Carlos Oliver, PhD

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SUMMARY

My expertise and interests span all aspects surrounding the question of understanding biomolecular structure & function. As a computer scientist, I approach this problem by combining machine learning and graph algorithms. Since my PhD, I have completed projects in a wide range of topics from *drug discovery*, *structure prediction*, and *pattern mining*.

WORK EXPERIENCE

Postdoctoral Researcher — October 2021 - Present
ETH Zürich — *full-time*
Basel, Switzerland

- **Department**: Machine Learning and Computational Biology Group, Department of Biosystems Science and Engineering
- **Advisor**: Karsten Borgwardt
- Researching graph machine learning methods and their applications to biological problems

Technical Advisor — May 2022 - Present
Simmunome Inc. — *remote, part-time*
Montreal, Canada

- Advisory board member for biotech startup focusing on disease modeling and drug discovery.

Consultant & Co-Founder — January 2019 - Present
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 with technical planning, troubleshooting, hiring and education.

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.
- Assessed startups on technical soundness and potential.

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

- Taught and prepared learning material 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 U. & Montreal Institute for Learning Algorithms (MILA)
Montreal, Canada — 2016-2021

- **Advisor(s):** Jerome Waldispuhl, William L. Hamilton
- **Thesis:** Origins, structure, and patterns of complex RNA structures.
- **Research Areas:** Computational Biology, Machine Learning on Graphs, Representation Learning, Network Science, Drug Discovery

M.Sc - Molecular Biology
McGill U.
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

B.Sc - Computer Science & Biology
McGill U.
Montreal, Canada — 2010-2014

- **Minor:** Italian Studies

RESEARCH HIGHLIGHTS

Fuzzy Network Motif Mining

- Fully automated tool for mining quasi-isomorphic and frequent network motifs in biological data.
- Integrates concepts from graph kernel methods, unsupervised graph representation learning, and exact graph algorithms (See [4] in Publications section)
- Source Code: `https://github.com/cgoliver/vernal`
- Motif Gallery: `http://vernal.cs.mcgill.ca`

Automated Drug Discovery for RNA

- First learning platform for target-based drug discovery on RNA molecules.
- Graph representation learning and kernel methods revealed insights for understanding key interactions in biomolecules (See [8] in Publications).

- Source Code: `https://github.com/cgoliver/vernal`
- Webserver: `http://rnamigos.cs.mcgill.ca`

PUBLICATIONS

1. Dexiong C., Fan B.., **Oliver, C.** & Borgwardt, K. (2022). "Joint Multidimensional Scaling" (NeurIPS 2022 submission, preprint in preparation)
2. **Oliver, C.**, Dexiong C., Mallet V., Philoppopoulos P., & Borgwardt, K. (2022). "Approximate Network Motif Mining Via Graph Learning" (NeurIPS 2022 submission, *arXiv preprint* arXiv:2206.01008.)
3. Mallet, V., **Oliver, C.**, Broadbent, J., Hamilton, W. L., & Waldispühl, J. (2022). "RNAglib: a python package for RNA 2.5 D graphs." *Bioinformatics*, 38(5), 1458-1459.
4. **Oliver, C.**, Mallet, V., Philippopoulos, P., Hamilton, W. L., & Waldispühl, J. (2022). "Vernal: a tool for mining fuzzy network motifs in RNA." *Bioinformatics*, 38(4), 970-976.
5. Mallet, V., **Oliver, C. G.**, & Hamilton, W. L. (2021). "Edge-similarity-aware Graph Neural Networks." *arXiv preprint* arXiv:2109.09432.
6. Boitreaud, J., Mallet, V., **Oliver, C.**, & Waldispühl, J. (2020). OptiMol: optimization of binding affinities in chemical space for drug discovery. *ACS Journal of Chemical Information and Modeling*, 60(12), 5658-5666.
7. Philippopoulos, P., Ricottone, A., & **Oliver, C. G.** (2020). "Difficulty Scaling in Proof of Work for Decentralized Problem Solving." *Ledger*, 5.
8. Sarrazin-Gendron, R., Yao, H. T., Reinharz, V., **Oliver, C. G.**, Ponty, Y., & Waldispühl, J. (2020, May). "Stochastic sampling of structural contexts improves the scalability and accuracy of RNA 3d module identification." *In International Conference on Research in Computational Molecular Biology* (pp. 186-201). Springer, Cham.
9. **Oliver, C.**, Mallet, V., Gendron, R. S., Reinharz, V., Hamilton, W. L., Moitessier, N., & Waldispühl, J. (2020). "Augmented base pairing networks encode RNA-small molecule binding preferences." *Nucleic Acids Research*, 48(14), 7690-7699.
10. **Oliver, C. G.**, Reinharz, V., & Waldispühl, J. (2019). "On the emergence of structural complexity in RNA replicators." *RNA*, 25(12), 1579-1591.
11. Vincent Mallet, **Carlos G. Oliver**, Nicolas Moitessier, Jérôme Waldispühl. "Leveraging binding-site structure for drug discovery with point-cloud methods". arXiv preprint arXiv:1905.12033 (2019)
12. Sarrazin-Gendron, R., Reinharz, V., **Oliver, C. G**., Moitessier, N., & Waldispühl, J. (2019). "Automated, customizable and efficient identification of 3D base pair modules with BayesPairing." *Nucleic Acids Research*, 47(7), 3321-3332.
13. Harris, J., Shadrina, M., **Oliver, C.**, Vogel, J., & Mittermaier, A. (2018). "Concerted millisecond timescale dynamics in the intrinsically disordered carboxyl terminus of γ-tubulin induced by mutation of a conserved tyrosine residue." *Protein Science*, 27(2), 531-545.
14. **Oliver, C.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).
15. Bouchard, Johnathan, **Carlos Oliver**, and Paul M. Harrison. "The distribution and evolution of Arabidopsis thaliana cis natural antisense transcripts." *BMC Genomics* 16.1 (2015): 444.

AWARDS

2017	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

- *Deep Graph Learning Library Developer Group* Virtual (Invited Talk)
- *RECOMB 2021* Virtual (Oral Presentation for [4])
- *RNA Society Meeting 2020 Online* Vancouver, Canada (Selected Talk)
- *Machine Learning in Drug Discovery 2018,* University of Leuven, Belgium (Selected Talk)
- *RiboClub Meeting 2018*, Sherbrooke, Candada (Selected Talk)
- *Computational Approaches to RNA Structure and Function*, Benasque, Spain 2018 (Invited Speaker)

OPEN SOURCE CONTRIBUTIONS

- GitHub: `https://github.com/cgoliver/`
- `torch-pdb`: co-creator and developer of largest deep learning-ready protein structure database; including newly published AlphaFold datasets.
- NetworkX (+ 4k users) graph comparison algorithms (WL-isomorphism, and Graph Edit Distance).
- Neural Subgraph Learning Library(+ 4k users) minor code enhancements.