

REACTION INTELLIGENCE FOR PROCESS CHEMISTRY

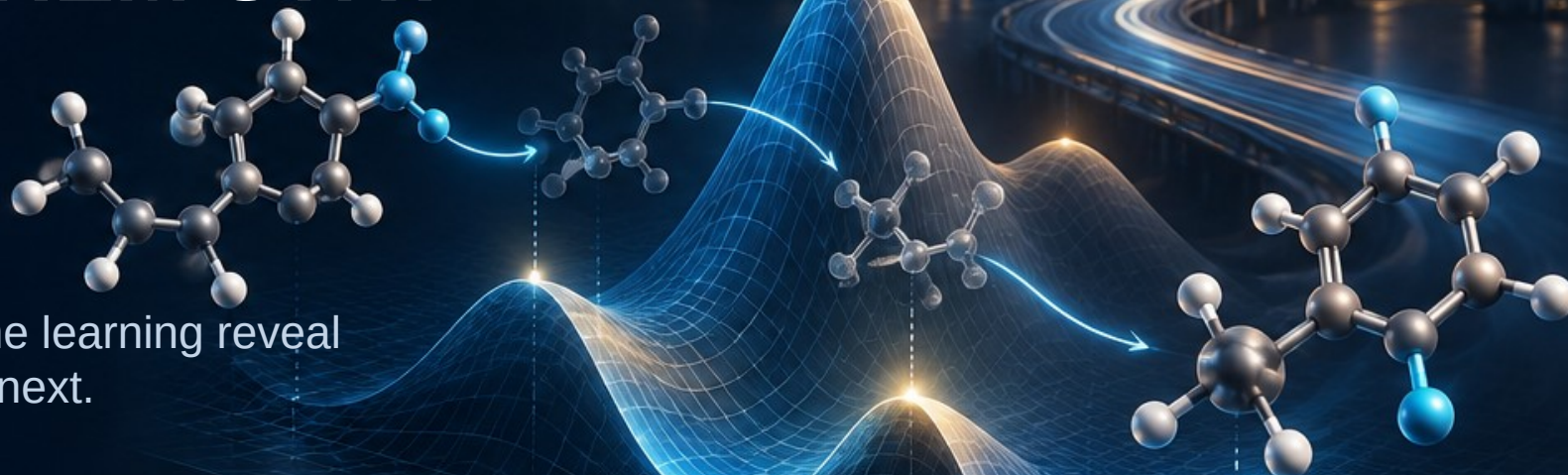
Physics-based simulation and machine learning reveal why reactions fail — and what to test next.

CLIENT TECHNOLOGY OVERVIEW

www.aiqimia.com

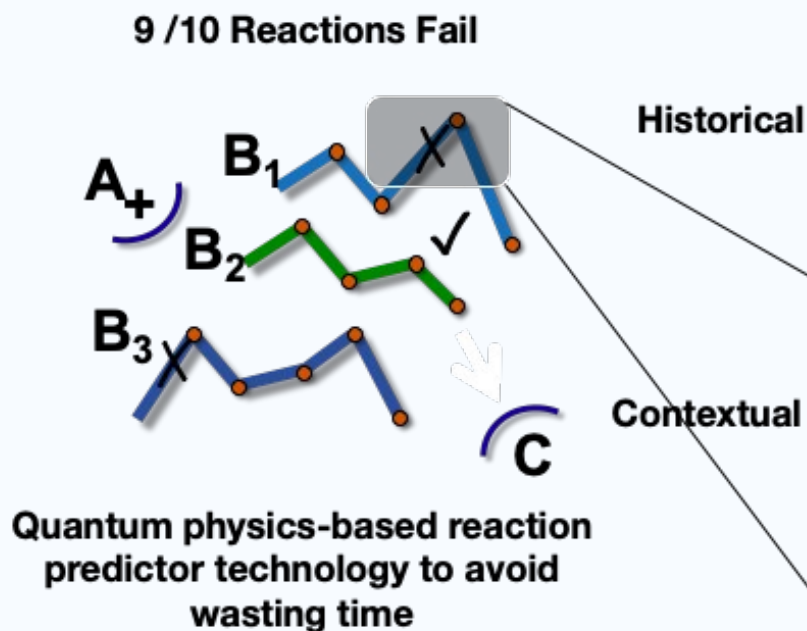
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Published conditions often fail when the chemistry changes

A workable recipe for one molecule may fail after a small structural, equipment or process change.



WHY TRANSFER FAILS

Literature conditions describe one substrate, one apparatus and one operating window.

A single atom can change protonation, selectivity or the rate-determining step.

