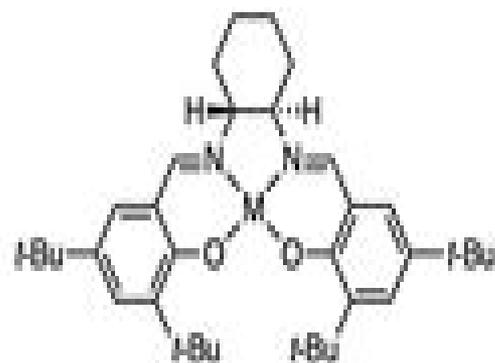
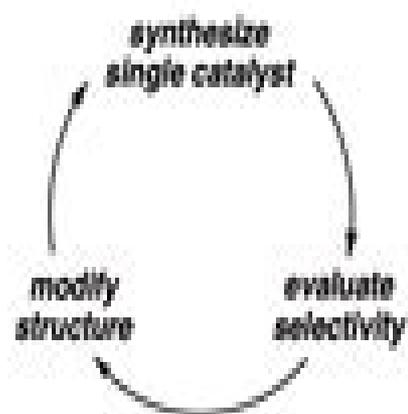
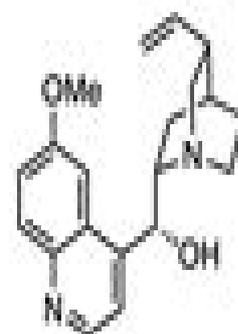


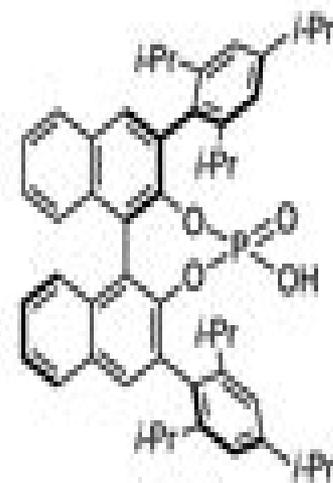
# A. Current method for catalyst design and representative privileged catalyst scaffolds



salen complexes

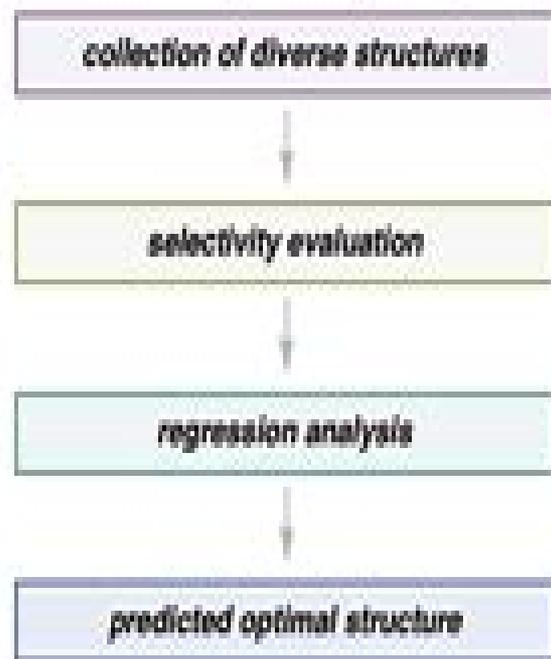


cinchona alkaloid derivatives

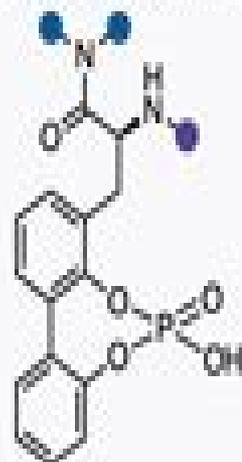


BINOL

# B. Alternative strategy for catalyst design using data science tools



## novel catalyst family



- conformationally flexible
- predictable NCIs
- readily diversifiable core

# C. Key catalyst features



intramolecular hydrogen bonding networks dictate shape of chiral pocket

# Advances In Catalyst Design

**ML Yell**



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