Exploring Molecular Dynamics for the Development of Bio-based Hybrid Molecules With Applications in Coloring and Preservation

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Introduction

Although substantial progress has been made in food additives, ongoing controversies surrounding some of them have driven research into the next generation of safer and healthier options. These additives can come from natural sources and confer health benefits beyond coloring or preserving, among others. However, issues of stability, sustainability, and cost-effectiveness often constitute limiting factors, highlighting the need for innovative solutions.[1]

Non-covalent complexation is a natural process and a crucial mechanism for stabilizing and enhancing blue, violet, and red colors in flowers, vegetables, and fruits. In this context, copigmentation with antioxidant and antimicrobial molecules can be explored. New cheminformatics tools and models can be used to support the development of unique dual-function hybrid compounds by predicting and verifying experimental results in order to develop new bio-based molecules as the next generation of food additives.[2]

Metodology

Molecular dynamics (MD) simulations were conducted to evaluate the interaction between several natural molecules, used as colorants, and two natural antioxidants (ascorbic acid and α-tocopherol) by calculating their binding affinity (ΔG). System minimizations were performed using the Sander program from the AMBER18 software package. For the equilibrium and production phases, PMEMD was used, followed by analysis using CPPTRAJ, both from the AMBER18 software package (**Fig. 1**).

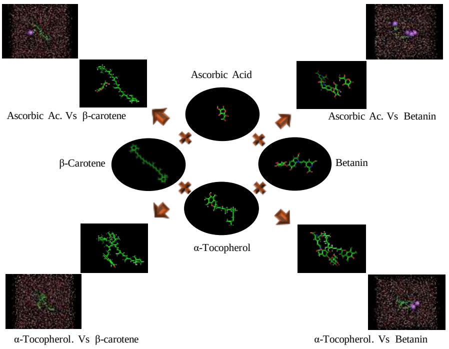

Fig. 1. Example of molecules evaluated and illustration of the preparation steps and crossing scheme used.

Results

Table 1. Average ΔG (kcal/mol) resulting from MD simulations of the crossings between molecules.

Preservatives / Colorants	Ascorbic Acid (E300)	α-Tocopherol (E307)
Curcumin (E100)	0,16 ± 0,02	-10,02 ± 0,11
Betanin (E162)	0,65 ± 0,03	-6,00 ± 0,10
β-Carotene (E160a)	0,21 ± 0,02	-8,30 ± 0,11

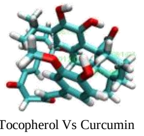

Fig. 2. Picture from the visualization of the MD simulation, with the VMD software.

Among all colorants, the interaction with the antioxidant showing the highest average ΔG was α-tocopherol, particularly notable in the case of curcumin (-10.02). For ascorbic acid, the ΔG values were around zero.

Conclusions and Perspectives for Future Work

Based on these results, further studies will be performed to assess the potential hybridization between the curcumin molecule and α-tocopherol, as also the effectiveness of the hybrid as a dual-function additive.

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References

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The mission and scientific challenge of this poster are aligned with Agenda 2030, specifically: the development of sustainable high-tech production systems for obtaining bio-based hybrid molecules with storage stability and high quality, ensuring food security and human nutrition (G2); recycling of agri-food waste and valorization of ugly/unsellable fruits/vegetables, reducing food losses along production and supply chains and enabling sustainable production and consumption (G12); and benefiting ecosystems and local populations through the promotion of sustainable exploitation of mountain crops (G15).

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