Oral solid dose

Modeling polymer interactions to improve amorphous solid dispersion stability

Computational modeling helped clarify polymer interactions and guide formulation strategies for poorly soluble drug candidates.

Development challenge

Poor solubility continues to be a major barrier to the development of many small-molecule drugs. Amorphous solid dispersions can improve solubility and bioavailability, but identifying stable polymer combinations often requires extensive experimental screening.

Understanding polymer interactions at the molecular level can help reduce formulation uncertainty and improve the stability of amorphous systems.

Applying molecular dynamics modeling

Predictive modeling techniques within the OSD Predict™ framework were used to evaluate polymer interactions and their role in stabilizing amorphous solid dispersions.

Molecular dynamics simulations provided insight into intermolecular interactions between polymers and drug molecules. The modeling approach helped characterize how different polymers interact, form complexes, and influence dispersion stability.

Guiding polymer selection

Simulation results provided a mechanistic understanding of polymer compatibility and their ability to stabilize amorphous systems. These insights helped narrow candidate materials and guide experimental formulation work.

By combining computational modeling with targeted laboratory studies, the development team was able to focus experimental work on the most promising polymer systems.

Development outcome

The modeling framework improved understanding of drug–polymer interactions and supported the development of more stable amorphous solid dispersions. This combined computational and experimental approach reduced the need for extensive formulation screening while providing a stronger scientific basis for polymer selection.

At a glance

Program focus

Understanding polymer interactions in spray-dried amorphous solid dispersions to improve stability of poorly soluble drugs.

Methods used

Molecular dynamics simulations, interaction energy calculations, and hydrogen-bond analysis combined with experimental validation using SEM, FTIR, and NMR spectroscopy.

Polymer system evaluated

Inter-polymer complexes between polyvinylpyrrolidone (PVP) and Eudragit polymers.

Key technical finding

Hydrogen bonding between hydroxyl groups of Eudragit and carbonyl groups of PVP drove stable inter-polymer complex formation.

Development impact

Combined computational and experimental analysis provided a mechanistic basis for polymer selection and enabled development of stable amorphous solid dispersions.

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