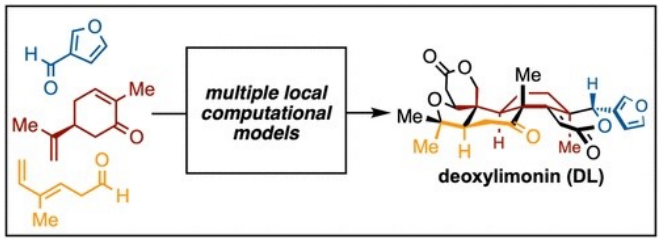
Development of Multiple Local Computational Models in Retrosynthetic Analysis: Total Synthesis of (-)-Deoxylimonin

Leanna M. Gharbaoui,* Jungmin Eun,* Yizhou: Zhao, and Timothy R.



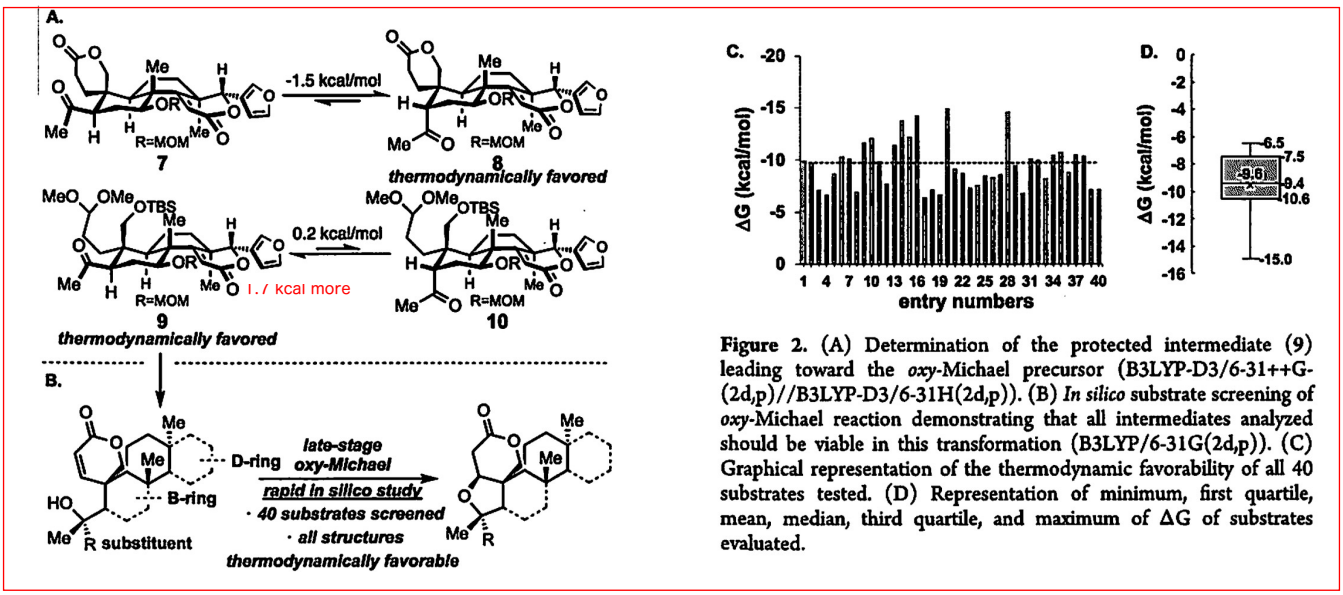
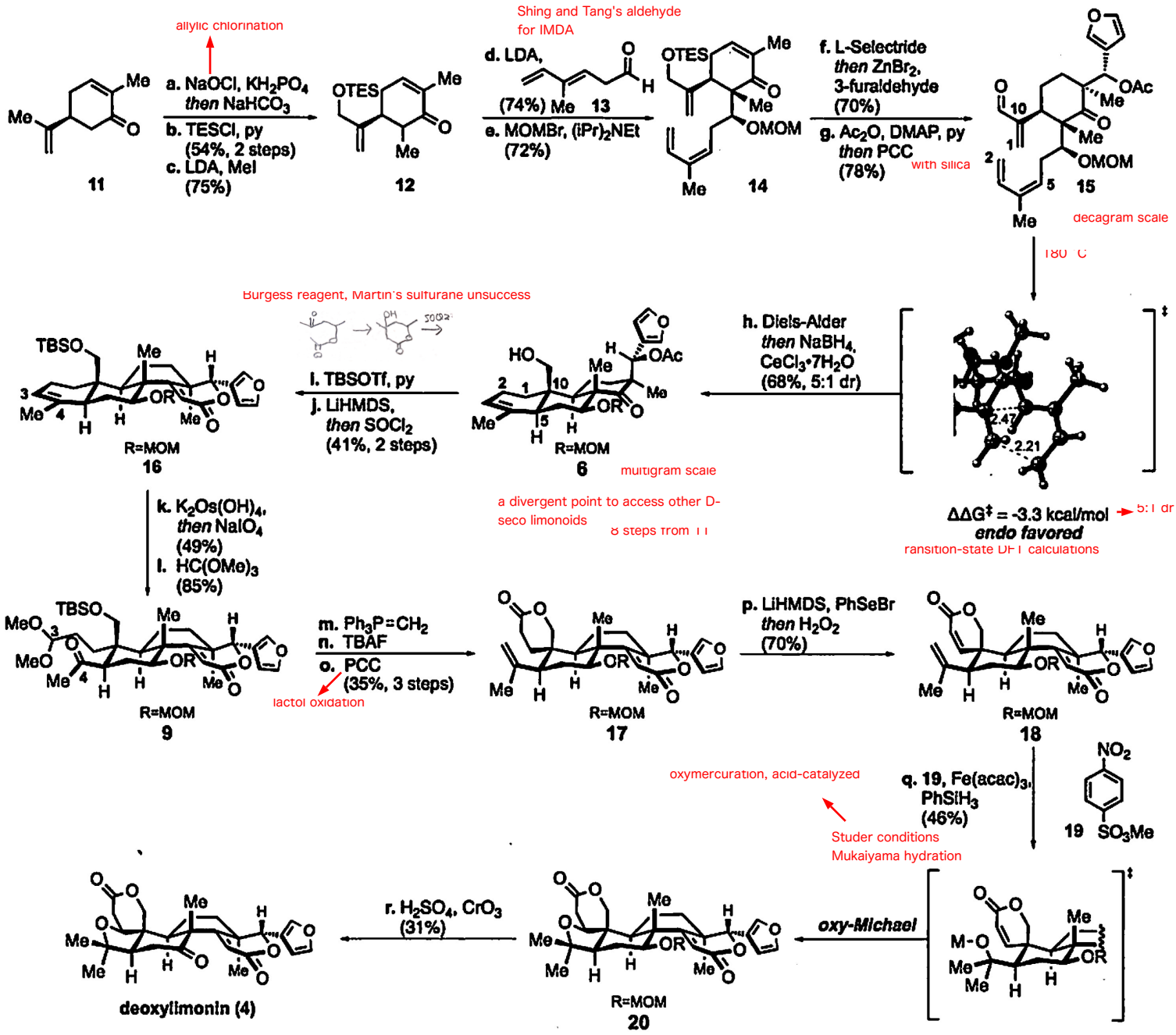



Figure 2. (A) Determination of the protected intermediate (9) leading toward the *oxy*-Michael precursor (B3LYP-D3/6-31++G-(2d,p)//B3LYP-D3/6-31H(2d,p)). (B) *In silico* substrate screening of *oxy*-Michael reaction demonstrating that all intermediates analyzed should be viable in this transformation (B3LYP/6-31G(2d,p)). (C) Graphical representation of the thermodynamic favorability of all 40 substrates tested. (D) Representation of minimum, first quartile, mean, median, third quartile, and maximum of ΔG of substrates evaluated.