Without a mechanism, chemists repeat broad screens to find the workable region again.

Representative campaign: 9 of 10 tested reactions failed

Ai.Qimia turns a synthesis question into decisions

A client does not receive another black-box score.
The output is an interpretable package a chemist can challenge, test and use

01

ROUTE

Which pathways and intermediates are viable?

Route feasibility • pathway risk • realistic intermediates

02

MECHANISM

What controls rate, failure and selectivity?

Transition states • rate-determining step • competing paths

03

CONDITIONS

What should the laboratory test next?

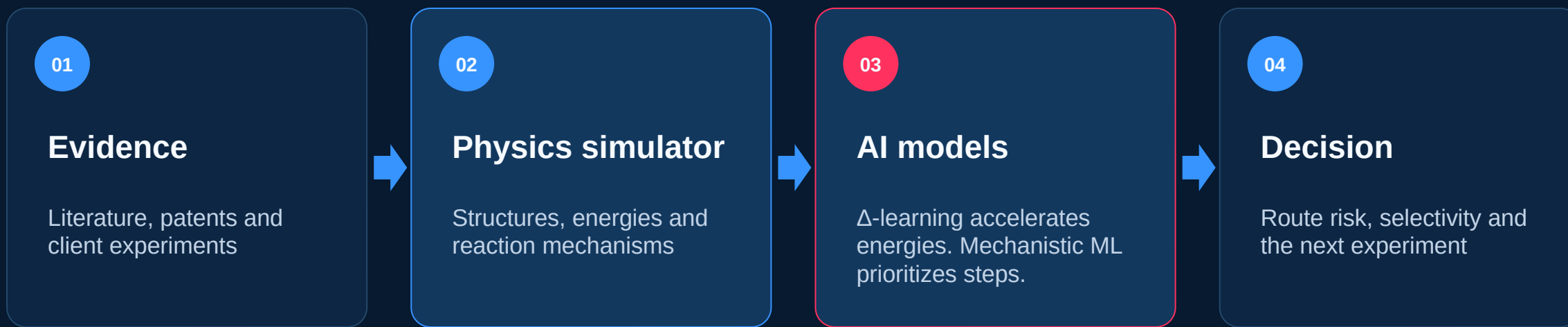
Selectivity drivers • key variables • prioritized experiments

DELIVERABLE • Mechanism, predictions and a laboratory validation plan

Physics and AI form a closed prediction loop

04

AI accelerates the expensive parts of simulation and directs where physics should look next



FEEDBACK

New experimental results improve the next prediction

The closed loop combines simulated ground truth with customer data while preserving a physics-based starting model.

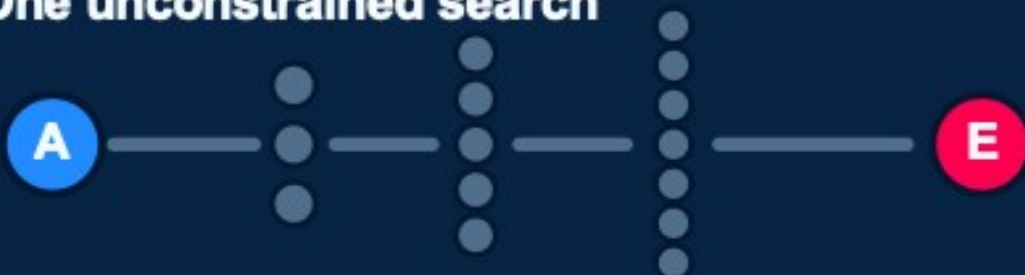
Model development with HES-SO and the University of Geneva

A learned midpoint divides the mechanism search

C constrains the route, but the platform must still discover B, D and the connecting transition states.

MECHANISM SEARCH

One unconstrained search



Search frontier grows by approximately b at each step

C divides the search



A to C, depth $d/2$

C to E, depth $d/2$

SEARCH-SPACE MATH

Example: $b = 20$, $d = 4$, 1 ms per state

Direct four-step breadth-first search

$$1 + 20 + 400 + 8,000 + 160,000$$

$$168,421 \text{ states} = 168.4 \text{ seconds}$$

Two searches of depth two

$$2 \times (1 + 20 + 400) = 842 \text{ states}$$

$$0.842 \text{ seconds}$$

approximately 200× faster

Energy predictions prune implausible branches before the expensive calculations.

