

# NGOC-QUANG NGUYEN

Ph.D. in Computer Science

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 Home

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## EDUCATION

### Korea University

Ph.D, Computer Science and Engineering, GPA: 93.5%

Sep 2020 - Aug 2024

Advisor: Jaewoo Kang

### Gachon University

MSc, Computer Science and Engineering, GPA: 80.6%

Sep 2017 - Jul 2019

Advisor: Sangwoong Lee

### Vietnam National University, Hanoi

BEng, Mechanical Engineering, GPA: 75.5%

Sep 2012 - Mar 2017

## EXPERIENCE

### AIGEN Sciences Inc.

CSE

Feb 2025 – Present

*Machine learning and AI researcher*

- Conducting molecular dynamics simulations using AI to study protein-ligand interactions, revealing binding mechanisms.
- Delving into the world of drug absorption, distribution, metabolism, excretion, and toxicity.

### DMIS lab

CSE

Sep 2020 – Jan 2025

*Machine learning and AI researcher*

- May 2023 - Dec 2023: Collaborated with **AIGEN Sciences** on predicting compound-protein interactions utilizing multi-level features.
- Mar 2022 - Mar 2023: Collaborated with **SK-Nexilis** on predicting material properties and making recipe recommendation systems.
- Analyzing large-scale datasets from various sources such as biochemical assays such as: BioLiP, PDBbind, DUD\_E, Davis, KIBA, Metz.
- Building multimodal models and algorithms predict protein-compound interactions mainly focusing on multimodal learning.
- Developing models to capture 3D geometric information with Equivariant neural networks.

### Voronoi Inc

CSE

Aug 2019 - Jul 2020

*Machine learning and AI researcher*

- Developed and applied reinforcement learning techniques for small molecule generation with high binding affinity by ReLeaSE (Reinforcement Learning for Structural Evolution).
- Predicted compound properties by the deep directed message passing neural network.
- Predicted compound toxicity by a deep neural network with multitask learning technique.
- Collaborated with biologists, chemists, and other researchers to design experiments, validate predictions, and optimize experimental conditions.

### PRML lab

CSE

Sep 2017 - Jul 2019

*Machine learning and AI researcher*

- Using multi-resolution fusion for medical imaging analysis (image segmentation for seeking lung, colon, and breast tumors).
- Classified the breast cancer histology images using incremental boosting convolution networks.
- Face recognition: automatic door recognition (adopted Google Facenet to make output for Arduino kit to open the lab door) [Here].

### NTQ Solution

ME

Jun 2015 - Sep 2015

*Robotic engineering intern*

- Built a guidance robot using a Raspberry Pi kit, which is controlled by a gaming remote.
- Developed and programmed a quadcopter thesis using an Arduino kit, integrating a radio control system with a transmitter and receiver.

## SELECTED PUBLICATIONS

## *Conference publications*

# PepTri: Tri-Guided All-Atom Diffusion for Peptide Design via Physics, Evolution, and Mutual Information

**ICLR, Rio de Janeiro, Brazil, 2026**

Colorectal segmentation using multiple encoder-decoder network in colonoscopy images

Ngoc-Quang Nguyen; Sang-Woong Lee AIKE, Laguna Hills, USA, 2018

## *Journal publications*

# EquiCPI: SE(3)-Equivariant Geometric Deep Learning for Structure-Aware Prediction of Compound-Protein Interactions

Ngoc-Quang Nguyen; Jaewoo Kang **Journal of Chemical Information and Modeling**, 2025

# MulinforCPI: enhancing precision of compound-protein interaction prediction through novel perspectives on multi-level information integration

**Briefings in Bioinformatics, 2024**

# PerceiverCPI: A nested cross-attention network for compound-protein interaction prediction

Ngoc-Quang Nguyen; Gwanghoon Jang; Hajung Kim; Jaewoo Kang **Bioinformatics, 2023**

# Contour-aware Polyp Segmentation in Colonoscopy Images using Detailed Upsampling Encoder-Decoder Networks

Ngoc-Quang Nguyen; Duc My Vo; Sang-Woong Lee IEEE Access, 2020

# Robust Boundary Segmentation in Medical Images Using a Consecutive Deep Encoder-Decoder Network

Ngoc-Quang Nguyen; Sang-Woong Lee IEEE Access, 2019

# MolPLA: a molecular pretraining framework for learning cores, R-groups and their linker joints

Mogan Gim et al.; Ngoc-Quang Nguyen; Jaewoo Kang **Bioinformatics**, 2024

# Classification of breast cancer histology images using incremental boosting convolution networks

Duc My Vo; Ngoc-Quang Nguyen; Sang-Woong Lee **Information Sciences, 2018**

## SELECTED PROJECTS

### **PepTri (3D, Tri-Guided Diffusion)**, [OpenReview\_Here]

*Duration:* May.2025– Dec.2026

*Project size:* 3–4 members

*Project description:* Development of PepTri, a novel generative framework that jointly produces peptide sequences and 3D structures using a tri-guided diffusion model. This model integrates physics-based structural guidance, evolutionary priors, and mutual information objectives to ensure designs are structurally stable, evolutionarily plausible, and sequence-structure coherent.

