

# Calum Hand

PHD STUDENT - CENTRE FOR SUSTAINABLE & CIRCULAR TECHNOLOGIES

Bath, United Kingdom

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## Skills

	<b>Research</b>	Design & analysis of experiments, Project management, Critical evaluation, Cross-disciplinary mindset
<b>Machine Learning &amp; Cheminformatics</b>		Scikit-learn, RDKit, Deepchem, GPy, GPFlow, Data visualisation
<b>Programming &amp; Development</b>		Python, OOP, Version control, Continuous integration, Automated testing, Environment Management

## Education

### EPSRC Centre for Sustainable & Circular Technologies - University of Bath

SUSTAINABLE CHEMICAL TECHNOLOGIES (CHEMICAL ENGINEERING)

Applying machine learning to accelerate in-situ discovery of highly performant materials

*Integrated PhD & MRes*

*Sept 2018 - Present*

### Imperial College London

GREEN CHEMISTRY

Conducted year long project on synthesis of novel organic molecules

*MRes (Distinction)*

*Sept 2016 - Aug 2017*

### University of St. Andrews

CHEMISTRY WITH MEDICINAL CHEMISTRY

Attended workshops given by AstraZeneca and GSK on their drug discovery process

*BSc (2.1)*

*Sept 2012 - June 2016*

## Research Experience

### Sustainable Circular Technologies

UNIVERSITY OF BATH - CENTRE FOR SUSTAINABLE & CIRCULAR TECHNOLOGIES

- "Bayesian Screening: Multi-test Bayesian Optimization Applied to in silico Material Screening" (arXiv:2009.05418)
- Developing a significant Python package, integrating active learning and molecular simulations for novel screenings
- Constantly researching and investigating novel chemical descriptors and kernels
- Work extensively with popular libraries like scikit-learn, including writing novel models / data transformers

*Integrated PhD & MRes*

*Sept 2018 - Present*

### Green Chemistry

IMPERIAL COLLEGE LONDON

- Successfully demonstrated bio-renewable materials utilisation as a synthetic precursor for solar cells
- Research combined DFT calculations and novel synthetic strategies to investigate and synthesise target materials
- Granted a high degree of autonomy, allowing development of strong, self-motivated research ethic

*MRes (Distinction)*

*Sept 2016 - Aug 2017*

### Chemistry with Medicinal Chemistry

UNIVERSITY OF ST. ANDREWS

- "The synthesis of Hibbert ketone structures in technical lignins" (Org. Biomol. Chem., 2016, 14, 10023 - 10030)
- Year long project investigating the synthesis of small molecules

*BSc (2.1)*

*Sept 2012 - June 2016*

## Professional & Work Experience

### RIMES Technologies (Financial data management)

ACCOUNT TEAM MEMBER

- Initially hired as part of a global team of analysts. Daily tasks included: being first point of contact for all of RIMES' 300 clients; efficiently analysing anomalies within client's data; and identifying and fixing errors within RIMES' in house coding language
- Due to my proficiency in problem solving, knowledge of the RIMES tools and experience with clients, I was promoted to the account team of RIMES' largest client after only six months
- This promotion allowed me to work on the more technical and challenging problems being faced by the client including working on the development and implementation of their new data feed system, the largest single project RIMES had undertaken in their company history
- Routinely worked across multiple departments requiring me to be an effective communicator for both clients and technical teams
- Due to the fast paced nature of the role, an ability to prioritise tasks and often work on multiple issues at once was a key skill I developed while at RIMES

*London*

*Sept 2017 - Aug 2018*

## The Big Issue

Glasgow

OUTREACH & OFFICE VOLUNTEER

July 2016 - Sept 2016

- Travelled extensively within the West of Scotland in order to help and build relationships with street vendors about problems they were experiencing relating to their work, and offering support to vendors who had experienced abuse or been victim to violent crime
- Assisted with the sale of magazines to vendors, allocating vending pitches for the week and ensuring records were maintained and up to date

## YMCA Camp Silver Beach

USA - Virginia

ALPINE TOWER STAFF & COUNSELLOR

May 2015 - Aug 2015

- Worked as staff for the rock climbing tower and counsellor to cabin of 13 campers
- We were responsible for setting up and maintaining all equipment used on the tower and zipline every day and making sure all equipment was safe to be used
- Expected to be autonomous in our day to day work caring for over 120 campers a week

## Development Experience

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### Significant Contributions

Aug 2018 - Present

- Published cheminformatics python library "ChemSci" on github which allows conventional and custom chemical features to be easily combined with scikit-learn / machine learning pipelines.
- Over 2.5 years of machine learning, python programming, and data analysis experience
- Routinely help colleagues and postgraduates with programming / data analysis queries
- During COVID-19 have gained significant experience collaborating on active code development and incorporating best practises like automated testing for continuous integration, and version control
- Have experience working with linux environments on HPC systems

### Other

Aug 2018 - Present

- Have began establishing an applied machine learning interest group at University of Bath
- Member of the teaching team for University "Research software skills" courses which teach postgraduates and academics best coding and development practises
- Attended the 2019 HPC Autumn Academy at Cambridge University, a 2 week course on writing efficient and parallel C++ code for distributed systems
- Have completed Andrew NG's Machine Learning course on coursera, implementing the discussed algorithms in python using base libraries to expand my knowledge of machine learning techniques

## Other Achievements & Interests

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### Achievements

Ongoing

- Took part in Entrepreneurial skills exchange with local companies to better develop community involvement (2021)
- Completed the Microsoft accredited course on "Azure Cloud Fundamentals" (2020)
- Abel & Imray prize for best research project (2019)
- Scottish Institute for Enterprise Get "Enterprising" National winner (2015)
- "Race 2 Budapest" Charity Hitchhike Logistics Officer (2015)
- University of St Andrews Jujitsu Club Treasurer & Equipment Officer (2013-2015)
- "Race 2 Berlin" charity hitchhike race from Glasgow to Berlin (2014)

### Interests

Ongoing

- Training in numerous martial arts (Jujitsu, Krav Maga, Systema, Taekwondo, Kickboxing)
- Playing bass guitar
- Bouldering & Rock Climbing
- Enjoying all the films I can get my hands on