

Lipid Track Terminated: 8 Months of Failure Compressed into 2 Hours

Executive Summary: Upadacitinib Topical Formulation Project

Chemical Outcome

NO GO

- Target: Topical Upadacitinib
- Verdict: Thermodynamic Instability
- SR9 Resonance: < 0.30 (Target > 0.80)
- Action: Project Closed

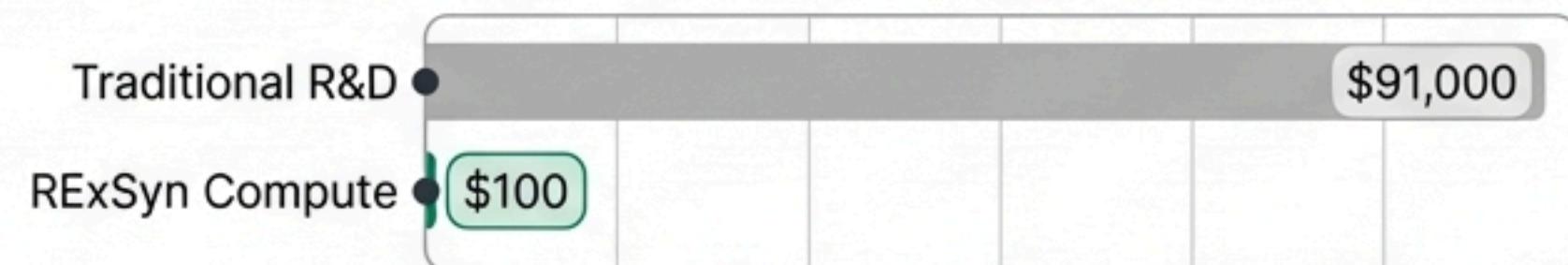
Operational Outcome

SUCCESS

