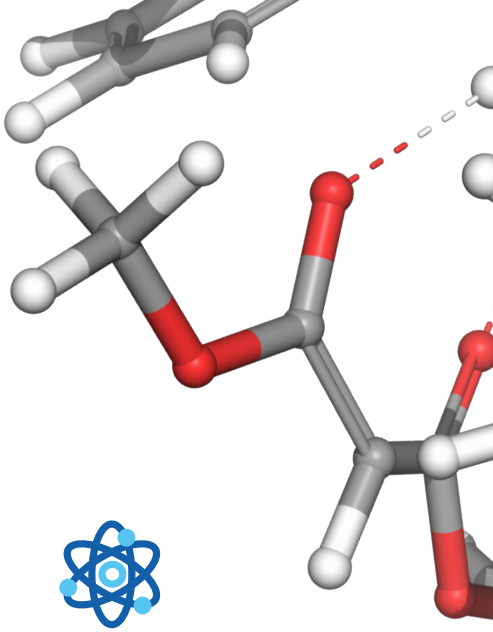
Nanoreactor

Automated potential energy surface (PES) sampling and sorting with extended tight-binding (xTB) and density functional theory (DFT)



Highlights

- Enhanced Nanoreactor with new features, expanding upon the tool developed by Grimme and co-workers[1], including improved energy refinement of results, sorting and integrated user interface
- Highly automated solution for indirect prediction of chemical degradation products

Use cases

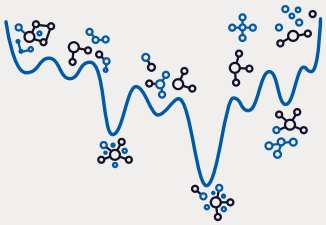
- Identify intermediates and products for any chemical reaction
- Predict products for chemical degradation of small molecules
- Simulate thermal decomposition, oxidation, hydrolysis, and photodegradation
- Perform PES sampling (restricted to minima states)

Key methods

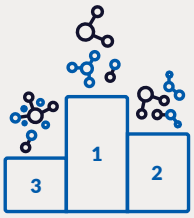
- Metadynamics
- Semiempirical GFN2-xTB extended tight binding quantum method
- Pseudospectral and composite DFT

Input (XYZ, SMILES)

- One or few molecules, ions, radicals
- Closed or open-shell system (conserves total spin)



Potential Energy Surface sampling and minima generation through GFN2-xTB metadynamics and optimization



Sorting

- GFN2-xTB Free Energies (default)
- DFT//GFN2-xTB Free Energies (optional)

E — geometry, thermochemistry

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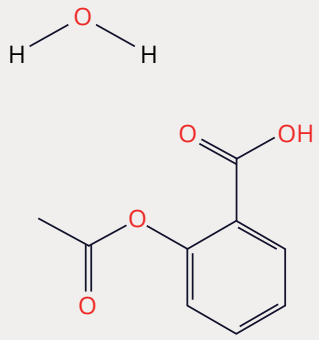
Example: Hydrolysis of aspirin

Predict plausible degradation products of active pharmaceutical ingredients using xTB metadynamics. Optionally identify their thermodynamic sorting with free energy refinement.

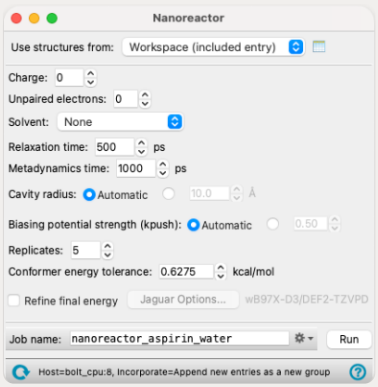
Highlights

- Simulation results align well with experiments
- Can be performed on laptop-type compute resources

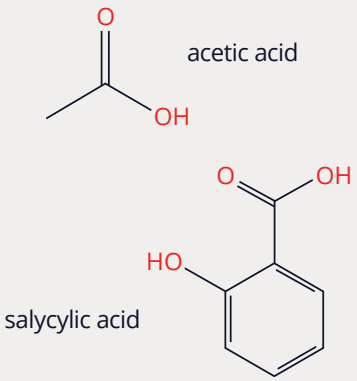
Input



Nanoreactor Panel



Output



Reference

1. Exploration of Chemical Compound, Conformer, and Reaction Space with Meta-Dynamics Simulations Based on Tight-Binding Quantum Chemical Calculations, Stefan Grimme, *J. Chem. Theory Comput.* 2019, 15, 5, 2847–2862.

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