

## Special Issue

# Computational and Experimental Approaches in Pharmaceutical Crystals

### Message from the Guest Editors

It is well known as solid-state analysis plays a key role in the study of compounds of pharmaceutical interest. In fact, it helps to understand a multiplicity of phenomena like polymorphism and pseudo-polymorphism, intermolecular interactions, solvation and desolvation et.al. On the other hand, an experimental approach alone may sometimes not be sufficient to deeply rationalize particular behavior of a pharmaceutical compound; in this case, the possibility to perform theoretical calculations is of great importance.

In addition to this, a computational approach may help in the design of compounds having desired properties, this kind of analysis is of fundamental importance for the crystal engineering of well performing APIs (Active pharmaceutical ingredients).

The special issue on “Computational and Experimental Approach in Pharmaceutical Crystals” is intended to cover both the fields of design and solid-state analysis, by an experimental and computational point of view, of compounds of pharmaceutical interest.

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### Guest Editors

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### Deadline for manuscript submissions

closed (16 December 2022)



## Crystals

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## About the Journal

### 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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### Editor-in-Chief

Prof. Dr. Alessandra Toncelli  
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