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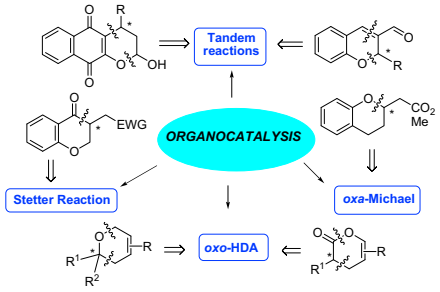
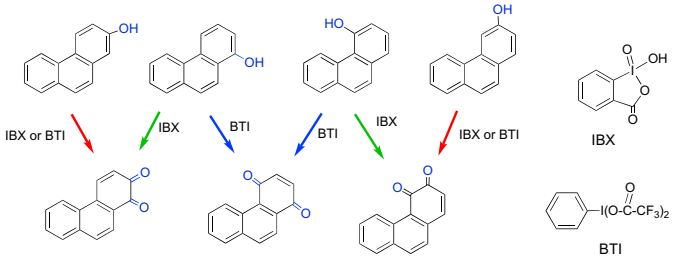
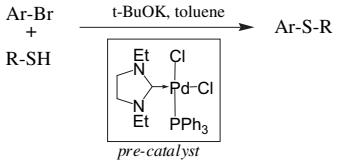
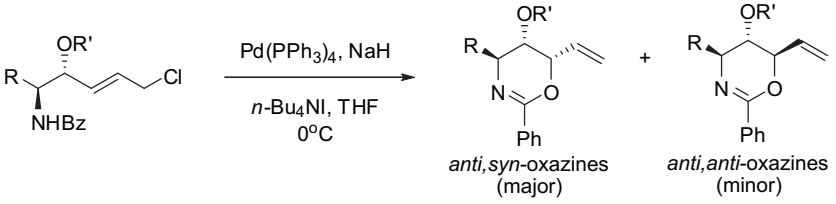
REPORT