Time Saved – Traditional vs RExSyn



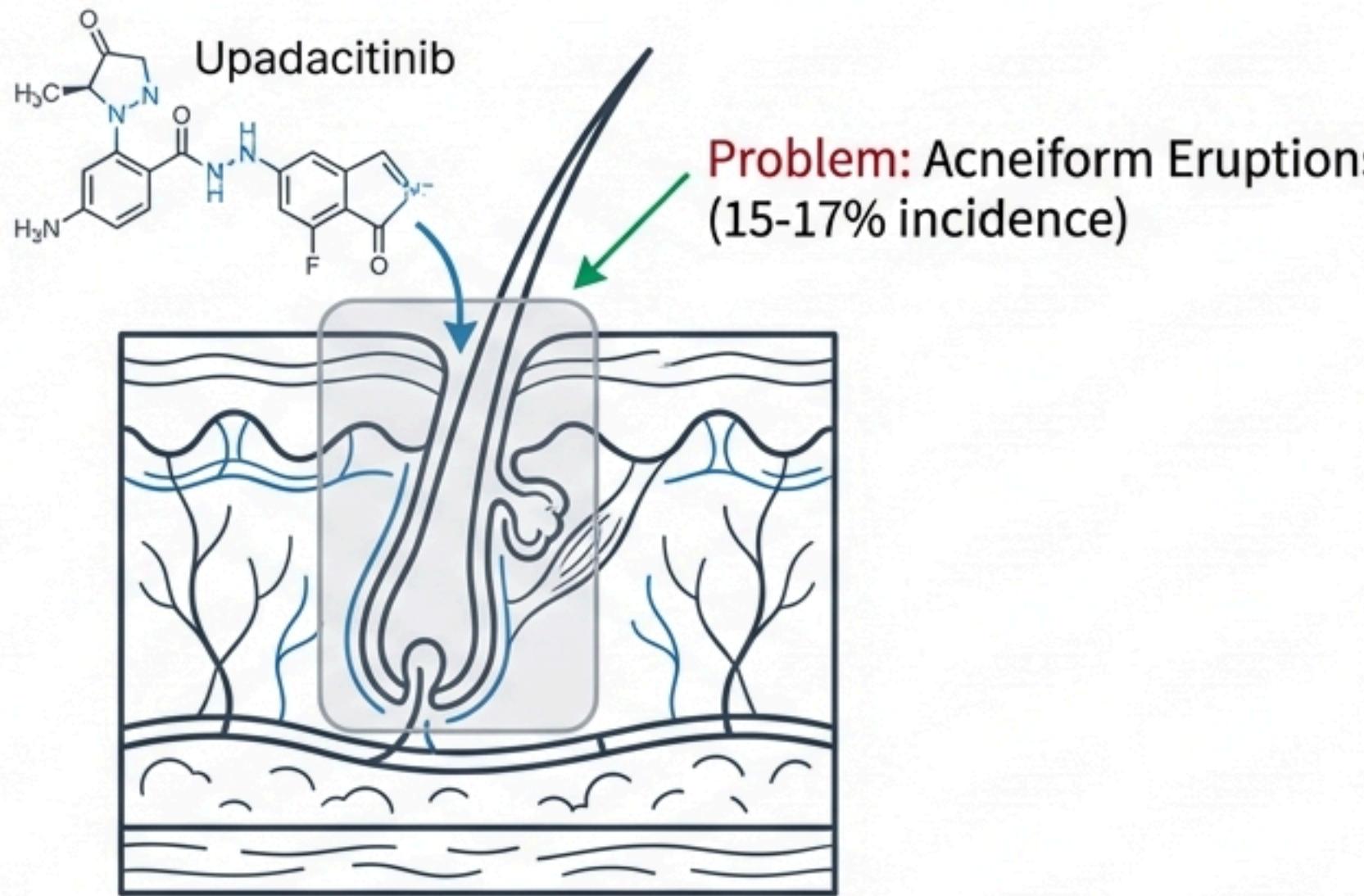
Cost Avoidance – Crimson RExSyn



Efficiency Gain: 99.8%

The Mission: Solving Upadacitinib's Cutaneous Side Effects

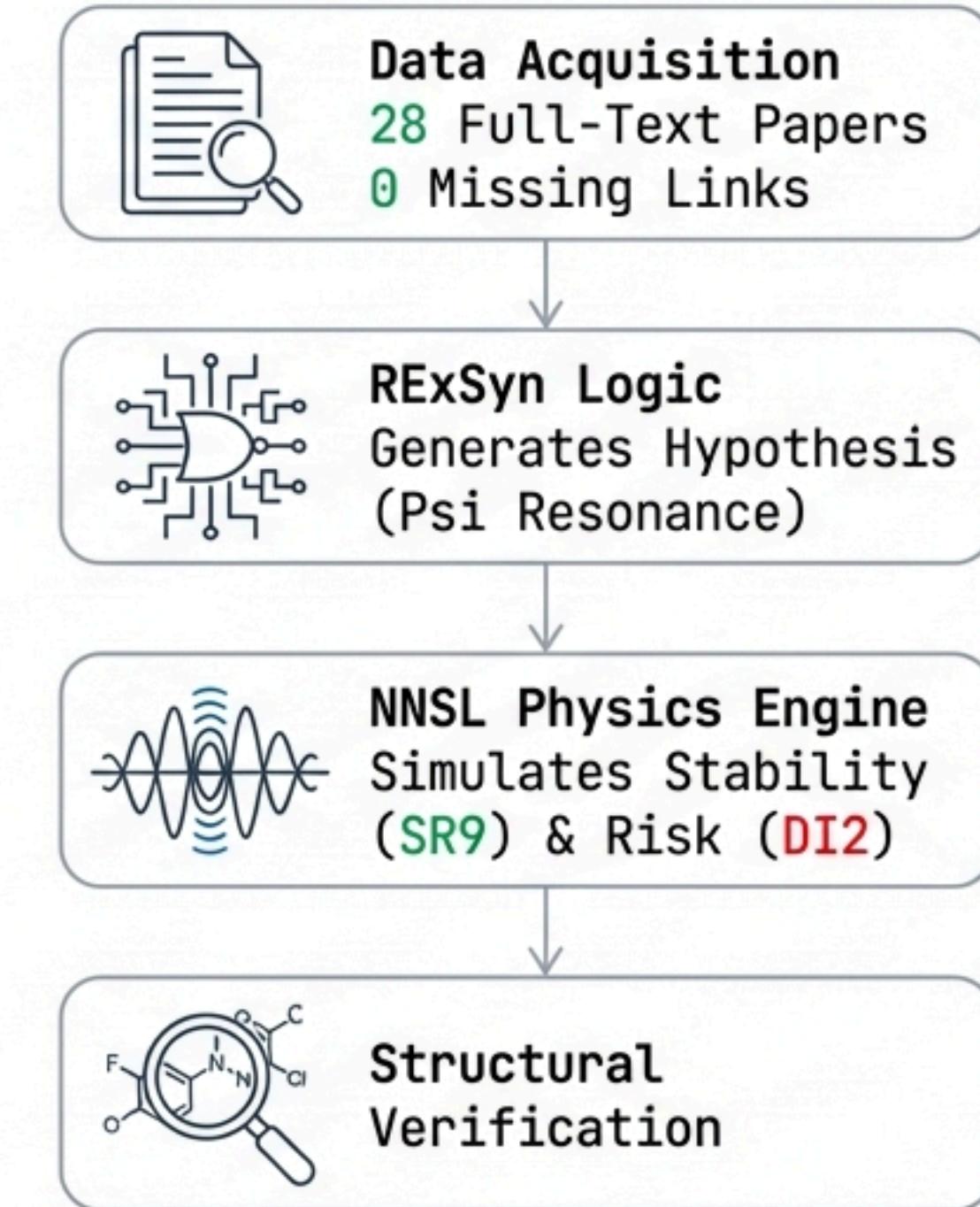
Medical Context



Objective: Encapsulate drug to minimize follicular intrusion while maintaining efficacy for Atopic Dermatitis.

