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Graph Neural Networks for Predicting and Ranking Drug Loading in Mesoporous Silica Nanoparticles

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Mesoporous silica nanoparticles (MSNs) are widely used as drug-carrier platforms because of their tunable pore structures, large surface areas, favorable biocompatibility, and the ease with which their surfaces can be chemically modified.[1-8] Among the various performance metrics used to evaluate MSN-based delivery systems, drug loading capacity (DLC) is especially important, as it directly influences formulation efficiency and the achievable therapeutic dose.[9] In practice, DLC is governed not by any single factor but by the coupled effects of drug structure, modifier chemistry, pore architecture, and loading conditions.[10-12] Because these factors interact, optimizing MSN formulations becomes a high-dimensional combinatorial problem that remains time-consuming to explore experimentally.

Data-driven strategies offer a promising route to accelerate formulation discovery,[13-20] but applying deep learning to MSN drug loading remains challenging, as it requires integrating not only molecular structures of drugs and modifiers but also carrier textural parameters such as pore size and surface area together with loading conditions.[21-23] Models that rely solely on molecular fingerprints or only on tabulated formulation variables are therefore unlikely to capture the full structure-property relationship governing loading behavior.[24-28] Unsupervised pretraining combined with transfer learning has been shown to improve the generalization of graph neural networks (GNNs) in small-data settings.[29-36] Nevertheless, an experimentally validated machine-learning framework specifically designed for MSN drug loading has not yet been established.

To meet this need, here we introduce a graph-learning-based Network for Drug-loading Ranking in MSNs (GNDR). GNDR is designed to support both quantitative DLC prediction and decision-oriented ranking of surface modifiers. GNDR builds on a graph neural network architecture that integrates molecular graph representations of drugs and modifiers with MSN textural descriptors and loading parameters through unsupervised pretraining, condition-aware transfer learning, and downstream

regression. Using this framework, we conduct high-throughput virtual screening across 128 drugs and 13 silane modifiers plus the unmodified control, followed by Bayesian optimization of formulation variables. As a screening-assisted validation, we further performed experiments on independently synthesized single-pore MSNs using representative systems based on APTES and MPTMS modifiers and model drugs including ibuprofen and dexamethasone.

To establish the predictive framework, two large molecular libraries were assembled from PubChem and ChEMBL, comprising 74,919 silane modifiers and 10,563 clinically advanced drugs, and 213 MSN-drug-modifier loading records were curated from the literature to construct a drug-modifier-condition dataset (Figure 1). The overall workflow combined self-supervised pretraining, condition-aware transfer learning, and downstream fine-tuning for DLC prediction. Pretraining was used to learn general molecular representations from the large drug and modifier libraries. These embeddings were then adapted through transfer learning with a pairing objective to better capture compatibility patterns relevant to drug loading. Finally, an end-to-end dual-stream predictor was trained to regress DLC by combining drug and modifier graph embeddings with experimental-condition descriptors.

The pretrained embeddings formed a shared representation space for drugs and modifiers. A 2D visualization using Uniform Manifold Approximation and Projection (UMAP) of the 256-D embeddings showed substantial overlap between the two sets (Figure 2a), even when the reducer was fit on drugs and applied to modifiers, indicating that the organization was driven primarily by structural similarity rather than dataset identity.[37, 38] Distinct neighborhoods were enriched in recurring structural motifs, suggesting that the pretrained space retained chemically meaningful structural relationships.[39] The effect of fine-tuning on the pretrained representation was examined after loading-related signals had been introduced through drug-modifier-MSN data. Drug and modifier embeddings were projected into two dimensions using the

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