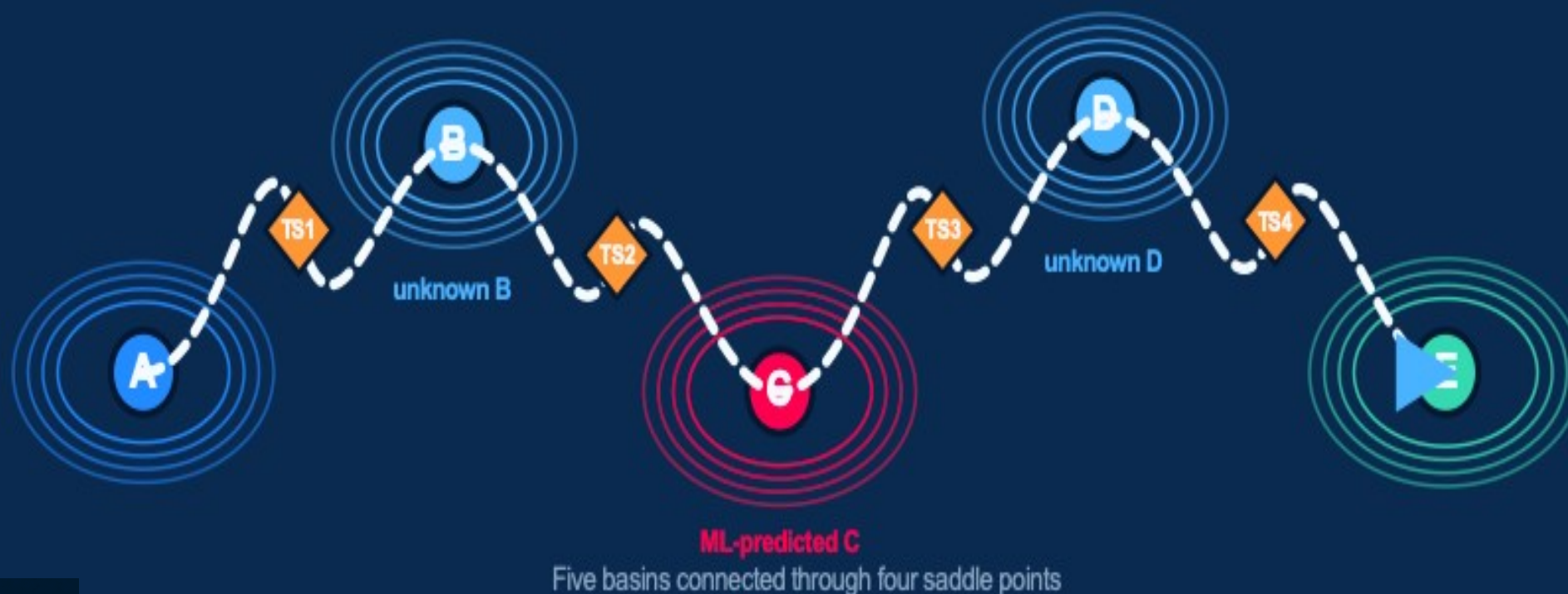
The simulator navigates the energy surface around the learned anchor

