BIO-SUSTENTABILIDADE E BIO-SEGURANÇA ALIMENTAR, INOVAÇÃO E QUALIDADE ALIMENTAR

23-26 de outubro de 2022

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XVI ENCONTRO DE QUÍMICA DOS ALIMENTOS

Bio-based hybrid molecules for coloring and preservative purposes

Novais C,[1,2] Molina AK,[1] Abreu RMV,[1] Santos-Buelga C,[2] Ferreira ICFR, [1] Pereira C,[1*] Barros L[1]

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The increasing urgency to feed the growing world population, along with growing consumer awareness and expectations, have driven the evolution of food production systems and the processes and products applied in the food industry. Although substantial progress has been made in food additives, the controversy in which some of them are still embroiled has encouraged research into the next safer and healthier generations. These additives can come from natural sources and confer health benefits, in addition to serving to color or preserve, among others.[1] Limiting factors of these additives are often related to stability, sustainability, and cost-effectiveness issues, which justify the need for innovative solutions. Finding compounds that can have both capabilities (colorant and preservative) and additionally exert bioactive functions may be a promising solution. However, to obtain benefits such as antioxidant or antimicrobial activity, the concentrations of these compounds are often high, not meeting the acceptable daily intake (ADI) requirement. In addition, such compounds may take time to become part of the additives authorized for use by regulators, remembering that in addition to the research for these new molecules, they must undergo thorough toxicity and safety evaluation before their use is allowed for consumption.[2]

The research and development of new molecules through new chemical approaches, such as the modification of natural molecules already known and of accepted use worldwide, so that they can develop a better and double performance (colorant plus preservative), may be a path to be followed to circumvent the difficulties and monetize the use of these additive molecules in the food industry. Non-covalent complexation is a natural process and an important mechanism responsible for stabilizing and enhancing the blue, violet, and red colors in flowers, vegetables, and fruits, as well as in food products derived from them. The increased interest in copigmentation has been remarkable, especially by the food industry, in order to enhance the color palette. In view of its mastery and use through the selection of the better copigments to be added to food products, precise (computer-aided) control of the supramolecular assemblies of non-covalent supramolecular copigments is essential. In this regard, copigmentation with antioxidant/antimicrobial molecules can be explored, and the use of new cheminformatics tools and models can support the development of unique hybrid compounds with dual function (coloring and preserving), based on the screening of numerous biomolecules so as to spawn new bio-based molecules as the next generation of food additives.[3]

In this regard, and with the observed advances in computers and computational methodologies for *in silico* experimental aid, their exploitation for the research and development of these safer and more efficient bio-based hybrid molecules with dual functionality by predicting and verifying the experimental results, allow the study of certain physical characteristics that are not easily examined in the laboratory and are very promising, which can help and accelerate research on a topic that is now fundamental.

Acknowledgements: The authors are grateful to the Foundation for Science and Technology (FCT, Portugal) for financial support through national funds FCT/MCTES to CIMO (UIDB/00690/2020); national funding by F.C.T. and P.I., through the institutional scientific employment program-contract for C.P. and L.B. contracts and C.N. (2021.05369.BD) and A.K.M. (2020.06231.BD) PhD grants. To FEDER-Interreg España-Portugal programme for financial support through the project TRANSCoLAB 0612_TRANS_CO_LAB_2_P; to ERDF through the Regional Operational Program North 2020, within the scope of Project Mobilizador Norte-01-0247-FEDER-024479: ValorNatural®. The GIP-USAL is financially supported by the Spanish "Ministerio de Ciencia and Innovación" (PID2019-106167RB-I00) and "Junta de Castilla y León" (SA093P20 and CLU-2018-04).

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1. N. Martins, C.L. Roriz, P. Morales, L. Barros, I.C.F.R. Ferreira, Trends Food Sci. Technol. 53 (**2016**) 1–15.
2. F.C.O.L. Martins, M.A. Sentanin, D. De Souza, Food Chem. 272 (**2019**) 732–750.
3. V.D. Paramita, S. Kasapis, Food Hydrocoll. 88 (**2019**) 301–19.

