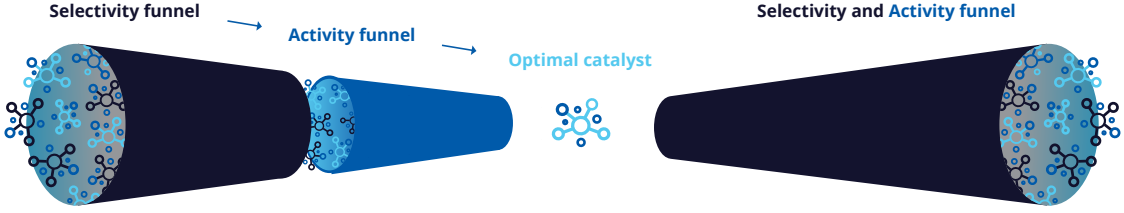
Automated Reaction Workflow

Massively parallel physics-based computational workflow for molecular catalyst design

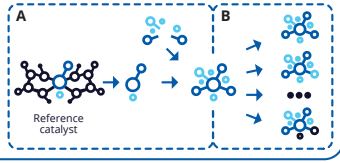
Two approaches available



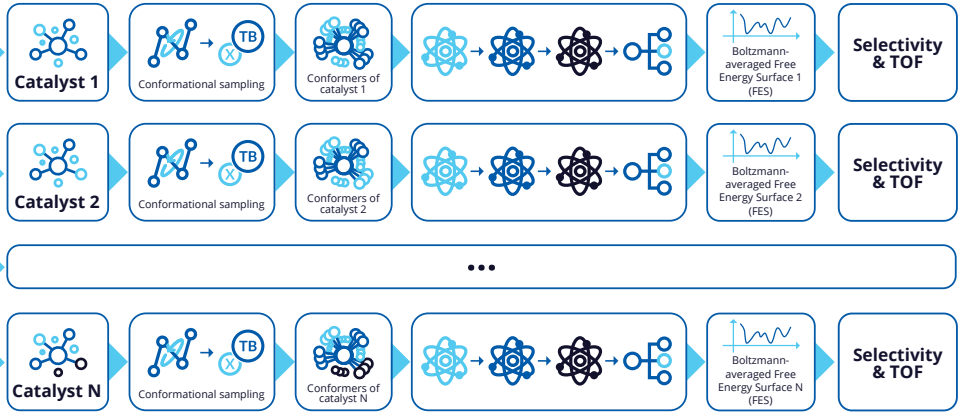
User-friendly GUI

1 **Knowledge of the catalytic reaction mechanism for reference "template" catalyst:**
- 3D structures for selectivity-determining TSs
- 3D structures for catalytic cycle

2 **Fragment swapping[A] + R-group libraries[B]**



3 **DFT method + basis set**



Force Field (optional) → xTB (optional) → DFT preoptimization → DFT optimization → DFT single point → Analysis

Schrödinger

For more information, please contact:
Pavel Dub, Sr Research Scientist, Product Manager and Scientific Lead for Reactivity and Catalysis
pavel.dub@schrodinger.com