

Hair Keratin Molecular Dynamics Studies

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The keratin is a key element of the hair, nails and skin in vertebrates. Understand the keratin features such its assembling in the mentioned structures, its interactions with some compounds or mechanical properties is of great interest in the fight against some diseases or in the development and optimization of cosmetic products.

Although molecular dynamics (MD) simulations provides unique information at molecular level in a dynamic way, there are only a few studies using this technique on the study of keratin. This is likely the result of the nonexistence of full length keratin crystallographic model. In the few published works the authors had to design and build the computational keratin model to perform the simulations of interest.

This work addresses some MD studies about hair keratin, from the physicochemical properties of the molecular models to the correlation of the simulations results with experimental data.

Our work on this field, with recently developed computational models of hair fibers, is also discussed. We built MD models able to reproduce in simulations some phenomena observed in experimental assays, providing important information at molecular level about the mechanisms that lead to the experimental results.

References

- [1] Antunes, E., Cruz, C. F., Azoia, N. G., Cavaco-Paulo, A. The effects of solvent composition on the affinity of a peptide towards hair keratin: experimental and molecular dynamics data, *RSC Adv.* 5, 12365–12371, 2015.
- [2] Antunes, E., Cruz, C. F., Azoia, N. G., Cavaco-Paulo, A. Insights on the mechanical behavior of keratin fibrils, *International Journal of Biological Macromolecules*, 89, 477-483, 2016.