Technical Note: Visualizations are conceptual schematics only
rendered structures may vary from exact chemical sequences.

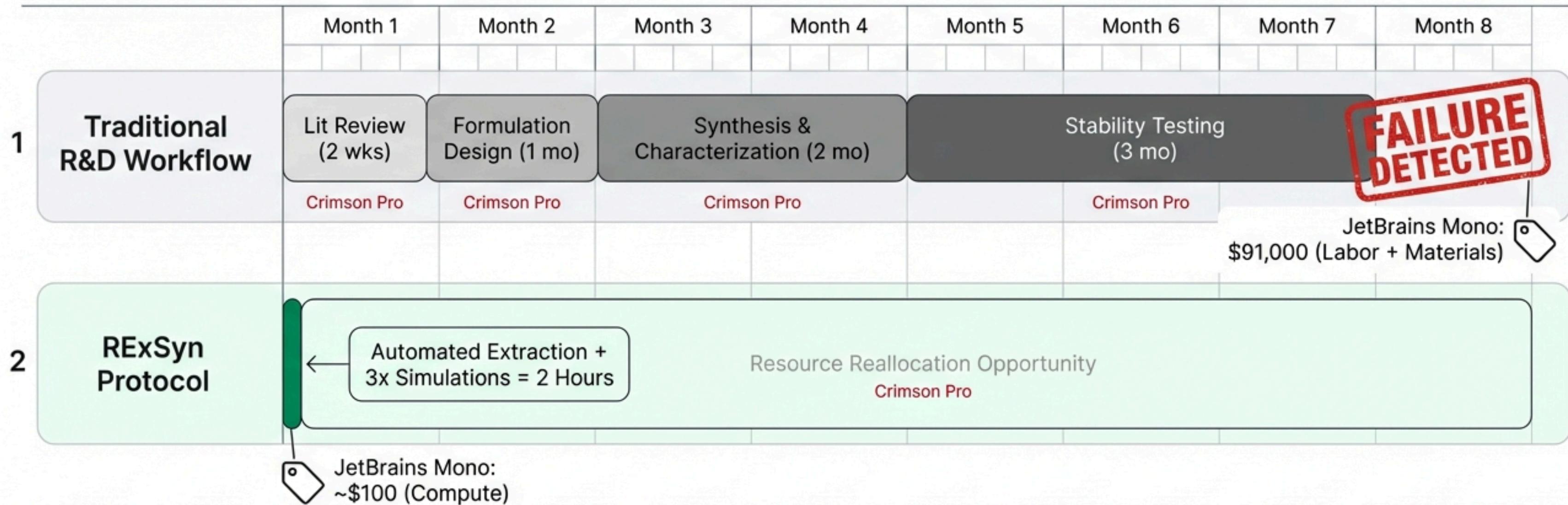
The Engine: RExSyn + NNSL



“Data → Hypothesis → Structural Verification → Physics Simulation”