*Responsibilities:*

- Research and implement all-atom diffusion models that generate peptide conformations and sequences in a unified SE(3)-equivariant latent space.
- Integrate three guidance signals: (i) differentiable physics constraints for molecular stability, (ii) evolutionary bias toward conserved motifs, and (iii) mutual information maximization between sequence and structure.
- Design and run benchmark evaluations on peptide design datasets such as PepBench, LNR, and PepBDB.
- Analyze binding affinity and structural accuracy improvements over baseline peptide generative models.

*Component neural networks:* Tri-guided diffusion model combining SE(3)-equivariant neural networks, differentiable physics modules, evolutionary embedding modules, and mutual information maximization networks.

### **EquiCPI (3D)**, [Github\_Here]

*Duration:* Dec.2023–Sep.2024

*Project size:* 2 members

*Project description:* Fully leveraging the 3D-generated structures derived from an existing sequence dataset using SE(3) neural networks enhances the accuracy of the CPI task with the help of multimodal techniques.

*Responsibilities:*

- Researching and utilizing the Special Euclidean Group in three dimensions.
- Implementing SE(3) to effectively extract and learn information from 3D structures considering translation, rotation, reflection.

*Component neural networks:* Euclidean neural networks, multiplayer perceptron neural network.

### **MulinforCPI (2,5D)**, [Github\_Here]

*Duration:* Jan.2023–Sep.2023

*Project size:* 3 members

*Project description:* Proposed a two-step deep learning strategy named MulinforCPI (utilizing multi-level information for compound–protein interaction prediction) that incorporates transfer learning techniques along with multi-level resolution features. The aim is to overcome the limitations associated with forecasting the interaction between compounds and proteins.

*Responsibilities:*

- Conducted an analysis of the impact of 3D information with a multimodal fusion technique on the CPI task.
- Designed a cross-cluster validation strategy to comprehensively assess model performance, with a specific emphasis on evaluating its effectiveness in predicting interactions with novel scaffold compounds.
- Proposed and implemented a novel architecture to address the challenge of limited availability of comprehensive and well-structured datasets.

*Component neural networks:*

Principal neighborhood aggregation graph neural network, message passing neural network, multiplayer perceptron neural network, 1D convolutional neural network, 2D convolutional neural network

### **PerceiverCPI (2D)**, [Github\_Here]

*Duration:* Sep.2021–Sep.2022

*Project size:* 3 members

*Project description:* Proposed the Perceiver CPI network, which adopts a cross-attention mechanism to fuse multimodal data for enhancing the representation learning of drug-target interactions. It also leverages information from extended-connectivity fingerprints to improve the performance of binding free energy prediction.

*Responsibilities:*

- Proposed main ideas to overcome the representation's simplification of molecular fingerprints and the current integration methods.
- Implemented the proposed architecture with a directed message-passing neural network and 1DCNN network.
- Analyzed the importance of atom features and bond features.
- Designed the performance evaluation strategies.

*Component neural networks:*

Directed message passing neural network, multiplayer perceptron neural network, 1D convolutional neural network

## 🏆 HONORS & AWARDS

<b>BK21 graduate innovation project scholarship (GAG-KU):</b> [Here]	Feb 2024, BK21FOUR
<b>Excellent paper award:</b> [Here]	Feb 2023, Korea University
<b>Research scholarship:</b> [Here]	Sep 2020 - Sep 2022, BK21FOUR
<b>Foreign natural sciences and engineering scholarship:</b> [Here]	Sep 2020 - Sep 2022, Korea University
<b>Full scholarship covering living expenses and tuition fees</b>	Sep 2017 - Jul 2019, Gachon University

## 🔧 SKILLS AND CERTIFICATES

Exploratory Data Analysis, Statistics, Modeling, Communication.

**Certificates:** AWS Fundamentals [Here], IBM Data Analyst [Here], Google Advanced Data Analytics [Here]

**Others:** Pytorch, Tensorflow, Geometric-pytorch, AWS Unix/Linux, working cross-functionally, GitHub, Gitlab.

**Languages:** English (advanced), Korean (beginner), Vietnamese (native).

## 🔗 REFERENCES

### Prof. Jaewoo Kang, Ph.D.

Address: Korea University, Seoul, Korea.

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Letter of recommendation: upon request

### Prof. Sangwoong Lee, Ph.D.

Address: Gachon University, Gyeonggi, Korea.

Tel: (+82) 3-1750-6918

Email: slee@gachon.ac.kr

Letter of recommendation: [Here]

### Mujeen Sung, PhD.

Address: Kyung Hee university, Gyeonggi, Korea.

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Email: mujeensung@khu.ac.kr

Letter of recommendation: [Here]