Chemo- and Diastereoselective Tandem Dual Oxidation of B(pin)-substituted Allylic Alcohols: Synthesis of B(pin)-substituted Epoxy Alcohols, 2-Keto-anti-1,3-diols and Dihydroxy-tetrahydrofuran-3-ones

Nusrah Hussain, Mahmud M. Hussain, Patrick J. Carroll and Patrick J. Walsh*

P. Roy and Diana T. Vagelos Laboratories, Department of Chemistry, University of Pennsylvania, 231 S. 34th Street, Philadelphia, PA 19104-6323
pwalsh@sas.upenn.edu

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Part 2

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Electronic Supplementary Material (ESI) for Chemical Science
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Figure S31. ORTEP drawing of 4-hydroxy-5-(hydroxyl(phenyl)methyl)-5-methyl-2-phenyldihydrofuran-3-(2H)-one (6k) with 30% probability thermal ellipsoids.
Preliminary Computational Studies:

All calculations were optimized using GAUSSIAN09, B3LYP or M06-2X functional with the 6-31G(d) or 6-311G(d,p), basis set in the gas phase and in dichloromethane using CPCM solvation model and UFF radii. Optimizing transition state structures using (U)B3LYP with guess=(mix, always) did not revealed any changes in spin state. Frequency analysis was used to characterize each stationary point as minima or transition state structure. Further, IRC calculations were carried out on model systems to connect transition state structures to minima.

Figure S31. Relative barriers for epoxidations of model alkenes. All structures were calculated using B3LYP/6-31G(d) in gas phase and in dichloromethane (CPCM;UFF radii), in parenthesis, using M06-2X/6-311G(d,p). Reported energies are in kcal/mol. Pinacolato ligand was modeled as C2H4O2.

References:
