

# Daniel J. Kowalski

Research Associate in  
Digital Chemistry



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djkowalski.github.io



dankowalskichm



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## Skills

### Coding / Data Science:

Primary language is Python. Comfortable with use of GitHub for versioning and collaboration.

- Statistical Analysis
- Machine Learning
- Data Engineering / Pipeline Automation
- Data Visualisation
- Digital Interpretation of Chemical Data
- Metric Design
- Some knowledge of R and SQL
- Limited experience of Gaussian / Orca
- LaTeX, HTML, Basic UI Construction

### Synthesis:

Experience with organic, coordination / organometallic, and nanochemical synthesis.

- Solution-Phase Synthesis
- Air-sensitive Techniques
- Solvothermal (Solid-State) Synthesis
- Construction and Operation of Chemical Robots

### Analytical Techniques:

Knowledge of the measurement and interpretation of the following:

- Spectroscopy: NMR, IR, UV-vis
- Mass Spectrometry (inc MS<sup>2</sup>, IM-MS)
- Diffraction: SCXRD, PXRD
- Other: DLS, Chromatography (Flash, HPLC, TLC, Automated)

### Other:

- MS Office (inc. Word, Excel, Power-Point)
- Remote Conferencing: Zoom, MS Teams
- Various Analytical Software Suites

## References

Available on request

## Research Experience

2022—

**Research Associate**  
*Glasgow, United Kingdom*

University of Glasgow

### Technical Achievements

- Application of deep learning to the prediction of synthetic conditions.
- Secondary research into the prediction of candidate success in medicinal chemistry and subsequent comparative data analysis.

### Broader Skills

- Skilled in client-focused problem-solving, as evidenced through data science-focused contributions to projects led by synthetic chemists (and in collaboration with a start-up), and the development of automated tools to mitigate labour-intensive admin tasks.

2018-2022

**Postgraduate Researcher**  
*Glasgow, United Kingdom*

University of Glasgow

### Technical Achievements

- Constructed and operated fluid-handling robots (using group infrastructure) for universal or medium-throughput inorganic synthesis.
- Purposed a variety of statistical and probabilistic machine learning techniques for the directed exploration of chemical search spaces in coordination chemistry.
- Built pipelines for extracting, transforming, and conditioning data, leveraging web scraping, APIs, and chemistry-specific analytical packages to capture input data.
- Designed metrics for the quantification of novelty in MS data, engaging with new techniques to allow the interpretation of complex spectra.

### Broader Skills

- Excellent teamwork and time management demonstrated by balancing participation in several small project teams. Led to the construction of multiple robotic platforms, and 2 publications in high-impact journals.
- Clear communicator of complex topics to diverse audiences, shown by award-winning presentations at international conferences, visual presentation of data and ideas through the production of publication-quality figures and regular update presentations, as well as production of educational videos for remote undergraduate teaching.
- Adaptable and attentive researcher, as evidenced by the revitalisation of an inactive project; identifying and solving issues with the existing data to produce an impactful publication with 38 citations over 3 years.
- Independent and reflective learner, as demonstrated through the self-directed development of machine learning knowledge from scratch to enable my required contributions to complex, data-driven projects.
- Compassionate and supportive colleague; mentoring a junior colleague through their Research Master's degree to secure a technical job.

2017-2018

**Masters Student**  
*Leeds, United Kingdom*

University of Leeds

### Technical Achievements

- Design and implementation of synthetic routes to complexes with proposed oncological activity, and diversification of these to a small library.
- Proficiency with the use of Schlenk lines and glove boxes.

2016-2017

**Roche Intern in Medicinal Chemistry**  
*Basel, Switzerland*

F. Hoffmann-La Roche AG

### Technical Achievements

- Synthesised analogues of a macrocyclic anti-infective candidate.
- Experienced with a broad range of organic synthesis, including solid-phase peptide synthesis, and the use of gas-phase reagents.

