

CURRICULUM VITAE

Gyu Rie Lee

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WORK EXPERIENCE

2023. 01 – present Research Specialist I, University of Washington and Howard Hughes Medical Institute, Advisor: David Baker
2022. 07 – 2023. 01 Acting instructor, University of Washington, Advisor: David Baker
2018. 02 – 2022. 06 Postdoctoral scholar, University of Washington, Advisor: David Baker
2017. 03 – 2018. 01 Postdoctoral researcher, Seoul National University, Advisor: Chaok Seok

EDUCATION

2011. 09 – 2017. 02 Ph.D. in Physical Chemistry, Seoul National University, Advisor: Chaok Seok
- Thesis: Development of protein modeling methods for structure refinement in the context of unreliable environments
2007. 03 – 2011. 08 B.S. in Chemistry Education, Seoul National University (*Cum Laude*)

RESEARCH INTERESTS

- Machine learning-assisted computational design and experimental screening of functional proteins; small-molecule binding proteins, enzymes, peptide binding proteins, design of protein-protein interfaces.
- Developing and utilizing deep-learning models for protein-ligand complex structure, function prediction, and sequence design.
- Development of systems for biological application using de novo designed proteins:
 - Sensors and biologics based on chemical induced dimerization
 - Detection of post-translational modifications
- Generating synthetic data using computational protein design for activity guided learning.

PUBLICATIONS

- **G. R. Lee**, C. Norn, I. Anischenko, [...], D. Baker, De novo design of biotin-binding proteins, *manuscript in preparation*
- **G. R. Lee** (co-first), S. J. Pellock, C. Norn, A. H-W. Yeh, [...], D. Baker, De novo design of small-molecule binders enables sensor development, *manuscript in preparation*
- J. Dauparas, **G. R. Lee**, R. Pecoraro, L. An, [...], D. Baker, LigandMPNN: backbone conditional protein sequence design with atomic context, *manuscript in preparation*
- R. Krishna, J. Wang, W. Ahern, P. Sturmfels, **G. R. Lee**, P. Venkatesh, I. Kalvet, [...], D. Baker, Generalized biomolecular modeling and design with RoseTTAFold all-atom, *manuscript in preparation*
- C. J. Glasscock, R. Pecoraro, R. McHugh, [...], **G. R. Lee**, [...], D. Baker, Computational design of sequence-specific DNA-binding proteins, *submitted*

- S. Mansoor, M. Baek, H. Park, **G. R. Lee**, D. Baker, Protein Ensemble Generation through Variational Autoencoder Latent Space Sampling, *bioRxiv* 2023.08.01.551540 (2023).
- H.-W. Yeh, C. Norn, Y. Kipnis, D. Tischer, S. J. Pellock, D. Evans, P. Ma, **G. R. Lee**, J. Z. Zhang, I. Anishchenko, [...], K. N. Houk & D. Baker, De novo design of high activity and specificity luciferases using deep learning, *Nature*, 614, 774–780 (2023).
- S. Vázquez Torres, P. J. Y. Leung, I. D. Lutz, P. Venkatesh, J. L. Watson, F. Hink, H.-H. Huynh, A. H.-W. Yeh, D. Juergens, N. R. Bennett, A. N. Hoofnagle, E. Huang, M. MacCoss, M. Expòsit, **G. R. Lee**, P. M. Levine, X. Li, M. Lamb, E. N. Korkmaz, [...], D. Baker, De novo design of high-affinity protein binders to bioactive helical peptides, *Nature*, *in press*
- S. Lee, S. Kim, **G. R. Lee**, H. Woo, C. Seok & H. Park, Evaluating GPCR modeling and docking strategies in the era of deep learning-based protein structure prediction, *Computational and Structural Biotechnology Journal*, 21, 158-167 (2023).
- M. Baek, F. Dimaio, I. Anishchenko, J. Dauparas, S. Ovchinnikov, **G. R. Lee**, J. Wang, Q. Cong, L. N. Kinch, [...], D. Baker, Accurate prediction of protein structures and interactions using a three-track neural network, *Science*, 373(6557):871-876 (2021).
- L. An and **G. R. Lee**, De novo protein design using the blueprint builder in Rosetta, *Current Protocols in Protein Science*, 102(1):e116 (2020).
- H. Park, **G. R. Lee**, D. E. Kim, I. Anishchenko, Q. Cong, D. Baker, High-accuracy refinement using Rosetta in CASP13, *Proteins: Structure, Function, and Bioinformatics*, 87(12):1276-1282 (2019).
- **G. R. Lee**, J. Won, L. Heo, and C. Seok, GalaxyRefine2: Simultaneous refinement of inaccurate local regions and overall protein structure, *Nucleic Acids Res.*, 47, Web Server issue W451–W455 (2019).
- I. Bang, H. R. Kim, A. H. Beaven, J. Kim, S. Ko, **G. R. Lee**, H. Lee, W. Im, C. Seok, K. Y. Chung, H.-J. Choi, Biophysical and functional characterization of Norrin signaling through Frizzled4, *Proc. Natl. Acad. Sci.*, 115 (35), 8787-8792 (2018).
- C. Keasar et al. (**G. R. Lee**, C. Seok) An analysis and evaluation of the WeFold collaborative for protein structure prediction and its pipelines in CASP11 and CASP12, *Sci. Rep.*, 8:9939 (2018).
- J. Won, **G. R. Lee**, H. Park, and C. Seok, GalaxyGPCRloop: Template-Based and Ab Initio Structure Sampling of the Extracellular Loops of G-Protein-Coupled Receptors, *J. Chem. Inf. Model*, 58 (6), 1234-1243 (2018).
- **G. R. Lee**, L. Heo, and C. Seok, Simultaneous refinement of inaccurate local regions and overall structure in the CASP12 protein model refinement experiment, *Proteins: Structure, Function, and Bioinformatics*, 86 (S1), 168-176 (2018).
- X. Shao, H. Kang, T. Loveless T, **G. R. Lee**, C. Seok, W. I. Weis, H. J. Choi, and J. Hardin, Structural and functional characterization of the α -catenin- β -catenin binding interface in *Caenorhabditis elegans* reveals conserved requirements for cell-cell adhesion in metazoans, *J. Biol. Chem.*, *in press* (2017).
- Q. Xu, Q. Tang, P. Katsonis, O. Lichtarge, D. T. Jones, S. Bovo, G. Babbi, P. L. Martelli, R. Casadio, **G. R. Lee**, C. Seok, A. Fenton, R. L. Dunbrack, Jr, Benchmarking predictions of allostery in liver pyruvate kinase in CAGI4, *Human Mutation*, *in press* (2017).
- H. Lee, M. Baek, **G. R. Lee**, S. Park, and C. Seok, Template-based modeling and ab initio refinement of protein oligomer structures using GALAXY in CAPRI Round 30, *Proteins: Structure, Function, and Bioinformatics*, 85, 399–407 (2017).
- **G. R. Lee** and C. Seok, Galaxy7TM: Flexible GPCR-ligand docking by structure refinement, *Nucleic Acids Res.* 44 (W1), W502-506 (2016).
- M. F. Lensik et al. (**G. R. Lee**, C. Seok), Prediction of homo- and hetero-protein complexes by protein docking and template-based modeling: a CASP-CAPRI experiment, *Proteins: Structure, Function, and Bioinformatics*, 84 (S1), 323-348 (2016).
- W. -H. Shin, **G. R. Lee**, and C. Seok, Evaluation of GalaxyDock based on the Community Structure-

