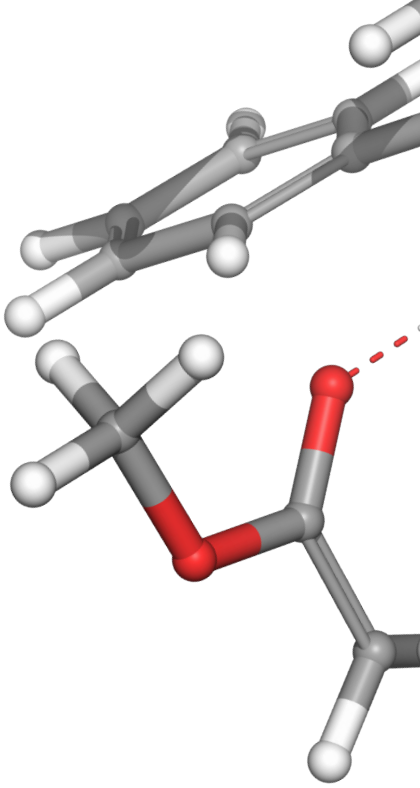
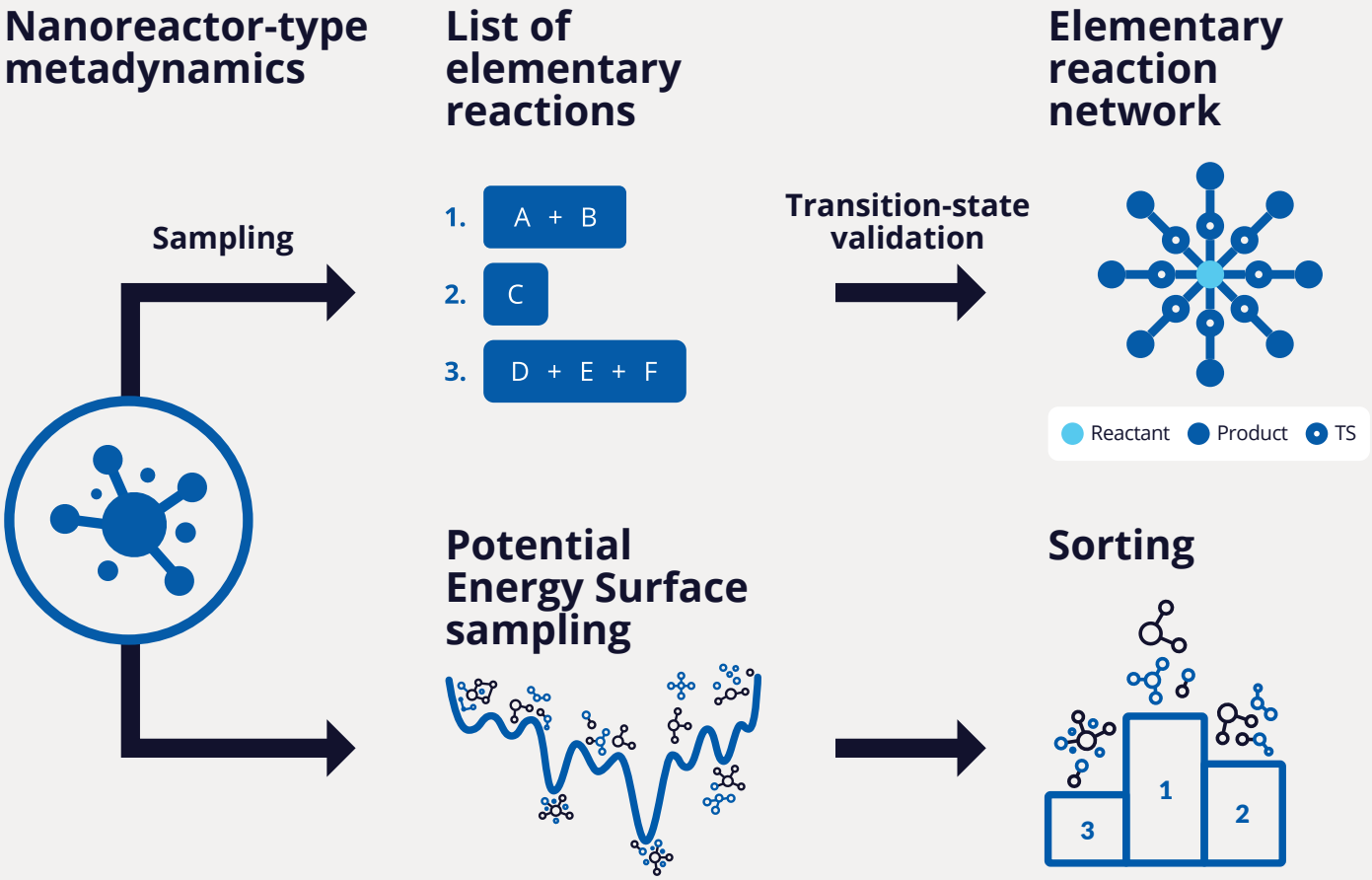
Nanoreactor