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The increasing urgency to feed the growing world population, along with growing consumer awareness and expectations, have driven the evolution of food production systems, processes and products applied in the food industry. Although substantial progress has been made in food additives, the controversy in which some of them are still embroiled has encouraged research into the next safer and healthier generations.

Additives from natural sources, in addition to coloring or preserving, may also confer health benefits, however, they are often related to stability, sustainability, and cost-effectiveness issues, which justify the need for innovative solutions.[1]

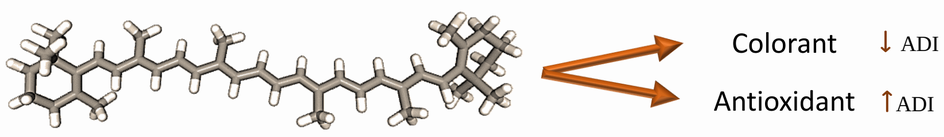

Fig.1. β-Caroten, example of a molecule with dual capacity.

Finding compounds that can have both capabilities (colorant and preservative) and additionally exert bioactive functions may be a promising solution. However, to obtain benefits such as antioxidant or antimicrobial activity, their concentrations of are often high, not meeting the acceptable daily intake (ADI) requirement (Fig.1). In addition, such compounds may take time to become part of the additives authorized for use by regulators, which, in addition to their research, they must undergo thorough toxicity and safety evaluation before their use is allowed for consumption.[2]

The research and development of new molecules through new chemical approaches, such as the modification of natural molecules already known and of accepted use worldwide (Fig.2), so that they can develop a better and double performance (colorant plus preservative), may be a path to be followed to circumvent the difficulties and monetize the use of these additive molecules in the food industry.

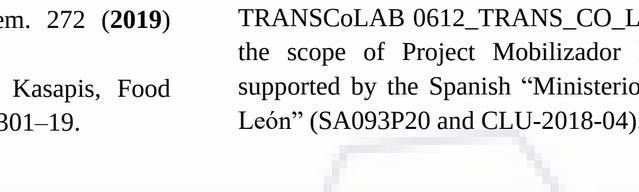

Fig.2. Example of additives approved by EFSA with different functions: a) Curcumin, colorant; and b) γ-Tocopherol, antioxidante.

Non-covalent complexation is a natural process and an important mechanism responsible for stabilizing and enhancing the blue, violet, and red colors in flowers, vegetables, and fruits, as well as in food products derived from them. The increased interest in copigmentation has been remarkable, especially by the food industry, in order to enhance the color palette.

In view of its mastery and use through the selection of the better copigments to be added to food products, precise (computer-aided) control of the supramolecular assemblies of non-covalent supramolecular copigments is essential (Fig.3). In this regard, copigmentation with antioxidant/antimicrobial molecules can be explored, and the use of new cheminformatics tools and models can support the development of unique hybrid compounds with dual function (coloring and preserving), based on the screening of numerous biomolecules so as to spawn new bio-based molecules as the next generation of food additives.[3]

