Modeling small drug molecules and the winding career path that got me here

Caitlin C. Bannan

Today, I am a Lead Scientific Software Developer at OpenEye, Cadence Design Systems. However, if you told me that in 2012 when I finished my BS in chemistry, I wouldn't have believed you. In this presentation, I will share my winding career path including an early dream of teaching high school science, work in inorganic and radiochemistry laboratories, to the decision to pursue a PhD in computational chemistry, and how that got me to OpenEye [1]. This journey will include my graduate research at the University of California, Irvine with David Mobley, and the Open Force Field Consortium (OpenFF) [2]. OpenFF's close connections with the pharmaceutical industry helped shape my goal to pursue a career in industry after school. In my job now, I have had the opportunity to build and manage quantum chemical (QC) workflows on Orion, OpenEye's cloud platform for drug discovery [3] and contribute to important research into small molecule crystal structure prediction [4]. Throughout this presentation I'll include an overview of the scientific research I've contributed too. This will include my work on cheminformatics fits into force field development and how my work on small molecule crystal structure prediction and QC calculations impacts the drug discovery pipeline.

Citation and context for each reference:

1. Ruggiu, F., Bannan, C. & Bootsma, A. Early Career Perspectives from Large Pharma, Software, and Start-up Companies. *J. Chem. Inf. Model.* **62**, 2631–2638 (2022). Doi: 10.1021/acs.jcim.1c01416
   This is a summary of different computational jobs written by members of the JCIM early career board. Our aim was to help provide the perspective on different industries that we wished we'd had when looking for work after our PhDs.
2. Mobley, D. L. *et al.* Escaping Atom Types in Force Fields Using Direct Chemical Perception. *J. Chem. Theory Comput.* **14**, 6076–6092 (2018). doi: 10.1021/acs.jctc.8b00640
   This is an overview paper of Open Force Field's work. It contains a lot of details about force fields, most of which is more detailed than I will get into in this presentation.
3. Sørensen, J. *et al.* Orion ® A Cloud-Native Molecular Design Platform. in *Computational Drug Discovery* (eds. Poongavanam, V. & Ramaswamy, V.) 579–615 (Wiley, 2024). doi:10.1002/9783527840748.ch24.
   This is OpenEye's contribution to the book Computational Drug Discovery. This work focuses on the impact of cloud computing in the pharmaceutical industry. It is more detail than I would cover in this presentation.
4. Bannan, C *et al.* Crystal Structure Prediction of Drug Molecules in the Cloud: A Collaborative Blind Challenge Study. *Under Review*
   White paper with the same methods as the one under review: Using Computational Crystal Structure Prediction (CSP) to Optimize Small Molecule Drug Formulation
   The white paper includes a good high level view of OpenEye's approach to computational small molecule crystal structure prediction. I can share the link to the paper when it is published, but will be more technical.