Abstracts

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計算を用いた医薬品開発における原薬形態開発の実例

新規医薬品化合物を医薬品活性成分（Active Pharmaceutical Ingredient/API）とする医薬品開発において、活性成分の結晶形、すなわち原薬形態の結晶多形制御は、製品の品質管理のための重要な要素である。そのために、研究段階から承認申請にかけて、塩・共結晶なども含めた適切な原薬形態の選択と結晶多形の全体像の理解は、欠かすことが出来ない項目である。
本発表では、演者が考える研究段階から開発段階にかけての原薬形態選択の戦略の全体像を概説し、さらにデザインスペースの構築に計算的手法を用いた共結晶スクリーニングと、結晶構造予測による原薬形態のリスク評価の実例を紹介する。

Mathew D. Halls

Senior Vice President
Materials Science
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Advancing Materials Science with Schrödinger: Latest Innovations, Future Roadmap, and Key Applications Impacting Personal Care, Foods and Fragrances, and Pharmaceutical Formulations

The development of advanced materials and formulations is crucial for driving toward improved products. Schrödinger's digital chemistry platform accelerates this development through atomic-scale modeling, enabling informed selection, discovery, and optimization of materials and processes. Recent advancements in physics-based simulations and machine learning enhance the accuracy, efficiency, and accessibility of Schrödinger software. In recent years, Schrödinger's key areas of development have led to powerful capabilities that impact multiple applications critical to the design, manufacturing, and optimization of consumer packaged goods and pharmaceutical products; examples include new machine learning frameworks that map individual ingredient properties to overall product performance, quantum chemistry solutions for optimized reactivity and catalysis for complex chemical synthesis and scale up production, molecular dynamics simulations to assess atomic-scale interactions in packaging and delivery, and new technologies for solid state morphology and crystal structure prediction. In this presentation, select recently added features and capabilities, major development areas, along with key applications related to drug formulation and cosmetics will be reviewed.

Shiva Sekharan

Senior Director
Schrödinger

Schrödinger's Modeling Platform and Solutions to Accelerate Drug Substance and Drug Product Formulation and Delivery Processes

Early assessment of stereoconfiguration, degradation, reactivity, catalysis, polymorphism and solubility of active pharmaceutical ingredients (API) is critical for small molecule drug discovery and development processes. We have developed automated computational platform leveraging physics-based methods, chemistry-informed AI and ML models to efficiently predict 1) Boltzmann-averaged spectra of small molecules without crystallizing the molecule or using X-ray spectroscopy, 2) bond dissociation energies and decomposition products to elucidate reaction mechanisms, 3) crystal polymorphs to aid selection of a stable solid form, 4) solubility enhancement via organic cosolvents using free energy perturbation (FEP+) method, 5) polymer excipients that can interact strongly with the API and reduces the risk of recrystallization, and 6) enable calculation of apparent pKa values of ionizable lipids and simulate the self-assembly and structural properties of lipid nanoparticles.

Pavel A. Dub

Product Manager
Catalysis and Reactivity
Schrödinger

Schrödinger Reactivity and Catalysis Tools for Pharma Formulation and Cosmetics

In this presentation, we will showcase our automated workflows for simulating reactivity and catalysis. We will illustrate their capabilities with tailored examples focused on pharma formulation and cosmetics.

Anand Chandrasekaran

Senior Principal Scientist
Schrödinger

Combined Physics-Based and Machine Learning Approaches in the Design of Complex Formulations

Machine learning (ML) is revolutionizing formulation design across pharmaceuticals, cosmetics, and consumer packaged goods by enabling data-driven predictions of critical properties such as solubility, viscosity, and stability. Chemistry-informed AI/ML models provide a powerful framework for accelerating materials innovation, extending beyond active ingredients to complex multi-component formulations. The ability of machine learning to analyze vast amounts of data and make predictions about novel formulations allows for the rapid exploration of extensive chemical spaces, significantly reducing reliance on traditional trial-and-error experimentation. Automated workflows and deep learning can integrate both chemical composition and molecular structure to generate predictive models, thereby optimizing formulation properties with enhanced speed and efficiency.
In this webinar, we will demonstrate how Schrödinger's integrated ML- and physics-based approaches are transforming formulation design. This includes:

- How an automated ML workflow, incorporating chemical principles and composition, can predict Active Pharmaceutical Ingredient (API) solubility in binary solvents.
- How ML models, augmented with physics-based descriptors, can be utilized to optimize viscosity predictions of organic molecules for improved formulation performance.
- Optimization of shampoo formulation properties, reducing the need for trial-and-error experimentation.

John C. Shelley

Fellow
Schrödinger

Enabling Formulation via Coarse-Grained Modeling: Application to Proteins Solutions and LNPs

Formulation science often encounters challenges arising from inhomogeneities at the supramolecular level in solution for applications involving drying, dispersions, solubility enhancement, aggregation, permeation, dissolution, concentrated solutions, and interactions with biological structures. Experimental characterization of the internal structure of the inhomogeneities is often intractable and the length-scales involved often preclude using atomistic simulations. Coarse-grained (CG) simulations can fill this gap and provide insight into the nature and evolution of these structures. This talk will highlight Schrödinger's recently deployed automated workflows for generating CG models and showcases their application to protein and lipid nanoparticle formulations.

Jeffrey M. Sanders

Product Manager and
Scientific Lead of
Consumer Goods
Schrödinger

Transforming Cosmetic Innovation with Physics-Based Modeling and AI

As machine learning and physics-based modeling become more prominent in cosmetic and personal care innovation, they offer a powerful framework for accelerating formulation and packaging development. Yet many applications of AI remain ad hoc, especially when working with limited or non-transferable datasets. By integrating machine learning with experimental results and simulation data, researchers can build more robust models that offer both performance and transparency—avoiding the "black box" pitfalls of traditional AI. Physics-based modeling, in particular, enables the generation of rich molecular descriptors, allowing for virtual screening of ingredients, evaluation of formulation morphology and stability, and analysis of interactions with biological surfaces or packaging materials. These methods provide a mechanistic understanding at the molecular level, guiding formulation design and reformulation efforts with greater precision. Case studies demonstrate how these tools support faster, more informed decisions—reducing trial-and-error, supporting sustainability goals, and bringing high-performing products to market more efficiently.