Digital Pharmaceutics: Model-Informed Pharmaceutical Products and Process Design

Guest Editor:

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Message from the Guest Editor

This Special Issue intends to compile top-level contributions in the form of research articles, opinions, and reviews from key academic and industrial opinion leaders and eminent groups dealing with the predictive science applied to pharmaceutical material, process, and product developments. We encourage the submission of case studies of applying a wide diversity of modeling and simulations, such as molecular simulations, crystals, and crystallization modeling (MD simulations, QM, QC calculations), contact mechanics, macroscopic modeling of particle and powder processes (e.g., CFD-DEM, LBM, FEM, PBE), physiologically-based absorption modeling (e.g., PBPK, PBB, IVIVC), machine learning/AI applied to pharmaceutical product and processes, etc. In addition, small-scale predictive experiments that generate predictive knowledge of processes and products at larger scales, as well as in vitro understanding that can predict the fate of drug product in vivo are also welcome.

Special Issue

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Message from the Editor-in-Chief

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