

Total Synthesis of Taxol Enabled by Intermolecular Radical Coupling and Pd-Catalyzed Cyclization

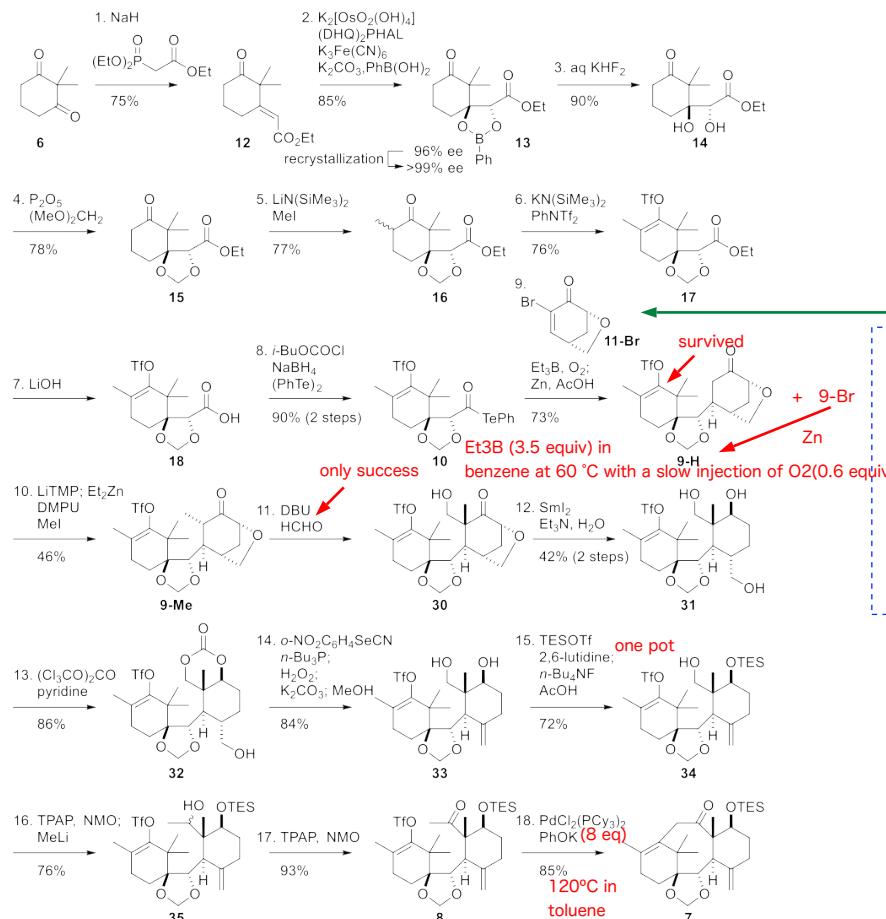
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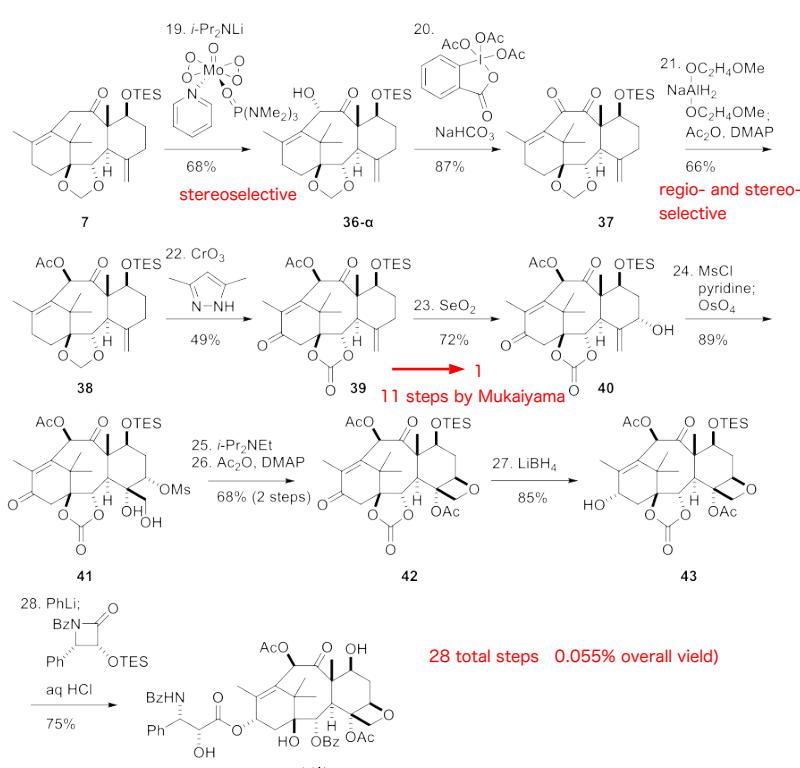
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11 total syntheses and 3 formal syntheses

