

Employment

Scientific Officer – Computational Structural Biology

Structural Biology Facility, UNSW

2023–present

Management of the computational resources of the SBF (scientific software & GPU compute). Mentoring scientists and end-users in computational techniques. Coordinating with computing providers to implement state-of-the-art computational structural biology workflows. Promoting the adoption of scientific services.

Bioinformatician

Australian Proteomics Analysis Facility

2022–2023

Working with R code for mass spectrometry proteomics analysis. Refactoring an existing experiment-specific codebase to be more modular, allowing easy addition of new analysis functions. Mentoring a final-year PhD candidate in refactoring code, while learning how to clean up terse R scripts. Retiring legacy systems.

Research Computing Support Officer

Research Technology Services, UNSW

2021–2022

HPC and research computing support, including day-to-day system administration. Installation and troubleshooting of scientific software. HPC outreach and uptake, including weekly 'Hacky Hour' sessions.

Postdoctoral Research Associate

School of Chemistry, USYD

2020–2021

Continuation of my PhD research. Multiconfigurational quantum chemistry calculations (CASSCF & CASPT2). Mentoring PhD candidates to submission and employment. Preparing research papers.

Casual Science Teacher

Matrix Education

2016–2020

Student experience questionnaire 2-year average : **4.7/5**

Top quality high school curriculum tuition. Classroom lessons, quiz marking, workbook development.

Postgraduate Teaching Fellow & Tutor

School of Chemistry, UNSW

2016–2018, 2019–2020

1st year tutorials, mentoring, 3rd year physical chemistry resource development, exam marking, outreach.

Laboratory Demonstrator

School of Chemistry, UNSW

2014–2015, 2020

Laboratory teaching, supervision, and marking, for 1st, 2nd and 3rd year chemistry students.

Education

PhD - Computational Chemistry

University of New South Wales

2016–2020

Thesis Title: [Structure–Activity Relationships for Carbonyl Photolysis](#)

Supervisors: Prof. Scott Kable, Prof. Meredith Jordan

Assessment: **A,A** — All categories 'Outstanding'

Thesis summary: Structure-activity relationships for carbonyl UV photochemistry were comprehensively elucidated for 38 molecules across seven structural classes, for ten unique reaction mechanisms, on all relevant ground (S_0) and excited (S_1 & T_1) states. Theoretical protocols for photolysis thresholds and excitation energies were extensively validated to the available spectroscopic and kinetic data for ± 10 kJ/mol accuracy.

B.Sc. (Adv.) - Chemistry - Honours Class 1 - Angyal Prize (Top Performance)

University of New South Wales

2011–2014

Dissertation Title: [Computational Studies on the Basis of 'Neighbour Exclusion' in a Series of Diacridine and Di-\(terpy\)Pt\(II\) Thiol Bisintercalators: combined MD & FMO approaches](#)

Supervisors: A/Prof. Graham Ball, A/Prof. Larry Wakelin, Dr Donald Thomas

Programming Experience

Python.....

- Developed resources for Python and Jupyter Notebooks instruction in 3rd year chemistry
 - 'Rising Star' award for introducing Jupyter Notebooks interactive coding lessons
 - Wrote 'Intro to Python and plotting' lessons for physical science students
- Molecular rotational constants calculator. Exploratory data analysis with pandas and matplotlib
- Developed code to process, search, and plot 1000s of pair-wise energies between DNA fragments

High Performance Computing.....

- 5+ years experience running within Linux and High Performance Computing environments
 - Bash scripting, environment modules, basic sys. admin., schedulers (PBS Pro)
 - Fundamental command line tools, vim, git, awk, ch(mod|own|grp), etc. Compilers
 - Attended regular ResTech seminars on computational research methods and data management

C.....

Undergraduate coursework

- Computational Bioinformatics (BINF3020, **HD**)
 - String alignment (DNA and protein sequences), Statistical modelling (HMM, Bayes net)
- Computer science (COMP1917, **DN**)
 - Memory allocation, algorithms and data structures, OOP (COMP1927 recordings)

Fortran.....

- Worked with 'Grow' in-house Fortran code for potential energy surface interpolation

Teaching and Mentorship

Postgraduate Teaching Fellowship.....