06

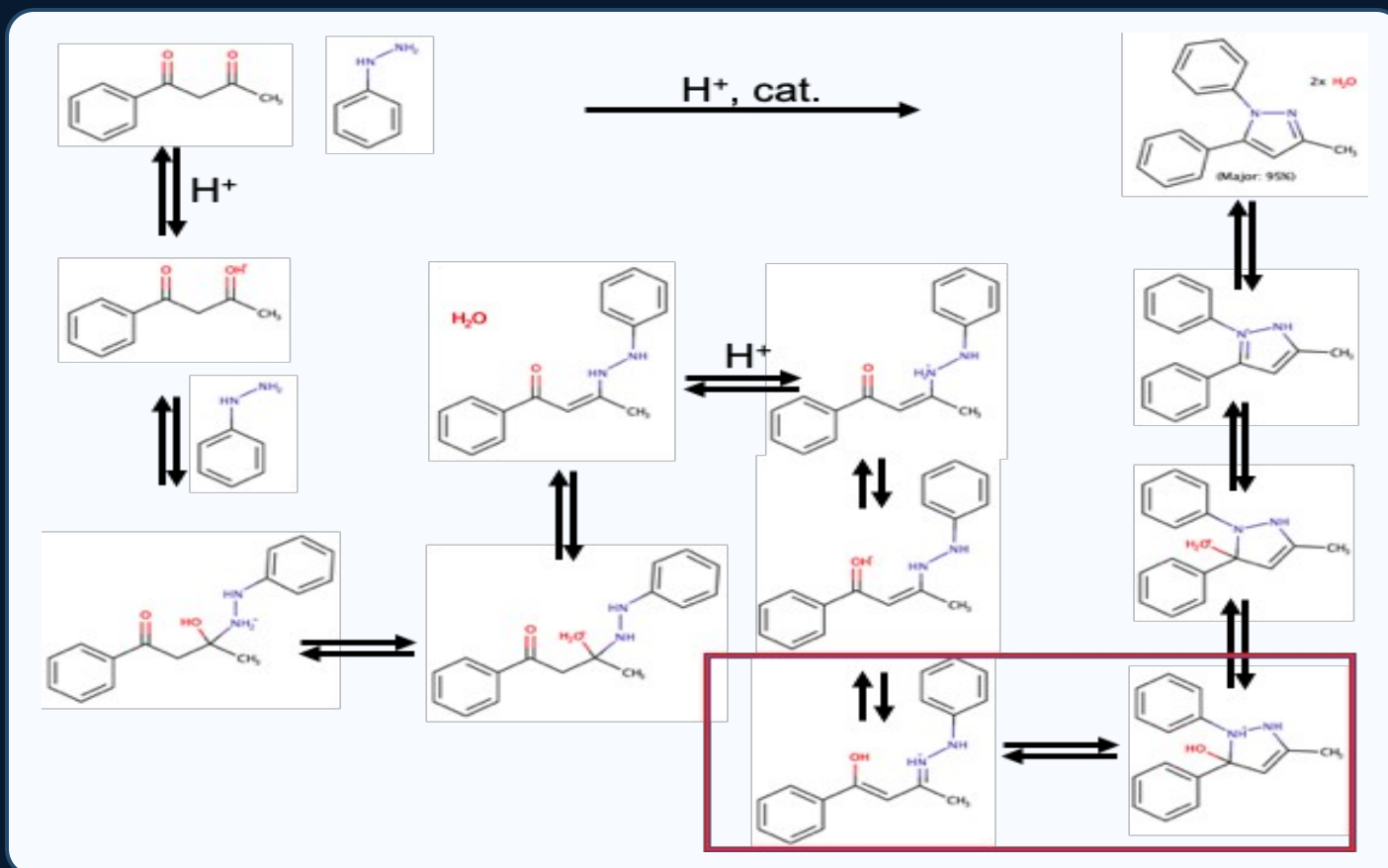
The search discovers B, D and four transition states while connecting A to E through C.

SCHEMATIC 2D PROJECTION OF THE ENERGY SURFACE

C is predicted; B, D and TS1–TS4 are discovered



Case study: mechanism and regiochemistry were both uncertain



THE DECISION

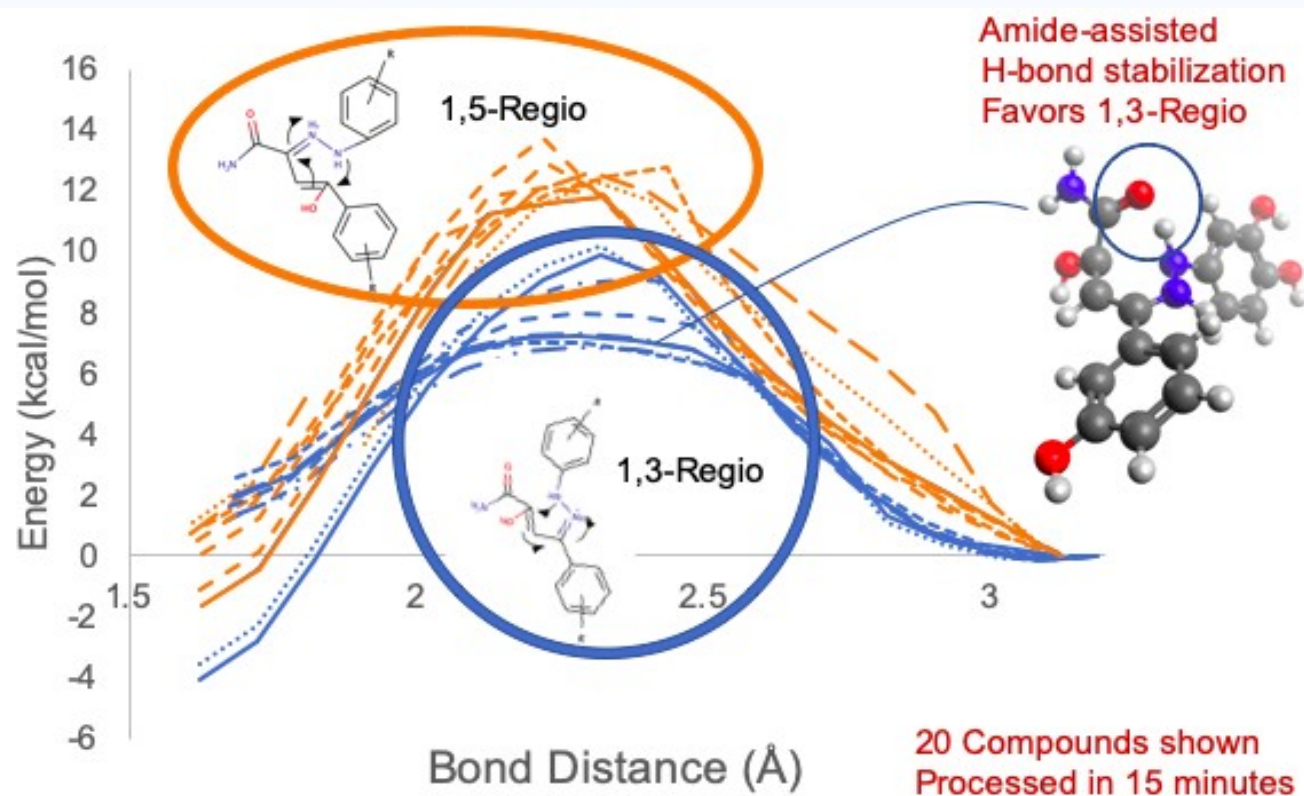
Which path is chemically viable?

