



EDUCATION

PhD 2023-	MIT, Massachusetts Institute of Technology, Cambridge <i>Coadvised by Tommi Jaakkola and Regina Barzilay.</i> <i>Robert T. Haslam (1911) MIT Presidential Fellow (100,000\$)</i> <i>Korea Foundation for Advanced Studies (KFAS) Fellow (13,000 \$/year, 5 years)</i>
BS 2016-2023	SNU, Seoul National University, Seoul, Korea <i>Double-major in CHEM/CSE, Summa Cum Laude</i> <i>Supported by Korea Student Aid Foundation (KOSAF), Korea Presidential Science Scholarship (11,000 \$/year).</i> <ul style="list-style-type: none"> ➤ 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

Conferences	<ul style="list-style-type: none"> - Choi MG and Lee C (2023), "Clinical Time Series Imputation using Conditional Information Bottleneck," <i>NeurIPS23 DGM4H (Deep Generative Models for Health) Workshop</i>. - Choi MG, Shin W, Lu Y and Kim S (2023), "Triangular Contrastive Learning on Molecular Graphs," <i>MoML23 : Molecular Machine Learning Conference</i>.
Journals	<ul style="list-style-type: none"> - 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," <i>Computational and Structural Biotechnology Journal</i>, 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," <i>Journal of the American Chemical Society</i>, 142(6);3013-3023.

RESEARCH HISTORY

Dry-lab Clinical AI	Decision Intelligence Lab Nov22-Jul23 <i>Principal Investigator : Prof. Changhee Lee</i> <ul style="list-style-type: none"> ➤ Leading project : Information-theoretically defined time series imputation - Conditional Information Bottleneck (CIB) - 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). 	CHUNG-ANG UNIVERSITY, Korea
Dry-lab Clinical AI	Centre for AI in Medicine Jan23-Feb23 <i>Principal Investigator : Prof. Mihaela van der Saar (Co-advised with Prof. Changhee Lee)</i> <i>Supported by SNU OIA : Scholarship for Independent Research Abroad (4,500 \$)</i>	CAMBRIDGE UNIVERSITY, UK
Dry-lab Drug Discovery	AIGENDRUG Co. Ltd Jun21-Oct22 <i>Principal Investigator : Dr. Sunho Lee</i> <i>Supported by SNU Liberal Education FAC : Scholarship for Undergraduate Independent Research (3,000 \$)</i> <ul style="list-style-type: none"> ➤ 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," <i>arXiv preprint</i>, arXiv:2205.13279., Presented at MOGAM AI for Drug Discovery Symposium (Jun 2022)). ➤ Devised a Tryptophan-Scanning algorithm that can predict drug-binding residues via mutating putative residues to tryptophan, inspired from alanine-screening method in biochemistry. 	SEOUL, Korea
Wet-lab Prebiotic Chem	Origins of Life Lab Jun19-Aug19 <i>Principal Investigator : Prof. Matthew Powner Mentor : Jasper Fairchild</i> <i>Supported by SNU Chemistry Dept : Scholarship for International Undergraduate Research (4,000 \$)</i> <ul style="list-style-type: none"> ➤ 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. 	UNIVERSITY COLLEGE LONDON, UK

Wet-lab Synthetic Chem	Stimuli-Responsive Chemical Systems Lab SEOUL NATIONAL UNIVERSITY, Korea Feb19-Jun19 <i>Principal Investigator : Prof. Dongwhan Lee Mentor : Hongsik Kim</i> <ul style="list-style-type: none"> ▶ 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 <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"> ▶ 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. ▶ Research 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," <i>Journal of the American Chemical Society</i>, 142(6);3013-3023.

HONORS AND AWARDS

Scholarships

S008	2023 - 2024	MIT	100,000 \$	Robert T. Haslam Fellow (MIT Presidential Fellowship)
S007	2023-	KFAS	13,000 \$/year	Doctoral Study Abroad Scholarship (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

Bio	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, 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

Teaching Assistant	5.111 Principles of Chemical Science Fall 2023 <i>Massachusetts Institute of Technology, Chemistry Department</i> <ul style="list-style-type: none"> ▶ Taking charge of recitation (2 hours / week, 25 undergrads) and holding office hours (2 hours / week). ▶ MITx team : editing and managing online problem sets written in Python and HTML.
Air Operations Manager	Republic of Korea Air Force September 2019 - June 2021 <i>Seoul Air Base</i> <ul style="list-style-type: none"> ▶ 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	034.020 General Chemistry 2017-2018 <i>Seoul National University</i> <ul style="list-style-type: none">➤ Answered for questions for freshman students in the general chemistry class (2 hours / week).
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