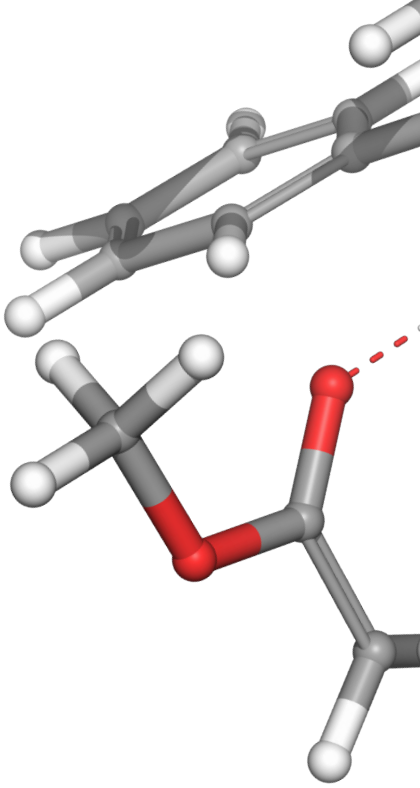
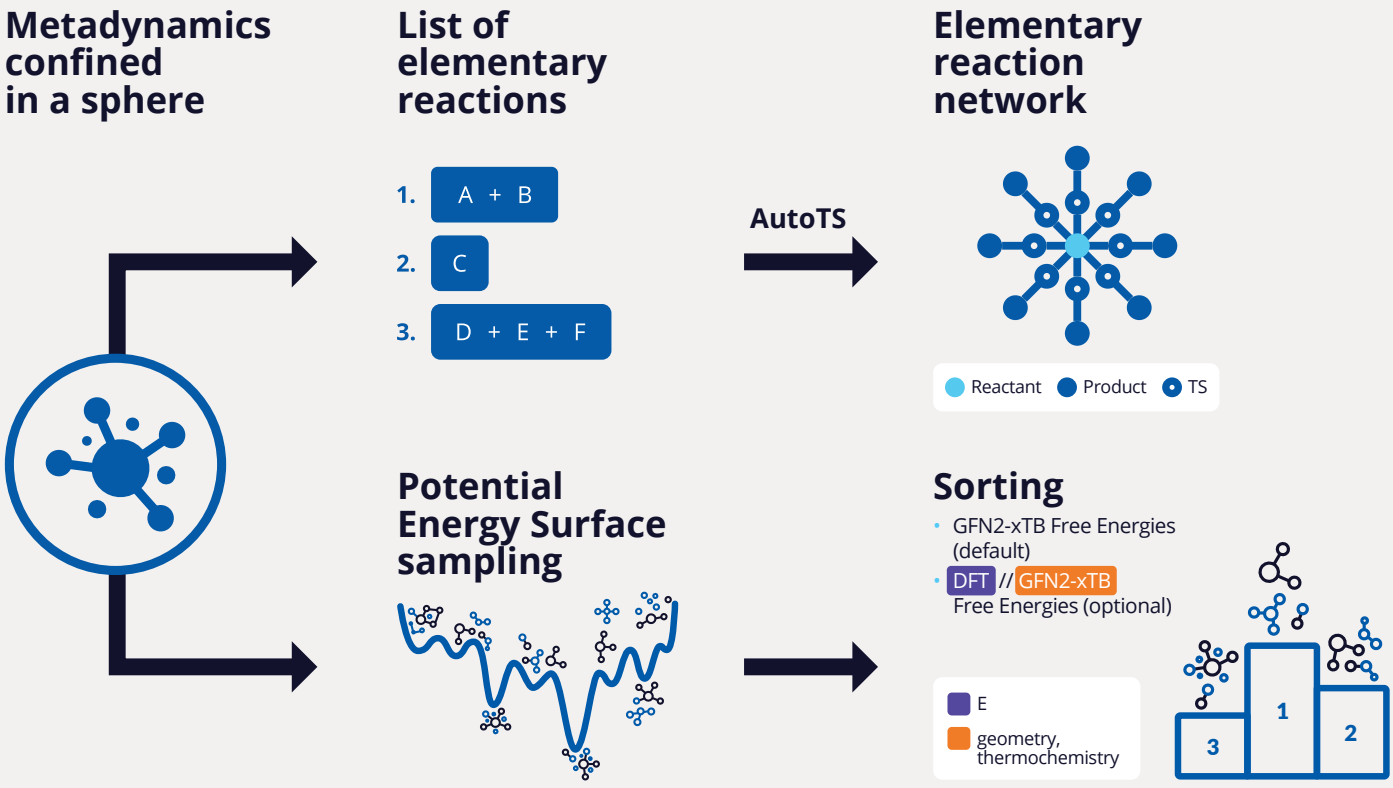
Nanoreactor



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 tool developed by Schrödinger, automates the identification of relevant elementary reactions starting from a known local minimum on the xTB potential energy surface (PES). Complementing this, **Potential Energy Surface Sampling-Sorting (PESS)** enhances Nanoreactor's capabilities by systematically exploring and ranking minima states on xTB (DFT, or MLFF) 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.



