

Total Synthesis of the Norcembranoid Scabrolide B and Its Transformation into Sinuscalide C, Ineleganolide, and Horiolide

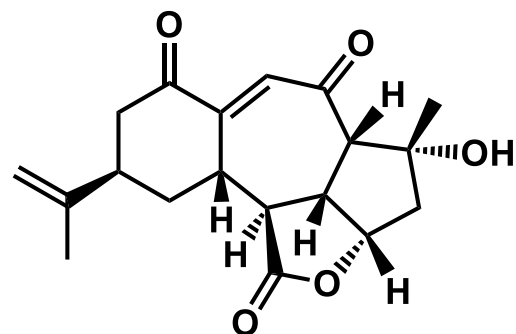
Davy S. Lin, Georg Späth, Zhanchao Meng, Lianne H. E. Wieske, Christophe Farès, and Alois Fürstner*



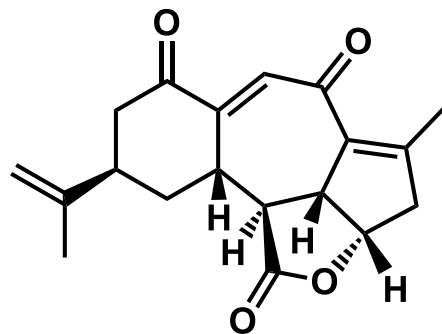
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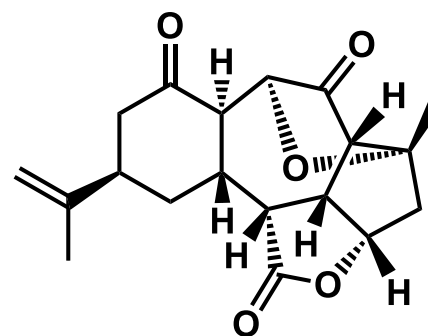
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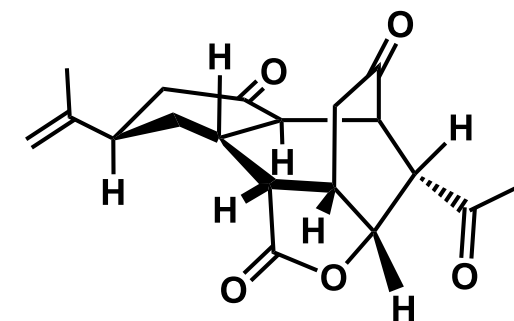
Scabrolide B (3)



Scabrolide C (4)



Ineleganolide (6)



Horiolide (34)