Activity Resource 2013 and 2014 Benchmark Studies, *J. Chem. Inf. Model*, 56 (6), 988-995 (2016).

- **G. R. Lee**, L. Heo, and C. Seok, Effective protein model structure refinement by loop modeling and overall relaxation, *Proteins: Structure, Function, and Bioinformatics*, 84 (S1), 293-301 (2016).
- H. Park, **G. R. Lee** (co-first author), L. Heo, and C. Seok, Protein loop modeling using a new hybrid energy function and its application to modeling in inaccurate structural environments, *PLoS ONE* 9 (11): e113811 (2014).
- W. -H. Shin, **G. R. Lee**, L. Heo, H. Lee, and C. Seok, Prediction of Protein Structure and Interaction by GALAXY protein modeling programs, *Bio Design*, 2 (1), 1-11 (2014).
- **G. R. Lee**, W. Shin, H. Park, S. Shin, and C. Seok, Conformational sampling of flexible ligand-binding protein loops, *Bull. Korean Chem. Soc.* 33 (3), 770-774 (2012).

ORAL PRESENTATIONS

- “Towards generalizable design of de novo small-molecule binders using deep learning”, RosettaCon2023, August 9th, 2023.
- “Re-engineering ORs: Identification and Interrogation of Odorant Receptors in Bio-Hybrid Systems for Disease Detection”, Decoding Olfaction Convening organized by Bill & Melinda Gates foundation, March 9th, 2023.
- “Xe Sensing via Insights from Noble Gas-Protein Interactions”, 2019 DTRA Life Sciences Technical Review meeting, July 16, 2019.
- “Automatic protein structure refinement with an improved energy function and diverse sampling of unreliable regions”, CASP12 meeting, Refinement category round table, December 11, 2016.
- “Galaxy7TM: a web server for flexible GPCR-ligand docking”, The 118th Korean Chemical Society Meeting, October 13, 2016.
- “Predicting allosteric regulation using GALAXY protein modeling programs”, CAGI4 conference, March 25, 2016.

HONORS AND AWARDS

- Washington Research Foundation Innovation Postdoctoral Fellowship (2018. 02-)
- Best poster presentation award, Korean Society for Structural Biology (2017)
- Best poster presentation award, The 16th KIAS Conference on Protein Structure and Function, KIAS (2016)
- Scholarship for the Next Generation of Academics in Basic Research, Seoul National University (2015. 03 - 2017. 02)
- CASP11 Conference Participation Fellowship (financial supports of the participation in CASP11 meeting) (2014)
- Best poster presentation award, The 13th KIAS Conference on Protein Structure and Function, KIAS (2013)
- Best poster presentation award, 2013 Structure Festival, Korean Society for Structural Biology (2013)
- Best poster presentation award, The 12th KIAS Conference on Protein Structure and Function, KIAS (2012)
- Best presentation award, The 11th KIAS Protein Folding Winter School, KIAS (2012)
- Best poster presentation award, The 11th KIAS Conference on Protein Structure and Function, Korea Institute for Advanced Study (KIAS) (2011)