- 3 year tenure, 75 hours commitment per year, tutorials, developed physical chemistry resources

University Subjects Taught.....

- 3rd year physical chem – demonstrator, coding facilitator — satisfaction rose from **65% to 94%**
- 2nd year physical chem – laboratory demonstrator
- 1st year chemistry – tutor and laboratory demonstrator — tutor feedback form average **4.6/5**

Academic Mentorship.....

- Mentored theoretical chemistry Honours students in performing computational chemistry research
- Mentored newer Teaching Fellows in effective chemistry tutorials and pedagogical techniques

Presentation Highlights

Group & 'Super-group' organiser: Organised weekly group and monthly 'super-group' meetings: sourcing academic speakers, coordinating schedules. Ran computing & visualisation masterclasses

APATCC 2019 (*volunteer, poster*)

USYD - Sydney

Asia-Pacific Association of Theoretical and Computational Chemists

Sep. 2019

ISTCP-X (*poster*)

UiT - Tromsø

10th Triennial Congress of the International Society of Theoretical Chemical Physics

Jul. 2019

QUACCS 3.0 (<i>talk</i>)	ANU Campus - Kioloa
Computational chemistry workshops & student 'chalk 'n talk' presentations	Dec. 2018
ACCOMC 2018 (<i>poster</i>)	CSIRO - Aspendale
Atmospheric composition & modelling conference for Australasian region	Dec. 2018

Awards

Rising Star - PhD Casual Teacher

School of Chemistry UNSW 2018
Awarded to casual PhD tutors who have demonstrated educational excellence

Poster presenter prize

Association of Molecular Modellers of Australia 2015
Best Honours-level poster presenter

Angyal prize

School of Chemistry UNSW 2014
Top mark in Chemistry Honours

Bosworth prize

School of Chemistry UNSW 2013
Equal 1st in third year Physical Chemistry

Computer Skills

Programming: Python, Bash, C

Analysis: Python, Pandas, Excel, R

Documents: Word, L^AT_EX, Overleaf

Figures: Matplotlib, Inkscape, GNU IMP

Publications (refer to my [Google Scholar](#) page)

1. — Rowell, K.; Kable, S.; Jordan, M., "An assessment of the tropospherically accessible photo-initiated ground state chemistry of carbonyls", *Atmospheric Chemistry and Physics*, (2022), doi:[10.5194/acp-22-929-2022](#)
2. — Juan, C.Z.T.; Syme, A-M.; Rowell, K.; *et al.*, "Infrared Spectroscopy of Phosphorus-containing Molecules", *Frontiers in Astronomy and Space Science*, (2021), doi:[10.3389/fspas.2021.639068](#)
3. — Rowell, K.; Thomas, D.; Ball, G.; Wakelin, L., "Molecular Dynamic Simulations of Diacridine Binding to DNA: Indications that C6 Diacridine can Bisintercalate Spanning Two Base Pairs", *Biopolymers*, (2020), doi:[10.1002/bip.23409](#)
4. — Rowell, K.; Kable, S.; Jordan, M., "Substituent Effects on the Norrish Type I α -bond Cleavage of Tropospherically Important Carbonyls", *The Journal of Physical Chemistry A*, (2020), doi:[10.1021/acs.jpca.9b05534](#)
5. — Harrison, A.; Kharazmi, A.; Shaw, M.; Quinn, M.; Lee, K.; Klaas, N.; Rowell, K.; Jordan, M.; Kable, S., "Dynamics and Quantum Yields of H₂ + CH₂CO as a Primary Photolysis Channel in CH₃CHO", *Physical Chemistry Chemical Physics*, (2019), doi:[10.1039/C8CP06412A](#)

Pre-prints.....

Rowell, K.; Kable, S.; Jordan, M., "Predicting Carbonyl Excitation Energies Efficiently Using EOM-CC Trends", doi:[10.26434/chemrxiv.12917369.v2](#)

Rowell, K.; Kable, S.; Jordan, M., "Structural Causes of the Singlet/Triplet Preferences of Norrish Type II Reactions in Carbonyls", doi:[10.26434/chemrxiv.12941702.v1](#)