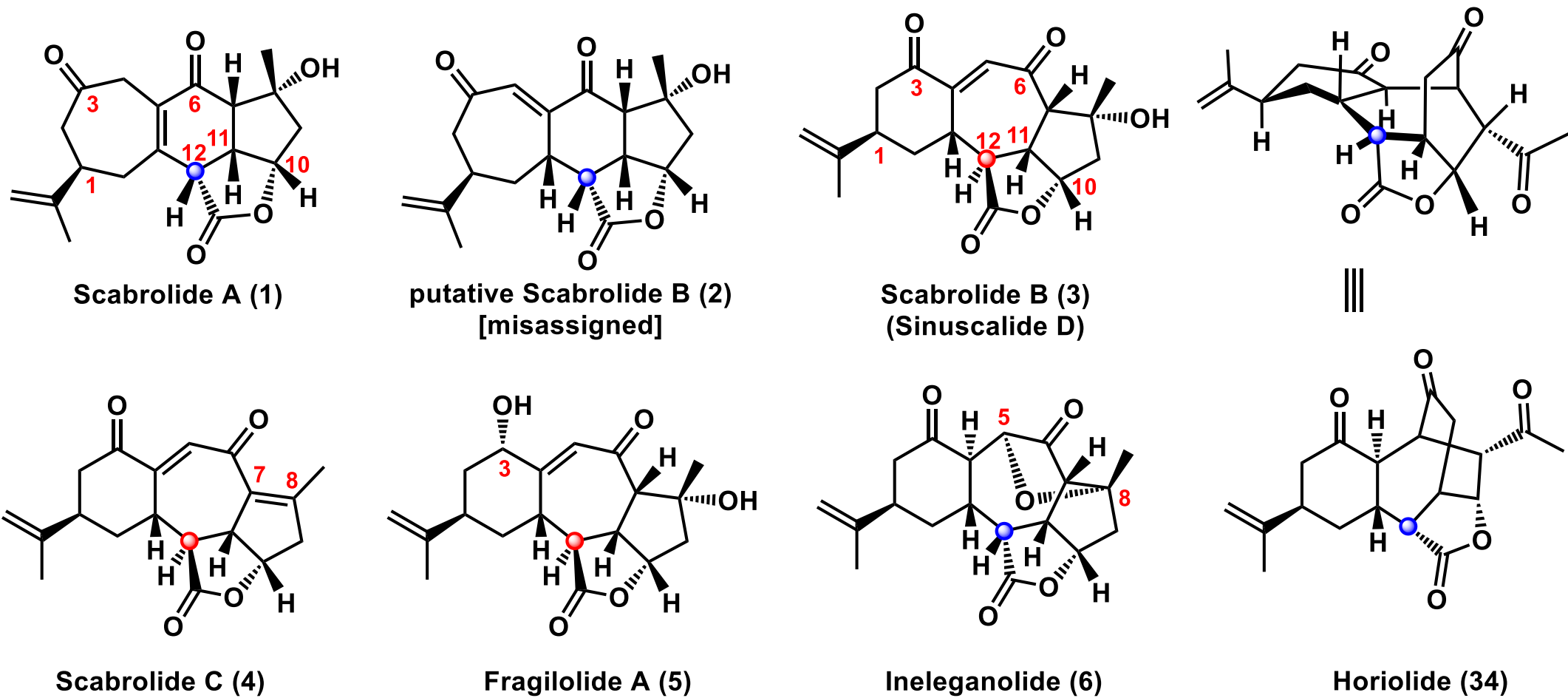
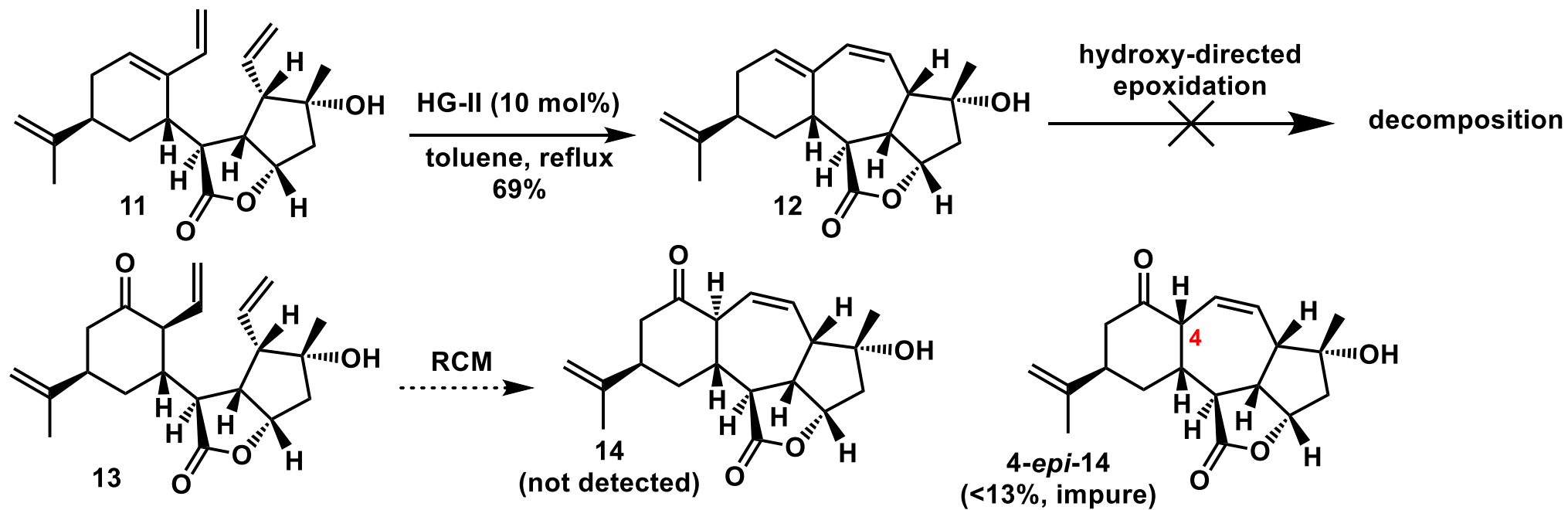
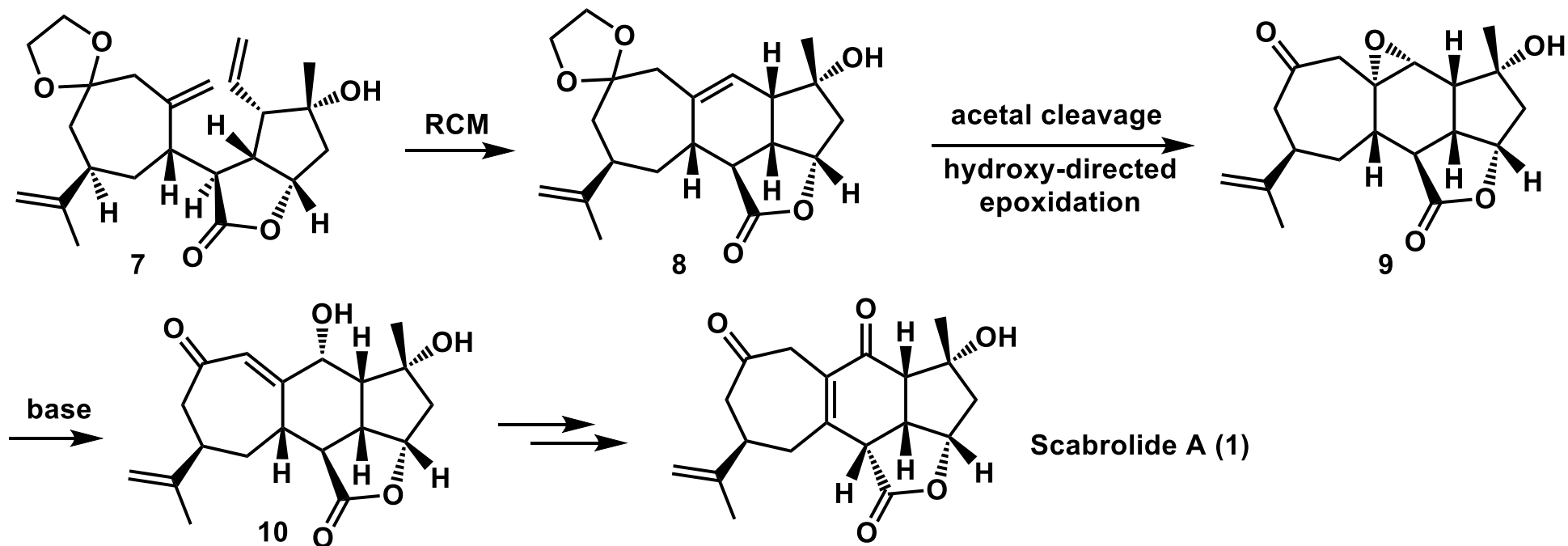
