Carlos Oliver, PhD
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WORK EXPERIENCE

Assistant Professor, Tenure Track January 2025 -
Vanderbilt University
Nashville, USA *full-time*

- **Department**: Molecular Physiology & Biophysics, Computer Science
- Core member of the Center for Artificial Intelligence in Protein Dynamics.
- Leading research lab with focus on geometric deep learning for structural biology and pattern mining algorithm development for structured and dynamics data.

Independent Contractor July 2024 - December 2024
McGill University
Montreal, Canada *full-time*

- **Department**: School of Computer Science
- Developing tools for artificial intelligence-aided RNA drug discovery.

Project Leader June 2023 - June 2024
Max Planck Institute of Biochemistry
Munich, Germany *full-time*

- **Department**: Machine Learning and Systems Biology
- Founded and leading the *Molecular Pattern Mining and Learning Group*
- Responsibilities along with conducting primary research include PhD and Postdoc supervision with the aim of algorithm development in deep learning for structural biology and network analysis.

Postdoctoral Researcher October 2021 - May 2023
ETH Zürich *full-time*
Basel, Switzerland

- **Department**: Machine Learning and Computational Biology Group, Department of Biosystems Science and Engineering
- **Advisor**: Karsten Borgwardt, Full Professor.

- Developing novel unsupervised machine learning algorithms for mining complex structured datasets.
- Leading projects on biological network motif mining through deep learning, deep representation learning for protein structures, clinical outcome prediction, and biological systems evolution.
- Teaching assistant for Data Mining I graduate course. Prepared teaching & examination materials, as well as presented tutorials.

Technical Advisory Board Member May 2022 - July 2024
Simmunome Inc. *remote, part-time*
Montreal, Canada

- Developed tech plan for translating clinical data into systems biology models for drug discovery.

Consultant & Co-Founder January 2019 - July 2024
Ozeki Inc. *remote, part-time*
Montreal, Canada

- Consultancy service for startups; specializing in AI and blockchain implementations and advising.

Lead Scientist in Residence March 2020 - August 2021
NextAI *part-time*
Montreal, QC, Canada

- Supporting incubator startups in multiple industries through technical advising consultations.
- Helped startups develop their core technology and understand how to leverage state of the art methodologies.

Expert AI Advisor *May 2021 - October 2021*
Creative Destruction Labs *remote, part-time*
Toronto, ON, Canada

- Conducted interviews with startup founders to select incubator cohort for largest Canadian startup incubator.
- Assessed startups on technical soundness and potential for innovation.

Expert AI Advisor August 2020 - July 2021
Québec Ministry of Immigration *remote, part-time*
Montreal, QC, Canada

- Evaluating Québec residence applications with respect to artificial intelligence proficiency.

Course Lecturer September 2018-2019
School of Computer Science, McGill University *part-time*
Montreal, Canada

- Designed courses and delivered lectures for undergraduate and graduate-level computer science courses ($>$ 600 students). Topics: 'Introduction to Computer Science', and 'Fundamentals of Programming for Biology'

EDUCATION

PhD - Computer Science
McGill University & Montreal Institute for Learning Algorithms (MILA)
Montreal, Canada 2016-2021

- **Advisor(s):** Jérôme Waldispühl, William L. Hamilton
- **Thesis:** Origins, structure, and patterns of complex RNA structures.
- **Research Areas:** Computational Biology, Algorithm Design, Machine Learning on Graphs, Representation Learning, Network Science, Drug Discovery
- **Contribution:** Developed the first supervised and unsupervised representation learning approaches for RNA 3D structures, demonstrated applications to drug discovery, significant substructure searching, and structure prediction.

MSc - Molecular Biology
McGill University
Montreal, Canada 2014-2016

- **Advisor(s):** Jackie Vogel
- **Thesis:** Molecular Dynamics of the γ-Tubulin C-Terminal Tail
- **Research Areas:** Molecular Dynamics, Intrinsically Disordered Proteins, Systems Biology
- **Contribution:** Carried out high throughput computational analysis of intrinsically disordered proteins to understand the effects of key point mutations on biological function.

BSc - Computer Science & Biology
McGill U.
Montreal, Canada 2010-2014

PUBLICATIONS (Google Scholar)

* co-first, † co-corresponding, ‡ last-last author

Journal Articles

4. Oliver, Carlos & Waldispühl, J. What's so hard about RNA-targeting drug discovery? Drug discovery. *Nature Computational Science,* 1–2 (2025).

6. Carvajal-Patiño, J. G., Mallet, V., Becerra, D., Niño Vasquez, L. F., Oliver, Carlos† & Waldispühl, J. RNAmigos2: accelerated structure-based RNA virtual screening with deep graph learning. *Nature Communications* **16,** 1–12 (2025).

8. Oliver, Carlos, Mallet, V. & Waldispühl, J. 3D-based RNA function prediction tools in rnaglib. *book chapter to appear in Methods in Molecular Biology, Springer Nature* (2024).

