

ALIREZA NOROOZI

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RESEARCH INTERESTS

- Peptide and protein binder design; generative models for biological sequences; discrete and insertion–deletion diffusion; evaluation of designed binders with molecular dynamics; protein–ligand cofolding at adaptive resolution.

EDUCATION

Koç University

MSc in Computational Sciences and Engineering

October 2025 – June 2027 (expected)

GPA: 3.48/4.0

Sharif University of Technology

Bachelor of Science in Computer Engineering

September 2020 – June 2024

GPA: 17.32/20 (3.46/4.0)

PUBLICATIONS AND PREPRINTS

- **A. Noroozi**, Ö. Keskin, A. Gürsoy, Y. Karami, and H. Khakzad, **IDPepDesign: Insertion-Deletion is All Peptide Design Needs**, preprint, 2026; ML4SM Workshop, NeurIPS 2026.
- **BinderEval**: evaluating designed protein binders with molecular dynamics data and COMPASS, with the DELTA team, Inria Nancy, preprint, 2026.
- M. Ghasemiagreh and **A. Noroozi**, **BoltzGen-ADC**: Generative Design of Universal Protease-Cleavable Peptide Linkers for Antibody–Drug Conjugates, Merck Challenge submission, July 2026.
- **A. Noroozi**, Ö. Keskin, and A. Gürsoy, **AMP-DiT**: Antimicrobial Peptide Design with AMP-classifier Conditional Diffusion Transformers, GenBio Workshop at ICML 2026 (poster). [paper](#) [code](#)
- M. Kalematis, **A. Noroozi**, A. Shahbakhsh et al., ParaAntiProt provides paratope prediction using antibody and protein language models, *Scientific Reports* 14, 29141 (2024). [link](#)
- J. Reyes, **A. Noroozi**, Y. Xiao, and M. Kersten-Oertel, Bridging the Gaps: Imputation of Parkinson’s Disease Clinical Assessments With Federated Learning, *IEEE Journal of Biomedical and Health Informatics* (2025). [link](#)

RESEARCH EXPERIENCE

DELTA Team, Inria Nancy | *Peptide Binder Design, Molecular Dynamics*

June 2026 – Present

- Research internship under the supervision of Hamed Khakzad and Yasaman Karami
- Developed **IDPepDesign**, a target-conditioned insertion–deletion diffusion model for peptide binder design, built on SCISOR with a pooled target representation injected through denoising and residue-level cross-attention; improved perplexity 17.1 → 11.3 and Fréchet protein distance 1.84 → 0.75, with competitive predicted interface quality across 11 benchmark targets
- Contributed to **BinderEval**, which evaluates designed binders using molecular dynamics data and COMPASS instead of single-structure confidence scores, and released a new version of **COMPASS**
- Invited talk at PhD Pizza Time, Inria Nancy (September 2026)

AMP-DiT, Koç University | *Discrete Diffusion, Generative Modeling*

October 2025 – Present

- Computational Sciences and Engineering; supervised by Prof. Attila Gürsoy and Prof. Özlem Keskin
- Built a conditional discrete diffusion framework that generates antimicrobial peptides directly in sequence space, avoiding the representation mismatch of protein language models trained on full-length proteins
- Used classifier conditioning from Macrel-derived activity and non-hemolytic safety scores; conditioning on a single predictor generalised across multiple AMP predictors, indicating learned antimicrobial features rather than scorer overfitting
- Accepted as a poster at the GenBio Workshop at ICML 2026; submitted to the AMP Challenge

AMP-BindGen, Koç University | *Targeted Binder Design, AMR*

2026 – Present

- Guided design of peptide-like binders and inhibitors against the clinically important carbapenemases **NDM-5** and **KPC-3**, in collaboration with KUISCID and the Koç University School of Medicine
- Designed a composite ranking scheme over interface confidence, catalytic-site engagement, predicted antimicrobial activity and toxicity filters for candidate selection
- Designed peptides have been validated experimentally in the lab, alongside metrics for peptide–protein interaction quality
- Presented as posters at ECCB 2026 (Geneva) and the Koç University AI Symposium

TED, Koç University / 310.ai | *Protein Domain Prediction, CATH Classification*

2024 – Present

- [Project link](#)
- End-to-end sequence-to-sequence transformer that predicts domain boundaries and CATH identifiers directly from sequence, removing the external search tools other methods depend on
- Trained on ~186M unique protein sequences from the TED database with LoRA fine-tuning over ESM-2 embeddings; ran large-scale preprocessing and fine-tuning on GPU clusters

BoltzGen-ADC | *Antibody–Drug Conjugates, Generative Design*

July 2026

- Pipeline over BoltzGen and ADFLIP that designs short protease-cleavable peptide linkers for an arbitrary antibody variable region and small-molecule payload given as isomeric SMILES, without retraining
- Added filters for Fc preservation, protease-cleavage liability, and Boltz-based validation of peptide–protease complexes; demonstrated on brentuximab–MMAE conjugates