Schrödinger

Nanoreactor - ERN

Thermal decomposition of amoxycillin

Predict the relevant elementary reaction network and associated organic_ MPNICE//xTB Free energies for the thermal decomposition of the antibiotic amoxicillin, using only its 2D structure as input. This reactivity corresponds to the predicted initial step of the drug's thermal degradation pathway. Transition state search and optimization are performed separately using AutoTS.

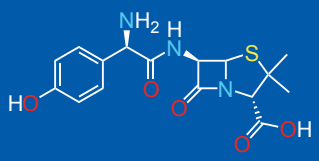
Google Cloud

High Performance Computing (HPC) Cluster

100 cores

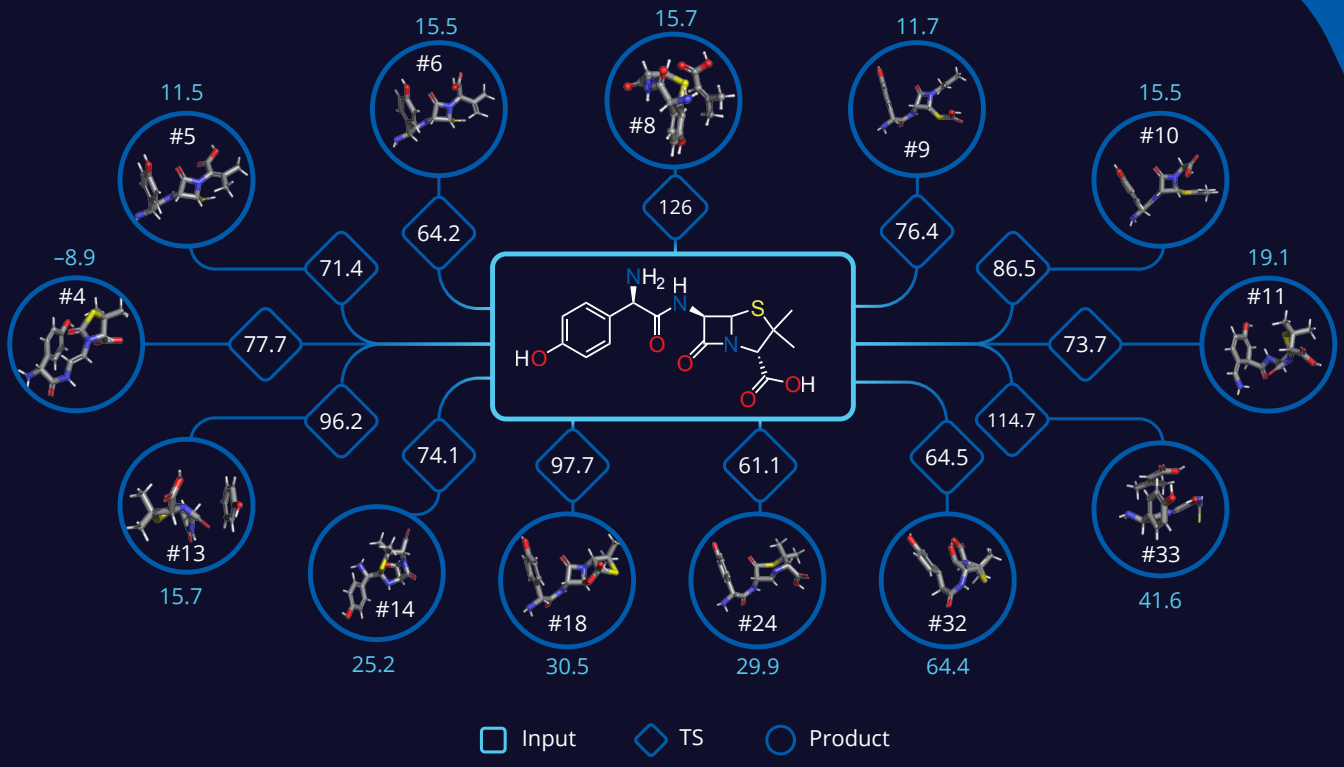