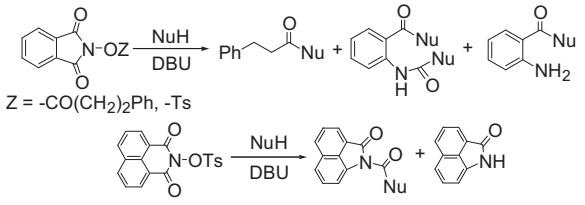


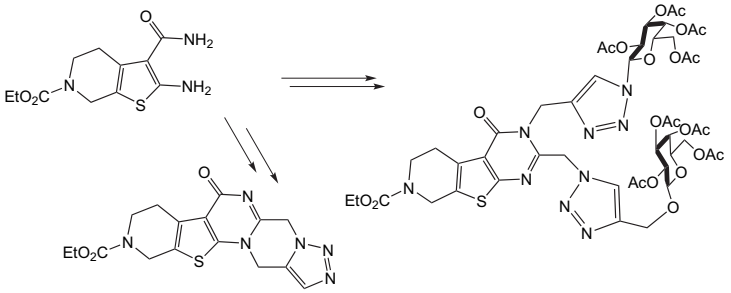
ARTICLES

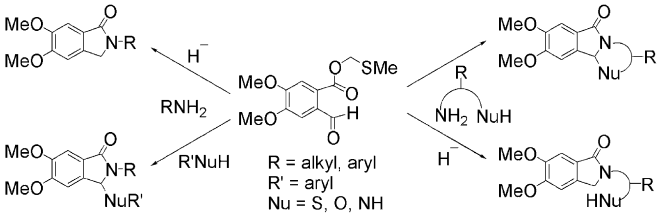


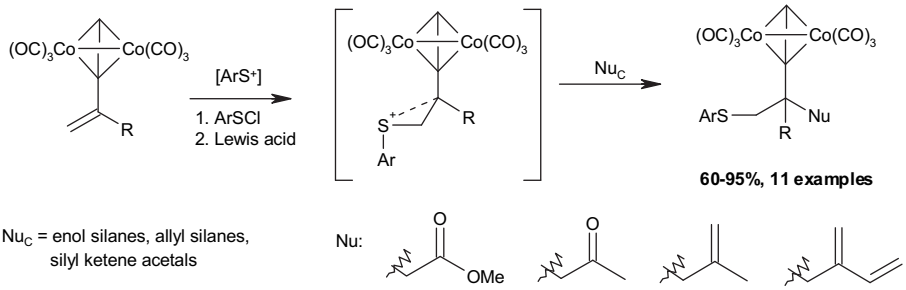


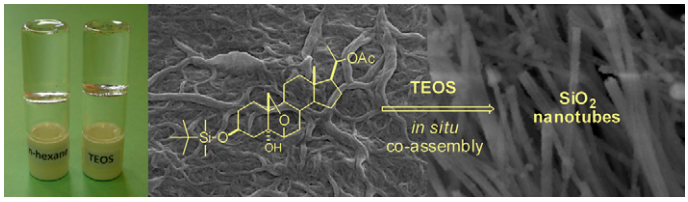


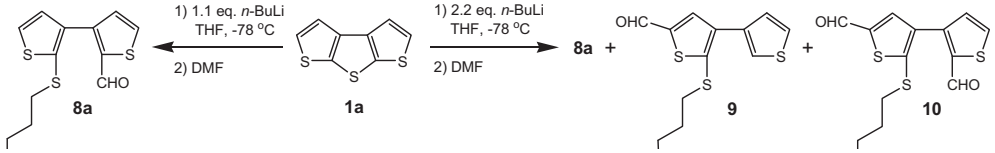


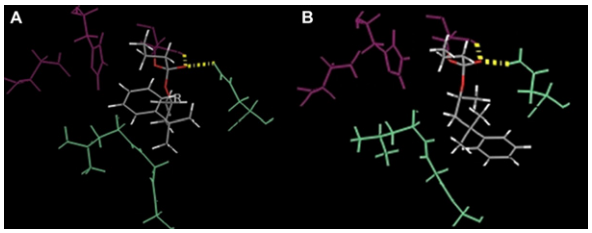




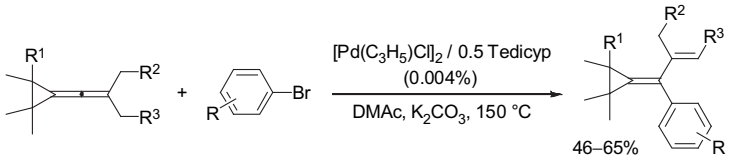


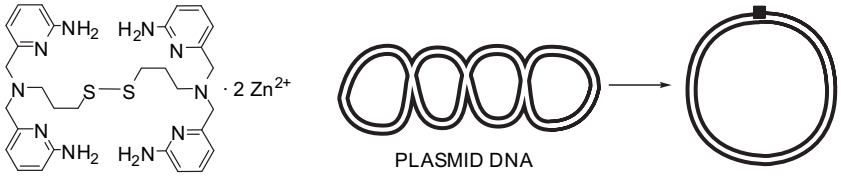




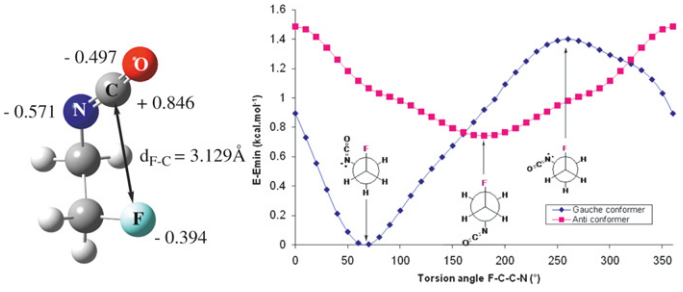


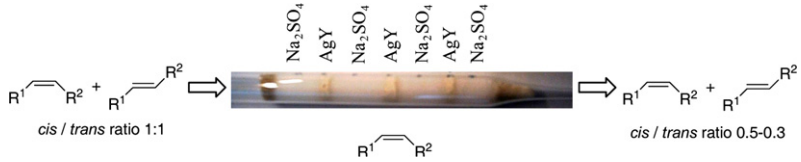
Modeling of the tetrahedral intermediates of (*R*)-**A** and (*S*)-**B** 4-methyl-4-phenyl-2-pentanol in the active site of subtilisin Carlsberg reveals the reason for high enantioselectivity (*E*=240).

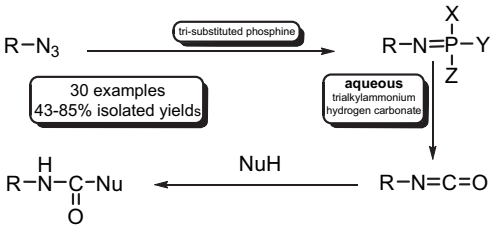




DFT derived conformational energy profiles of a series of 2-substituted fluoroethanes (F–CH_2CH_2–X) have been explored relative to 1,2-difluoroethane, a compound which exhibits a *gauche* preference. Steric, electrostatic and NBO interactions were explored. In the event the *gauche* preference for 1,2-difluoroethane is largely hyperconjugative in origin, whereas the conformational preference for the remaining structures is most reasonably explained as a balance between hyperconjugative, steric and electrostatic effects.







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Supplementary data available via ScienceDirect

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