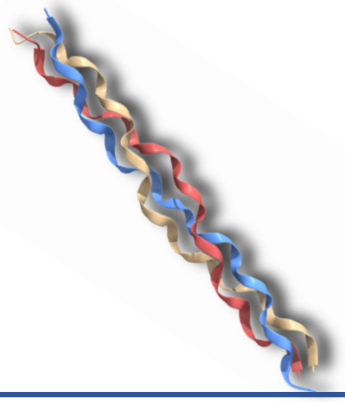
Computational engineering of novel collagen-mimetic biomaterials



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Background: Collagen is the most abundant protein in the human body, forming the structural framework for tissues such as skin, bones, tendons, and ligaments. It can self-assemble into highly organized fibrillar structures, which help maintain the integrity and function of these tissues. Hence, collagen serves as a foundational template for the development of novel biomaterials with applications in tissue engineering, wound healing and regenerative medicine.

Rationale: Understanding the interplay between collagen structure, chemical modifications, and self-assembly is essential for advancing both fundamental science and the development of novel biomaterials.

Goals:

- Understand the impact of mutations on collagen self-assembly
- Develop a novel collagen-mimetic biomaterial

Research questions

1. What is the impact of chemical modification in the collagen structure and dynamics?
2. What are the aggregation mechanisms of collagen-mimetic peptides?

Research approaches

1. Molecular dynamics simulations
2. Parametrization of non-natural residues
3. Close collaboration with experimental colleagues for validation (with UTwente)

Literature

G. Giubertoni et al. Elucidating the role of water in collagen self-assembly by isotopically modulating collagen hydration, PNAS, 121, e2313162121 (2024)