Numerical simulations of proteins

Ramirez Palacios, Carlos

DOI:
10.33612/diss.196789826

List of publications

- Souza, P. C. T.; Thallmair, S.; Conflitti, P.; **Ramírez-Palacios, C.**; Alessandri, R.; Raniolo, S.; Limongelli, V.; Marrink, S. J. Protein–Ligand Binding with the Coarse-Grained Martini Model. *Nat Commun* **2020**, *11* (1), 3714. https://doi.org/10.1038/s41467-020-17437-5.
- Meng, Q.; **Ramírez-Palacios, C.**; Capra, N.; Hooghwinkel, M. E.; Thallmair, S.; Rozeboom, H. J.; Thunnissen, A.-M. W. H.; Wijma, H. J.; Marrink, S. J.; Janssen, D. B. Computational Redesign of an ω-Transaminase from *Pseudomonas jessenii* for Asymmetric Synthesis of Enantiopure Bulky Amines. *ACS Catal.* **2021**, *11*, 10733–10747. https://doi.org/10.1021/acscatal.1c02053.
- **Ramírez-Palacios, C.**; Wijma, H. J.; Thallmair, S.; Marrink, S. J.; Janssen, D. B. Computational Prediction of ω-Transaminase Specificity by a Combination of Docking and Molecular Dynamics Simulations. *J. Chem. Inf. Model.* **2021**, *61* (11), 5569–5580. https://doi.org/10.1021/acs.jcim.1c00617.
- **Ramírez-Palacios, C.** Super High-Throughput Screening of Enzyme Variants by Spectral Graph Convolutional Neural Networks. *Thesis chapter, and manuscript in preparation*. **2021**
- **Ramírez-Palacios, C.** Binary Classification of Molecular Dynamics Trajectories using Neural Networks. *Thesis chapter*. **2021**
- Yakovlieva, L.; **Ramírez-Palacios, C.**; Marrink, S. J.; Walvoort, M. T. C. Semiprocessive Hyperglycosylation of Adhesin by Bacterial Protein N-Glycosyltransferases. *ACS Chem. Biol.* **2021**, *16* (1), 165–175. https://doi.org/10.1021/acschembio.0c00848.
- Marjanovic, A.; **Ramírez-Palacios, C. J.**; Masman, M. F.; Drenth, J.; Otzen, M.; Marrink, S.-J.; Janssen, D. B. Thermostable D-Amino Acid Decarboxylases Derived from *Thermotoga maritima* Diaminopimelate Decarboxylase. *Protein Engineering, Design and Selection* **2021**, *34* (gzab016). https://doi.org/10.1093/protein/gzab016.
- Dong, L.; Meng, Q.; **Ramírez-Palacios, C.**; Wijma, H. J.; Marrink, S. J.; Janssen, D. B. Asymmetric Synthesis of Optically Pure Aliphatic Amines with an Engineered Robust ω-Transaminase. *Catalysts* **2020**, *10* (11), 1310. https://doi.org/10.3390/catal10111310.