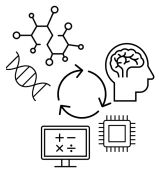
MinGyu **CHOI**

Seoul, Korea +82 10 9508 5488 chemgyu@mit.edu chemgyu.github.io



Education

PhD 2023-
MIT, Massachusetts Institute of Technology, Cambridge
Accepted for the Chemistry PhD program.
Supported by Korea Foundation for Advanced Studies (KFAS), Doctoral Study Scholarship (13,000 $/year)

BS 2016-2023
SNU, Seoul National University, Seoul, Korea
Double-major in CHEM/CSE, Summa Cum Laude
Supported by Korea Student Aid Foundation (KOSAF), Korea Presidential Science Scholarship (11,000 $/year).
- BSc in Chemistry (Major GPA 4.22/4.3) and Computer Science and Engineering (Major GPA 3.83/4.3)
- 2 years Mandatory Military Leave of Absence : Sep2019-June2021, Republic of Korea Air Force.

Publications

Journals
- Lu Y, Lim S, Park S, **Choi MG**, Jo C, Kim S (under revision), "EnsDTI-kinase:A Web-server for Ensemble Prediction of Kinase-inhibitor Interactions."
- Lim S, Lee S, Piao Y, **Choi MG**, Bang D, Gu J, Kim S (2022), "On Modeling and Utilizing Chemical Compound Information with Deep Learning Technologies : A Task-oriented Approach," *Computational and Structural Biotechnology Journal*, 20 ;4288-4304.
- Lee H, **Choi MG**, Park J-U, Roh H, Kim S (2020), "Genome Mining Reveals High Topological Diversity of w-Ester-Containing Peptides and Divergent Evolution of ATP-Grasp Macrocyclases," *Journal of the Americal Chemical Society*, 142(6) ;3013-3023.

Preprints
- **Choi MG**, Shin W, Lu Y (2022), "Triangular Contrastive Learning on Molecular Graphs," *arXiv preprint*, arXiv:2205.13279.

Research History

Dry-lab Clinical AI
Decision Intelligence Lab — Chung-Ang University, Korea
Nov22-Present | Principal Investigator : Prof. Changhee Lee (Co-advsed with Prof. Mihaela van der Saar)
- Developing an algorithm for efficient analysis of **time-series clinical data** - cellular/organismic level.

Dry-lab Clinical AI
Centre for AI in Medicine — Cambridge University, UK
Jan23-Feb23 | *Principal Investigator : Prof. Mihaela van der Saar (Co-advised with Prof. Changhee Lee)*
Supported by SNU OIA : Scholarship for Independent Research Abroad (4,500 $)
- Leading project : Classification of measured features in time-series, having coarse(limited) information about fine-grained class. Especially application for clinical AI.

Dry-lab Drug Discovery
AIGENDRUG Co. Ltd — Seoul, Korea
Jun21-Oct22 | Principal Investigator : Dr. Sunho Lee
Supported by SNU Liberal Education FAC : Scholarship for Undergraduate Independent Research (3,000 $)
- Leading project : Devised a Triangular Area Loss, which integrates three different views about molecule - 1D string, 2D graph, and 3D conformer. SOTA performances on the MoleculeNet benchmark dataset (**Choi MG**, Shin W, Lu Y (2022), "Triangular Contrastive Learning on Molecular Graphs," *arXiv preprint*, arXiv:2205.13279.)
- Participating project : Devised an **Tryptophan-Scanning** algorithm that can predict drug-binding residues via mutating putative residues to tryptophan, **inspired from alanine-screening** method in biochemistry. (Lu Y, Lim S, Park S, **Choi MG**, Jo C, Kim S (in preparation), "EnsDTI-kinase : A Web-server for Ensemble Prediction of Kinase-inhibitor Interactions.")

Wet-lab Prebiotic Chem
Origins of Life Lab — University College London, UK
Jun19-Aug19 | Principal Investigator : Prof. Matthew Powner | Mentor : Jasper Fairchild
Supported by SNU Chemistry Dept : Scholarship for International Undergraduate Research (4,000 $)
- Leading project : Explored and assessed three independent reaction schemes for prebiotic synthesis of homocystamine, a core metabolic intermediate for peptide ligation in water without enzymes.
- Trained in the application of cystamine for **thiol-catalyzed prebiotic peptide ligations in water**.

