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Cocrystallization as effective tool for driving the release of natural active compounds

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The use of pesticides for chemical treatment of plants and soil is still an alarming issue since contributes to the accumulation of harmful by-products in the environment [1]. Some of most sustainable and effective alternatives have been found in essential oil (EOs), which are natural compounds based on terpenoids and directly produced by plants. EOs have been shown antibacterial, antifungal and insecticide effects, but their physical properties, such as low melting point and high volatility, have limited their application in agrochemical industry.
Cocrystallization has proved to be a practical solution for tuning the physical properties of EOs [2], giving new crystalline materials with an enhanced thermal stability and able to deliver the active compounds in a more prolonged way. Cocrystals are indeed multi-component crystalline compounds obtained by the interaction of two or more different molecules, called coformers, in a defined stoichiometric ratio. However, the coformers often have just played a rule of "co-builders" of a new crystalline scaffold, remaining their molecular properties untapped for further applications [3].
The purpose of this work is thus to exploit cocrystallization to drive the release of EOs and control their availability. We here report an example of cocrystal, prepared through a mechanochemical reaction, where the release of the active component is triggered by an external stimulus and monitored along the time. To this end, X-ray powder diffraction (XRPD) and UV-vis measurements were performed before and after the triggering and were compared between the individual conformer and its cocrystal. Raman spectra were also collected using micro-focused laser on single crystals samples. At last, physical properties of the cocrystal and coformer were opportunely described by calorimetric measurements (DSC) and further characterized with single crystal X-ray diffraction (SCXRD).

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