

Publication List

Juan Francisco Carrascoza Mayén, Ph.D.

Institute of Computing Science, Poznań University of Technology
European Centre of Biology and Informatics (ECBiG), Polish Academy of Sciences

ORCID: 0000-0003-4311-5951

Peer-Reviewed Journal Articles

1. **Carrascoza, F.**, Lukasiak, P., Nowak, W., & Blazewicz, J. (2023). Ab Initio Study of Glycine Formation in the Condensed Phase: Carbon Monoxide, Formaldimine, and Water Are Enough. *Life*, *13*(10), 2023.
2. **Carrascoza, F.**, & Silaghi-Dumitrescu, R. (2022). The dynamics of hemoglobin-haptoglobin complexes: Relevance for oxidative stress. *Journal of Molecular Structure*, *1250*(1), 131829.
3. **Carrascoza, F.**, Antczak, M., Miao, Z., Westhof, E., & Szachniuk, M. (2022). Evaluation of the stereochemical quality of predicted RNA 3D models in the RNA-Puzzles submissions. *RNA*, *28*(3), 250–262. <https://doi.org/10.1261/rna.078685.121>
4. **Carrascoza, F.**, Brânzanic, A.M.V., & Silaghi-Dumitrescu, R. (2021). The dynamics of hemerythrin and hemerythrin derivatives. *Studia Universitatis Babeş-Bolyai Chemia*, *66*(4), 77–88.
5. **Carrascoza Mayén, J.F.**, & Błażewicz, J. (2020). Recent Results on Computational Molecular Modeling of The Origins of Life. *Foundations of Computing and Decision Sciences*, *45*(1), 21–40.
6. **Carrascoza, F.**, Surducan, M., Eriksson, L.A., & Silaghi-Dumitrescu, R. (2020). Interaction of cobalt and iron hydroperoxo bleomycin with deoxyribonucleic acid (DNA): Dynamic vs. electronic structure considerations. *Inorganica Chimica Acta*, *509*, 119682. <https://doi.org/10.1016/j.ica.2020.119682>
7. **Carrascoza Mayén, J.F.**, Rydzewski, J., Szostak, N., Blazewicz, J., & Nowak, W. (2019). Prebiotic Soup Components Trapped in Montmorillonite Nanoclay Form New Molecules: Car-Parrinello Ab Initio Simulations. *Life*, *9*(2), 46. <https://doi.org/10.3390/life9020046>
8. **Carrascoza Mayén, J.F.**, Lupan, A., Cosar, C., Kun, A.-Z., & Silaghi-Dumitrescu, R. (2015). On the roles of the alanine and serine in the β -sheet structure of fibroin. *Biophysical Chemistry*, *197*, 10–17. <https://doi.org/10.1016/j.bpc.2014.11.001>
9. **Carrascoza, F.**, Zarić, S.D., & Silaghi-Dumitrescu, R. (2014). Computational study of protein secondary structure elements: Ramachandran plots revisited. *Journal of Molecular Graphics and Modelling*, *50*, 125–133. <https://doi.org/10.1016/j.jm gm.2014.04.001>
10. Lupan, A., Kun, A.-Z., **Carrascoza, F.**, & Silaghi-Dumitrescu, R. (2013). Performance comparison of computational methods for modeling alpha-helical structures. *Journal of Molecular Modeling*, *19*(1), 193–203. <https://doi.org/10.1007/s00894-012-1531-z>

Publication Summary

- **Total peer-reviewed publications (2013–2023):** 10
- **First-author publications:** 8
- **Publications since 2019:** 7
- **Research areas:** Quantum molecular dynamics, *ab initio* molecular dynamics, prebiotic chemistry, RNA structure prediction, QM/MM methods, protein structure, computational biochemistry

Key Research Contributions

Origins of Life & Prebiotic Chemistry:

- Glycine formation mechanisms in condensed phase (2023)
- Car-Parrinello AIMD simulations of montmorillonite nanoclay catalysis (2019)
- Computational molecular modeling review for origins of life (2020)

Structural Biology & Bioinformatics:

- RNA 3D structure prediction quality assessment (RNA-Puzzles, 2022)
- Protein secondary structure computational analysis (2014, 2015)
- β -sheet structures in oligopeptides and fibroin (2004, 2015)

Metalloprotein Dynamics & Drug Mechanisms:

- Bleomycin-DNA interactions via QM/MM dynamics (2020)
- Hemoglobin-haptoglobin complex dynamics (2022)
- Hemerythrin and spin-labeled derivatives (2021)

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