Automated reaction discovery lies at the heart of predictive chemistry, enabling chemists to design chemical processes that are smarter, faster, cleaner, and more efficient. **Nanoreactor – Elementary Reaction Network (ERN)**, a workflow developed by Schrödinger, automates the identification of products arising from kinetically accessible elementary reactions starting from a known local minimum on the potential energy surface (PES), using nanoreactor-type molecular dynamics-based enhanced sampling coupled with an integrated workflow for automated transition-state identification.

Complementing this, **Potential Energy Surface Sampling-Sorting (PESS)** enhances Nanoreactor's capabilities by systematically exploring and ranking minima on PES. Since chemical reactions tend to follow the downhill path on the free energy surface, this feature focuses on pinpointing the most probable final products from a thermodynamic perspective.



Schrödinger

Nanoreactor - ERN

Thermal decomposition of amoxycillin

Predict the kinetically acccessible elementary reaction network for the thermal decomposition of the antibiotic amoxicillin, using only its 2D structure as input. This reactivity corresponds to the predicted first step of the drug's thermal non-radical (heterolytic) degradation pathway.

Google Cloud

High Performance Computing (HPC) Cluster

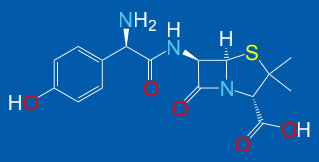
500 trajectories sampled

40 kcal/mol filter (wrt reactant, Free Energy)