The Efficiency Paradigm: 99.8% Resource Reduction

Gantt Chart vs. Timestamp

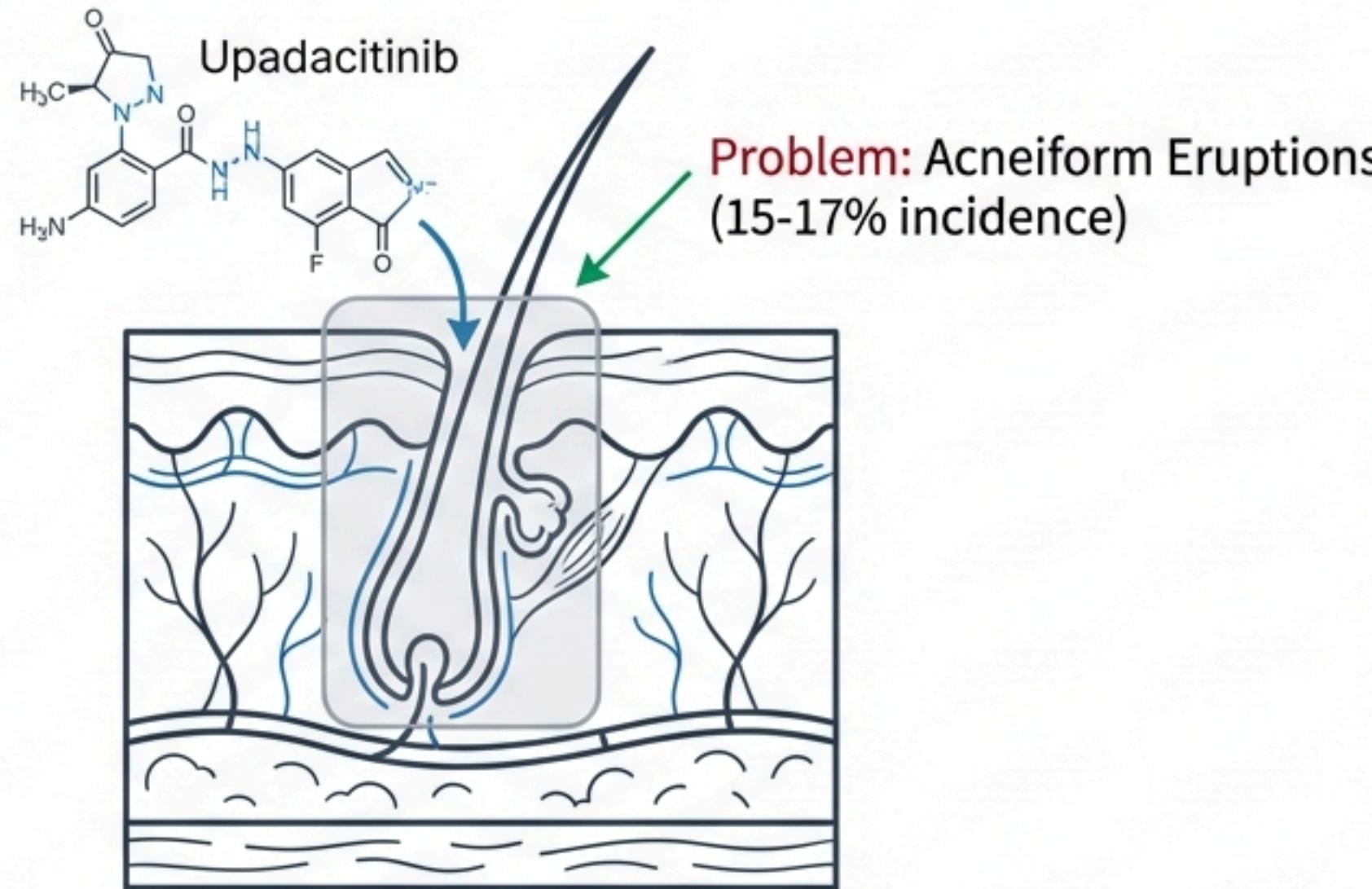


Zero False Positives.

The system avoided 8 months of “dead end” wet-lab work by predicting failure immediately.

