

Daniel J. Kowalski

Research Associate in
Digital Chemistry



+44 776 2709573



14kowalskid@gmail.com



djkowalski.github.io



dankowalskichm



0000-0003-0397-871X

Skills

Coding / Data Science:

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

- Statistical Analysis
- Machine Learning
- Data Wrangling and Visualisation
- Automation of Data Pipelines
- Digital Interpretation of Spectral 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 some solid state synthesis.

- Solution-Phase Synthesis
- Air-sensitive Techniques
- Solvothermal 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 MS², IM-MS)
- Diffraction: SCXRD, PXRD
- Other: DLS, Chromatography (Flash, HPLC, TLC, Automated)

Other:

- MS Office
- 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

- Synthesis generation via literature-informed deep learning.

Broader Skills

- Effective and communicative problem-solver as evidenced through the development of data-driven workflows, built and refined around specifications provided by synthetic chemists.

2018-2022

Postgraduate Researcher
Glasgow, United Kingdom

University of Glasgow

Technical Achievements

- Constructed, designed, and operated fluid-handling robots (using group infrastructure) for universal or medium-throughput synthesis.
- Purposed a variety of statistical and probabilistic machine learning techniques (e.g. Bayesian Optimisation) for the direction of exploration in chemical search spaces on automated platforms.
- Built pipelines for the extraction, transformation, and conditioning of data, leveraging web scraping, APIs, and chemistry-specific analytical packages to capture input data.
- Designed metrics for the quantification of novelty in MS data, introducing techniques for the deconvolution of highly complex spectra.

Broader Skills

- Excellent teamwork and collaboration skills demonstrated by participation in several small project teams (as both leader and member) leading to the construction of multiple robotic platforms, publication of 2 research papers, and discovery of a family of novel species.
- 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.
- Clear communicator of complex topics to diverse audiences, shown by 2 award-winning presentations at international conferences, and an educational video series produced for undergraduates during lockdown.
- Flexible and effective learner both independently, through self-guided development of programming skills, and collaboratively, through organisation of a series of peer-led problem sessions.
- Able to think creatively and identify opportunities for meaningful contribution, resulting in data-driven tools for chemical risk management inspired by shortcomings in the existing inventory system.
- Compassionate and supportive colleague; mentored 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

- Designed and implemented synthetic routes to complexes with proposed oncological activity, and diversification of these to a small library.
- Built proficiency with common air-sensitive synthetic techniques, including 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.
- Experience 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 in an international industrial environment, with a strong understanding of discovery workflows and the drug discovery pipeline.

Education

2018-2022	PhD, Digital Chemistry <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	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)	Wirral Grammar School for Boys

Selected Teaching and Voluntary Positions

2022—	Ordinary Board Member <i>Glasgow, United Kingdom</i> Involved in the organisation and operation of events to strengthen industry-academia links	Society of Chemical Industry Scotland Group
2018-2022	Graduate Teaching Assistant <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	Local Organiser <i>Glasgow, United Kingdom</i> As part of a small team, organised a raft of speakers for a pub-based, national outreach event. Event was ultimately cancelled due to the national lockdown.	Pint of Science UK
2017-2018	Safety, Health, and Environment Committee Secretary <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	Student-Staff Forum Representative <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, 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