

Proposal for the Development of Bio-Based Hybrid Molecules: Exploring Molecular Dynamics for Coloring and Preservation of Molecules

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Introduction

Despite the considerable progress in the field of food additives, the controversy in which some of them are still involved has encouraged research into the next generation of safer and healthier counterparts. These additives can come from natural sources and confer health benefits beyond coloring or preserving, among others. Issues of stability, sustainability, and cost-effectiveness are often related limiting factors that justify the need for innovative solutions.¹

Non-covalent complexation is a natural process and an important mechanism responsible for the stabilization and enhancement of blue, violet, and red colors in flowers, vegetables, and fruits. In this context, copigmentation with antioxidant/antimicrobial molecules can be explored, and the development of unique dual-function hybrid compounds, with the support of new cheminformatics tools and models, predicting and verifying experimental results, could culminate in the next generation of food additives.²

Methodology

Molecular dynamics (MD) simulations were performed considering the crossover of several natural molecules, used as colorants, against natural antioxidants. The initial positioning of the molecules was performed with Packmol, so that each atom of the molecules was at least 10 Å away from the edge of the periodic box. The system minimizations were performed using the Sander program from the AMBER18 software package; for the equilibrium and production phases, PMEMD was used; the subsequent analysis was performed using CPPTRAJ, and the calculation of the ΔG association by MM-GBSA. All from the AMBER18 software package (**Fig. 1**).

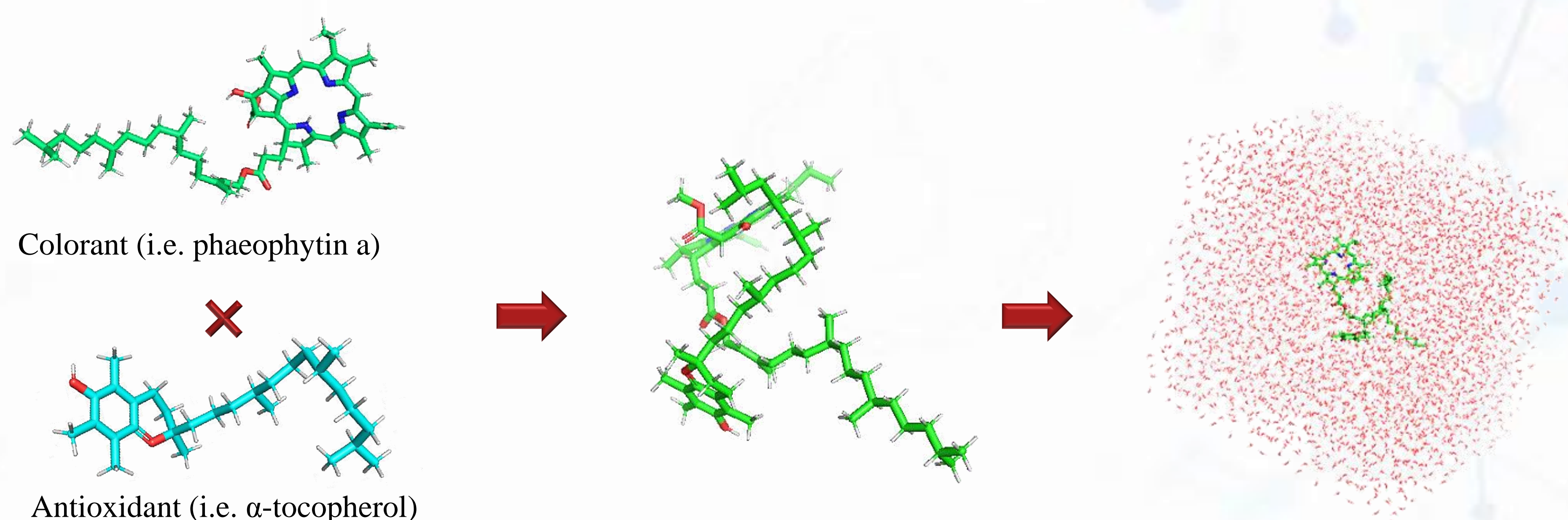


Fig. 1. Illustration of the preparation steps and the crossing scheme used, for the studied molecules.