UMA_SM_OMOL v 1.1

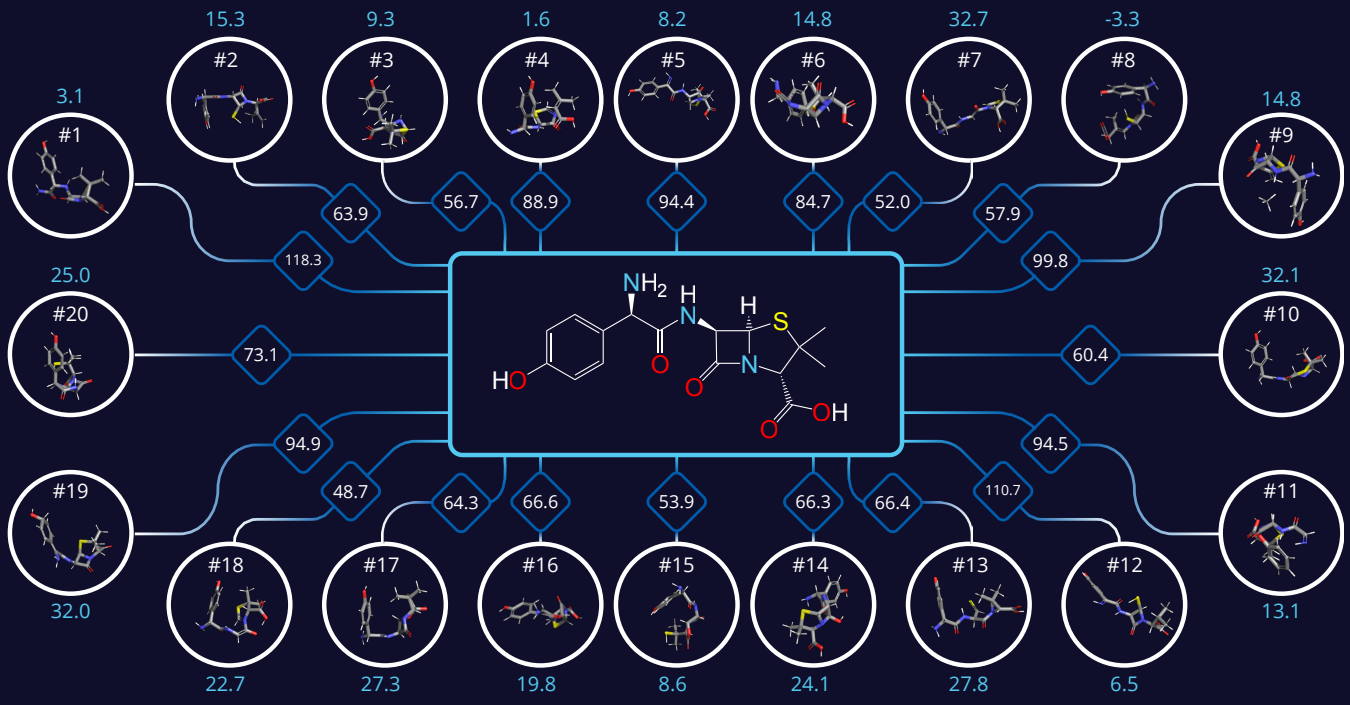
~ 24 hrs

Amoxicillin



Relevant elementary reactions

Energies in kcal/mol



Nanoreactor - ERN

Thermal decomposition of perfluorooctanoic acid

Predict the kinetically acccessible elementary reaction network for the thermal decomposition of PFOA. This reactivity corresponds to the predicted first step of the PFOA's non-radical (heterolytic) degradation pathway.

Google Cloud

High Performance Computing (HPC) Cluster

1000 trajectories sampled

40 kcal/mol filter (wrt reactant, Free Energy)