### Broader Skills

- Able to communicate and build strong relationships with a range of colleagues, developed through collaboration with related teams, specialist separation scientists, and regular presentations to the project team.
- Experience with sensitive IP in an international industrial environment.
- Strong understanding of drug discovery workflows.

## Education

2018-2022	<b>PhD, Digital Chemistry</b> <i>Glasgow, United Kingdom</i>  <i>Submission:</i> November 2022 (Awaiting viva) <i>Provisional Title:</i> Digital Discovery Strategies for Inorganic Chemistry <i>Advisor:</i> Prof. Leroy Cronin	University of Glasgow
2014-2018	<b>MChem BSc, Chemistry with a Year in Industry</b> <i>Leeds, United Kingdom</i>  <i>Thesis:</i> Cytotoxic Ruthenium Complexes for Anti-proliferative Cancer Treatment <i>Advisor:</i> Prof. Patrick C. McGowan  <i>Industrial Project:</i> Target-Oriented Synthesis of Peptidic Macrocycles for Anti-Infection Applications <i>Host Company:</i> F. Hoffmann-La Roche Ltd.	University of Leeds
2009-2014	<b>A Levels / GCSEs</b> <i>Merseyside, United Kingdom</i>  <i>A Level:</i> Chemistry (A*), Biology (A), Physics (B), General Studies (A). AS levels in French and Critical Thinking. <i>GCSE:</i> 12 A*-B with 10 at A* (inc. Maths, English Language, Chemistry, Biology, Physics, Astronomy)	Wirral Grammar School for Boys

## Selected Voluntary and Teaching Positions

2022—	<b>Ordinary Board Member</b> <i>Glasgow, United Kingdom</i>  Involved in the organisation of events to strengthen industry-academia links.	Society of Chemical Industry Scotland Group
2018-2022	<b>Graduate Teaching Assistant</b> <i>Glasgow, United Kingdom</i>  Responsible for supervising and teaching groups of 8-20 undergraduates across experiments in organic, inorganic, and physical chemistry.	University of Glasgow
2019-2020	<b>Local Organiser</b> <i>Glasgow, United Kingdom</i>  As part of a small team, organised a raft of speakers for the local branch of a national outreach event. Event was ultimately cancelled due to the national lockdown.	Pint of Science UK
2017-2018	<b>Safety, Health, and Environment Committee Secretary</b> <i>Leeds, United Kingdom</i>  Inaugural member. Responsible for meeting records and operating an anonymised laboratory reporting scheme.	Department of Chemistry, University of Leeds
2014-2018	<b>Student-Staff Forum Representative</b> <i>Leeds, United Kingdom</i>  Peer representative, responsible for communicating feedback to departmental management at regular meetings.	Department of Chemistry, University of Leeds

## Publications

- Kowalski, Cronin; “**Review: Discovery Strategies in Chemistry**” *In preparation*
- Kowalski, MacGregor, Long, Bell, Cronin; “**Automated Library Generation and Serendipity Quantification Enables Diverse Discovery in Coordination Chemistry**” *J. Am. Chem. Soc.* 2023, ASAP (DOI: 10.1021/jacs.2c11066)
- Porwol, Kowalski, Henson, Long, Bell, Cronin; “**An autonomous chemical robot discovers the rules of inorganic coordination chemistry without prior knowledge**” *Angew. Chem. Int. Ed.* 2020, **59**(28), 11256-11261 (DOI: 10.1002/anie.202000329)

## Awards and Honours

- **RSC Advances Best Talk Prize**, RSC Scottish and North of England Dalton Meeting, August 2021
- **Sir Geoffrey Wilkinson Prize**, CIC GIDW Virtual Poster Competition, July 2020
- **Robert Macrae Prize for Inorganic Chemistry**, University of Leeds, July 2018
- **Dean's List for Outstanding Academic Achievement**, University of Leeds, July 2018
- **Headmaster's Award for Services to the School**, Wirral Grammar School for Boys, July 2014