The Mission: Solving Upadacitinib's Cutaneous Side Effects

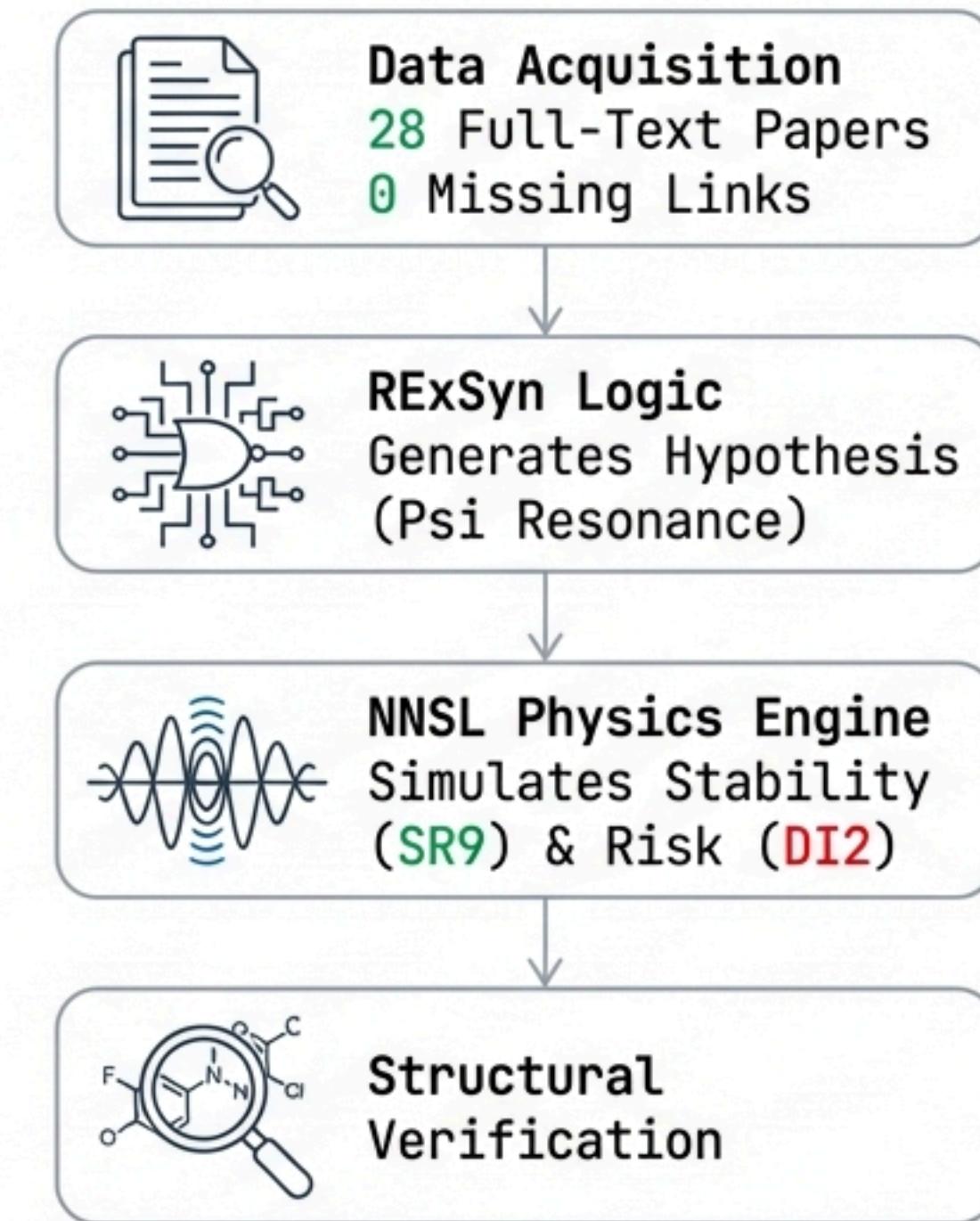
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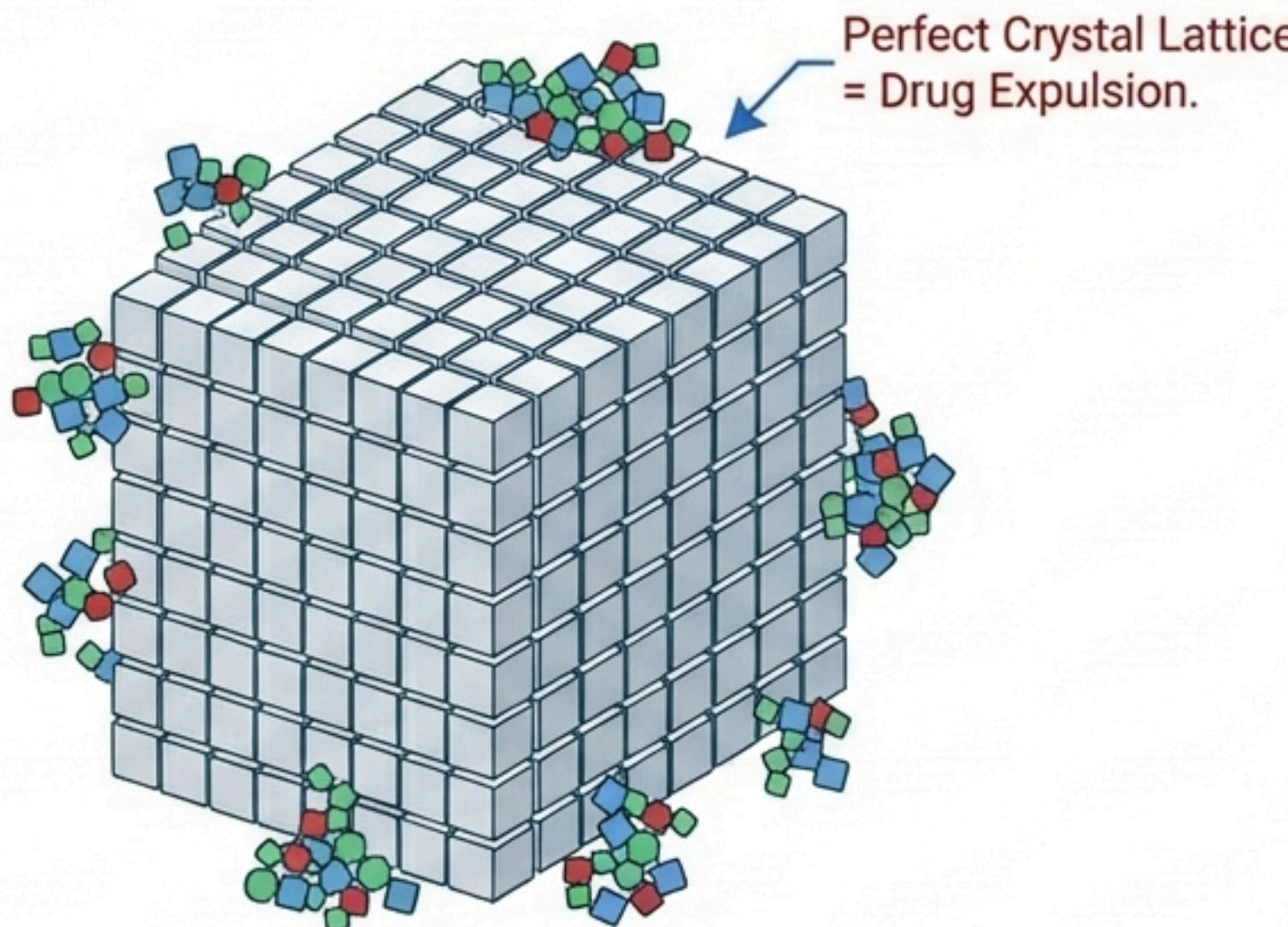


