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Configuring material properties by crystal engineering

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Crystal engineering is a powerful tool to design materials with high technological added value to address health and environment protection through mild and nature friendly components and methods. Some compounds relevant to human health and nutrition are liquid at ambient conditions (L-API); widely known examples are propofol, vitamin E, nicotine, and terpenoids and phenolic derivatives used as natural antioxidants such as carvacrol, eugenol, eucalyptol, and valproic acid. A practical way to manufacture some of these compounds in a solid dosage form is to modify their molecular structures by synthetic derivatization, or to turn them into salts, provided that the molecule may be reacted with a convenient acid or base, and that these are acceptable from a regulatory point of view. However, not all the molecules may become salts, and derivatization may alter molecular bioavailability. Recently, cocrystallization has proven to be a powerful method to control the release of liquid ingredients in the environment, thanks to the engineering of ad hoc intermolecular interactions which strengthen or weaken the tendency of the ingredient to be retained inside the solid matrix. [1-2]. Similarly, L-API have been encapsulated within adaptable cavities of Metal Organic Frameworks purposely designed to uptake such guests; the evolution in time of the supramolecular arrangement of the nano-confined guests in the cavities has been monitored by SCXRD and related to the observed selectivity of the material towards different L-API guests [3-4].

We here present some proofs of concept that a rational design of crystalline materials such as MOFs and cocrystals capable to store and release L-API guests is feasible (Figure 1), and that the release profile can be related to the solid state arrangement of the material, offering a strong and rational tool to afford a vast range of materials capable of controlled release of L-APIs.

References

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Figure 1.

