Isaiah Betinol

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Education

2021 - Expected 2026 PhD (Cheminformatics), **The University of British Columbia**
2016 - 2021 BSc with First Class Honours (Chemistry), **University of Alberta**

Research Experience

The University of British Columbia with Dr. Jolene Reid Sep 2021 - Present

- Developed workflows to probe the mechanism and performance of asymmetric catalysts using machine learning and chemical informatics. Key projects include developing a quantification scheme for asymmetric catalyst generality (*JACS* **2023**), and using ML for data-driven mechanistic insights (*OBC* **2022**, *ChemRxiv* **2024**).
- Side projects include using ML to predict extraction conditions for the large scale recovery of cannabinoids (*Digital Discovery* **2024**), predicting the impacts of peptide structure in lipid nanoparticles for mRNA transportation using graph neural networks (In preparation), and computational studies to explain chemical reactivity (*ACS Catal.* **2023**)

University of Alberta with Dr. Sheref Mansy Jan 2020 - Apr 2021

- Elucidated the effects of side-chain structure on prebiotically plausible nicotinamide reductions by metabolic α-Ketoacids and demonstrated that amphiphillic nicotinamide biomimetics could transfer electrons across a protocellular membrane (Undergraduate Thesis).
- Developed a program that automates the spectral decomposition of iron-sulfur clusters using Microsoft Excel (*Anal. Biochem.* **2021**)

University of Alberta with Dr. Arthur Mar Sep 2019 - Dec 2019

- Synthesized novel ternary intermetallic compounds using solid-state techniques.

University of Calgary with Dr. Jeff Van Humbeck May 2019 - Sep 2019

- Planned and developed the syntheses of perylene diimide variants for use in organic photovoltaics.

Publications

12. Betinol, I.O., Kuang, Y., Lai, J., Yousofi, C., Reid, J.P. Machine Learning Enables A Top-Down Approach to Mechanistic Elucidation, *ACS Catal.* **2025**. Accepted.

11. Betinol, I.O., Demchenko, A., Reid, J.P. Evaluating Predictive Accuracy in Asymmetric Catalysis: A Machine Learning Perspective on Local Reaction Space. *ACS Catal.* **2025**, 15, 8, 6067-6077. DOI:10.1021/acscatal.5c01051

10. Betinol, I.O., Kuang, Y., Mulley, B.P., Reid, J.P. Controlling Stereoselectivity with Non-covalent Interactions in Chiral Phosphoric Acid Catalysis, *Chem. Rev.* **2025**, 125, 8, 4184–4286. DOI: 10.1021/acs.chemrev.4c00869

9. Plommer, H., Betinol, I.O., Dupree, T., Roggen, M., Reid. J.P. Predicting Extraction Conditions for the Large Scale Recovery of Cannabinoids. *Digital Discovery* **2024**, 3, 155-162. DOI: 10.1039/D3DD00176H

8. Goonesinghe, C., Jung, H., Betinol, I.O., Gaffen, J., Garrard, C.N., Chang, J., Hosseini, K., Roshandel, H., Patrick, B.O., Baumgartner, T., Caputo, C.B., Reid, J.P., Mehrkhodavandi, P. Rethinking

the Lewis acidity of cationic gallium and indium complexes. *ACS Catal.* **2023**, 13, 24, 16148–16157. DOI: 10.1021/acscatal.3c04918

7. Reid, J.P., Betinol, I.O., Kuang, Y. Mechanism to Model: A Physical Organic Chemistry Approach to Reaction Prediction. *Chem. Commun.* **2023**, 59, 10711-10721. DOI: 10.1039/D3CC03229A

6. Betinol, I.O.‡, Lai, J.‡, Thakur, S., Reid, J.P. A Data Driven Workflow for Assigning and Predicting Generality in Asymmetric Catalysis. *J. Am. Chem. Soc.* **2023**, 145, 23, 12870–12883. DOI: 10.1021/jacs.3c03989

5. Lai, J., Li, J., Betinol, I.O., Kuang, Y., Reid, J.P. A Statistical Modeling Approach to Catalyst Generality Assessment in Enantioselective Synthesis. *ChemRxiv* **2022**, DOI: 10.26434/chemrxiv-2022-80fgz

4. Betinol, I.O., Reid, J.P. A Predictive and Mechanistic Statistical Modelling Workflow for Improving Decision Making in Organic Synthesis and Catalysis. *Org. Biomol. Chem.* **2022**, 20, 6012-6018. DOI: 10.1039/d2ob00272h

3. Betinol, I.O., Kuang, Y., Reid, J.P. Guiding Target Synthesis with Statistical Modeling Tools: A Case Study in Organocatalysis. *Org. Lett.* **2022**, 24, 7, 1429-1433. DOI: 10.1021/acs.orglett.1c04134 *Featured on the front cover of *Organic Letters*