Taxonomy Lineage Generation, 310.ai | *Transformers, Protein Language Models*

2024 – 2025

- Built a transformer that generates full taxonomy lineages from protein sequences
- Designed training pipelines, tokenisation strategies, and loss functions to stabilise sequence generation
- Addressed token collapse and improved generalisation with curriculum learning and embedding regularisation

IgG1 Binder Design, 310.ai | *Protein Design, Structural Modeling*

2024 – 2025

- Designed IgG1 antibody binders using generative protein models and sequence design pipelines
- Integrated structural constraints and protein language model embeddings to guide binder specificity and stability

OPL, Sharif University | *Transfer Learning, Antibody, Paratope Prediction*

June 2023 – September 2024

- Department of Computer Engineering; bachelor project under the supervision of Dr. Koohi
- **ParaAntiProt**: transfer learning for paratope prediction from sequence alone
- Improved paratope prediction accuracy using antibody and protein language models; published in *Scientific Reports*

apLab, Concordia University | *Federated Learning, Medical ML*

June 2023 – September 2023

- Department of Computer Science, Montreal, Canada; internship under the supervision of Dr. Kersten-Oertel
- Compared and implemented federated learning algorithms for data imputation on Parkinson’s disease clinical assessments; published in *IEEE JBHI*
- Implemented PW, FedAvg, and FedOpt in PyTorch, including work on a convergence proof for PW
- Developed federated algorithms for non-identically distributed data, and used GANs for prediction from distributed data

OPL, Sharif University | *Attention Models, MHC–Peptide Binding Affinity*

December 2022 – March 2023

- Department of Computer Engineering; bachelor student under the supervision of Dr. Koohi
- MHC–peptide binding prediction using attention mechanisms

TALKS AND POSTERS

- Talk, **PhD Pizza Time**, Inria Nancy, September 2026.
- Posters, **ECCB 2026**, Geneva — AMP-BindGen and AMP-DiT, September 2026.
- Posters, **Koç University AI Symposium**, April 2026 — AMP-BindGen and TED; joint talk on treatment options for carbapenem resistance and AMP design with AI.
- Poster, **GenBio Workshop at ICML 2026** — AMP-DiT.

WORKING EXPERIENCE

310.ai | *AI Engineer in Computational Biology*

September 2024 – October 2025

- Deep learning models for protein design, including taxonomy prediction and binder design pipelines
- Developed an AI chatbot backend using LLM tool calling

Ershan Total Solution | *PHP, Back-end, Web Developer*

June 2022 – September 2022

- Developed a stock trading website using the Laminas framework in PHP
- Built an Excel and PDF generator for all reports

AI Medical | *Deep Learning, Medical Imaging*

June 2021 – September 2021

- Summer internship in machine learning for medical data and medical imaging

Salam High School | *Mathematics Olympiad Tutor*

September 2021 – March 2023

- Taught mathematical olympiad topics (geometry, algebra, combinatorics, number theory)

HONORS

- Awarded the 2025 Presidential Fellowship at Koç University for MSc entrance.
- Awarded the 2024 Vector Scholarship for MSc entrance at York University, valued at 17,500 CAD (deferred).
- Ranked 31st among 150k+ participants in Iran's national university entrance exam in 2020 (Konkur).
- Silver (2019) and Bronze (2018) medals in **Iran's National Mathematical Olympiad**.

REVIEWING

- Reviewer, GenBio Workshop (Generative and Agentic AI for Biology), ICML 2026
- Reviewer, ML4SM Workshop, NeurIPS 2026

TEACHING ASSISTANT EXPERIENCE

- Teaching Assistant, Python Programming, Koç University
- Head of Teaching Assistant Team, Probability and Statistics, 2 semesters (lecturer: Dr. Sharifi-Zarchi)
- Head of Teaching Assistant Team, Compiler Design (lecturer: Dr. Hosseinmardi)
- Projects Head, Teaching Assistant Team, Introduction to Bioinformatics
- Teaching Assistant, Discrete Structures and Basic Programming in Python

TECHNICAL SKILLS

- **Languages:** Python, C++, JavaScript, PHP
- **Machine learning:** PyTorch, Hugging Face, scikit-learn, distributed and multi-GPU training, SLURM clusters
- **Structural biology:** Boltz, BoltzGen, ADFLIP, AlphaFold-class predictors, RFdiffusion, ESM-2/ESM-C, ProtT5, Biopython, molecular dynamics analysis
- **Other:** Git, Docker, Linux

LANGUAGE PROFICIENCY

- Persian: Native
- English: Fluent, TOEFL (T: 97, R: 26, L: 25, S: 25, W: 21)