Schrödinger's software and services capabilities to accelerate drug substance and drug product development processes

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A thorough characterization of the active pharmaceutical ingredient (API) is critical in the early-stage drug development process. Evaluating and defining the physicochemical properties is a regulatory requirement that helps identify APIs that meet safety and bioavailability requirements. In this presentation, I will demonstrate how Schrodinger leverages decades of experience in combining physics-based modeling with machine learning methods to offer reliable software tools and solutions to support API manufacturing, pre-formulation, formulation and delivery experiments and ensure success and consistency at all stages of the drug substance and drug product development processes.

Applications of Coarse-Grained Simulations to Drug Formulation

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Many drug formulations contain supramolecular structures such as clusters or micelles or these may appear during processing or delivery. These structures are hard to characterize experimentally and the limited understanding of their structure and behavior limits
the development of composition-structure-performance relationships. Coarse-grained modeling can be useful for simulating the formation and evolution of such structures providing information that complements experimental data. In this presentation we will provide background on coarse-grained modeling and go through 3 case studies employing it in drug formulation:

1. Complexation of drugs by cyclodextrin
2. Dissolution of amorphous solid dispersions
3. The self-assembly of lipid nanoparticles