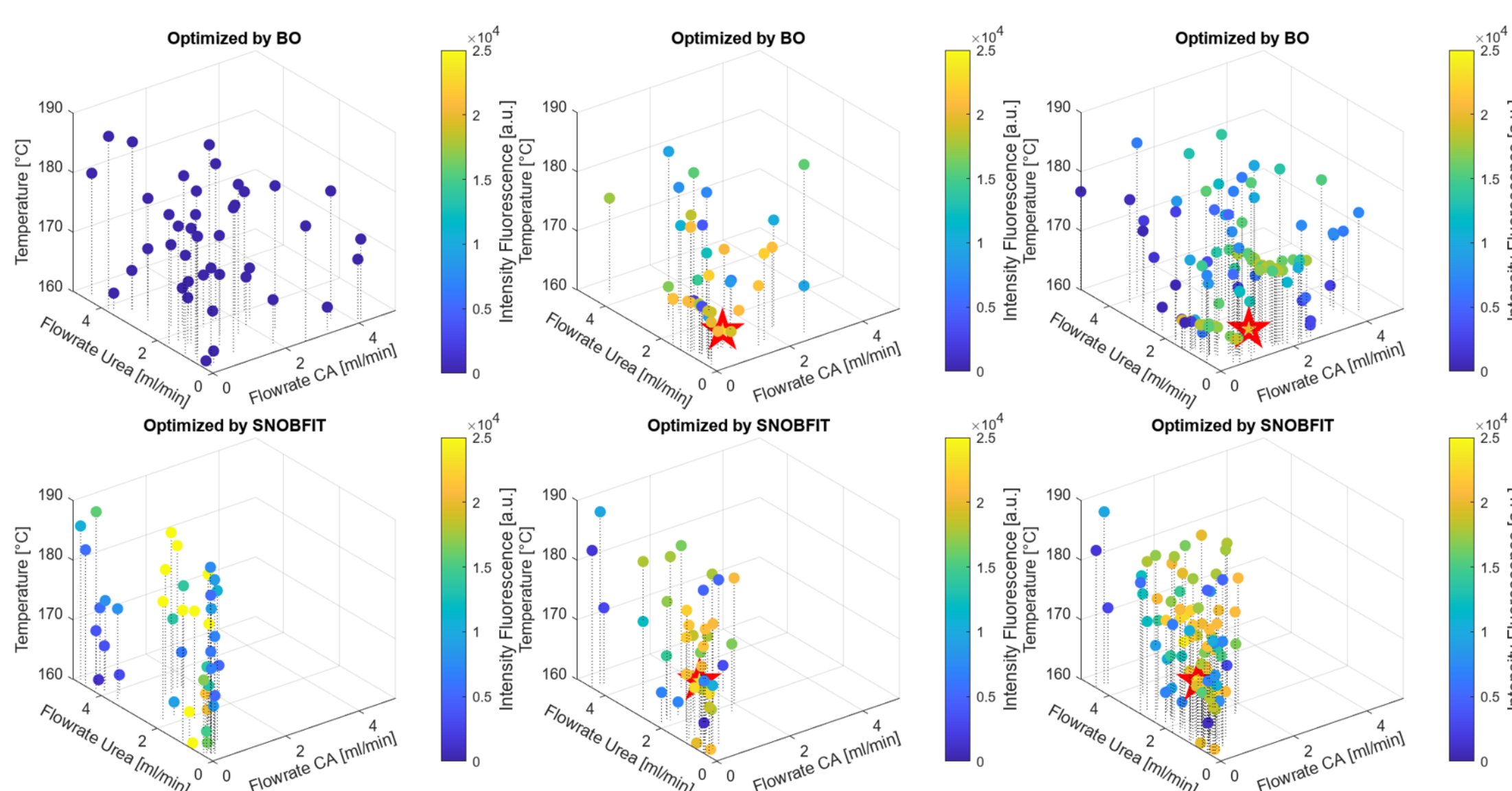


FIGURES & RESULTS

Pre-tests (mixing of 2 dyes) were carried out to set up the algorithms



Synthesis of CQDs was optimized by SNOBFIT and BO



CONCLUSIONS

- » Successful application of optimization algorithms to the preactor system
- » Comparison between algorithms possible
- » Algorithms successfully increased the fluorescence intensity automatically



OUTLOOK

- » Hyperparameter BO
- » Analyse product
- » Other educts
- » Influence of other parameters



Further readings

Clayton et al., React. Chem. Eng., 2019
 McMullen et al., Org. Process Res. Dev., 2010
 Huyer et al., SNOBFIT -- Stable Noisy Optimization by Branch and Fit., ACM Trans. Math. Softw. 35, 1–25, 2008
 Krishnadasan et al., Lab Chip, 2007

Libraries

https://github.com/jdmgroup/SNOBFit_for_chemical_optimisations
<https://github.com/bayesian-optimization/BayesianOptimization>

Further information

Master thesis - supervised by HiTec Zang GmbH and RWTH Aachen University

Please feel free to get in touch with me if you have any further questions:
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