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Title: Collagen Type I Fibril Assembly

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Abstract: Many previous works have tried to shed light on collagen self-assembly and its distinct D- periodicity. However, despite this effort, a complete understanding of this phenomenon has yet to be developed. In this work, we look at this problem through computational means. We first develop various molecule designs from

Type I collagen, which are smaller and suited for efficient computations. Following that, we ran various Molecular Dynamics sim- ulations to test these designs for fibril assembly. Gaining insights from these, we develop an artificial molecule that can show periodic assembly. Furthermore, we look at the amino acid sequence of various types of collagen α chains to understand the role of amino acid distribution in the assembly process. Ultimately, we lay out a plan to further

investigate this periodic feature.

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