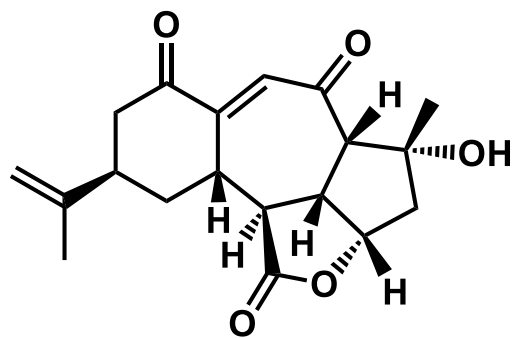
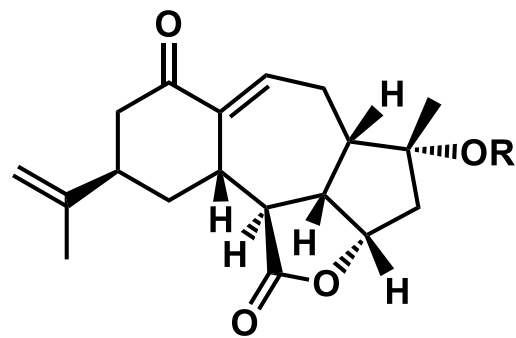
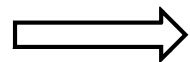