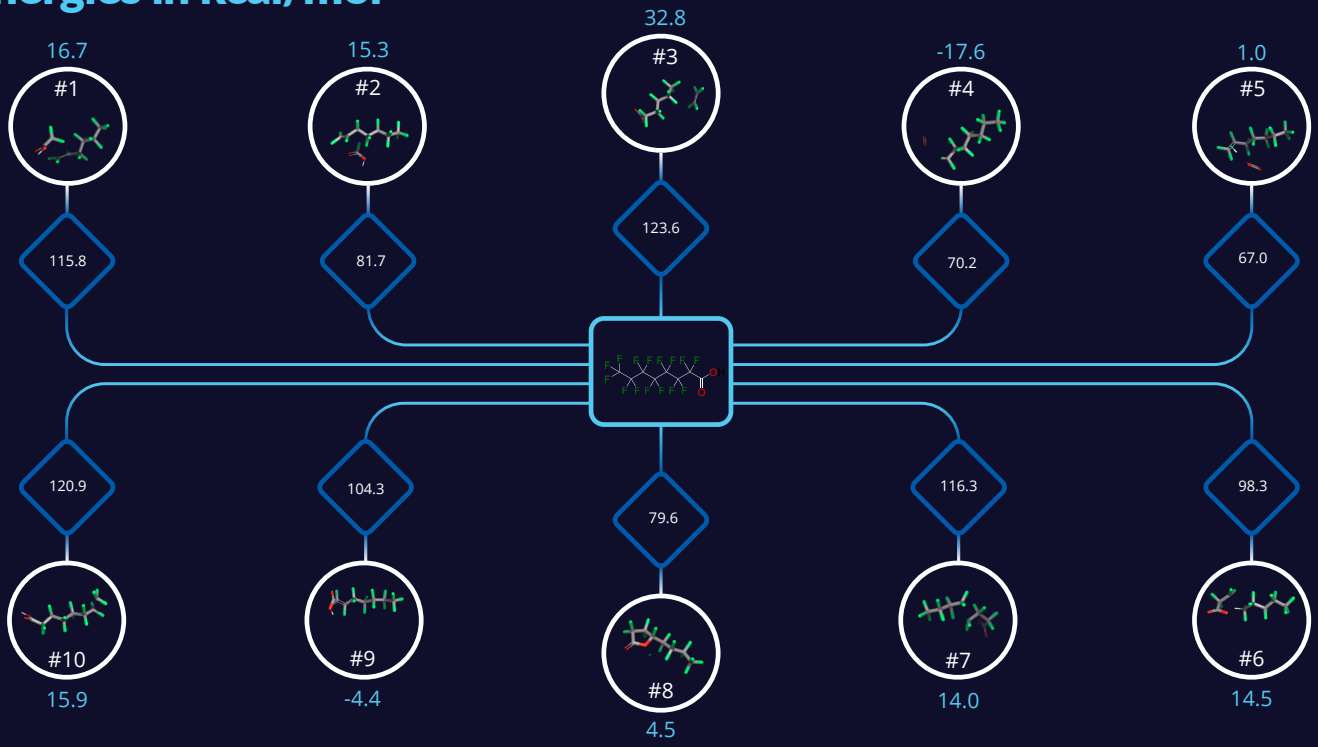
UMA_SM_OMOL v 1.1

~ 24 hrs

PFOA

Relevant elementary reactions

Energies in kcal/mol

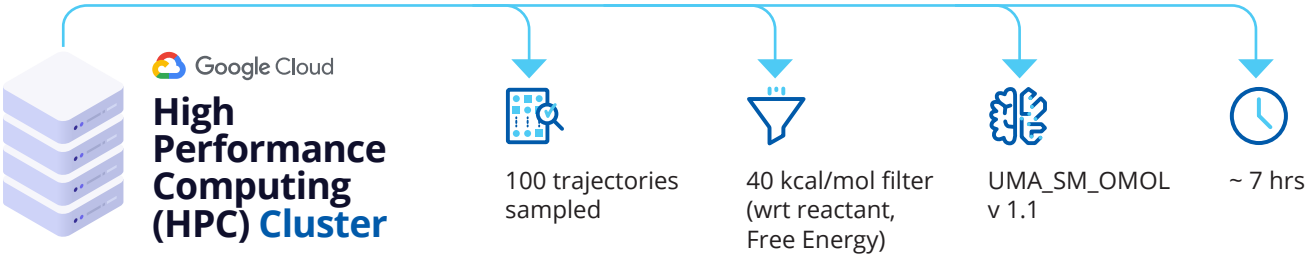


Reactant TS Product

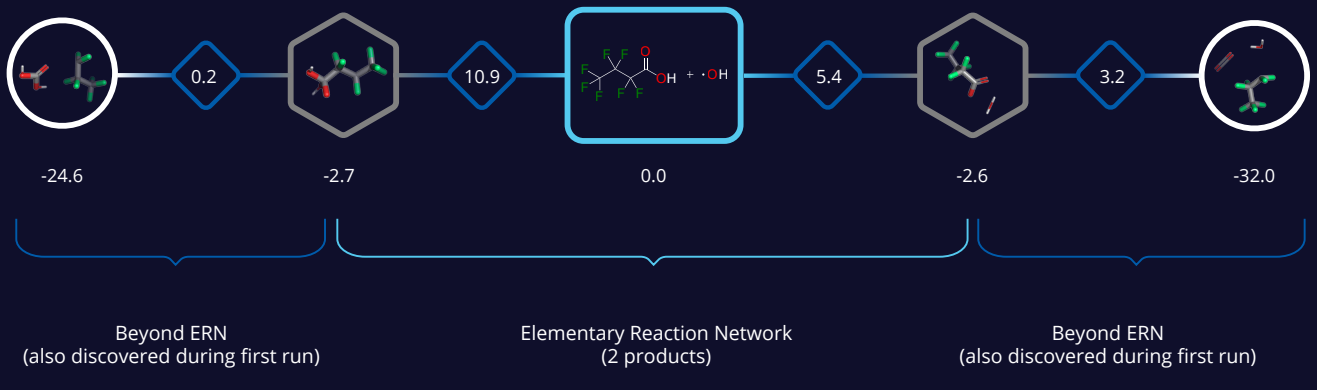
ΔG, kcal/mol

Nanoreactor - ERN

Reaction of HFBA acid with the HO· radical



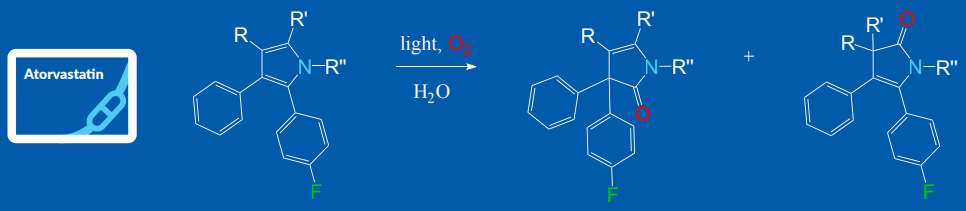
Energies in kcal/mol



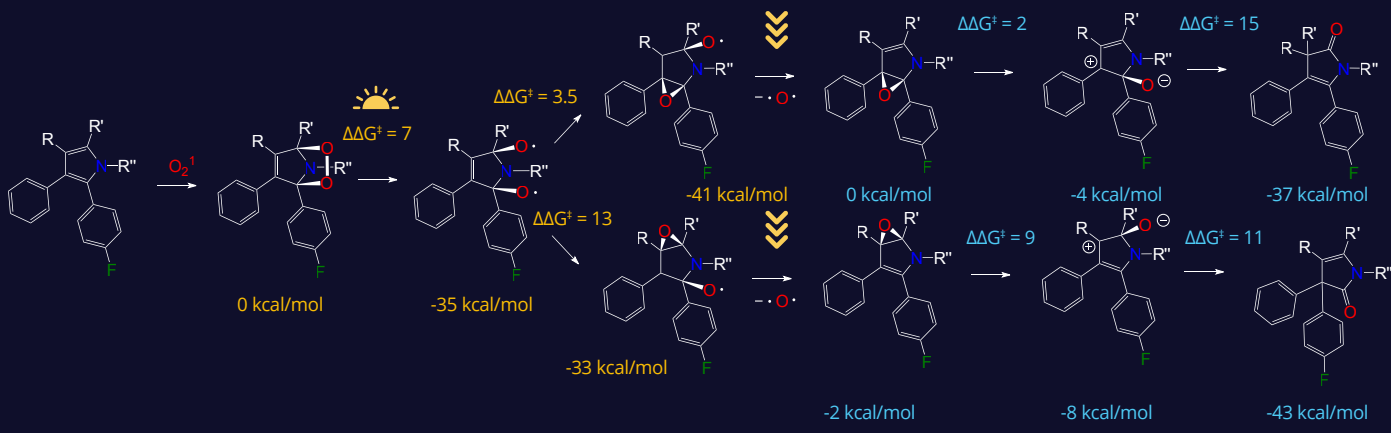
Nanoreactor-ERN (sampling) + AutoTS for mechanism discovery

Oxidative degradation of Atorvastatin

Challenge: unknown reaction mechanism



Solution: discovered reaction mechanism



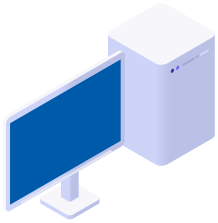
sunlight-induced

excited-to-ground state relaxation

Nanoreactor - PESS

Aspirin thermal hydrolysis

Predict plausible degradation products of active pharmaceutical ingredients, for example, the thermal hydrolysis of aspirin.

