Sun Choi

CMI-P-22

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Research Keywords

AI and computer-aided drug design, Computational medicinal chemistry, Drug discovery

Academic Career

[Academic and Professional Career]
• Assistant, Associate, Professor, College of Pharmacy and Graduate School of Pharmaceutical Sciences, Ewha Womans University (2005-present)
• Department Chair, Department of Pharmacy,College of Pharmacy, Ewha Womans University (2015-2017)
• Director, “Global AI Drug Discovery Center” (2020-present)
• Fellow, the Korean Academy of Science and Technology (FKAST) (2024-present)
• American Chemical Society ‘ACS Medicinal Chemistry Letters’ Associate Editor (2023-present)
• Council Member, the Asia Pacific Protein Association (APPA) (2025-present)
• Postdoctoral Fellow, Department of Chemistry and the Drug Discovery Program, Northwestern University, USA (1997-2001)
• Molecular Modeler / Computational Chemist, Tripos, Inc., USA (2001-2005)

[Leadership and Service to the Scientific Community]
• Presidential Advisory Council on Science and Technology, Chair of the Expert Committee on Life Sciences and Medicine (2021-2024)
• National Supercomputing Committee Member, Ministry of Science and ICT (2019-2021)
• President, the Korean Biophysical Society (KBPS) (2022-2024)
• President, the Korean Society for Protein Science (KSPS) (2018-2019)

Selected Publications

"GolpHCat (TMEM87A), a unique voltage-dependent cation channel in Golgi apparatus, contributes to Golgi-pH maintenance and hippocampus-dependent memory” H. Kang, A. Han, A. Zhang, ... S. Choi*, H. M. Kim*, and C. J. Lee*, Nat. Commun. 2024, 15, 5830.

"Employing Automated Machine Learning (AutoML) Methods to Facilitate the In Silico ADMET Properties Prediction” H. Han†, B. Shaker†, J. H. Lee†, S. Choi†, S. Yoon†, ..., S. Kang, M. S. Yeom*, and S. Choi*, Journal of Chemical Information and Modeling, 2025, 65(7), 3215-3225.

“Dynamic allosteric networks drive adenosine A1 receptor activation and G-protein” M.A.M. Solano*, S. Choi*, eLife, 2023, 12(3), 31a.

“GPCR Agonist-to-Antagonist Conversion: Enabling the Design of Nucleoside Functional Switches for the A2A Adenosine Receptor” A. Shiriaeva, D. Park, G. Kim, Y. Lee, ... L. S. Jeong*, S. Choi*, and V. Cherezov*, J. Med. Chem. 2022, 65(17), 11648-11657 (Cover).

"Subtle Chemical Changes Cross the Boundary between Agonist and Antagonist: New A3 Adenosine Receptor Homology Models and Structural Network Analysis Can Predict This Boundary," Y. Lee, X. Hou, J. H. Lee, A. ... K. A. Jacobson, S. Choi*, and L. S. Jeong*, J. Med. Chem. 2021, 64(17), 12525-12536 (Cover).

"N-terminus-independent activation of c-Src via binding to a tetraspan(in) TM4SF5 in hepatocellular carcinoma is abolished by the TM4SF5 C-terminal peptide application," H. E. Song, Y. Lee, ... S. Choi*, J. W. Lee*, Theranostics, 2021, 11(16), 8092-8111.

"Transmembrane 4 L Six Family Member 5 Senses Arginine for mTORC1 Signaling" J. W. Jung, S. J. Y. Macalino, M. Cui, J. E. Kim, H. J. Kim, D. G. Song, S. H. Nam, S. Kim, S. Choi*, J. W. Lee*, Cell Metabolism 2019, 29(6), 1306-1319.

"In Vivo Albumin Traps Photosensitizer Monomers from Self-Assembled Phthalocyanine Nanovesicles: A Facile and Switchable Theranostic Approach" X. Li, ... J.-D. Huang*, S. Choi*, K. T. Nam*, and J. Yoon*, J. Am. Chem. Soc. 2019, 141(3), 1366-1372 (Cover).

Why My Lab?

My lab can offer...

The research work in the Choi group is focused on Artificial Intelligence (AI)/Computer-Aided Drug Design (CADD) and drug discovery, molecular modeling, cheminformatics and computational medicinal chemistry. Using computational methods, we develop strategies for drug discovery involving cancer, virus, cardiovascular disease, neuropathic pain, etc.

In-silico technologies, such as molecular modeling, CADD and virtual screening, when used in conjugation with experimental methods, significantly reduce the time and money required for drug discovery. Based on multiple disciplines required for drug discovery, the Choi group is involved in several international, active collaborations and scientific exchanges.

Based on the high-quality and extensive research outcomes, we are continuously publishing articles in world-renowned journals, such as Nature Communications, Cell Metabolism, Journal of the American Chemical Society, Angewandte Chemie, Journal of Medicinal Chemistry, and Theranostics, etc. It was selected as the National Leading Research Laboratory (NLRL) funded by the Korean government, and has engaged in active research activities, leading the Global AI Drug Discovery Center.

[Research Areas]
- Computer-Aided Drug Design (CADD) Methods and Applications, including Docking
- Protein-Ligand Interaction & their Mechanism of Action Studies
- Molecular Design, Combinatorial Library Design, Virtual Screening
- Drug Discovery Research for Various Diseases in Cell Signaling
- Biomolecular Simulations: Protein Motion and Allostery
- Theoretical Studies of Enzymatic & Chemical Reactions
- Big Data Analysis and Artificial Intelligence (AI)-based Drug Discovery