Which transition state controls the rate?

Why does one regioisomer win?

A connected mechanism resolves viability, rate and regioselectivity.

The model explained the regioselectivity



MECHANISTIC INSIGHT

Amide-assisted H-bond stabilization favors the 1,3-regioisomer.

20 related compounds

processed in 15 minutes

Mechanistic insight explains the observed selectivity across related compounds.

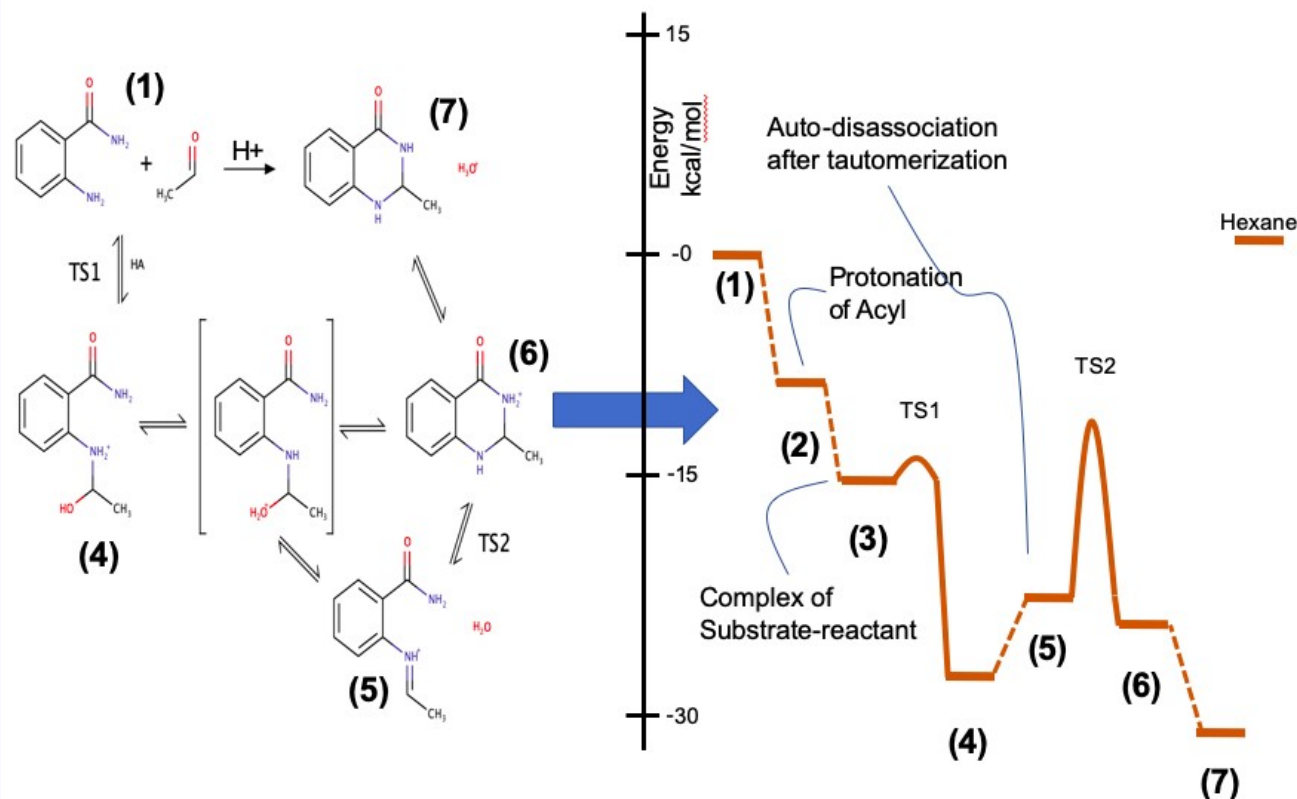
From a 2D hypothesis to a quantitative mechanism

