

Evaluation of the unbinding kinetics of Mineralocorticoid (MR) receptor steroid agonist Cortisol (COL) , Aldosterone (AS4), and Progesteron (STR) ligands

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Abstract

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References

- [1] Chantal Hellal-Levy, Jérôme Fagart, Anny Souque, and Marie-Edith Rafestín-Oblin. Mechanistic aspects of mineralocorticoid receptor activation. *Kidney International*, 57(4):1250–1255, 2000.
- [2] Marie-Edith Rafestín-Oblin, Anny Souque, Brigitte Bocchi, Gregory Pinon, Jerome Fagart, and Alain Vande-walle. The Severe Form of Hypertension Caused by the Activating S810L Mutation in the Mineralocorticoid Receptor Is Cortisone Related. *Endocrinology*, 144(2):528–533, 02 2003.
- [3] David S. Geller, Anita Farhi, Nikki Pinkerton, Michael Fradley, Michael Moritz, Adrian Spitzer, Gretchen Meinke, Francis T. F. Tsai, Paul B. Sigler, and Richard P. Lifton. Activating mineralocorticoid receptor mutation in hypertension exacerbated by pregnancy. *Science*, 289(5476):119–123, 2000.
- [4] Jérôme Fagart, Jessica Huyet, Grégory M. Pinon, Marina Rochel, Claudine Mayer, and Marie-Edith Rafestín-Oblin. Crystal structure of a mutant mineralocorticoid receptor responsible for hypertension. *Nature Structural & Molecular Biology*, 12(6):554–555, Jun 2005.
- [5] K. Belfon I.Y. Ben-Shalom J.T. Berryman S.R. Brozell D.S. Cerutti T.E. Cheatham III G.A. Cisneros V.W.D. Cruzeiro T.A. Darden R.E. Duke G. Giambasu M.K. Gilson H. Gohlke A.W. Goetz R. Harris S. Izadi S.A. Izmailov K. Kasavajhala M.C. Kaymak E. King A. Ko-valenko T. Kurtzman T.S. Lee S. LeGrand P. Li C. Lin J. Liu T. Luchko R. Luo M. Machado V. Man M. Manathunga K.M. Merz Y. Miao O. Mikhailovskii G. Monard H. Nguyen K.A. O’Hearn A. Onufriev F. Pan S. Pantano R. Qi A. Rahnamoun D.R. Roe A. Roitberg C. Sagui S. Schott-Verdugo A. Shajan J. Shen C.L. Simmerling N.R. Skrynnikov J. Smith J. Swails R.C. Walker J. Wang J. Wang H. Wei R.M. Wolf X. Wu Y. Xiong Y. Xue D.M. York S. Zhao D.A. Case, H.M. Aktulga and P.A. Kollman (2022). *Amber 2022*. University of California, San Francisco.
- [6] Yinglong Miao, Apurba Bhattarai, and Jinan Wang. Ligand gaussian accelerated molecular dynamics (ligamd): Characterization of ligand binding thermodynamics and kinetics. *Journal of Chemical Theory and Computation*, 16(9):5526–5547, 2020. PMID: 32692556.
- [7] Yinglong Miao, Apurba Bhattarai, and Jinan Wang. Ligand gaussian accelerated molecular dynamics (ligamd): Characterization of ligand binding thermodynamics and kinetics. *bioRxiv*, 2020.
- [8] Heloisa dos Santos Muniz and Alessandro S. Nascimento. Ligand- and receptor-based docking with libela. *Journal of Computer-Aided Molecular Design*, 29(8):713–723, Aug 2015.
- [9] Pablo R. Arantes, Marcelo D. Polêto, Conrado Pedebos, and Rodrigo Ligabue-Braun. Making-it-rain, August 2021.
- [10] Matthew M. Copeland, Hung N. Do, Lane Votapka, Keya Joshi, Jinan Wang, Rommie E. Amaro, and Yinglong Miao. Gaussian accelerated molecular dynamics in openmm. *The Journal of Physical Chemistry B*, 126(31):5810–5820, 2022. PMID: 35895977.
- [11] Jinan Wang, Pablo R. Arantes, Apurba Bhattarai, Rohaine V. Hsu, Shristi Pawnikar, Yu-ming M. Huang, Giulia Palermo, and Yinglong Miao. Gaussian accelerated molecular dynamics: Principles and applications. *WIREs Computational Molecular Science*, 11(5):e1521, 2021.
- [12] Geraldo Rodrigues Sartori and Alessandro S. Nascimento. Comparative analysis of electrostatic models for ligand docking. *Frontiers in Molecular Biosciences*, 6, 2019.
- [13] Heloisa S. Muniz and Alessandro S. Nascimento. Towards a critical evaluation of an empirical and volume-based solvation function for ligand docking. *PLOS ONE*, 12(3):1–19, 03 2017.
- [14] Tamar Schlick. *Molecular Modeling and Simulation: An Interdisciplinary Guide*, volume 21 of *Interdisciplinary Applied Mathematics*. Springer New York, NY, Berlin, Heidelberg, 2 edition, August 2010.
- [15] A.R. Leach. *Molecular Modelling: Principles and Applications*. Prentice Hall, 2 edition, 2001.