

## CONFERENCE PRESENTATIONS & TALKS

- 1. CCP5 General Meeting, Manchester, UK**  
I.Ismail, A. Shafiq, R. Mahmood, N. Aziz, A. Akinshina & M.Seaton Sep 2018  
"Interactions of terpenes in water and aqueous alcohol solutions."
- 2. Women in Chemistry Conference, Nottingham, UK**  
I.Ismail & S.Habershon Mar 2019  
"Optimising catalytic design using automated reaction path sampling."
- 3. RSC Online Conference, UK**  
I.Ismail & S.Habershon Mar 2019  
"Optimising catalytic design using automated reaction path sampling."
- 4. Computational Molecular Science Meeting (CMS), Coventry, UK**  
I.Ismail & S.Habershon Mar 2019  
"Optimising catalytic design using automated reaction path sampling."
- 5. International Meeting on Atomic and Molecular Physics and Chemistry, Madrid, Spain**  
I.Ismail, C.Robertson, & S.Habershon Jun 2019  
"Optimising catalytic design using automated reaction path sampling."
- 6. Research Harambee Conference, Coventry, UK**  
I.Ismail & S.Habershon Jun 2019  
"Optimising catalytic design using automated reaction path sampling."
- 7. RSC Theoretical Chemistry Group Graduate Meeting, Nottingham, UK**  
I.Ismail & S.Habershon Jul 2019  
"Automatic prediction and construction of complex chemical reaction routes."
- 8. Alumni Talk, Salford, UK- *\*invited speaker\****  
I.Ismail Nov 2019  
"Journey into postgraduate research."
- 9. Women in Chemistry Conference, Nottingham, UK**  
I.Ismail, C.Robertson, & S.Habershon Mar 2020  
"Connect the dots: In Silico Prediction of Heterogeneous Reaction Mechanisms."
- 10. HetSys Summer Conference, Coventry, UK**  
I.Ismail & S.Habershon Jul 2020  
"Connect the dots: In Silico Prediction of Heterogeneous Reaction Mechanisms."
- 11. ScotCHEM2020 Computational Chemistry Virtual Symposium, Online**  
I.Ismail & S.Habershon Aug 2020  
"Connect the dots: In Silico Prediction of Heterogeneous Reaction Mechanisms."
- 12. Machine Learning, Online Conference**  
I.Ismail & S.Habershon Oct 2020  
"Accelerating the prediction of complex multi-step reaction mechanisms using novel stochastic graph-based methods."
- 13. Reaction mechanisms in catalysis, Faraday Discussions, Online Conference, UK**  
I.Ismail & S.Habershon Feb 2021  
"Accelerating the prediction of complex multi-step reaction mechanisms using novel stochastic graph-based methods."
- 14. RSC, Online Conference, Online**  
I.Ismail & S.Habershon Mar 2021  
"Accelerating the prediction of complex multi-step reaction mechanisms using novel stochastic graph-based methods."
- 15. HetSys Summer Conference, Virtual Conference, Coventry, UK - [Talk Prize]**  
I.Ismail Jul 2021

"Accelerating the prediction of complex multi-step reaction mechanisms using novel stochastic graph-based methods."

**16. PTC-Virtual Seminar, Chemical Institute of Canada, Canada - *\*invited speaker***

I.Ismail

Jan 2022

"Automated Discovery of Multi-Step Elementary Reactions."

**17. ACS Spring 2022 Meeting, San Diego, US**

I.Ismail & S.Habershon

Mar 2022

"High-throughput screening of mechanistic hypotheses using machine-learning and multi-criteria decision making."

**18. Warwick Postgrad Chemistry Symposium, Coventry, UK**

I.Ismail & S.Habershon

May 2022

"High-throughput screening of mechanistic hypotheses using machine-learning and multi-criteria decision making."

**19. Midlands Computational Chemistry Meeting, Manchester, UK - [Talk Prize]**

I.Ismail

May 2022

"High-throughput screening of mechanistic hypotheses using machine-learning and multi-criteria decision making."

**20. CompChemURG: Forging New Pathways, Online- *\*invited speaker***

I.Ismail

Jun 2022

"Jack of all trades, master of what? Blurring disciplinary boundaries in science."

**21. Project Invisible Conference, Coventry, UK**

I.Ismail

Jul 2022

"High Throughput Screening of Mechanistic Hypotheses Using Machine Learning and Multi-Criteria Decision Making."

**22. HetSys Summer Conference, Coventry, UK**

I.Ismail

Jul 2022

"Successes and challenges in using machine-learned activation energies in kinetic simulations."

**23. Psi-k 2022 Conference, Lausanne, Switzerland**

I.Ismail

Aug 2022

"High Throughput Screening of Mechanistic Hypotheses Using Machine Learning and Multi-Criteria Decision Making."

**24. Alan Turing CDT Conference, Manchester, UK**

I.Ismail

Nov 2022

"Automated Graph-Driven Reaction Discovery."

**25. MIT Research Seminar, Virtual- *\*invited speaker***

I.Ismail

Mar 2023

"High-throughput Screening of Mechanistic Hypotheses Using Graph-Based Methods and Machine Learning."

**26. ETH Zurich Research Seminar, Virtual- *\*invited speaker***

I.Ismail

May 2023

"High-throughput Screening of Mechanistic Hypotheses Using Graph-Based Methods and Machine Learning."