# Keratin Molecular Dynamics Models

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## Abstract

The keratin is a key element of the hair, nails and skin in vertebrates. Understand the keratin features such as its assembling in the mentioned structures, its interaction 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.

Molecular dynamics modelling is the only technique able to provide information at atomic and molecular level in a dynamic way, which can greatly help in the study of these features. However there are only a few studies using molecular dynamics simulations. This is likely to the non-existence of full length crystallographic structure models of keratin. In the few works published about keratin using molecular dynamics simulations the authors had to design and build the computational keratin model, to make the simulations of interest.

This work addresses the different keratin models developed, from its physicochemical properties to the correlation of the simulations results with experimental data. One big computational model of a truncated protofibril (8 chains of keratin), which was able to predict the increase of peptide absorption by hair shaft in response to alcohol based formulations, is also discussed.