Daniel J. Kowalski

Research Associate in
Digital Chemistry

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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 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 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^2, IM-MS)
- Diffraction: SCXRD, PXRD
- Other: DLS, Chromatography (Flash, HPLC, TLC, Automated)

Other:

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

References

Available on request

Research Experience

2022— **Research Associate** — University of Glasgow
Glasgow, United Kingdom

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** — University of Glasgow
Glasgow, United Kingdom

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 for the directed exploration of chemical search spaces.
- 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 skills demonstrated by balancing participation in several small project teams. Led to the construction of multiple robotic platforms, and timely publication of 2 primary research papers.
- 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** — University of Leeds
Leeds, United Kingdom

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** — F. Hoffmann-La Roche AG
Basel, Switzerland

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	**PhD, Digital Chemistry**	University of Glasgow

Glasgow, United Kingdom

Submission: November 2022 (Awaiting viva)
Provisional Title: Digital Discovery Strategies for Inorganic Chemistry
Advisor: Prof. Leroy Cronin

2014-2018	**MChem BSc, Chemistry with a Year in Industry**	University of Leeds

Leeds, United Kingdom

Thesis: Cytotoxic Ruthenium Complexes for Anti-proliferative Cancer Treatment
Advisor: Prof. Patrick C. McGowan

Industrial Project: Target-Oriented Synthesis of Peptidic Macrocycles for Anti-Infection Applications
Host Company: F. Hoffmann-La Roche Ltd.

2009-2014	**A Levels / GCSEs**	Wirral Grammar School for Boys

Merseyside, United Kingdom

A Level: Chemistry (A*), Biology (A), Physics (B), General Studies (A). AS levels in French and Critical Thinking.
GCSE: 12 A*-B with 10 at A* (inc. Maths, English Language, Chemistry, Biology, Physics, Astronomy)

Selected Voluntary and Teaching Positions

2022—	**Ordinary Board Member**	Society of Chemical Industry Scotland Group

Glasgow, United Kingdom

Involved in the organisation of events to strengthen industry-academia links.

2018-2022	**Graduate Teaching Assistant**	University of Glasgow

Glasgow, United Kingdom

Responsible for supervising and teaching groups of 8-20 undergraduates across experiments in organic, inorganic, and physical chemistry.

2019-2020	**Local Organiser**	Pint of Science UK

Glasgow, United Kingdom

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.

2017-2018	**Safety, Health, and Environment Committee Secretary**	Department of Chemistry, University of Leeds

Leeds, United Kingdom

Inaugural member. Responsible for meeting records and operating an anonymised laboratory reporting scheme.

2014-2018	**Student-Staff Forum Representative**	Department of Chemistry, University of Leeds

Leeds, United Kingdom

Peer representative, responsible for communicating feedback to departmental management at regular meetings.

Publications

- <u>Kowalski</u>, Cronin; "***Review: Discovery Strategies in Chemistry***" *In preparation*

- <u>Kowalski</u>, MacGregor, Long, Bell, Cronin; "***Automated Library Generation and Serendipity Quantification Enables Diverse Discovery in Coordination Chemistry***" J. Am. Chem. Soc. 2023, ASAP (<u>DOI</u>: 10.1021/jacs.2c11066)

- Porwol, <u>Kowalski</u>, 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 (<u>DOI</u>: 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