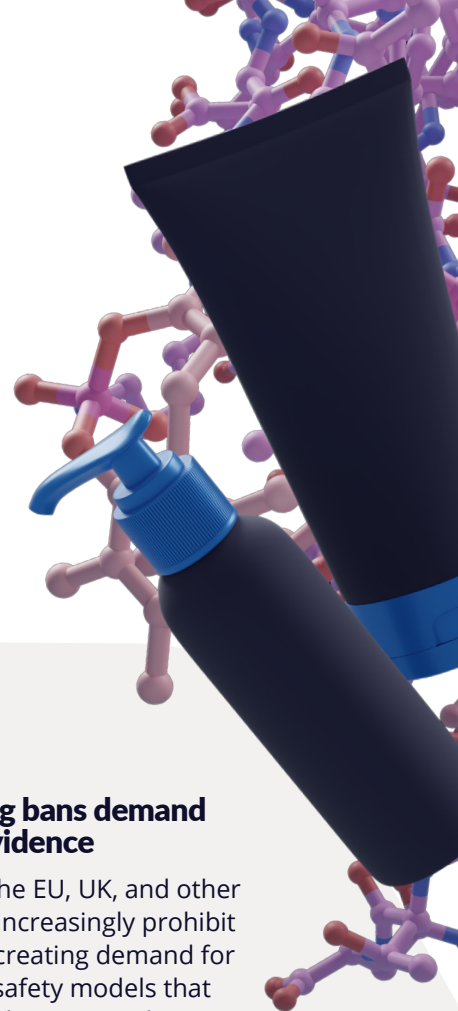


Predict skin products safety and efficacy computationally — ahead of the lab

As global animal testing bans expand, benchwork alone is no longer enough to meet modern safety benchmarks. Schrödinger's advanced molecular modeling and physics-informed AI platform predicts permeation, photostability, and ingredient performance — empowering teams to exceed regulatory expectations and slash development timelines from years to months.



The Problems You Face



Sunscreen development is a regulatory bottleneck

Every UV filter candidate must prove broad-spectrum protection, chemical and physical stability, and minimal skin penetration simultaneously. Testing all three properties empirically is prohibitively slow. Simulation evaluates these requirements computationally, allowing teams to screen candidates before a single prototype is made.



Animal testing bans demand new safety evidence

Regulations in the EU, UK, and other global markets increasingly prohibit animal testing, creating demand for computational safety models that provide the mechanistic evidence regulators accept for sensitization, irritation, and phototoxicity risk.



Finding effective active ingredients takes too long

Screening natural compounds against anti-aging targets with benchwork takes months per candidate. Virtual screening ranks thousands of candidates against key targets for brightening, anti-wrinkle, and firmness, delivering high-potential candidates in days, not quarters.



Emulsion stability failures waste resources

Creams and serums that pass early testing fail in accelerated stability tests because the molecular behavior at oil-water interfaces is invisible at the bench. Simulation reveals instability mechanisms at oil-water interfaces, helping teams design more robust formulations before prototyping.

The Solutions Schrödinger Offers

Validated workflows to predict, screen, optimize ingredients and formulations

Timely and dedicated scientific support from Schrödinger experts in skin care applications

Contract research services available — no software, hardware, or computational team resources needed



Schrödinger

What You Get



Actives delivery performance before any experiments

Validated computational skin barrier models predict how actives penetrate, adsorb, and are retained, evaluating delivery performance for hundreds of ingredient candidates before any physical experiment.



Photostable sunscreen candidates, fast-tracked

Screen UV absorption spectra, photostability, and degradation pathways computationally, narrowing dozens of filter candidates to a validated shortlist before regulatory submission work begins.



Thousands of actives ranked in days, not quarters

Virtual screening ranks natural and synthetic compounds against brightening, anti-wrinkle, and firmness targets, delivering experimentally validated leads in days instead of months.



Formulation optimization across the full design space

ML models trained on your data predict SPF, viscosity, stability, and sensory attributes simultaneously, screening formulation space computationally before a single prototype.



Safety evidence that satisfies regulators

Computational toxicity models, both physics-based and AI-enabled, provide the mechanistic safety evidence regulators accept — without animal testing.

Case Studies

Schrödinger Human Tyrosinase Model

First accurate and validated model of human tyrosinase (hTYR) oxy state that predicts inhibitor binding affinities with assay-like accuracy, enabling R&D teams to design, screen, and optimize next-generation depigmenting agents before any physical experiment. Built on AlphaFold2 and mechanism-informed binding states to accurately rank potency for inhibitors with suicide inactivation mechanism, such as thiamidol (the most potent depigmenting agent to date).

Schrödinger Skin Barrier Model

Validated computational models of the skin barrier that predict how cosmetic ingredients permeate, adsorb, and are retained - enabling R&D teams to evaluate moisturizer and active ingredient delivery performance before any physical experiment. Backed by step-by-step tutorials for immediate adoption.



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Ready to accelerate your skin care pipeline?

Schedule a consultation to see how Schrödinger's platform applies to your specific formulation and ingredient challenges.