2. Valer, L., Rossetto, D., Scintilla, S., Hu, Y.J., Tomar, A., Nader, S., Betinol, I.O., Mansy, S.S. Methods to Identify and Characterize Iron-Sulfur Oligopeptides in Water. *Can. J. Chem.* **2022**, 100, 475-483. DOI: 10.1139/cjc-2021-0237

1. Betinol, I.O.‡, Nader, S.‡, Mansy, S.S. Spectral Decomposition of Iron-Sulfur Clusters. *Anal. Biochem.* **2021**, 629, 114269. DOI: 10.1016/j.ab.2021.114269

‡Authors contributed equally

Awards and Scholarships

2023	Brian and Jane James Graduate Scholarship in Catalysis Research
2023	UBC Chemistry Graduate Research Excellence Award
2022	Sandra Morris and Richard Tillyer Scholarship in Chemistry
2022	UBC Chemistry Graduate Research Symposium - Poster Presentation Award Winner
2022 - 2025	NSERC Postgraduate Scholarship – Doctoral program (PGSD)
2022 - 2025	University of British Columbia Four Year Doctoral Fellowship (4YF)
2021	NSERC Alexander Graham Bell Canada Graduate Scholarship – Master's program (CGSM)
2021 - 2025	Gladys Estella Laird Research Fellowship
2021	University of Alberta Gold Medal in Chemistry (Highest GPA in graduating chemistry class)
2021	University of Alberta Dean's Silver Medal in Science
2021	University of Alberta Chemistry 401 Prize (Best undergraduate chemistry thesis)
2020	Reuben Benjamin Sandin Memorial Achievement Scholarship in Chemistry
2019	NSERC Undergraduate Student Research Award (USRA)
2018	Robert Tegler Undergraduate Scholarship
2017 - 2020	Jason Lang Scholarship
2017 - 2020	University of Alberta Faculty of Science Dean's Honour Roll
2016	Alexander Rutherford Scholarship

Presentations

Betinol, I.O., Reid, J.P. Machine Learning Enables a Top-Down Approach to Mechanistic Elucidation. *Canadian Chemistry Conference and Exhibition (CSC)*, Ottawa, Canada. June **2025**. Symposium.

Betinol, I.O., Reid, J.P. Machine Learning Enables a Top-Down Approach to Mechanistic Elucidation. *APEC Young Chemistry Leaders Forum*, Suwon, South Korea. April **2025**. Symposium.

Betinol, I.O., Lai, J., Thakur, S., Reid, J.P. Assigning Generality in Asymmetric Catalysis. *Canadian Chemistry Conference and Exhibition (CSC)*. June **2023**. Poster Presentation.

Betinol, I.O., Kuang, Y., Reid, J.P. Statistical Models for Reaction Design and Synthetic Campaigns. *UBC Chemistry Graduate Research Symposium*. September **2022**. Poster Presentation.

Betinol, I.O., Kuang, Y., Reid, J.P. Statistical Models for Reaction Design and Synthetic Campaigns. *12th Triennial Congress of the World Association of Theoretical and Computational Chemists (WATOC)*. July **2022**. Poster Presentation.

Betinol, I.O., Mansy, S.S. Natural vs Artificial: A Comparison of NAD and NAD Variants in Protometabolic Reductions. *University of Alberta Undergraduate Seminar Series.* April **2021**. Presentation.

Betinol, I.O., Mansy, S.S. Protometabolic Reductions of Nicotinamide Biomimetics. *University of Alberta Undergraduate Seminar Series.* December **2020**. Presentation.

Betinol, I.O., Turnbull, D., Welch, G.C., Van Humbeck, J.F. Synthesis of Semiconducting Materials for Organic Photovoltaics. *University of Calgary Undergraduate Symposium*. August **2019**. Poster Presentation.

Teaching Experience

Organic Chemistry Laboratory TA (UBC Chem 235, 245) 2021, Winter 2022

- Set up and supervised experiments, and graded student lab reports.
- Consistently achieved excellent teaching evaluations from students and supervisors.

Organic Chemistry Lecture TA (UBC Chem 233, 260) Fall 2022, 2023, 2024

- Ran tri-weekly office hours and bi-semester review sessions for undergraduate students, graded student quizzes and exams.

Organic Chemistry Laboratory TA (UAlberta Chem 266/267) Winter 2021

- Gave weekly talks on the background and theory of experiments, set up and supervised experiments, and graded student lab reports.
- Consistently achieved excellent teaching evaluations from students and supervisors.

Other Roles

Dec 2021 - Present	Reid Lab Sustainability Representative
Dec 2021 - Sep 2022	Reid Lab Safety Representative

Skills

Programming	Proficient in python with extensive use of machine learning packages (sklearn, PyTorch) and related workflows and libraries (e.g. pandas, numpy, rdkit). Experience with MATLAB and Visual Basic programming languages.
Synthetic Chemistry	Experience with synthetic techniques and principles of organic synthesis and catalysis.