"Data → Hypothesis → Structural Verification → Physics Simulation"

Iteration 2: Solid Lipid Nanoparticles (SLN)

STATUS: FAIL

Simulation Visual



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The Data & Logic

Pivot Strategy

Liquid → Solid. Used Cetyl Palmitate for rigid core.

Experiment:	EXP-02
SR9 (Stability):	0.27
Total MGU (Energy):	28.93 ↑
GOO Metric:	-29.37

The Pivot Logic:

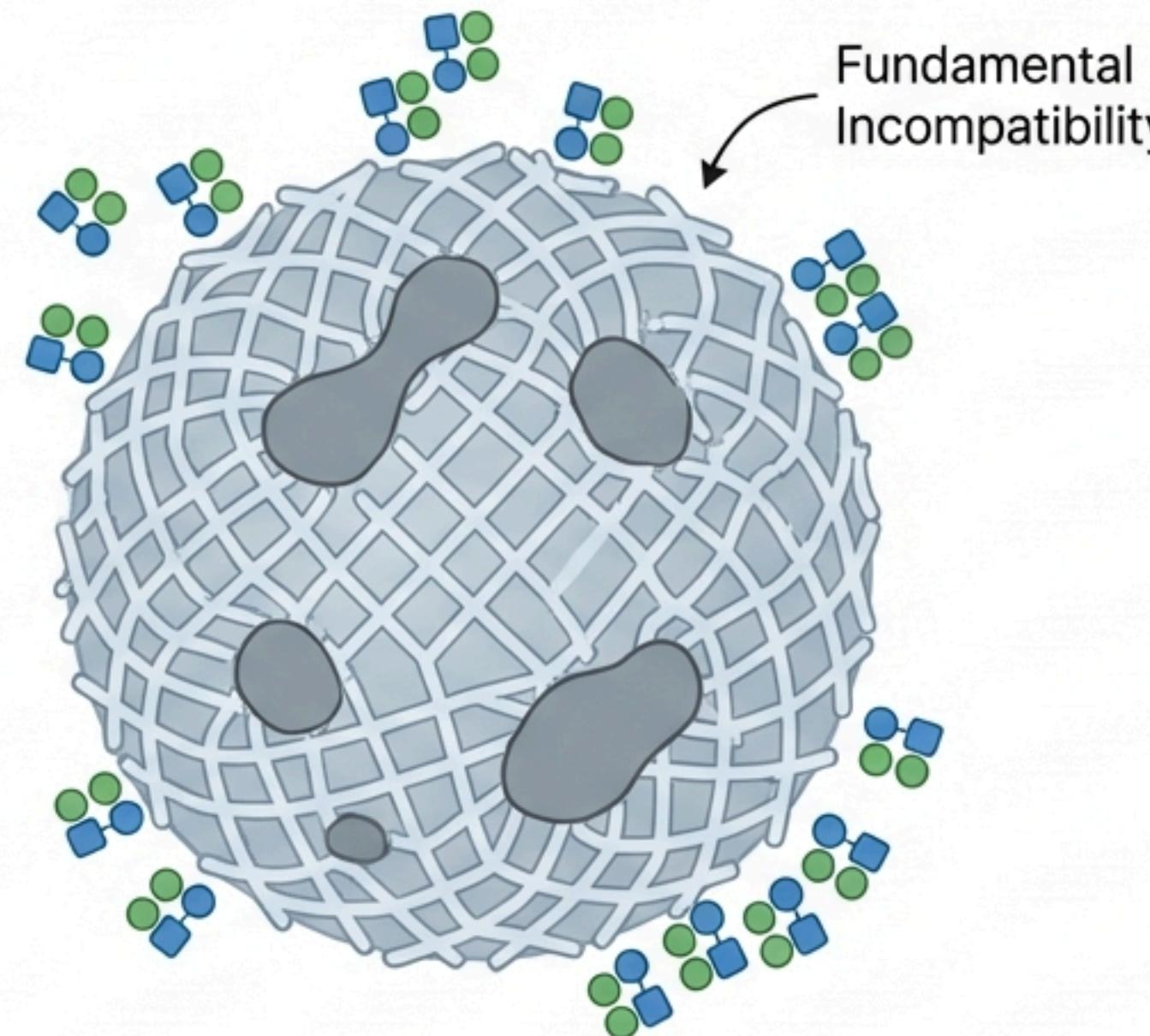
Problem: The Perfect Crystal. Lattice is too ordered to accommodate the drug.

