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QUALITY BY DESIGN APPROACH USED IN DEVELOPMENT OF NOVEL CRYSTALLINE FOOD PACKAGING MATERIALS

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Food waste is an issue of importance to global food security and good environmental governance, directly linked to environmental, economic and social impacts. In the EU, an estimated 20% of the total food produced is lost or wasted, while 43 million people cannot afford a quality meal every second day [1].
Currently, all the actors of the food chain (farmers, food manufacturers, retailers and consumers) are involved in preventing and reducing food waste. A way to reduce food waste can be related to the increase of the shelf-life of food as a result of improving the package type. An interesting approach to prevent food deterioration is the incorporation of antioxidants or antimicrobial agents in the packaging. Essential oils (EOs) are natural ingredients produced from plants with known antibacterial, antiviral, antifungal and insecticide properties [2] commonly used to this purpose. The aim of this study was to extend the use of natural products for packaging applications with cocrystallization. A further aim was to apply a Quality by Design (QbD) approach to optimize the inhibition of selected microorganisms involved in food deterioration. Even though cocrystals are largely known among the scientific community, their use has not systematically moved beyond pharmaceutical applications [3,4]. Cocrystals are multicomponent solid crystalline materials made by different chemical entities (i.e. the main ingredient and the coformer) with a given stoichiometric ratio. The presence of the conformer in the structure induces changes in the chemical environment of the EO in the solid providing a stable intermolecular network. The structure of a crystalline compound determines many fundamental physical properties of the material, and in the case of EOs, cocrystallization increases the melting point of the material thus inducing the stabilization of a liquid ingredient in a solid form. This is a really important matter since liquid or low-melting point compounds are not useful for industrial applications.
Our attention was focused on eugenol, carvacrol, cinnamaldehyde and thymol, which are mainly liquid at room temperature, thus requiring a way to stabilize them into the solid state to produce plastic films characterized by antimicrobial properties. New cocrystals were synthetized to tune the oil release profile at different environmental conditions (room temperature and refrigerated conditions), thus investigating their antibacterial properties

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against microorganisms commonly detected in fruit and vegetables and comparing the achieved results with those of the pure oils.

Since data deriving from time kill assays (TKA) revealed that the required broad antimicrobial effect could be achieved only by using a mixture of the investigated EOs, a QbD approach was used to optimize the simultaneous inhibition of the selected microorganisms. QbD is a science- and risk-oriented quality paradigm [5] based on multivariate tools, which could facilitate process, product or method development and could lead to important advantages in terms of gained knowledge and risk management. QbD was applied for in-depth investigating the effect of critical parameters (CPs), represented by the concentration values of the selected EOs in a mixture, on critical attributes (CAs) related to the percentage of inhibition of the selected microorganisms. A Face Centered Design was used for estimating the coefficients of the quadratic models that correlate the CPs with the CAs; contour plots were drawn, allowing significant interactions and quadratic effects to be evidenced. A target value for the CAs was set and Monte-Carlo simulations were used to draw probability maps, showing how the CPs settings could be varied around a selected set-point, still guaranteeing an adequate level of probability that the desired requirements for all the CAs are fulfilled. This multidimensional optimum zone, identified as the Design Space, represents the core of QbD approach and is defined in terms of variation range of each CP under study. The design space was validated by a Plackett-Burman design and the obtained results showed that in every verification point the complete inhibition of all the considered bacteria was observed. Finally, the optimized packaging was characterized in terms of release of EOs and increased shelf-life of fruit and vegetable samples.

References

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