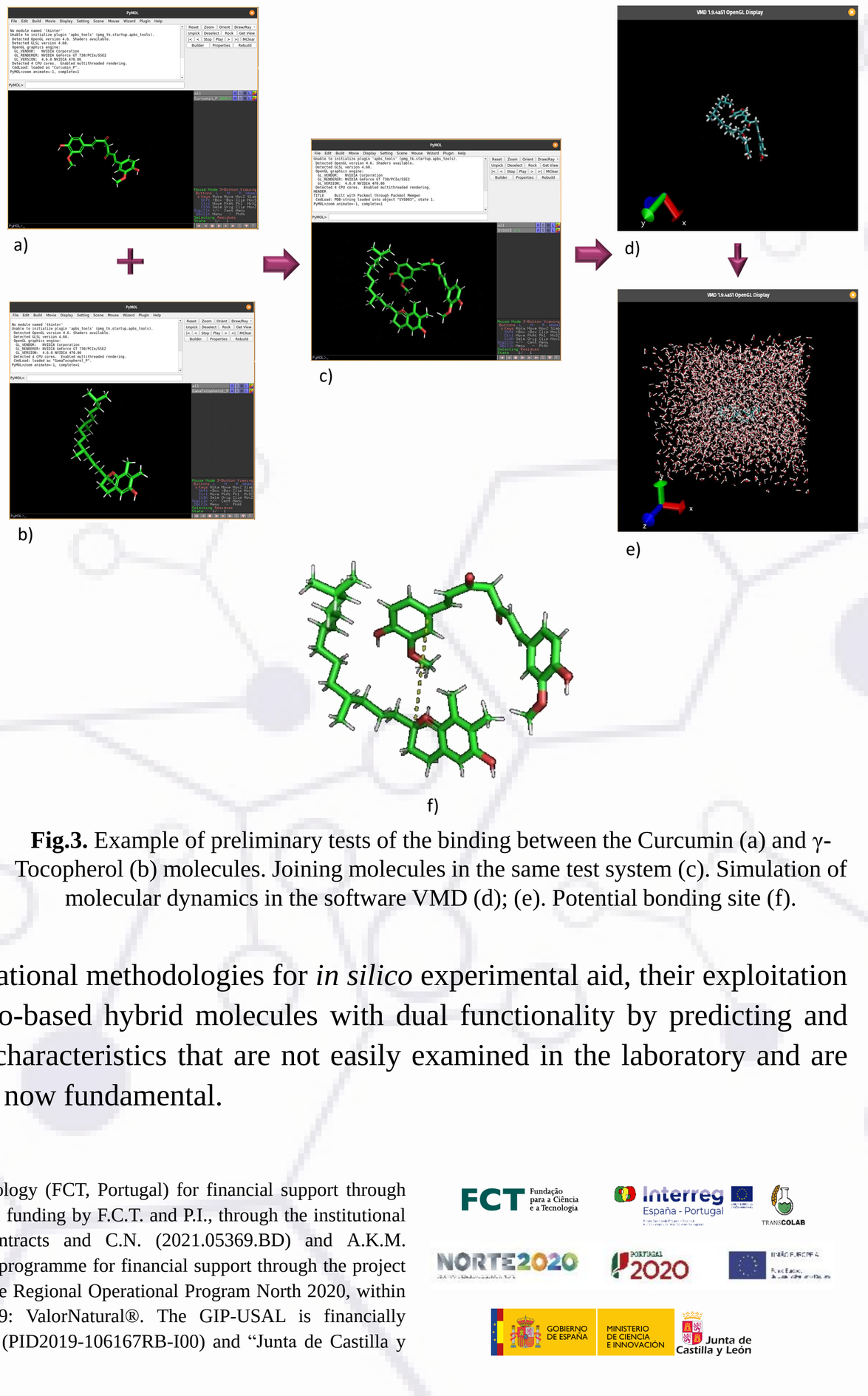

Fig.3. Example of preliminary tests of the binding between the Curcumin (a) and γ-Tocopherol (b) molecules. Joining molecules in the same test system (c). Simulation of molecular dynamics in the software VMD (d); (e). Potential bonding site (f).

In this regard, and with the observed advances in computers and computational methodologies for *in silico* experimental aid, their exploitation for the research and development of these safer and more efficient bio-based hybrid molecules with dual functionality by predicting and verifying the experimental results, allow the study of certain physical characteristics that are not easily examined in the laboratory and are very promising, which can help and accelerate research on a topic that is now fundamental.

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no/a XVI Encontro de Química dos Alimentos - na IPCB - Castelo Branco, de 23 a 26 outubro 2022

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