

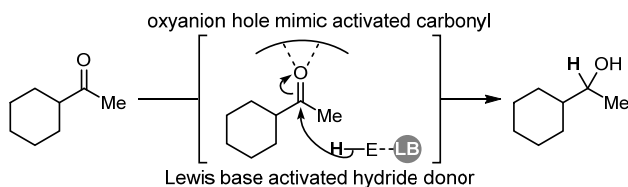
SYNTHETIC KETOREDUCTASE MIMICS

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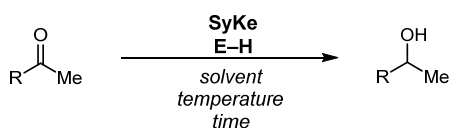
Efficient and selective reduction of carbonyl groups is a fundamental challenge in synthetic chemistry. While current synthetic methods often rely on rare transition-metals and harsh conditions, in Nature, reductions of ketones proceed under ambient aqueous conditions with outstanding selectivities. The use of bifunctional foldamer-type catalysts as synthetic ketoreductase (SyKe) mimics for this purpose has been investigated. Rigid catalyst scaffold forms an enzyme-like catalytic pocket for the substrate and the reductant. Initial results show proof-of-concept level enantioselectivity. Further optimization is driven by linear-free energy relationship modeling.

Enzyme-like bifunctional catalyst concept

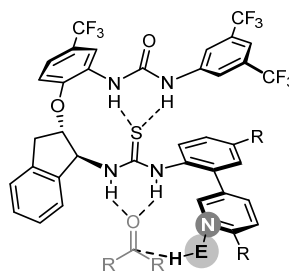


- dual activation of both the electrophilic carbonyl and the nucleophilic hydride
- tethering the two catalytic sites into a single catalyst provides full control of the reactive site

Reaction optimization



Tailored foldamer-type SyKe catalyst



Main-group element hydrides (E-H)