MECHANISTIC MODEL

We transform your 2D hypothesis into quantitative thermodynamic and kinetic data.

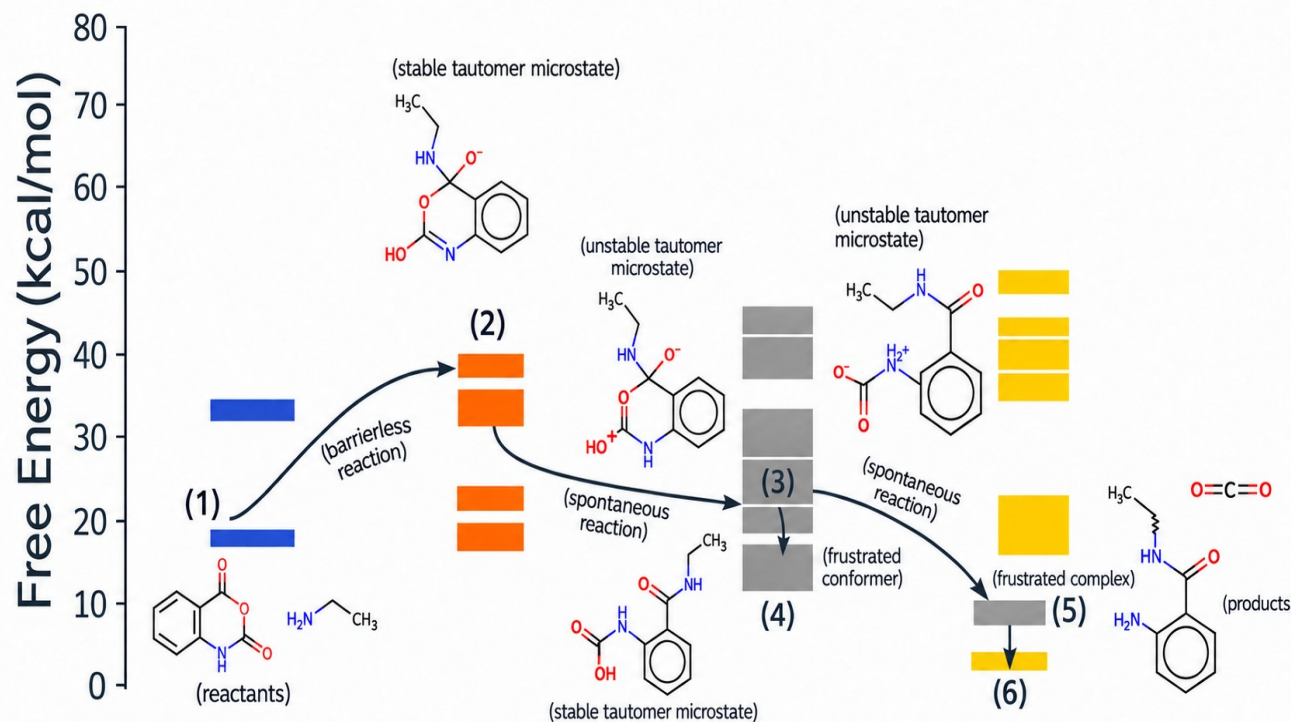
Thermodynamics ranks intermediates and pathways.

Kinetics identifies the controlling barriers and competing steps.



A quantitative definition of how the reaction works

Elementary steps across the microstate ensemble



FULLY ATOMISTIC

Each elementary step is resolved down to the microstate.

Tautomers, stereoisomers and conformers contribute according to their populations.