10. Chen, D., Pellizoni, P., Hartout, P., Oliver, Carlos & Borgwardt, K. Endowing protein language models with structural Knowledge. *Bioinformatics,* btaf582 (2025).

11. Visonà, G., Duroux, D., Miranda, L., Sükei, E., Li, Y., Borgwardt, K. & Oliver, Carlos. Multimodal learning in clinical proteomics: enhancing antimicrobial resistance prediction models with chemical information. *Bioinformatics,* btad717 (2023).

15. Oliver, Carlos*, Mallet, Vincent*, Philippopoulos, P., Hamilton, W. L. & Waldispühl, J. Vernal: a tool for mining fuzzy network motifs in RNA. *Bioinformatics* **38,** 970–976 (2022).

16. Mallet, V., Oliver, Carlos, Broadbent, J., Hamilton, W. L. & Waldispühl, J. RNAglib: a python package for RNA 2.5 D graphs. *Bioinformatics* **38,** 1458–1459 (2022).

18. Oliver, Carlos, Mallet, V., Gendron, R. S., Reinharz, V., Hamilton, W. L., Moitessier, N. & Waldispühl, J. Augmented base pairing networks encode RNA-small molecule binding preferences. *Nucleic acids research* **48,** 7690–7699 (2020).

19. Boitreaud, J., Mallet, V., Oliver, Carlos & Waldispuhl, J. OptiMol: optimization of binding affinities in chemical space for drug discovery. *Journal of Chemical Information and Modeling* **60,** 5658–5666 (2020).

20. Philippopoulos, P., Ricottone, A. & Oliver, Carlos G. Difficulty Scaling in Proof of Work for Decentralized Problem Solving. *Ledger* **5** (2020).

22. Oliver, Carlos G, Reinharz, V. & Waldispühl, J. On the emergence of structural complexity in RNA replicators. *RNA* **25,** 1579–1591 (2019).

23. Sarrazin-Gendron, R., Reinharz, V., Oliver, Carlos G, Moitessier, N. & Waldispühl, J. Automated, customizable and efficient identification of 3D base pair modules with BayesPairing. *Nucleic acids research* **47,** 3321–3332 (2019).

25. Harris, J., Shadrina, M., Oliver, Carlos, Vogel, J. & Mittermaier, A. Concerted millisecond timescale dynamics in the intrinsically disordered carboxyl terminus of γ-tubulin induced by mutation of a conserved tyrosine residue. *Protein Science* **27,** 531–545 (2018).

27. Bouchard, J., Oliver, Carlos & Harrison, P. M. The distribution and evolution of Arabidopsis thaliana cis natural antisense transcripts. *BMC genomics* **16,** 1–9 (2015).

Conference Proceedings

9. Pellizzoni, P., Oliver, Carlos* & Borgwardt, K. *Structure-and Function-Aware Substitution Matrices via Learnable Graph Matching* in *International Conference on Research in Computational Molecular Biology* (2024), 288–307.

12. Kucera, Tim*, Oliver, Carlos*, Chen, D. & Borgwardt, K. *ProteinShake: Building datasets and benchmarks for deep learning on protein structures* in *Thirty-seventh Conference on Neural Information Processing Systems Datasets and Benchmarks Track* (2023).

14. Chen, D., Fan, B., Oliver, Carlos & Borgwardt, K. Unsupervised Manifold Alignment with Joint Multidimensional Scaling. *Proceedings of the International Conference for Learning Representations* (2022).

21. Sarrazin-Gendron, R., Yao, H.-T., Reinharz, V., Oliver, Carlos G, Ponty, Y. & Waldispühl, J. *Stochastic sampling of structural contexts improves the scalability and accuracy of RNA 3d module identification* in *International Conference on Research in Computational Molecular Biology* (2020), 186–201.

Workshop Proceedings

3. Wang, X., Shi, K. & Oliver, Carlos. BioBlobs: Unsupervised Discovery of Functional Substructures for Protein Function Prediction. *arXiv preprint arXiv:2510.01632, (Accepted, Workshop on Machine Learning for Structural Biology)* (2025).

5. Wyss, L., Mallet, V., Borgwardt, K. & Oliver, Carlos‡. *A standardized library for benchmarks of RNA 3D structure analysis* in *ICLR AI4NA Workshop 2025* (2025).

7. Pellizzoni, P., Oliver, Carlos & Borgwardt, K. *Structure- and Function-Aware Substitution Matrices via Differentiable Graph Matching* in *2nd Differentiable Almost Everything Workshop at the 41st International Conference on Machine Learning,* (2024).

Pre-prints

1. Shi, K. & Oliver, Carlos. ENSEMBITS: an alphabet of protein conformational ensembles. *arXiv preprint arXiv:2605.13789* (2026).

