USE CASE

Accelerate Formulation Development for Liquid Home Care Product

Precision and efficiency in predicting fragrance evaporation profiles using science-based AI (SBAI)

Target

Predict evaporation profile of a liquid home care product to ensure it produces consistent odor over planned lifetime and meets regulatory requirements for advertised evaporation profile.

Challenge

Determining the evaporation rate for one single complex formulation typically requires experimental testing of 6 weeks. Each formulation contains up to 100 ingredients, making it infeasible/unaffordable to test all possible options.

Solution

Train a Science-Infused ML model in NobleAI Reactor that captures the chemical interactions within a formulation, the structure-function relationship for each ingredient, models the diffusion of each ingredient through a wick and its evaporation rate under a range of temperature and humidity conditions.

Reactor can use language models to read chemical formulas and infer chemical structures and formulation impact of chemicals outside the original training set.

The model can be used to quickly search through a large range of chemicals to find combinations with a high likelihood of success, ensuring that laboratory resources a re dedicated to validation, not exploration.

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