



## EDUCATION

PhD 2023-	MIT, Massachusetts Institute of Technology, Cambridge Chemistry PhD program. Robert T. Haslam MIT Presidential Fellow (100,000\$) Korea Foundation for Advanced Studies (KFAS) Fellow (13,000 \$/year, 5 years)
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). <ul style="list-style-type: none"> <li>➤ BSc in Chemistry (Major GPA 4.22/4.3) and Computer Science and Engineering (Major GPA 3.83/4.3)</li> <li>➤ 2 years Mandatory Military Leave of Absence : Sep2019-June2021, Republic of Korea Air Force.</li> </ul>

## PUBLICATIONS

Journals	<ul style="list-style-type: none"> <li>- Lim S, Lee S, Piao Y, <b>Choi MG</b>, Bang D, Gu J, Kim S (2022), "On Modeling and Utilizing Chemical Compound Information with Deep Learning Technologies : A Task-oriented Approach," <i>Computational and Structural Biotechnology Journal</i>, 20;4288-4304.</li> <li>- Lee H, <b>Choi MG</b>, 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," <i>Journal of the American Chemical Society</i>, 142(6);3013-3023.</li> </ul>
Preprints	- <b>Choi MG</b> , Shin W, Lu Y (2022), "Triangular Contrastive Learning on Molecular Graphs," <i>arXiv preprint</i> , arXiv:2205.13279.

## RESEARCH HISTORY

Dry-lab Clinical AI	Decision Intelligence Lab Nov22-Jul23   Principal Investigator : Prof. Changhee Lee <ul style="list-style-type: none"> <li>➤ Leading project : Information-theoretically defined time series imputation - <b>Conditional Information Bottleneck (CIB)</b> - and derived its variational approximation, resulting a combination of ELBO and contrastive loss. Conditional Information Bottleneck Approach for Time Series Imputation. Injecting inductive bias using temporal kernels (cauchy, periodic).</li> </ul>	CHUNG-ANG UNIVERSITY, Korea
Dry-lab Clinical AI	Centre for AI in Medicine 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 \$)	CAMBRIDGE UNIVERSITY, UK
Dry-lab Drug Discovery	AIGENDRUG Co. Ltd Jun21-Oct22   Principal Investigator : Dr. Sunho Lee Supported by SNU Liberal Education FAC : Scholarship for Undergraduate Independent Research (3,000 \$) <ul style="list-style-type: none"> <li>➤ 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 (<b>Choi MG</b>, Shin W, Lu Y (2022), "Triangular Contrastive Learning on Molecular Graphs," <i>arXiv preprint</i>, arXiv:2205.13279., Presented at MOGAM AI for Drug Discovery Symposium (Jun 2022)).</li> <li>➤ Devised a <b>Tryptophan-Scanning</b> algorithm that can predict drug-binding residues via mutating putative residues to tryptophan, <b>inspired from alanine-screening</b> method in biochemistry.</li> </ul>	SEOUL, Korea
Wet-lab Prebiotic Chem	Origins of Life Lab Jun19-Aug19   Principal Investigator : Prof. Matthew Powner   Mentor : Jasper Fairchild Supported by SNU Chemistry Dept : Scholarship for International Undergraduate Research (4,000 \$) <ul style="list-style-type: none"> <li>➤ 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.</li> <li>➤ Trained in the application of cystamine for <b>thiol-catalyzed prebiotic peptide ligations in water.</b></li> </ul>	UNIVERSITY COLLEGE LONDON, UK

Wet-lab Synthetic Chem	<b>Stimuli-Responsive Chemical Systems Lab</b> <b>SEOUL NATIONAL UNIVERSITY, Korea</b> Feb19-Jun19   <i>Principal Investigator : Prof. Dongwhan Lee   Mentor : Hongsik Kim</i> <ul style="list-style-type: none"> <li>▶ 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).</li> <li>▶ Introduced new C-N bonds via <b>C-N Palladium cross-coupling</b> and SNAr reactions (Yield=30%).</li> <li>▶ 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 <b>X-ray crystallography</b>.</li> </ul>
Wet-lab Biochemistry	<b>Lab of Proteolytic Systems</b> <b>SEOUL NATIONAL UNIVERSITY, Korea</b> Sep17-Oct18   <i>Principal Investigator : Prof. Seokhee Kim   Mentor : Dr. Hyunbin Lee</i> Supported by SNU Natural Science College : <i>Scholarship for UROP (1,000 \$)</i> <ul style="list-style-type: none"> <li>▶ Participating project : Characterized OEPs, a subgroup of Ribosomally Synthesized and Post-translationally modified Peptides (RiPPs) using <b>HPLC, MALDI-TOF</b> with Hydrolysis and Methanolysis.</li> <li>▶ Independent topic : <b>Explored four non-natural PTMs</b> via generating 50 chimeric protein-peptide pairs by substituting enzyme recognition sites using recombinant DNA technique.</li> <li>▶ Skilled in biochemistry techniques from DNAs to proteins; this includes <b>bacterial cloning, E.coli cell culture, His-tag protein purification, and fluorescence assay</b>.</li> <li>▶ Research outcome : Lee H, <b>Choi MG</b>, 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," <i>Journal of the American Chemical Society</i>, 142(6);3013-3023.</li> </ul>

## HONORS AND AWARDS

### Scholarships

S008	2023 - 2024	MIT	100,000 \$	<b>Robert T. Haslam Fellow</b> (MIT Presidential Fellowship)
S007	2023-	KFAS	13,000 \$/year	<b>Doctoral Study Abroad Scholarship (five years)</b>
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	<b>Korea Presidential Science Scholarship</b>
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 ( <i>E. Coli</i> ), Protein Purification, Western Blot
Organic	Substitution, Elimination, Aromatic Substitution, <b>Pd-Coupling</b> , Prebiotic Peptide Synthesis
Analytic	<b>MALDI-TOF</b> , HPLC, NMR, Fluorescence, <b>X-ray Crystallography</b> (Protein, Small-molecule)
Software Language	Python, C/C++, JAVA, Assembly Language (x86-64), LaTeX
Machine Learning	PyTorch, Tensorflow

## OTHER EXPERIENCES

Teaching Assistant	<b>5.111 Principles of Chemical Science</b> Fall 2023   <i>Massachusetts Institute of Technology, Chemistry Department</i> <ul style="list-style-type: none"> <li>▶ Taking charge of recitation (2 hours / week, 25 undergrads) and holding office hours (2 hours / week).</li> <li>▶ MITx team : editing and managing online problem sets written in Python and HTML.</li> </ul>
Air Operations Manager	<b>Republic of Korea Air Force</b> September 2019 - June 2021   <i>Seoul Air Base</i> <ul style="list-style-type: none"> <li>▶ 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 &amp; language.</li> <li>▶ Best Airmans Award (Top 10 in the whole 804th generation), Best Air Traffic Control Award (Top 1 in majoring Air Traffic Control, 804th generation).</li> </ul>

Teaching Assistant | 034.020 General Chemistry  
2017-2018 | *Seoul National University*  
➤ Answered for questions for freshman students in the general chemistry class (2 hours / week).