Carter J. Wilson

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About me

I am a second-year student at The University of Western Ontario pursuing a M.Sc. in Applied Mathematics. For the past three years I have had the privilege of working under Dr. James (Wing-Yiu) Choy, and for the past two years, under Dr. Mikko Karttunen. I am particularly interested in studying bio-macromolecular systems using computational methods, in particular the development of therapeutic peptides/small molecules and the effects of disease causing point mutations on protein stability and binding affinity. Most of my work makes use of molecular dynamics simulations implemented in GROMACS, and over the past year I have begun to make extensive use of enhanced sampling techniques (metadynamics, eABF, replica-exchange, etc.) to augment this research.

Education

The University of Western Ontario (UWO) — London, Canada

M.Sc. Applied Mathematics (94.0; 94.0 *) — *May '21 – Present*

Supervisors: Dr. Mikko Karttunen and Dr. Wing-Yiu Choy

The University of Western Ontario (UWO) — London, Canada

BMSc. (Hons.) Computational Biochemistry & BSc. (Maj.) Applied Mathematics (87.3; 87.7 *) — *2016 – 2021*

4th year thesis: Keap1 cancer mutants: A large-scale molecular dynamics study of protein stability.

3rd year project: Investigating a novel protein docking method using the disordered binding partners of CBP.

Experience

Computational Biomolecular Dynamics Group
(Max Planck Institute for Multidisciplinary Sciences) — Göttingen, Germany

Research Assistant — *May '22 – Nov '22*

Working under the supervision of Drs. Bert de Groot and Vytautas Gapsys.

SoftSimu and Choy Lab Research Groups (UWO) — London, Canada

Graduate Student Researcher — *May '21 – Present*

Working under the supervision of Dr. Mikko Karttunen jointly with Dr. James (Wing-Yiu) Choy.

Choy Lab and SoftSimu Research Groups (UWO) — London, Canada

Undergraduate Student Researcher — *Jan. '19 – May '21*

Working under the supervision of Dr. James (Wing-Yiu) Choy jointly with Dr. Mikko Karttunen.

Departments of Biochemistry and Biostatistics (UWO) — London, Canada

COVID-19 Transition Team Intern — *June '20 – May '21*

Helped to coordinate the initial transition from an in-person to online course setting. Continue to provide ongoing logistical, planning, and developmental support directly to faculty in both the Biochemistry and Biostatistics departments.

Denninger's Bistro and Grocery — Oakville, Canada

Assistant Manager (Bistro Department) — *May '18 – Sept. '18*

Self-employed — Burlington, Canada

Private Swim Instructor and Lifeguard — *May '17 – Sept. '18*

Town of Oakville — Oakville, Canada

Swim Instructor and Lifeguard — *Sept. '14 – Sept. '16*

Students supervised

Chery Ma — 4th Year Thesis

Hybrid solvation applied to disordered protein systems — *Sept. '21 – May. '22*

Janvi Shah — Summer student

Developing small molecules that bind TPR2A — *May. '21 – Sept. '21*

Lisa Hong (Co-supervisor: Megan Chang) — 4th Year Thesis

Stability study of the Kelch family of proteins — *Sept. '19 – May. '20*

Teaching assistantships

NMM 1414B: Calculus for Engineers II — Winter 2022

NMM 1412A: Calculus for Engineers I — Fall 2021

Phys 3926F: Computer Simulations in Physics — Fall 2021

*cGPA; final 2 years GPA

Publications

First-author

[1] Chang, M.[†], Wilson C. J.[†], Karunatilleke, N. C., Moselhy, M. H., Karttunen, M., and Choy W-Y. Exploring the conformational landscape of the Neh4 and Neh5 domains of Nrf2 using two different force fields and circular dichroism. *J. Chem. Theory Comput.*, **2021**, 17(5), 3145–3156; 10.1021/acs.jctc.0c01243

[2] Wilson, C. J., Chang, M., Karttunen, M., and Choy W-Y. KEAP1 Cancer Mutants: A Large-Scale Molecular Dynamics Study of Protein Stability. *Int. J. Mol. Sci.*, **2021**, 22(10), 5408; 10.3390/ijms22105408

[3] Salem, A.[†], Wilson, C. J.[†], Rutledge, B. S., Dilliott, A., Farhan, S., Choy W-Y and Duennwald, M. L. Matrin3: Disorder and ALS Pathogenesis. *Front. Mol. Biosci.*, **2021**, 22(10), 5408; 10.3389/fmolb.2021.794646

[4] Wilson, C. J., Choy W-Y and Kattunen, M. AlphaFold2: A Role for Disordered Protein/Region Prediction. *Int. J. Mol. Sci*, **2022**, 23(9), 4591; 10.3390/ijms23094591

Conferences

Western Undergraduate Research Conference — London, Canada

Invited Speaker — *March '21*

Exploring the conformational landscape of Nrf2 using molecular dynamics simulations and circular dichroism.

Western Undergraduate Research Conference — London, Canada

Invited Speaker[‡] — *March '20*

Keap1 cancer mutants: A large-scale molecular dynamics study of protein stability.

Harold Stewart Research Showcase — London, Canada

Poster — *Jan. '20*

Keap1 cancer mutants: A large-scale molecular dynamics study of protein stability.

Awards and Scholarships

The University of Western Ontario — London, Canada

Western Graduate Research Scholarship — *May '22*

Value: $6,750; Duration: 12 months

Western Graduate Research Scholarship — *May '21*

Value: $6,750; Duration: 12 months

Western Gold Medal — *April '21*

Attained the highest average in a degree module (HSP Computational Biochemistry).

Graduation with Distinction — *April '21*

Maintained standing on the Dean's List over the course of my degree program.

Western Scholar — *April '21*

Admitted with a +90% average and maintained standing on the Dean's List.

Western Scholarship of Excellence — *Sept. '16*

Merit based admission scholarship ($2,500).

Natural Sciences and Engineering Reserach Council of Canada — Ottawa, Canada

Canadian Graduate Scholarship (CGS) (Master's) — *May '21*

Value: $17,500; Duration: 12 months

CGS: Michael Smith Foregin Study Supplement — *May–Nov. '22*

Value: $6,000; Duration: 6 months

Government of Ontario — Toronto, Canada

Ontario Graduate Scholarship (OGS) (Master's) — *May '22*

Value: $15,000; Duration: 12 months

Skills and Graduate Courses

Natural languages: English (*mother tongue*), French (*memorized proficiency*)

Programming languages: Python (*mother tongue*), LaTeX(*mother tongue*), C++ (*professional working proficiency*), Java (*professional working proficiency*), MATLAB (*professional working proficiency*), Markdown (*limited working proficiency*), HTML (*limited working proficiency*)

Courses: Scientific Computing (Winter 2022; 0.5 credit), Statistical Mechanics (Winter 2022; 0.5 credit)

[†]Equal contribution.
[‡]Cancelled due to COVID-19.