

Mengrong Li

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EDUCATION

Nanjing Agricultural University, Nanjing, Jiangsu, China	2019.09-2023.09
College of Life Sciences	PhD: Biochemistry and Molecular Biology
Henan Normal University, Xinxiang, Henan, China	2016.09-2019.06
College of Aquaculture	M.S: Aquiculture
Nanning Normal University, Nanning, Guangxi, China	2012.09-2016.06
College of Environmental and Life Sciences	B.S: Biological Science

SKILLS

Familiarity with the theory and application of molecular dynamics simulations

Research Interests: Computational structural biology, protein dynamics, modeling and docking, molecular dynamics simulation, enhanced sampling, allosteric regulation, allosteric modulators

PROJECT & RESEARCH EXPERIENCE

Postgraduate Research & Practice Innovation Program of Jiangsu Province 2021.4-2022.3

PUBLICATIONS

1. **Li M.**, Bao Y, Xu R, Li M, Xi L, Guo J*. Understanding the allosteric modulation of PTH1R by a negative allosteric modulator. *Cells*. 2023, 12, 41.
2. **Li M.**, Bao Y, Li M, Zhang Y, Liu H, Guo J*. GPCR allostery: a view from computational Biology. *Curr Med Chem*. 2023, 30, 4533–4553.
3. **Li M.**, Bao Y, Xu R, Zhang X, La H, Guo J*. Mechanism of enhanced sensitivity of mutated β -adrenergic-like octopamine receptor to amitraz in honeybee *Apis mellifera*: An insight from MD simulations. *Pest Manag Sci*. 2022, 78, 5423–5431.
4. **Li M.**, Li M, Guo J*. Molecular mechanism of Ca^{2+} in the allosteric regulation of human parathyroid hormone receptor-1. *J Chem Inf Model*. 2022, 62, 5110–5119.
5. **Li M.**, Bao Y, Xu R, La H, Guo J*. Critical extracellular Ca^{2+} dependence of the binding between PTH1R and a G-protein peptide revealed by MD simulations. *ACS Chem Neurosci*. 2022, 13, 1666–1674.
6. Guo J*, **Li M.**, Zhang Y, Xi L, Cui F. Conformational dynamics is critical for the allosteric inhibition of cGAS upon acetyl-mimic mutations. *Phys Chem Chem Phys*. 2021, 23, 2154–2165.

* corresponding authorship

PERSONAL INTERESTS

- Exercise such as walking or going to the gym
- Reading books, articles and publications
- Travelling and meeting new people

HONORS & AWARDS

- National scholarship for doctoral students
- Outstanding graduates
- Triple-A outstanding student