## Daniel L. Parton

email danny.parton@gmail.com mobile 319-631-9146

website dannyparton.github.io

## **Technical Skills**

Python 7 years experience; numerical/scientific computing, data handling, parallel computing,

bioinformatics; packages—numpy, pandas, scikit-learn, Flask, SQLAlchemy, lxml, mat-

plotlib, mpi4py, setuptools, nosetests.

Other languages JavaScript, bash. Some experience with C, C++, R, MATLAB, CUDA.

 $\textbf{Web development} \hspace{0.3cm} 2 \hspace{0.1cm} \text{years experience; HTML5, CSS3, Bootstrap, knockout.js, Python Flask, Apache, nginx.} \\$ 

General GitHub, git, svn, Travis CI, Docker, Amazon AWS, IATFX, OS X, Linux, Windows.

## Experience

2012-pres

MEMORIAL SLOAN KETTERING CANCER CENTER, NEW YORK, NY

Postdoctoral Research Fellow, Computational Biology Center

Advisor: John D. Chodera

 Investigation of conformational networks in cancer-associated proteins using clustering techniques and Markov models.

- Developed MSMSeeder—pipeline for generating millions of simulation starting configurations.
- Developed TargetExplorer—database application for storing, presenting and querying biological data for a target protein family, with RESTful API and frontend web client (in development).
- Implemented a custom sorting and filtering scheme for data-driven selection of kinase sequences suitable for bacterial expression.
- 3 first-author papers in preparation.

2011-2012

University of Chicago

Postdoctoral Scholar, Department of Chemistry

Advisor: Gregory A. Voth

• Applied advanced computer simulation techniques and free energy calculations to the study of the actin cytoskeleton. One paper submitted as first author (in review).

2007-2011

University of Oxford

Graduate Student Researcher, Department of Biochemistry

Advisors: Mark S. P. Sansom (Oxford) and Ross Nobes (Fujitsu Laboratories of Europe)

- Studied complex membrane protein systems and viruses using physics-based molecular simulations.
- Developed various software tools for simulation analysis, and contributed to MDAnalysis.
- Organized and taught organic chemistry tutorials for a class of 3 undergraduates.
- Co-authored 5 papers, 3 as first author. Results presented at many national and international conferences, and in national scientific magazines.

2005 – 2007

UNIVERSITY OF BRISTOL AND GLAXOSMITHKLINE, UK

Undergraduate Researcher / Industrial Placement Student

Advisor: Chris Willis

• Conducted the design and synthesis of drug candidates, as a member of medicinal chemistry teams at Bristol (6 months) and GSK (1 year). Co-authored one paper.

## Education

2007–2011 D.PHIL. in Biochemistry, University of Oxford, UK 2003–2007 M.Sci. in Chemistry with Industrial Experience, University of Bristol, UK