Single-state rate

$$k_i = \kappa(kBT/h) \exp[-(G_i^\ddagger - G_i)/RT]$$

Boltzmann population

$$p_i = \exp[-\Delta G_i/RT] / \sum_j \exp[-\Delta G_j/RT]$$

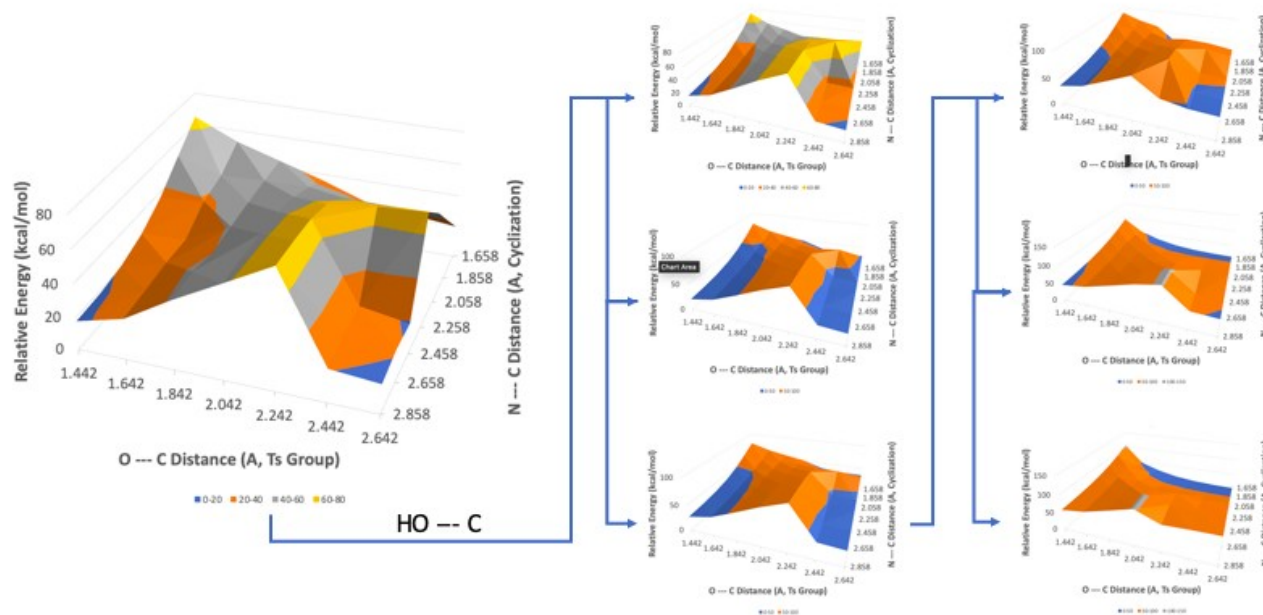
Observed ensemble rate

$$k_{obs} = \sum_i p_i k_i$$

The reactive ensemble can differ from the lowest-energy structure alone.

Mechanistic insight changed the experimental decision

Neutral Mechanism Results – Hypersurface is represented as layered surfaces at fixed HO --- C Lengths



NEUTRAL PATH

>40 kcal/mol

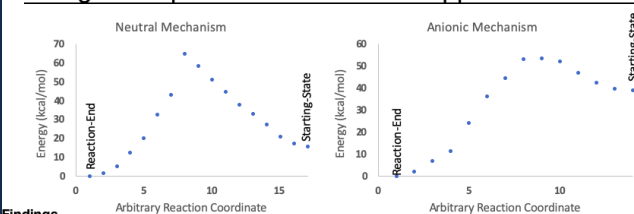
Forward barrier prohibits the proposed neutral mechanism.

ANIONIC PATH

≈15 kcal/mol

Viable at r.t.; prioritize conditions consistent with this pathway.

Reaction Barriers – Hypersurface is Traversed Using a Steepest Descent / Ascent Approach



