

## Employment

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### 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, Macquarie University*

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

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

### Laboratory Demonstrator

*School of Chemistry, UNSW*

2014–2015, 2020

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

## Education

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### 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  $\pm 10$  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

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### Python.....

- Developed resources for Python and Jupyter Notebooks instruction in 3<sup>rd</sup> 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

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### Postgraduate Teaching Fellowship.....

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

### University Subjects Taught.....

- 3<sup>rd</sup> year physical chem – demonstrator, coding facilitator — satisfaction rose from **65% to 94%**
- 2<sup>nd</sup> year physical chem – laboratory demonstrator
- 1<sup>st</sup> 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

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**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

*10<sup>th</sup> Triennial Congress of the International Society of Theoretical Chemical Physics*

Jul. 2019

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

## Awards

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<b>Rising Star - PhD Casual Teacher</b>	
<i>School of Chemistry UNSW</i>	2018
Awarded to casual PhD tutors who have demonstrated educational excellence	
<b>Poster presenter prize</b>	
<i>Association of Molecular Modellers of Australia</i>	2015
Best Honours-level poster presenter	
<b>Angyal prize</b>	
<i>School of Chemistry UNSW</i>	2014
Top mark in Chemistry Honours	
<b>Bosworth prize</b>	
<i>School of Chemistry UNSW</i>	2013
Equal 1 <sup>st</sup> in third year Physical Chemistry	

## Computer Skills

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<b>Programming:</b> Python, Bash, C	<b>Analysis:</b> Python, Pandas, Excel, R
<b>Documents:</b> Word, L <sup>A</sup> T <sub>E</sub> X, Overleaf	<b>Figures:</b> Matplotlib, Inkscape, GNU IMP

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

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1. — Rowell, K.; Kable, S.; Jordan, M., "An assessment of the tropospheric accessible photo-initiated ground state chemistry of carbonyls", *Atmospheric Chemistry and Physics*, (2022), doi:[10.5194/acp-22-929-2022](https://doi.org/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](https://doi.org/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](https://doi.org/10.1002/bip.23409)
4. — Rowell, K.; Kable, S.; Jordan, M., "Substituent Effects on the Norrish Type I  $\alpha$ -bond Cleavage of Tropospheric Important Carbonyls", *The Journal of Physical Chemistry A*, (2020), doi:[10.1021/acs.jpca.9b05534](https://doi.org/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 H<sub>2</sub> + CH<sub>2</sub>CO as a Primary Photolysis Channel in CH<sub>3</sub>CHO", *Physical Chemistry Chemical Physics*, (2019), doi:[10.1039/C8CP06412A](https://doi.org/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](https://doi.org/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](https://doi.org/10.26434/chemrxiv.12941702.v1)