Figure 1. Selected polycyclic norcembranoid diterpenoids from *Sinularia* and related soft corals.

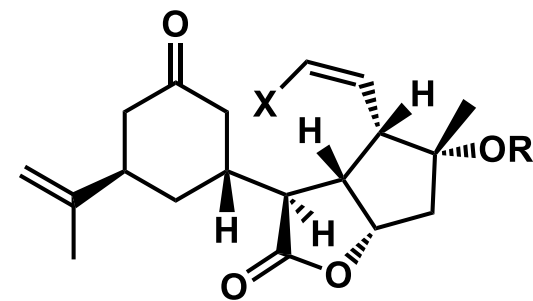
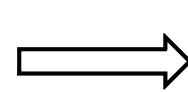




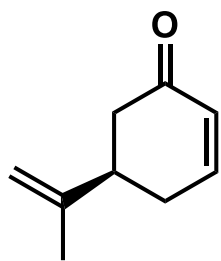
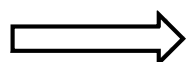
Scabrolide B (3)



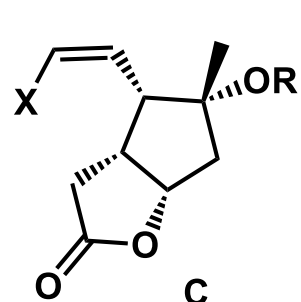
A



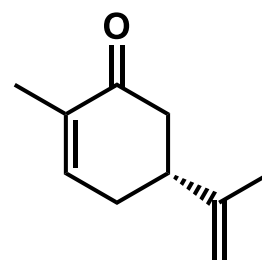
