

Marta K. Dudek

ASSOCIATE PROFESSOR – CMMS PAS · HEAD OF CRYSTAL CHEMISTRY AND ENGINEERING TEAM – CMMS PAS

Currently held positions Centre of Molecular and Macromolecular Studies of the Polish Academy of Sciences Łódź Associate Professor Łódź Centre of Molecular and Macromolecular Studies of the Polish Academy of Sciences Łódź Head of Crystal Chemistry and Engineering Team Lódź

Scientific profile and collaborations

Understanding crystallization. This part of my research is focused on the understanding of the crystallization of organic molecules with an aim to predict its outcome and influence it according to our needs. To that purpose my group is exploring new, easier to control approaches to crystallization in comparison with classical solution crystallization methods and complements them with crystal structure prediction calculations (CSP) to understand and harness molecules tendencies to crystallize in their specific forms. In this aspect my group is collaborating with Prof. Izabela Madura from Technical University of Warsaw and prof. Edyta Pindelska from Warsaw Medical University. We are also actively participating in BEST-CSP COST action.

Polymorphism and cocrystals. This part of my research is focused on understanding, crystallization and structural characteristic of new polymorphs, with an emphasis on pharmaceutical cocrystals.

CSP and NMR crystallography. To characterize and solve difficult structural problems my group is constantly developing methods based on solid-state NMR (NMR crystallography) and its joint use with CSP. This part of our research is conducted in a close collaboration with dr Piotr Paluch from CMMS PAS, as well as with prof. Luis Mafra from University of Aveiro, Portugal.

Structural characterization of natural products. In a collaboration with prof. Anna Kiss, prof. Sebastian Granica and prof. Jakub Piwowarski from Medical University of Warsaw, as well as dr Jan Glinski (Planta Analytica, Inc., USA) and prof. Michał Gleńsk from Wrocław Medical University I'm using NMR spectroscopy in solution and solid-state to structurally characterize compounds isolated from natural sources.

Selected publications _

- 2025 SCXRD, CSP-NMRX and microED in the quest for three elusive polymorphs of meloxicam [link]
- 2023 Crystallization of elusive polymorphs of meloxicam informed by crystal structure prediction [link]
- 2021 *Virtual Cocrystal Screening Methods as Tools to Understand the Formation of Pharmaceutical Cocrystals—A Case Study of Linezolid, a Wide-Range Antibacterial Drug [link]*

Research grants _____

Principal Investigator: 4 grants: Fuga NCN, Sonata NCN, Sonata Bis NCN, Mobility Plus MNiSW **Co-Investigator:** 3 grants: NCN, EU COST Action

Obtained patents

1 patent given by Polish Patent Office

International research stays _____

UK, University of Southampton, team of Prof. Graeme Day