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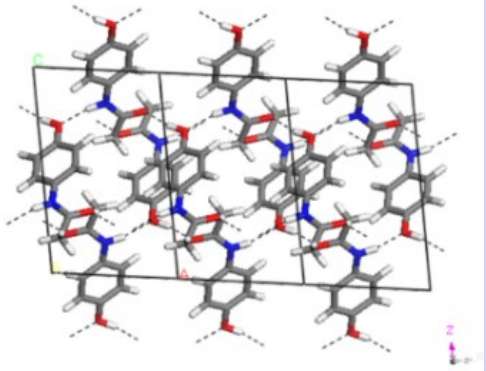
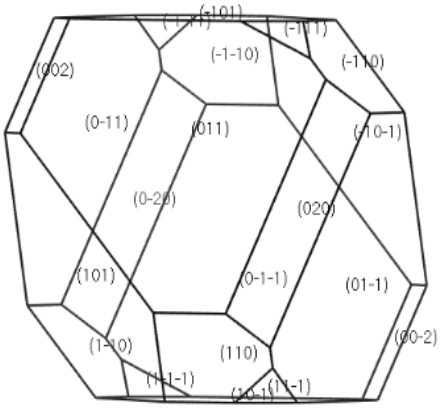
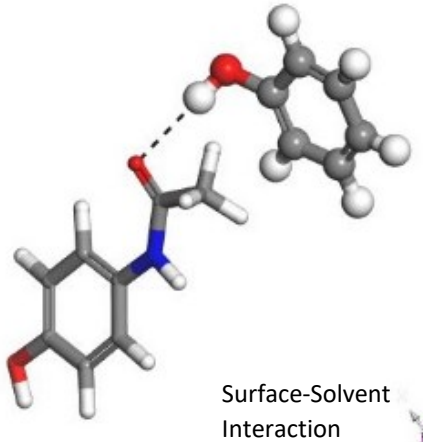
Tailoring Crystal Morphology of Paracetamol Using a Computational Approach



Paracetamol



Crystal Morphology



Surface-Solvent Interaction

Crystal shape, or morphology, plays a critical role in pharmaceuticals. Unwanted crystal shapes can create challenges in manufacturing processes like filtration, flowability and compressibility. This ultimately affects the final product's quality, including its dissolution rate and stability. This research tackles the challenge of predicting and controlling crystal morphology during crystallisation processes by modifying solvents. The unique aspect lies in using computational approach to analyse interactions between solvents and specific crystal surfaces of paracetamol. The findings revealed that the solute-solvent interactions can be dominated by non-bonded interactions, such as van der Waals forces, electrostatic forces, and hydrogen bonds, depending on the solvents used. This is due to the nature of the solvent functional groups, whose strength of interaction with paracetamol surfaces determines the preferential growth of certain surfaces, ultimately influencing the overall crystal shape.

Notably, the findings aligned with observed crystal morphology, i.e., prism-shaped crystals, when using a specific solvent, highlighting the accuracy of the approach. Such findings aid in achieving precise control over morphology, which is crucial for pharmaceutical development. This also provides a powerful tool for researchers to engineer desired crystal shapes to avoid downstream manufacturing failure issues, potentially leading to drugs with optimised dissolution rates, bioavailability, and stability. This translates to improved drug efficacy and potentially fewer side effects, impacting patient health and treatment outcomes. This research paves the way for a more rational design of crystallisation processes in pharmaceutical manufacturing. Beyond immediate drug development, the approach could be applied to other materials where crystal morphology is critical, such as pigments, catalysts, and functional materials. This opens doors for innovation in various scientific and technological fields.

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