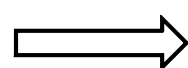
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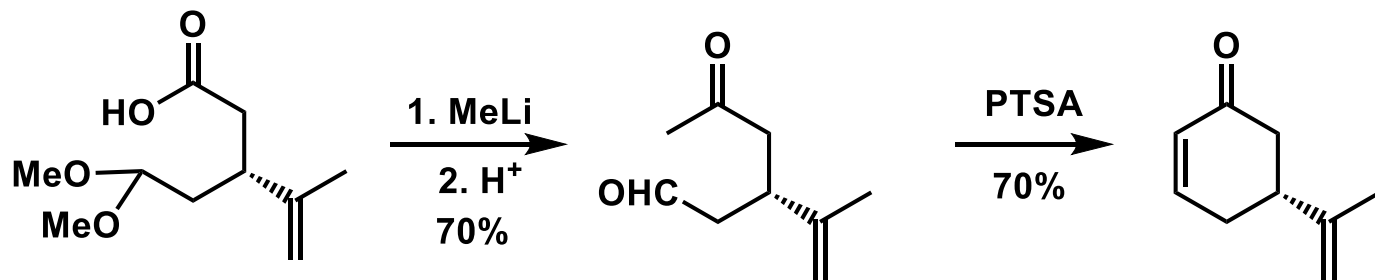
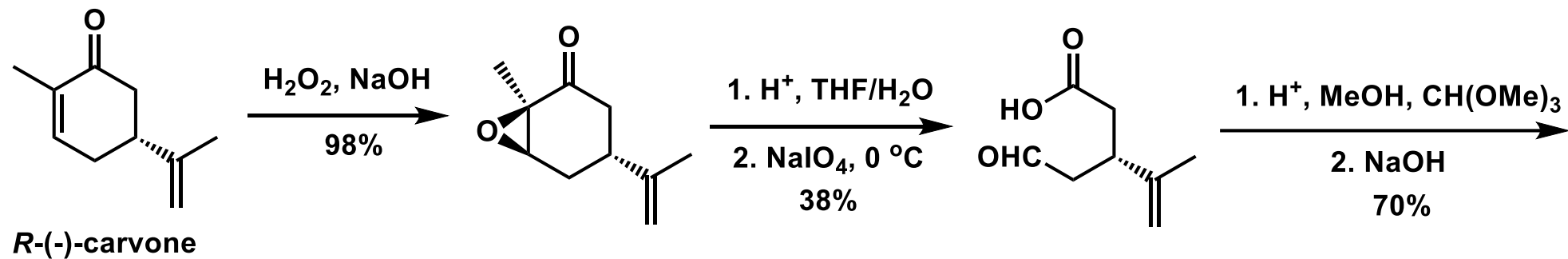
D

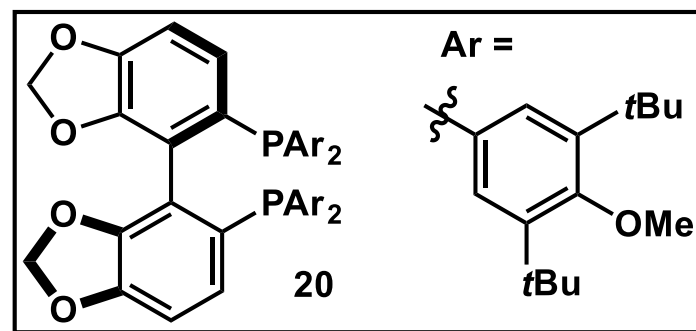
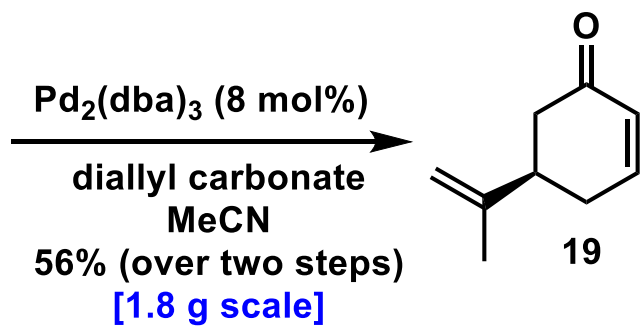
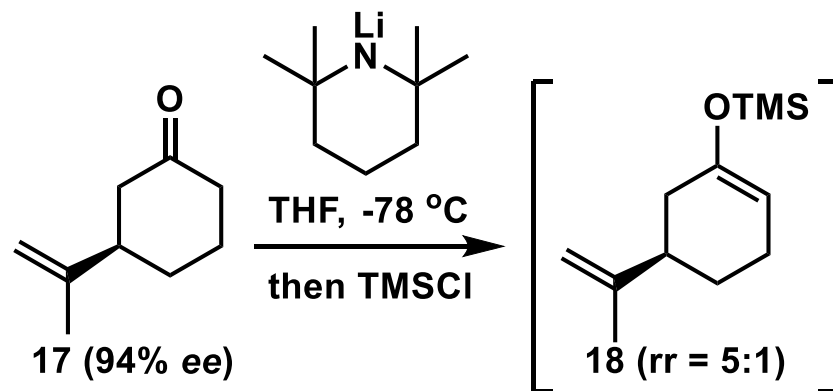
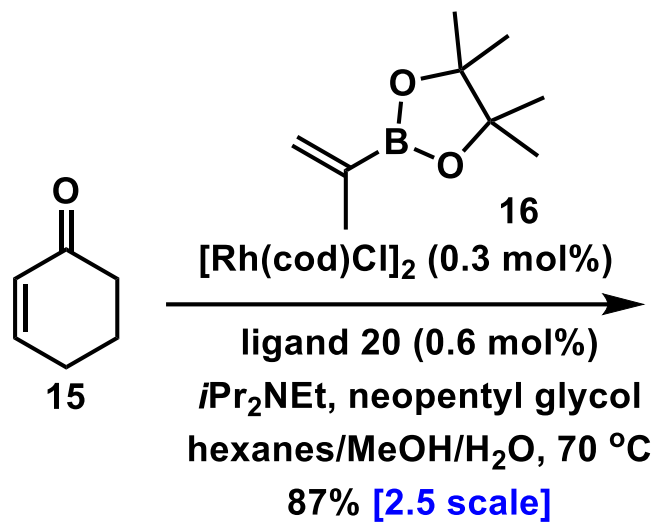