~15 min

Amoxicillin



Relevant elementary reactions

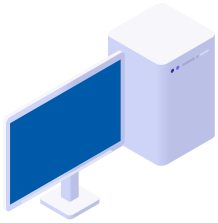
Energies in kcal/mol



Nanoreactor - PESS

Aspirin thermal hydrolysis

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

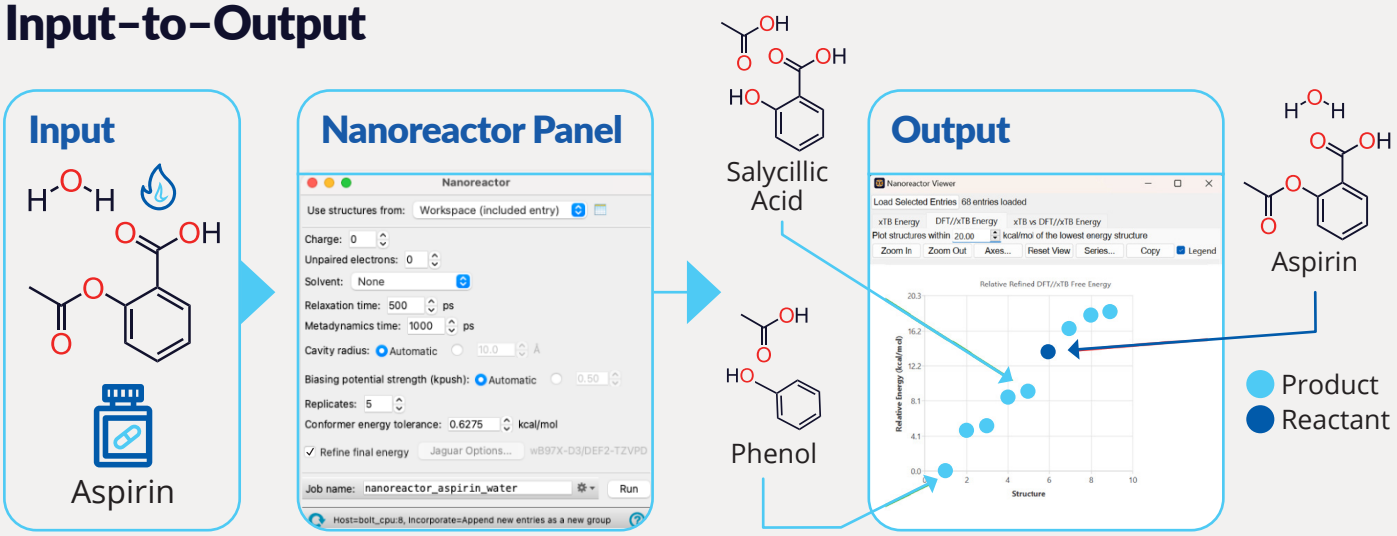


Personal Computer

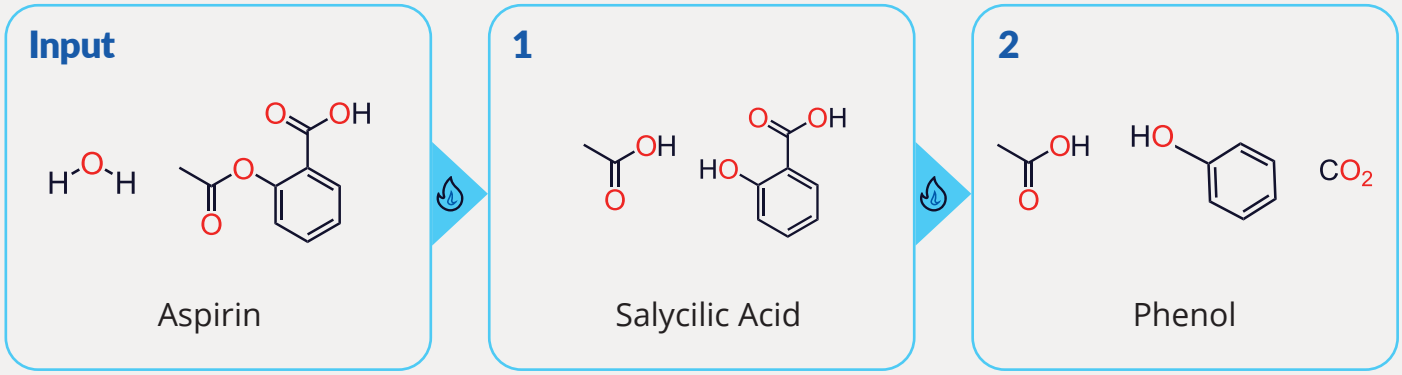
16 cores

~17 hours

Input–to–Output



Input–to–Interpretation



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Learn more: www.schrodinger.com/platform/products/ms-reactivity

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Connect with an expert to learn more