2. Karroucha, W., Oliver, Carlos, Stoven, V. & Mallet, V. Machine learning for RNA-targeting drug design. *arXiv preprint arXiv:2512.15645* (2025).

13. Oliver, Carlos, Chen, D., Mallet, V., Philippopoulos, P. & Borgwardt, K. Learning to Mine Approximate Network Motifs. *arXiv preprint arXiv:2206.01008* (2022).

17. Mallet, V., Oliver, Carlos G & Hamilton, W. L. Edge-similarity-aware Graph Neural Networks. *arXiv preprint arXiv:2109.09432* (2021).

24. Mallet, V., Oliver, Carlos G, Moitessier, N. & Waldispuhl, J. Leveraging binding-site structure for drug discovery with point-cloud methods. *arXiv e-prints,* arXiv–1905 (2019).

26. Oliver, Carlos G, Ricottone, A. & Philippopoulos, P. Proposal for a fully decentralized blockchain and proof-of-work algorithm for solving NP-complete problems. *arXiv preprint arXiv:1708.09419* (2017).

AWARDS

2017	Quebec FRQNT Doctoral Fellowship	$60k
2017	John D. Thompson TechIdea Pitch Competition	3rd Place
2016	Graduate Excellence Award	$10k
2014	Cellular Dynamics Graduate Fellowship	$35k
2014	Dean's Multidisciplinary Undergraduate Researcher List	

INVITED & REFEREED TALKS & MEETINGS

- *AI in Translational Research* (Vanderbilt Life Science Showcase, Vanderbilt University, July 2026, Invited Talk)
- *Structure-Based Machine Learning for RNA Drug Discovery: The Story So Far* (D2R Seminar Series, McGill University, May 2026, Invited Talk)
- *Taming the Biomolecular Structure Revolution — Representation Learning for dynamics, RNA, and substructures* (Yale Biomedical Informatics & Data Science Rising Star Seminar, 2026, Invited Talk)
- *Bio+ML Reading Group at Montreal Institute for Learning Algorithms, 2024* (Invited talk)
- *ProteinShake: Building Datasets and Benchmarks for Deep Learning on Protein Structures* (ISMB 2023, Lyon, France)
- *Roche InsightsLab Research Camp Paris 2022* (Invited Participant)
- *ETH Zurich Systems Biology Graduate Workshop, 2022* (Invited Lecturer)
- *ISMB/ECCB 2021 - Tools for the analysis of RNA 3D structures (Accepted talk)*
- *Deep Graph Learning Library Developer Group* Virtual (Invited Talk, [16])
- *International Conference on Research in Computational Molecular Biology (RECOMB) 2021* Virtual (Oral Presentation for [15])
- *RNA Society Meeting 2020 Online* Vancouver, Canada (Selected Talk, [18])

- *Machine Learning in Drug Discovery 2018,* University of Leuven, Belgium (Selected Talk, [18])
- *RiboClub Meeting 2018*, Sherbrooke, Candada (Selected Talk, [18])
- *Computational Approaches to RNA Structure and Function*, Benasque, Spain 2018 (Invited Speaker)

MENTEES

- *Vincent Mallet* (M.Sc, McGill University, Ecole Polytechnique Paris): representation learning for protein and RNA drug discovery [15]
- *Jonathan Broadbent* (B.Sc, McGill University) : software tools and datasets for RNA 3D structure learning [16]
- *Jacques Boitreaud* (M.Sc, McGil University, Ecole Polytechnique Paris): Chemical space optimization [19]
- *Juan Guillermo Carvajal Patiño* (PhD, McGill University): learning from molecular docking for RNA small molecule affinity prediction (submitted, RECOMB 2024)
- *Tim Kucera* (PhD, ETH Zürich): deep representation learning for massive protein datasets [12]
- *Yiran Li* (M.Sc., ETH Zürich): proteomic and chemical space modeling for antimicrobial resistance prediction [11]

COMMUNITY CONTRIBUTIONS
(GitHub)

- Reviewer for : Nature Biotechnology, Nature Computational Science, Bioinformatics Journal (OUP), Research in Computational Molecular Biology, Intelligent Systems for Molecular Biology, Journal of Machine Learning Research, American Chemical Society, Nature Communications Chemistry, Nucleic Acids Research, International Conference on Learning Representations, Neural Information Processing Systems Conference
- Track Chair Graph Models for Learning and Recognition (GMLR) at The 38th ACM/SIGAPP Symposium On Applied Computing (SAC 2023)
- `proteinshake`: co-creator and developer of largest deep learning-ready protein structure database; including newly published AlphaFold datasets.[12] **Maintainer**
- NetworkX (+ 4k users) graph comparison algorithms (WL-isomorphism, and Graph Edit Distance). **Contributor**

- `pytorch-geometric` (+ 4k users) Weisfeiler Leman Graph Convolution. **Contributor**
- Neural Subgraph Learning Library(+ 4k users) minor code enhancements. **Contributor**
