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Computational Research into Pharmaceutical Crystals

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Message from the Guest Editors

Pharmaceutical solids can be either amorphous, exhibiting only close-range orders, or characterized by molecular arrangements displaying long-range orders in all directions (crystalline) or in one or two directions (liquid crystals). Further, solid drugs can be classified as single or multicomponent compounds, such as crystalline solvates (including solid hydrates), cocrystals and salts. Variations of pharmaceutical solid forms can result in alternations of the physicochemical properties of a drug product, which, as a consequence, may affect drug effectiveness, safety and processing. The physical and chemical properties of solid-state APIs, resulting from the arrangement of molecules in the solid state, are related to their stability, solubility, bioavailability and formulatability. Therefore, the possibility to accurately predict and describe those properties using molecular modeling methods is both interesting, from the purely scientific point of view, but also of a great practical importance in the pharmaceutical industry.

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Message from the Editor-in-Chief

Welcome to *Crystals*, the journal dedicated to the fascinating world of crystallographic research! Crystals are more than mere decorative elements; they hold the key to understanding the fundamental structure of matter. Our mission is to explore the crucial significance of this research across various fields. From medicine to technology, chemistry to geology, crystals play a vital role. Their structure provides insights into new advanced materials, innovative drugs, and groundbreaking technologies. Through *Crystals*, we delve into the microscopic world to discover solutions that will shape the future. Join us on a journey through the *Crystals*, where science merges with beauty and innovation.

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