# YI-YUAN LEE

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### **EDUCATION**

## M.S., Carnegie Mellon University, Pittsburgh, PA

May 2020

Master of Science in Computational Biology, School of Computer Science Awarded Academic Achievement Fellowship

# B.S., National Taiwan University, Taipei, Taiwan

June 2014

Bachelor of Science in Biochemical Science and Technology

#### Relevant Course List:

Introduction to Deep Learning, Introduction to Machine Learning, Biological Modeling and Simulation, Computational Methods for Proteogenomics and Metabolomics, Algorithm and Advanced Data Structure, Introduction to Computer Systems, Bioinformatics Data Integration Practicum, Immunology, Physiology, Statistics.

### **PUBLICATIONS**

- Yi-Yuan Lee, Haodong Liu, Neel Mittal, Stephanie Eristoff, Liu Cao, Hosein Mohimani, "hypoNPAtlas: an atlas of hypothetical natural product for mass spectrometry database search". [06/15/2021 submitted to Nature Microbiology, https://bit.ly/37lTlJj]
- Liu Cao, Mustafa Guler, Azat Tagirdzhanov, **Yi-Yuan Lee**, Alexey Gurevich, Hosein Mohimani, "MolDiscovery: Learning Mass Spectrometry Fragmentation of Small Molecules". [06/04/2021 accepted, Nature Communications]
- Michelle et. al, including **Yi-Yuan Lee**, "A community resource for paired genomicand metabolomic data mining", Nature Chemical Biology, 2021.
- W.C. Su, S.-F. Hsu, Y.-Y. Lee, et al., "A Nucleolar Protein, Ribosomal RNA Processing 1 Homolog B (RRP1B), Enhances the Recruitment of Cellular mRNA in Influenza Virus Transcription", Journal of Virology, 2015.
- Tzu-Hui Hsu, Yu-Chan Chang, Yi-Yuan Lee, Chi-Long Chen, Michael Hsiao, Fan-Ru Lin, Li-Han Chen, Chun-Hung Lin, Takashi Angata, Fu-Tong Liu and Kuo-I Lin, "B4GALT1-depednent galectin-8 binding with TGFβ receptor suppresses colorectal cancer metastasis". [in preparation]

# RESEARCH EXPERIENCE

#### Computational Biology Department, Carnegie Mellon University

Sep 2018 - Now

Graduate Research Associate

Prof. Hosein Mohimani Ph.D.

- Developed deep neural networks for discovering novel ribosomally synthesized and post-translationally modified peptides (RiPPs), a class of natural products from microbial genomes. Both models are written in PyTorch and outperform the-state-of-the-art models in similar tasks.
- Implemented a subgraph-isomorphism-based chemical structure predictor, which generates hypothetical structures given a core peptide and a list of tailoring enzymes. Written in C++ and Rust.
- Mentoring three undergraduate students in research of in silico natural product discovery.

#### Genomics Research Center, Academia Sinica, Taiwan

Aug 2015 - May 2018

Research Assistant

Prof. Kuo-I Lin Ph.D.

- Project 1: "The role of B cell receptor (BCR) signaling in chronic lymphocytic leukemia (CLL)."
  - Established four drug-resistant clones for drug-resistance study.
  - Identified a kinase responses to BCR activity and stimulates the downstream transcriptional factor activation.
- Project 2: "The role of diSia motif in B cell immunity."
  - Identified the role of alpha-2,8-sialyltransferase 6 (ST8-6) in acute inflammatory response.
- Project 3: "The function of galectin-8 in colon cancer."
  - Performed extra splenic injection to confirm the anti-cancerous activity of galectin-8 with IVIS system.
  - Conducted animal experiments for lab members, and trained new lab members experimental techniques.

# National Taiwan University, Taiwan

Jan 2013 - June 2014

Undergraduate Volunteer

Prof. Bi-Fong Lin, Ph.D., Bor-Luen Chiang, M.D./Ph.D.