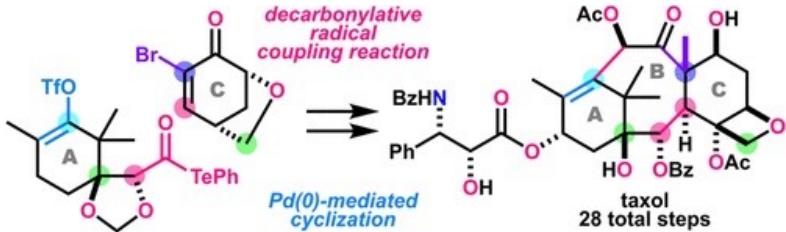
high functional group tolerance of an Et₃B/O₂-promoted decarbonylative radical reaction of α -alkoxyacyl tellurides



Scheme S1. Synthesis of taxane skeleton 7



Scheme S2. Total synthesis of taxol (1)

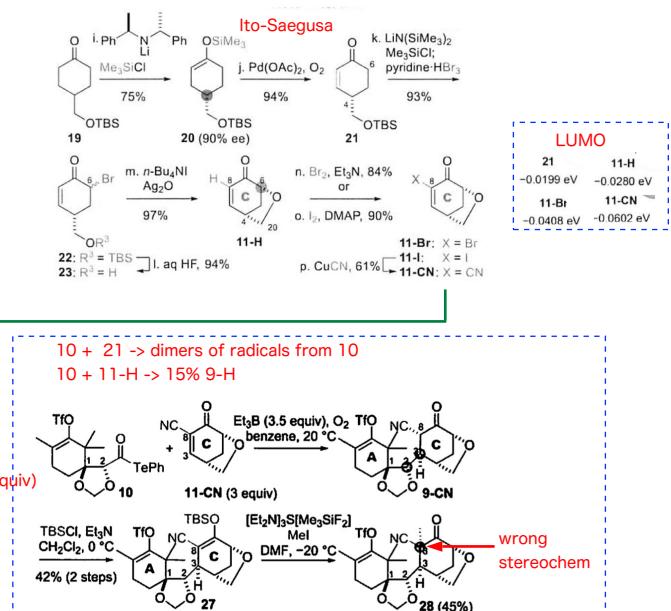


Pd(0)-mediated cyclization

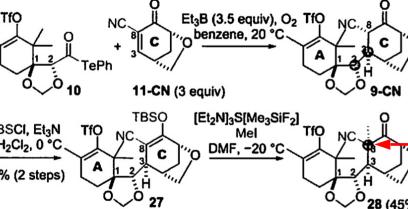
taxol
28 total steps

LUMO

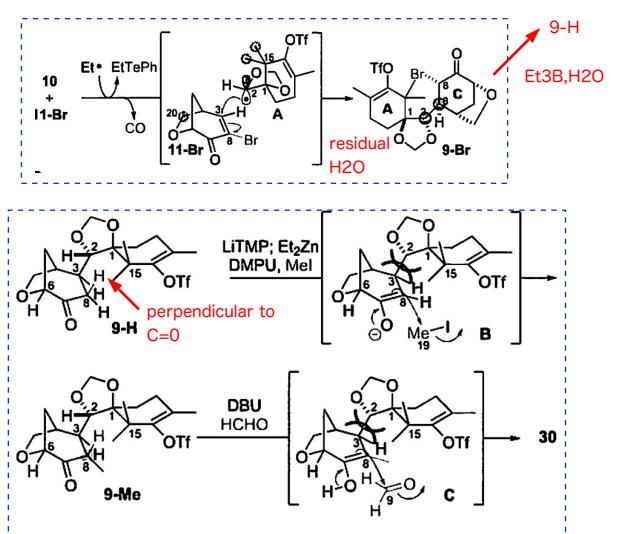
21 -0.0199 eV
11-H -0.0280 eV
11-Br -0.0408 eV
11-CN -0.0602 eV



10 + 21 → dimers of radicals from 10
10 + 11-H → 15% 9-H

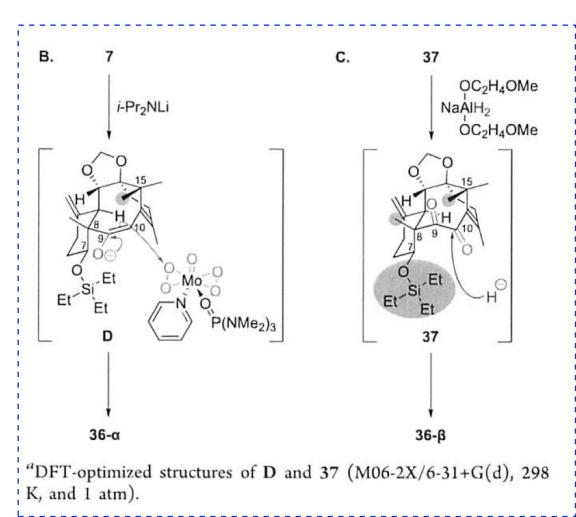


wrong stereochem



ether bridge of the C-ring :

- enhances the reactivity as the radical acceptor
- controls the C3-stereoselectivity
- controls the C8-site selectivity



DFT-optimized structures of D and 37 (M06-2X/6-31+G(d), 298 K, and 1 atm).