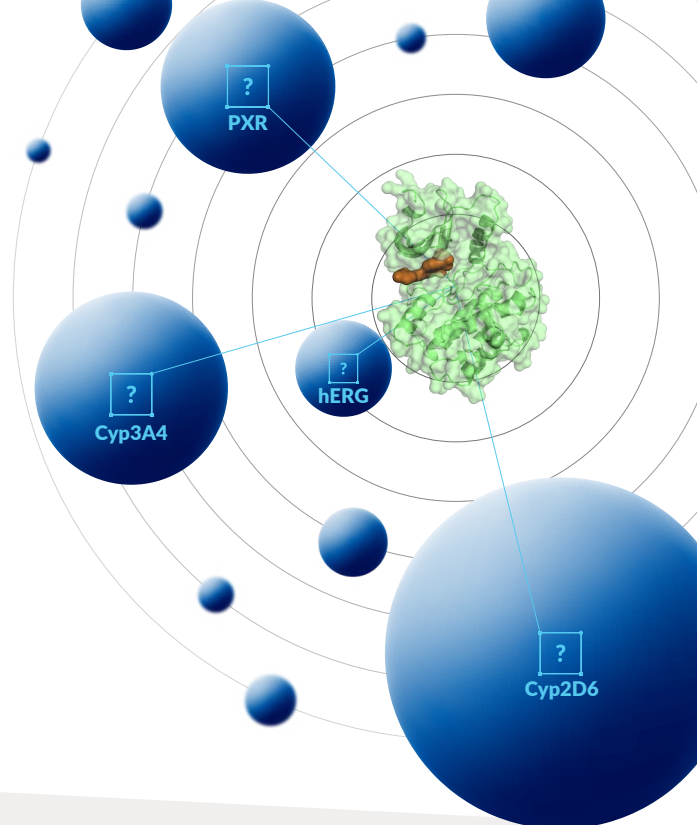


Predictive Toxicology

Have a hERG/CYP/PXR problem and don't know how to address it?

Late-stage discovery failures due to hERG, CYP, or nuclear receptor liabilities cost teams months of chemistry cycles and millions in downstream assays. Schrödinger's Predictive Toxicology Solution enables early, physics-based identification and rational mitigation of tox liabilities—before they derail your program.



Don't just flag off-targets—leverage atomic structural models to design out the liability



3X
Cost Savings



>10X
Faster to fit into your DMTA cycles

2 Modes of Access

Mitigate Known Liabilities

Targeted at: hERG, CYP, PXR problems in active programs.

- **Input:** Your congeneric series.
- **Output:** An all-atom, explicit solvent binding hypothesis that rationalizes your SAR in 3 days.
- **Result:** Perform surgical changes to chemical matter without sacrificing potency.

Pricing Evaluation Available

✓
Push button SaaS solution

✓
Credit based

Identify Unknown Liabilities

Targeted at: Early-stage de-risking and lead selection.

- **Input:** Just your 2D ligands.
- **Output:** Affinity predictions and binding hypotheses for anti-targets in 24hrs.
- **Result:** Identify the “cleanest” path forward before the first wet-lab assay is even scheduled.



Schrödinger

Stop Guessing at Tox. Start Designing Around It.

More than just binary predictions

Move beyond pass/fail with actionable, comprehensive readouts in a single day to supercharge your design process in lead optimization

De-risk from the get-go

Rapidly dial out liabilities with atom-level toxicity attribution required to not just fix a compound, but to design the superior compound from the start

What's in the panel?

Protein Family	Representative Targets	Organ System Library
Enzymes (CYP450s)	CYP3A4, CYP2D6, CYP2C9	Liver injury, drug drug interactions (DDI)
Kinases and Receptor Tyrosine Kinases (RTKs)	55 kinases, EGFR, ABL, VEGFR2, BRAF JAK2, BTK, PI3K	Bone marrow suppression, immune, skin, heart, vascular, cardiac
Ion Channels	hERG (KCNH2) Nav1.5, Cav1.2, Kv7.2	Cardiac arrhythmia, CNS seizures
Nuclear Receptors	PXR, ER CAR, LXR, AhR, FXR, GR	Hepatic enzyme induction, metabolic disruption
G-Protein Coupled Receptors (GPCRs)	H1R, 5-HT2B, β 1AR, α 1AR, M2R	Cardiac, CNS, GI

Available now

Coming soon



Finding out a tox liability does not have to be the end of your project, tap into Schrödinger's turnkey Predictive Toxicology Solution today to see immediate project impact!

Contact us: sales@schrodinger.com

Learn more: www.schrodinger.com/platform/products/predictive-toxicology