• Confirmed the effect of additional nutrients on mesenchymal stem cells' (MSCs) immunoregulatory ability.

# National Institute of Genetics (NIG), Japan

July 2012 - Sep2012

 $Summer\ Intern$ 

Prof. Inoue Ituro, M.D.

 $\bullet$  Identified the mutation of KDM5B is one of the causalities of ovarian cancer.

# Institute of Molecular Biology, Academia Sinica, Taiwan

Jan 2012 - June 2012

Undergraduate Volunteer

Prof. Michael M.C. Lai, M.D./Ph.D.

• Supported the postdoctoral researcher to identify the role of human gene RRP1B in the infection and replication of *influenza A virus*. The result was published on Journal of Virology in 2015.

## Institute of Molecular Biology, Academia Sinica, Taiwan

July 2011 - Sep 2011

Summer Intern

Prof. Meng-Chao Yao, Ph.D.

• Verified the chromosome breakage executing time is later than dsRNA guided DNA deletion in *Tetrahymena* thermophila duplication.

#### **PROJECTS**

ChiGAN: A deep generative neural network to discover new chemical flavor compounds using a deep generative neural network with chemical structure data from FooDB.

SimCLL: A signaling and transcriptional factor network to simulate responses of healthy B cells, and Ibrutinib treated CLL cell with BioNetGen.

**VireTap:** A viral gene detection pipeline in human disease transcriptomes, by integrating bioinforamtics tools such as TopHat, Trinity, and Blastn.

**ProLang:** A high level programming language parser and simulator to convert a code into cell-like structures. Written in Golang.

#### LEADERSHIP AND ACTIVITIES

### Department of Life Science, National Taiwan University

Feb 2014 - June 2014

Teaching Assistant in Biotechnological Core Techniques Course

• Coached students to complete molecular biology experiments.

Department of Information Management, Executive Government, Taiwan Substitutive Military Service

Aug 2014 - July 2015

Supervisor: Ming-Chung Lee

- Launched the guiding system and official website of History Exhibit in Executive Yuan.
- Solved problems of exigent program and system, and managed SVN subversion system.

### iGEM NTU-Taiwan Team, Hong Kong

Dec 2012 - Oct 2013

Team-leader

Advisor: Chern, Edward Yen-Rong

- Established a new iGEM team, recruited interdisciplinary members in NTU and raised funding.
- Awarded silver medal in the competition. Designed a biological heating device by transformed *SrUCP* into *Saccha-romyces cerevisiae* and simulated the regulation circuit with different types of promoters by computational model. Enhanced about 150% heat production in our device. (Website: 2013.igem.org/team:NTU\_Taiwan/index.html)

### Novartis Biocamp, Taiwan

May 2014 - May 2014

Participant

Organizer: Novartis Taiwan

- Only 30 students was selected out each year in Taiwan from various backgrounds.
- Acquired knowledge about how pharmaceutical industry works and worked with group members to create a business plan of hypertension drug.

# **SKILLS**

Programming Language

Python, C, C++, Rust, Go, Bash, R

Bioinformatics
Deep Learning

HMMER, BLAST, RDKit, Dereplicator+, MolDiscovery, BWA, SAMtools, NGS

PyTorch, TensorFlow, Numpy, Scipy, Sklearn, modAL

Development Tools
Wet lab skills

Linux, AWS, Git, Slurm, LATEX, VIM, tmux

mouse breeding and handling, simple survival surgery in mice and blood collection, primary B cell isolation, cell line and primary cell culture, flow cytometry, plasmid construction, point mutation, protein purification, genotyping, PCR, qRT-PCR, transfection, western blotting, virus preparation

Language

English (fluent), Mandarin Chinese (native speaker), Japanese (conversational)

# TEST SCORE

**TOEFL:** 111/120 (Reading: 29, Listening: 30, Speaking: 27, Writing: 25)

Sep 2019

GRE: Verbal 152/170, Quantitative 167/170, Analytic Writing Analysis: 3.5/6.0

Nov 2017