Daniel J. Kowalski

Postgraduate Researcher
Digital Chemistry

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Skills

Synthesis:

Experience in organic, coordination, and nanochemistry syntheses

- Solution-Phase Synthesis
- Air-sensitive Techniques
- Solvothermal Techniques

Analytical Techniques:

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

Coding/Software:

- Python
- GitHub
- LaTeX
- MS Office
- Origin
- Various Proprietary Analytical Software (e.g. TopSpin, Compass DataAnalysis)

References

Dr. Phil Kitson
Acting Group Coordinator
Research Fellow
Team Leader

philip.kitson@glasgow.ac.uk

Dr. Sebastian Manzano
Research Associate
Team Leader

sebastian.manzano@glasgow.ac.uk

Education

2018— **PhD, Digital Chemistry** University of Glasgow
Glasgow, United Kingdom

Expected Completion Date: September 2022
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 Bisquinaldamide ruthenium dichloride and Ruthenocenyl β-diketonate Complexes for Cancer Treatment
Advisor: Prof. Patrick C. McGowan

Research Experience

2018— **Postgraduate Researcher** University of Glasgow
Glasgow, United Kingdom

- Built and operated robotic semi-batch systems using group infrastructure. Optimised the automated synthesis of a variety of coordination compounds and metastable polymorphs of calcium carbonate. Used a higher-throughput platform in the exploration of chemical search spaces.
- Experienced with the use of machine learning techniques to explore chemical search spaces - including Gaussian Process Bayesian Optimisation, Evolutionary Algorithms, and Quasi-random Sampling methods.
- Developed data science techniques to probe complex systems encountered during unconstrained explorations of chemical search space. Project required digital interpretation of characterisation data, including data cleaning; matrix decomposition methods; and exploratory data analysis required both outlier detection and similarity measurement.
- Currently responsible for database construction to inform exploration of a chemical search space of hybrid nanostructures. Project has involved work with the CAS API to search and download literature sources; data encoding; and surface-level work with natural language processing and neural networks.
- Heavily involved in relocating the laboratory to new a facility, taking responsibility for organising the chemical inventory; resetting analytical equipment; and some new laboratory signage.
- Additionally: ran a series of inorganic problem sessions; organised external guest speakers; regularly presented at and engaged with group meetings; completed minor coding projects to automate admin or analyse hazard data on the group chemical inventory; and ran outreach events for a wide range of school-age pupils.

2017-2018 **Masters Student** University of Leeds
Leeds, United Kingdom

- Developed molecular targets with potential oncological application and designed synthetic routes to these.
- Built proficiency with common air-sensitive synthetic techniques, including use of Schlenk lines and glove boxes.

2016-2017 **Roche Intern in Medicinal Chemistry** F. Hoffmann-La Roche AG
Basel, Switzerland

- Worked as a member of a 3-person lab team to deliver novel analogues of a semi-peptidic macrocyclic anti-infective. Collaborated with and communicated across other labs using the same molecule class for different targets and with specialist separation scientists.
- Gained experience in a multi-national industrial environment, developing my understanding of discovery chemistry workflows, and the entire drug discovery pipeline.
- As part of the Internship programme, attended fortnightly problem sessions to build organic synthesis and presentation skills.

Teaching and Mentorship

2020, 2022— **Cronin Group Problem Sessions** University of Glasgow
Glasgow, United Kingdom

- Ran fortnightly Inorganic Problem Sessions, and have contributed to Organic Problem Sessions.
- Wrote and delivered sessions on: Organometallic Chemistry; C-H Activation; Crystal Field Theory; Ion Pairing; s-Block Reagents; UV-vis Spectroscopy

2018-2022 **Graduate Teaching Assistant / Laboratory Demonstrator** University of Glasgow
Glasgow, United Kingdom

- Supervised undergraduate students during physical and remote (during lockdowns) laboratory sessions. Responsible for teaching concepts and techniques pertinent to the experiments and enforcing good laboratory practice.
- Laboratory techniques taught included: solution-phase coordination chemistry, solution-phase organic chemistry, solid-state synthesis of zeolites, UV-vis spectroscopy, IR spectroscopy, NMR spectroscopy, HPLC, TLC, flame photometry
- Independently produced a series of videos during Covid-19 lockdowns to enable online teaching. Responsible for planning, filming, and editing the videos; performing the experiment; scripting and delivering narration.
- Helped deliver workshops for first year students (including under socially-distanced conditions), teaching concepts from all areas of the first year course.

2020-2021 **Supervisor to a Research Masters Student** University of Glasgow
Glasgow, United Kingdom

2020 **Undergraduate Chemistry Tutor** University of Glasgow
Glasgow, United Kingdom

Publications

- Kowalski, MacGregor, Long, Bell, Cronin; "***Coordination chemistry robots for generation of libraries and autonomous exploration of self-assembly and reaction space***" In preparation
- 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

Presentations

- Kowalski, Bell, Cronin; "***Automated Synthesis of Coordination Complexes***" RSC Scottish and North of England Dalton Division Meeting, Contributed Talk, August 2021, [Online]
- Kowalski, Asche, Mehr, ALife and Complexity Team, Cronin; "***Converging on a Long-Term Goal: Chemical Selection Engines***" RSC Twitter Poster Competition, March 2021, [Online]
- Kowalski, Porwol, Henson, Long, Bell, Cronin; "***Autonomous Chemical Robot Discovers the Rules of Coordination Chemistry***" CIC GIDW Virtual Poster Competition, July 2020, [Online]
- Kowalski, Porwol, Henson, Long, Mathis, Cooper, Cronin; "***The Role of Information in the Exploration of Metallosupramolecular Chemical Spaces***" University of Scotland Inorganic Conference, August 2019, Glasgow, United Kingdom
- Asche, Kowalski, Marshall, Doran, Mathis, Cooper, Cronin; "***Automating the Discovery of Artificial Life***" RSC Twitter Poster Competition, March 2019, [Online]

Awards and Honours

- **RSC Advances Best Talk Prize**, RSC Scottish and North of England Dalton Meeting, August 2021
- **Honourable Mention**, RSC Twitter Poster Competition, March 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