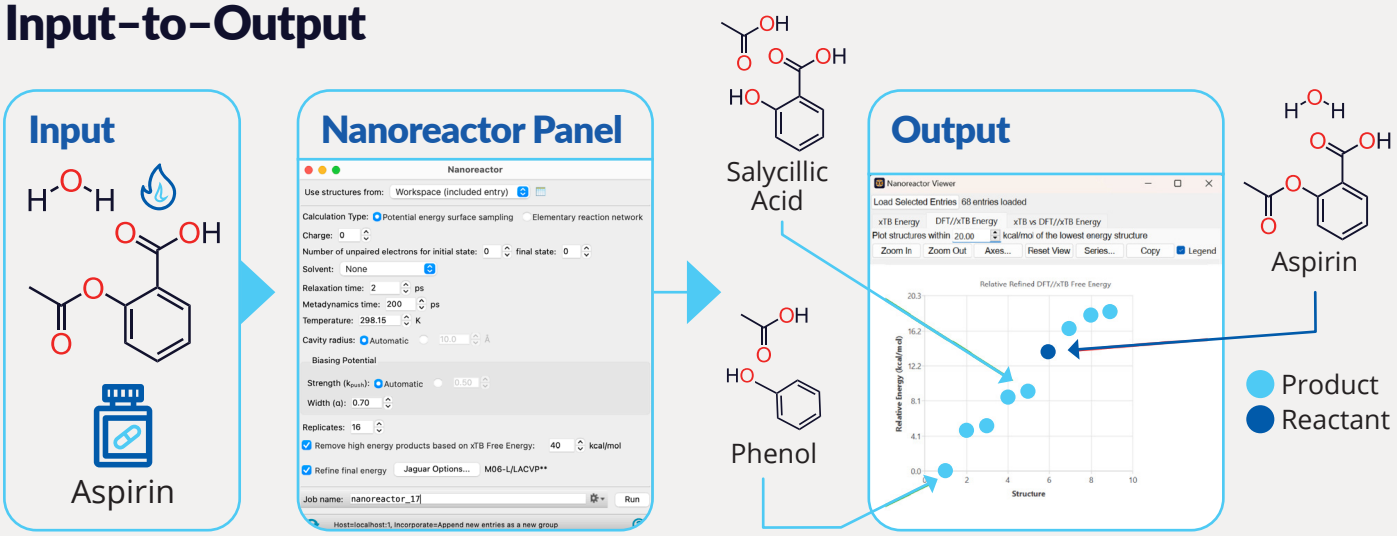


Personal Computer

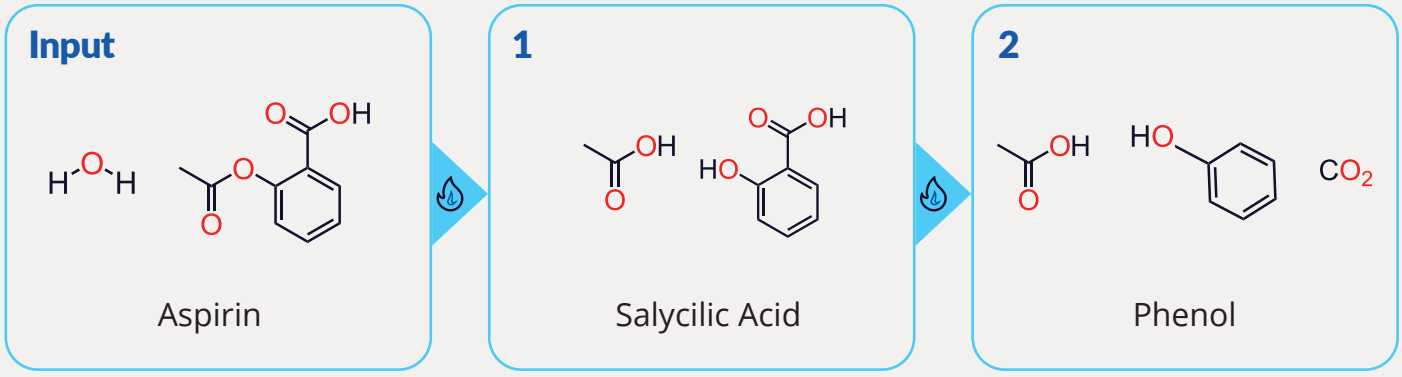
16 cores

~17 hours

Input–to–Output



Input–to–Interpretation



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