Nicholas Michelarakis
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WORK EXPERIENCE

Senior Scientist, Sanofi, Biopharmaceutical Drug Product Development **01/2025-present**

Research Areas: Predictive formulation development, management of data and infrastructure, computer-aided drug design, computational structural biology, molecular modeling

- Initiated, designed, and developed the digital strategy for the department. Identified current needs and gaps where digital tools could enhance efficiency. Decided on and prioritized areas and projects for digital development. Allocated resources and set up the teams to be working on the projects.
- Acquired necessary computational power to support digital initiatives.
- Established data governance and data management pipelines to ensure data integrity and accessibility.
- Set up molecular modeling pipelines of biologics to enable predictive formulation development and modeling capabilities int he department.
- Leading the creation of an interdepartmental database integrating wet lab and corresponding in-silico data. Deciding on data and metadata to be stored, ensuring relevance for future modeling and AI initiatives. Directing the generation of necessary wet lab experiments to fill data gaps.
- Developed an automated data parser and report generation tool using Python and Streamlit. Rolled it out to the department.
- Designed the curriculum for digital training in the department at all levels, from lab technicians to head of departments.

Post Doctoral Research Fellow, Boehringer-Ingelheim **10/2022-12/2024**

Research Areas: Computational Structural Biology, Molecular Modelling, Predictive Formulation Development, Data Management

- Spearheaded the molecular modeling initiatives across the entire Development Biologics department. I was responsible for project prioritization and resource allocation, strategic planning and fostering cross-functional synergies throughout the pipeline. This begins with Research and Discovery and extends to leveraging our existing toolset for broader applications.
- Tasked with the evaluation of ongoing pipeline projects, I utilized our existing computational resources while also identifying present and prospective pipeline requirements. I guided the development of innovative tools to meet these evolving needs.
- Managed the creation of a predictive formulation tool, necessitating the alignment of diverse teams across multiple departments. This role improved my proficiency in data management and digital landscape navigation while also improving my skills in stakeholder management and technical team coordination.

- Developed and evaluated existing computational tools to predict the viscosities of high-concentration liquid formulations. Evaluating the applicability of these tools in our internal pipeline projects. Establish industry collaborations to guide the development of innovative tools that meet our requirements more effectively.
- In partnership with colleagues in cell line development, I utilized molecular modeling techniques to decipher the mechanism of action of internally developed Glutamine Synthetase variants (active vs non-active). Patent application and publication submissions currently in progress.
- Contributed to shaping the department's overall data management strategy as a Subject Matter Expert (SME), identifying necessary data and metadata types required and generated by our team, while ensuring compliance with approved data standards. Coordinated with other departments to determine the storage locations of such data and establish sharing methods.
- Entrusted with the growth of the molecular modeling team, involving the recruitment of interns, master, and potential PhD students. Responsibilities include conducting interviews, selection, project design, and providing supervision/management.

Post Doctoral Research Fellow, Heidelberg Institute for Theoretical Studies

with Prof. Dr. Frauke Graeter **04/2019-09/2022**

Research Areas: Computational Material Science and Computational Structural Biology

- In collaboration with Toyota Motor Europe I designed and implemented a coarse grained molecular dynamics based protocol to predict the physical properties of Nafion solutions under ink-jet printing conditions.
- As part of a multidisciplinary team, I used simulation results to guide the membrane printing process leading to proton exchange membranes with improved properties.
- Developed a simulation protocol to model solvent evaporation under drying conditions.
- Identified the molecular mechanism governing the shear enhanced VAR2CSA-CSA interaction, an important vaccine target against malaria. Revealed a secondary, cryptic CSA binding site which becomes accessible over force exertion.

PhD Researcher, University of Oxford with Prof. Mark Sansom **2014-2018**

Research Areas: Computer Aided Drug Design and Computational Structural Biology

- Developed a molecular dynamics based modelling protocol for applications in structure based drug design, in collaboration with UCB. This protocol allows for the exploration of ligand binding sites along with identifying the moieties which drive ligand binding.
- Seconded to the UCB site, I applied the methodology to ongoing projects and targets, identifying regions for possible fragment linking and expansion as well as regions towards which expansion was not possible.
- Using publicly available crystal structures I successfully extended the simulation protocol in identifying lipid binding sites on membrane proteins such as GPCRs and other high value targets.

EDUCATION

DPhil in Computer Aided Drug Design 2014-2018

University of Oxford

Supervisors: Mark Sansom, Phillip Stansfeld, Zara Sands. Examiners: Christopher Reynolds (Essex) Frank von Delft (Oxford)

MRes in Computational Biology 2013-2014
University of York

BSc in Biochemistry with Molecular Biology 2010-2013
University of Leeds

COMPUTATIONAL RESEARCH SKILLS

Methods
Molecular Dynamics (MD) Simulations, fragment-based drug design, structure based and ligand based drug design, protein homology modeling, docking, free energy perturbation (FEP), method and algorithm development

Programming Languages
Python, Bash, Tcl

Modelling and Simulation Software
GROMACS, Schröndiger Suite, MOE, NAMD, Modeller, Plumed

Simulation/Structure Visualisation
VMD, PyMOL, Chimera

Simulation Analysis Packages
MDAnalysis, MDTraj, CHAP, PyLipID, Gromaps

Operating Systems
Linux, MacOS, Windows

High performance computing
Local clusters and national super-computing facilities

Presentation and text editing
Microsoft Office (Word, Excel, Powerpoint), LaTeX, Keynote, Inkscape

SELECTED PUBLICATIONS

- **Mechanical forces control the valency of the malaria adhesin VAR2CSA by exposing cryptic glycan binding sites**. Roessner, R., **Michelarakis, N.**, Gräter, F. and Aponte, C. , *PLOS Computational Biology* 19(12): e1011726., 2023; https://doi.org/10.1371/journal.pcbi.1011726
- **Longitudinal Strand Ordering Leads to Shear Thinning in Nafion**. **Michelarakis, N.**, Franz, F., Gkagkas, K. and Gräter, F., *Phys. Chem. Chem. Phys.*, 2021,23, 25901-25910; https://doi.org/10.1039/D1CP02024B
- **Martini 3 Coarse-Grained Force Field for Poly(para-phenylene ethynylene)s**. Brosz, M., **Michelarakis, N.**, Bunz, U., Aponte, C. and Gräter, F., *Phys. Chem. Chem. Phys.*, 2021; https://doi.org/10.1039/D1CP04237H

SELECTED TALKS AND PRIZES

- Invited talk at the PEGS Summit, Boston, 2024.
- Selected for a talk at the 62nd Annual Conference of the Biophysical Society, San Francisco, 2018. "Towards Dynamic Pharmacophore Models by Coarse Grained Molecular Dynamic Simulations". Travel grant awarded.
- First place in the BBSRC Grand Challenges for Technologies and Methods for Drug Discovery Skills School, Abingdon, 2018.

SUPERVISION, TEACHING AND OUTREACH

- Trained and supervised summer interns, bachelor, master and PhD candidates (Oxford and Heidelberg).
- Practical class Demonstrator for the Wellcome Trust: Structural Biology and MD simulations tutorials. Designed and delivered teaching material.
- Nominated by colleagues and won the HITS Award for enhancing the social and professional life of the institute and promoting communication and collaboration between the different groups.
- Represented the computational biochemistry in departmental open days (Oxford). Participated in the "Jugend präsentiert Summer School" of the Klaus Tschira foundation, presenting my research to a cohort of twenty high-school students (Heidelberg).
- Joined the BI soccer team in the Pharma Cup and helped the PDB soccer team to first place in Schuetzenkick.