AI Recommendation: Introduce chaos. Investigate Nanostructured Lipid Carriers (NLC).

Iteration 3: Nanostructured Lipid Carriers (NLC)

STATUS: TERMINATED

Simulation Visual



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The Data & Logic

Pivot Strategy

Solid + Liquid Chaos. Added Oleic Acid to create
lattice imperfections.

Data Panel

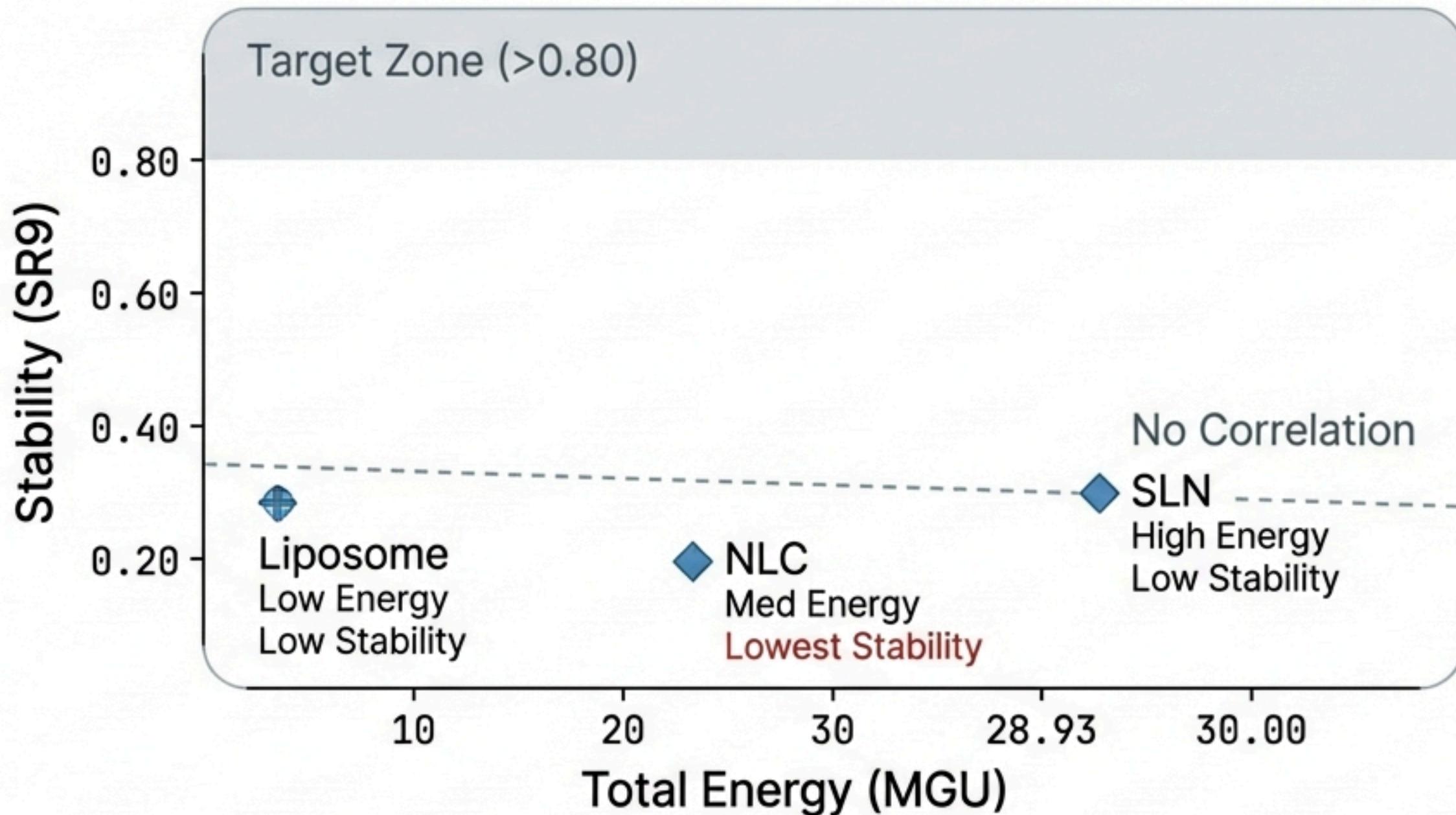
Experiment:	EXP-03
SR9 (Stability):	0.22 (Lowest Score Red)
Total MGU (Energy):	22.45
Coherence:	1.0

Critical Insight

Lipid is not the answer. Even with induced lattice
imperfection, Upadacitinib is thermodynamically rejected.

