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Achieving the Sustainable  
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## EXPLORING MOLECULAR DYNAMICS FOR THE DEVELOPMENT OF BIO-BASED HYBRID MOLECULES WITH APPLICATIONS IN COLORING AND PRESERVATION

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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].

For that purpose, molecular dynamics (MD) simulations were conducted to evaluate the interaction between several natural molecules, used as colorants, and two natural antioxidants (ascorbic acid and  $\alpha$ -tocopherol) by calculating their binding affinity ( $\Delta G$ ). 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. Among all colorants, the interaction with the antioxidant showing the highest average  $\Delta G$  was  $\alpha$ -tocopherol, particularly notable in the case of curcumin (-10.02). For ascorbic acid, the  $\Delta G$  values were around zero. Based on these results, further studies will be performed to assess the potential hybridization between the curcumin molecule and  $\alpha$ -tocopherol, as also the effectiveness of the hybrid as a dual-function additive.

**Keywords:** Natural food additives, Colorants, Preservatives, Copigmentation, Molecular dynamics.

### References

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