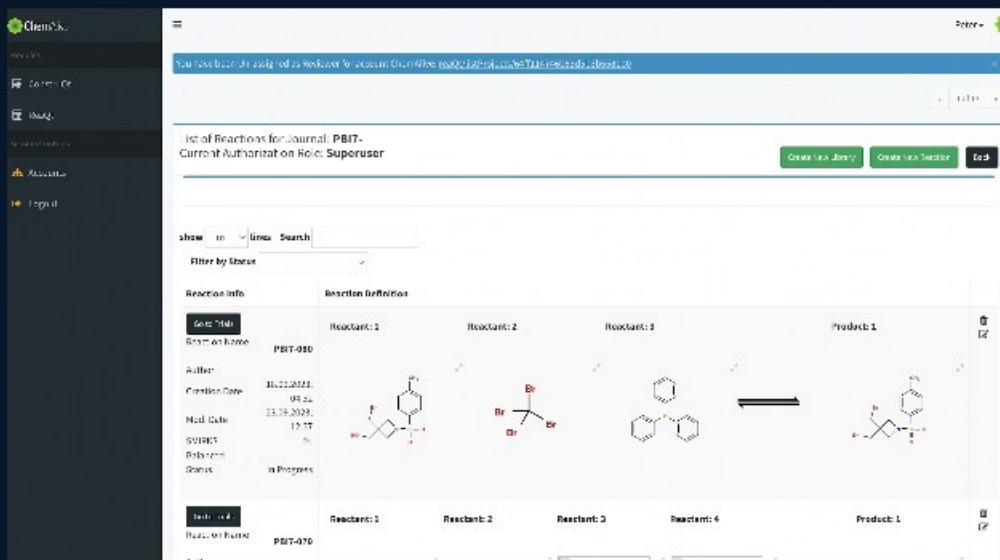
Findings

- Neutral mechanism is prohibited by unstable oxonium formed on cyclization with a forward barrier over 40 kcal/mol.
- Anionic mechanism should be available at room temperature with a forward barrier of ca. 15 kcal/mol.
- Both mechanism are thermally exothermic and essentially non-equilibrium reactions

Outcome: deprioritize the neutral route and focus validation on the anionic mechanism.

Ten years solving difficult industrial chemistry problems

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The screenshot displays the ChemScribe web application. On the left is a dark sidebar with navigation icons for Home, Projects, My Org, My Recent, My Alerts, and Logout. The main content area shows a 'List of Reactions for Journal: PB17-' with a 'Current Authorization Role: Superuser'. Below this, there's a 'Filter by Status' dropdown and a 'show' button. The interface is divided into two sections: 'Reaction Info' and 'Reaction Definition'. The 'Reaction Info' section for reaction PB17-010 lists details like Author, Creation Date (11/11/2024), Modification Date (11/11/2024), and Status (In Progress). The 'Reaction Definition' section shows a chemical reaction scheme with Reactants 1 through 4 and Product 1, represented by chemical structures and arrows.

OPERATING EXPERIENCE

Our team has supported industrial chemistry decisions for more than a decade

Chemistry-aware reaction workflows

Infrastructure designed to scale and preserve results

SELECTED INDUSTRIAL PARTNERS

SpiroChem

**Danone /
evian**

Puraffinity

Aurorium

SSE

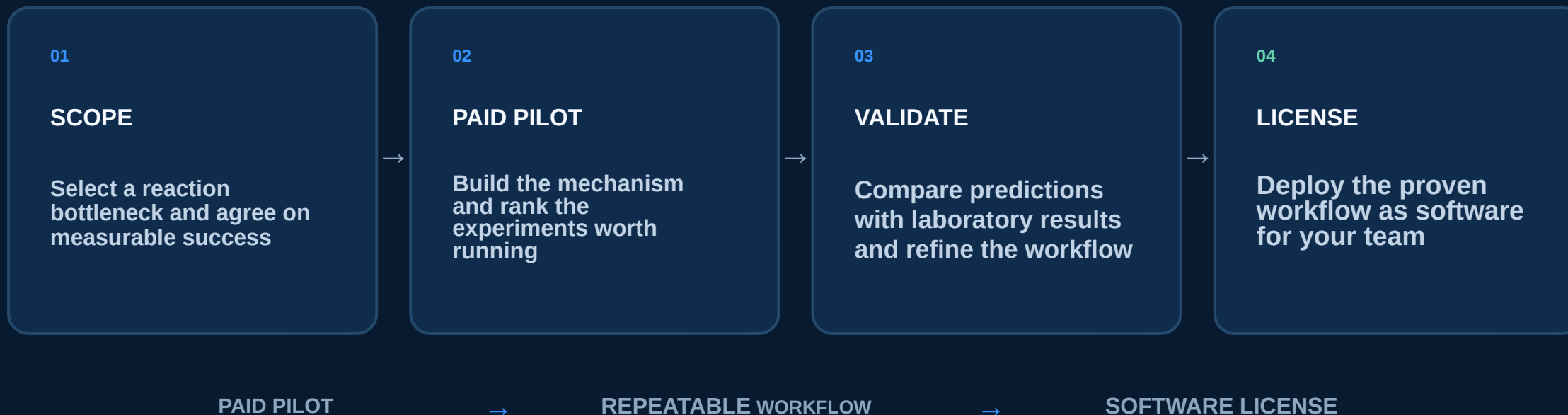
PIPELINE



AI.Qimia converts this experience into a focused product and commercial platform

Paid pilots establish fit before software licensing

We solve one real reaction problem with your team. Once the workflow performs on your chemistry, we license the platform for repeat use.



Have a reaction challenge? Please get in touch.

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