Verdict: STOP all lipid tracks.

Physics of Failure: Why Upadacitinib Rejects Lipids.



Synthesis: Increasing system energy (SLN) failed to improve stability.
The molecule fights the carrier geometry regardless of state.

Metric Tensor		
g_{00} :	g_{00} :	-29.37
g_{11} :		3.39
g_{22} :		0.27

Metric Tensor
confirms geometric incompatibility.

System Audit: Reliability & Limitations

B- (72/100)

Approved for Limited Use (Early Screening)

The Truthful Null (Positives)

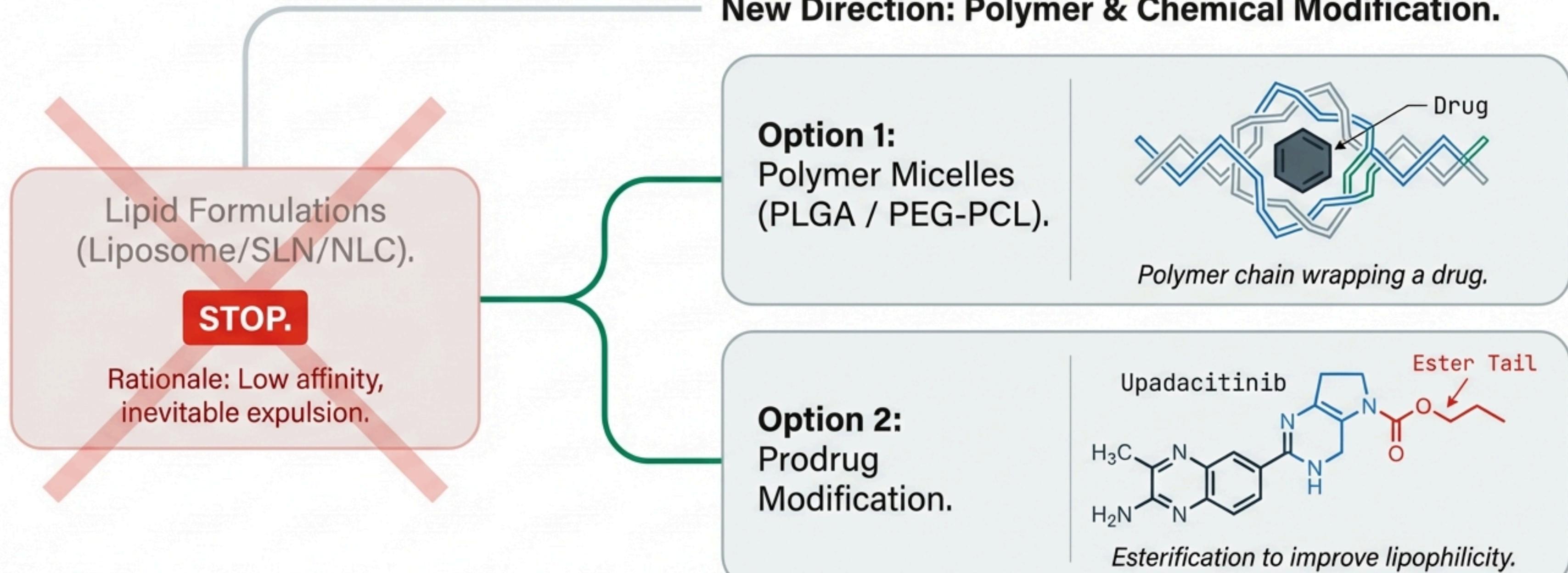
- ✓ Zero Hallucinations.
- ✓ 28 Papers Processed / 0 Missing Links.
- ✓ Pivot Logic (SLN vs NLC) verified as scientifically accurate.

The Phi Matrix Issue (Negatives)

- ⚠ Numerical Instability: Condition Number $> 10^{13}$.
- ⚠ High Uncertainty in exact SR9 values.
- ⚠ Not suitable for final regulatory submission.

Verdict: Excellent for binary '**No-Go**' decisions. Insufficient for precision regulatory data.

Strategic Pivot: The Way Forward.



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Immediate Action: Initiate RExSyn screening for Polymer tracks.

Project Status: Closed & Archived.

Date: 2026-01-24

Project: RExSyn Verification Series (Upadacitinib)

Outcome: **3** Tracks Evaluated, **3** Tracks Rejected.



For Early-Stage Screening.

***Perfect is the enemy of fast. We traded precision
for speed, and saved 8 months.***