

Daniel J. Kowalski

Research Associate in
Digital Chemistry



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Skills

Synthetic Chemistry:

- Solution-Phase Organic and Inorganic Synthesis
- Air-sensitive Techniques
- Solvothermal (Solid-State) Synthesis

Analytical Chemistry:

- Spectroscopy: NMR, IR, UV-vis
- Mass Spectrometry (inc MS², IM-MS)
- Diffraction: SCXRD, PXRD
- Other: DLS, Chromatography (Flash, HPLC, TLC, Automated)

Chemical Robotics:

- Construction, Operation and Maintenance of Fluid-Handling Platforms
- Operation of and Troubleshooting for Analytical Instruments

Coding / Data Analysis:

- Python
- GitHub
- Data Science & Visualisation
- Pipeline Automation
- Statistical Analysis
- Machine Learning
- Digital Interpretation of Chemical Data
- Some knowledge of R, HTML, & SQL

Software:

- MS Office (Word, PowerPoint, Excel)
- Conferencing: Zoom, MS Teams
- LaTeX
- 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.
- Development of novelty-directed exploration techniques.
- Conducted exploratory data analysis and generated dashboard visualisations to interrogate medicinal chemistry data.

Broader Skills

- Demonstrated client-focused problem-solving skills through data science contributions to synthetic projects, and by developing automated tools to reduce labour-intensive administrative tasks.
- Showcased self-motivation and adaptability by acquiring proficiency in unfamiliar deep learning techniques within a tight deadline.

2018-2022

Postgraduate Researcher
Glasgow, United Kingdom

University of Glasgow

Technical Achievements

- Designed and conducted exploratory experiments using machine learning to direct process optimisation and the discovery of novel coordination complexes.
- Constructed and operated fluid-handling robots (using group infrastructure) for medium-throughput inorganic synthesis.
- 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 enable the interpretation of complex spectra.

Broader Skills

- Demonstrated excellent teamwork and time management skills, resulting in the construction of several robotic platforms and the publication of two papers in high-impact journals.
- Recognised for clear communication of complex topics to diverse audiences through award-winning presentations at international conferences and instructional videos for practical teaching during lockdown.
- Showcased adaptability and attention to detail by revitalising an inactive project, resulting in an impactful publication with 40+ citations over 3 years.
- Exhibited self-directed, reflective learning by mastering machine learning skills through independent study, enabling leadership of data-driven projects and exhibiting self-directed, reflective learning.
- Effectively mentored a junior colleague through a Research Masters degree to their securing a technical job.

2017-2018

Masters Student
Leeds, United Kingdom

University of Leeds

Technical Achievements

- Design and implementation of synthetic routes to a library of Ruthenium complexes with proposed oncological activity.
- 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

- Collaborated with cross-functional teams and presented progress regularly, demonstrating excellent communication and relationship-building skills.
- International industry experience involving sensitive IP.

Education

2018–2022	PhD, Digital Chemistry <i>Glasgow, United Kingdom</i> Pending Viva: Date set for 6th April 2023 <i>Thesis:</i> Digital Discovery Strategies for Inorganic Chemistry (Provisional) <i>Advisor:</i> Prof. Leroy Cronin	University of Glasgow
2014–2018	MChem BSc, Chemistry with a Year in Industry <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	A Levels / GCSEs <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). 2 short courses at A*/A.	Wirral Grammar School for Boys

Selected Voluntary and Teaching Positions

2022—	Ordinary Board Member Involved in the organisation of events to strengthen industry-academia links.	Society of Chemical Industry Scotland Group
2019–2020	Local Organiser 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 national lockdown.	Pint of Science UK (Glasgow)
2018–2022	Graduate Teaching Assistant Responsible for supervising and teaching groups of 8–20 undergraduates across experiments in organic, inorganic, and physical chemistry. Produced videos for remote teaching during lockdown.	University of Glasgow
2017–2018	Safety, Health, and Environment Committee Secretary Recorded meetings and operated an anonymised reporting scheme for teaching laboratories.	University of Leeds
2015–2018	Peer-Assisted Learning (PAL) Mentor Delivered problem-based learning sessions for small group of Level 1 students with a partner mentor.	University of Leeds
2014–2018	Student-Staff Forum Representative Peer representative, responsible for communicating feedback to departmental management at regular meetings.	University of Leeds

Publications

- Kowalski, Cronin; “**Discovery Strategies in Chemistry**” [Review] *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