Wet-lab Synthetic Chem

Stimuli-Responsive Chemical Systems Lab — Seoul National University, Korea
Feb19-Jun19 | Principal Investigator : Prof. Dongwhan Lee | Mentor : Hongsik Kim

- Leading project : Devised a novel synthetic pathway for a geometrically perpendicular organic turn motif, BT[8]DBA, via 8-step organic reactions (Overall yield=2%, 64% per step).
- Introduced new C-N bonds via **C-N Palladium cross-coupling** and SNAr reactions (Yield=30%).
- Obtained needle-shaped crystal of BT[8]DBA by using vapor diffusion method, characterized 106-degree angle between arms and book stack-like packing structure through **X-ray crystallography**.

Wet-lab Biochemistry

Lab of Proteolytic Systems — Seoul National University, Korea
Sep17-Oct18 | Principal Investigator : Prof. Seokhee Kim | Mentor : Dr. Hyunbin Lee
Supported by SNU Natural Science College : Scholoarship for UROP (1,000 $)

- Participating project : Characterized OEPs, a subgroup of Ribosomally Synthesized and Post-translationally modified Peptides (RiPPs) using **HPLC, MALDI-TOF** with Hydrolysis and Methanolysis.
- Independent topic : **Explored four non-natural PTMs** via generating 50 chimeric protein-peptide pairs by substituting enzyme recognition sites using recombinant DNA technique.
- Skilled in biochemistry techniques from DNAs to proteins; this includes **bacterial cloning, E.coli cell culture, His-tag protein purification, and fluorescence assay**.
- Researh outcome : Lee H, **Choi MG**, Park J-U, Roh H, Kim S (2020), "Genome Mining Reveals High Topological Diversity of w-Ester-Containing Peptides and Divergent Evolution of ATP-Grasp Macrocyclases," *Journal of the Americal Chemical Society*, 142(6);3013-3023.

Honors and Awards

Scholarships

S007	2023-	**KFAS**	| 13,000 $/year |	**Doctoral Study Abroad Scholarship (confirmed, five years)**
S006	2023	SNU OIA	| 4,500 $ |	Scholarship for Independent Research Abroad (Cambridge, UK)
S005	2022	SNU FLE	| 3,000 $ |	Scholarship for Undergraduate Independent Research
S004	2016 - 2021	**KOSAF**	| 11,000 $/year |	**Korea Presidential Science Scholarship**
S003	2019	SNU	| 4,000 $ |	Scholarship for International Undergraduate Internship (UCL, UK)
S002	2017 - 2018	SNU	| 1,000 $ /year |	Scholarship for Undergraduate Research Opportunity Program
S001	2015	Hansung	| 3,500 $ |	Scholarship for Talented High-School Students

Awards

A004	2023	Undergraduate Independent Research Award : 3rd Prize | SNU, Faculty of Liberal Education
A003	2019	Undergraduate Research Award : 1st Prize | SNU, Chemistry Dept. and LG Chemical
A002	2018	Undergraduate Research Award : 2nd Prize | SNU, Chemistry Dept.
A001	2015	Samsung HumanTech Paper Award : Silver Prize | 3,500 $ | Samsung Electronics

Skills

Biochem	Bacterial Cloning, PCR, Miniprep, Gel electrophoresis (agarose, SDS-PAGE), Bacterial Cell Culture (*E. Coli*), Protein Purification, Western Blot
Organic	Substitution, Elimination, Aromatic Substitution, **Pd-Coupling**, Prebiotic Peptide Synthesis
Analytic	**MALDI-TOF**, HPLC, NMR, Fluorescence, **X-ray Crystallography** (Protein, Small-molecule)
Software Language	**Python**, C/C++, JAVA, Assembly Language (x86-64), LaTeX
Machine Learning	**PyTorch**, Tensorflow

Other Experiences

Air Operations Manager

Republic of Korea Air Force
September 2019 - June 2021 | Seoul Air Base

- Help planning the operation of aircraft necessary for national events and cooperating with relevant departments, including international events. Supported and developed a scheduler which automatically plans aircraft take-off and landing time, in security environment & language.
- Best Airmans Award (Top 10 in the whole 804th generation), Best Air Traffic Control Award (Top 1 in majoring Air Traffic Control, 804th generation).

Teaching Assistant

General Chemistry
2017-2018 | Seoul National University

- Answered for questions for freshman students in the general chemistry class (2 hours / week).