Results

The preservative/colorant crossover with the lowest predicted ΔG values was α -tocopherol/phaeophytin *a*, followed by natamycin/phaeophytin *a* (**Fig. 2**).

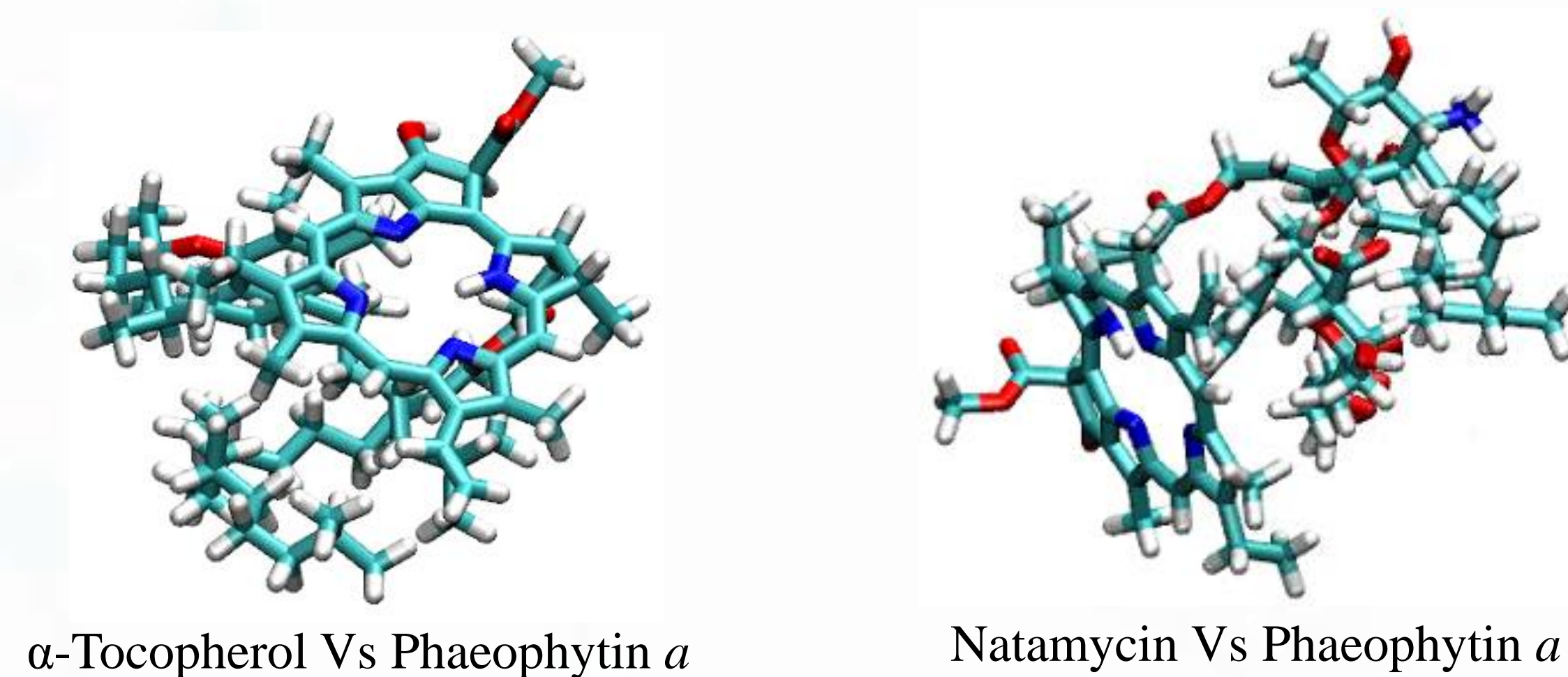


Fig. 2. Pictures from the visualization of the MD simulation, with the VMD software.

References

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2. V.D. Paramita, S. Kasapis, *Food Hydrocoll.* 88 (2019) 301–319.

Conclusions and Perspectives for Future Works

The results are quite interesting and promising, supporting the possibility of exploring the hybridization between phaeophytin *a*, as colorant, and α -tocopherol, as preservative, as well as between phaeophytin *a* and the preservative natamycin. A next step will involve performing and optimizing molecular hybridization protocols and testing the dual functionality of the hybrids.