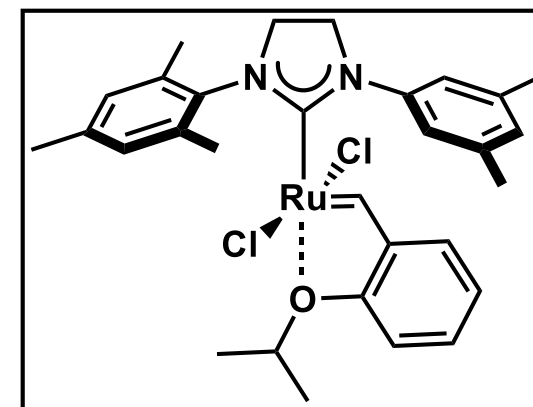
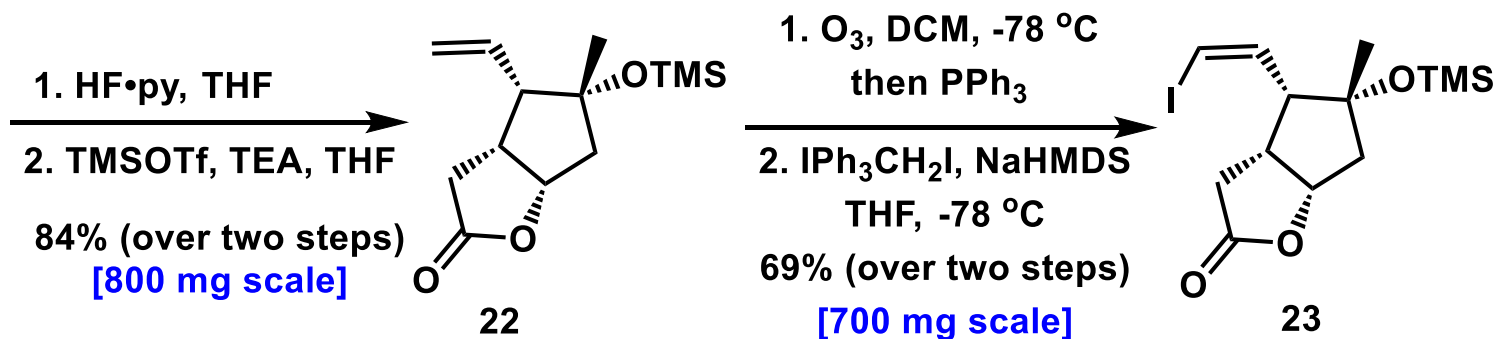
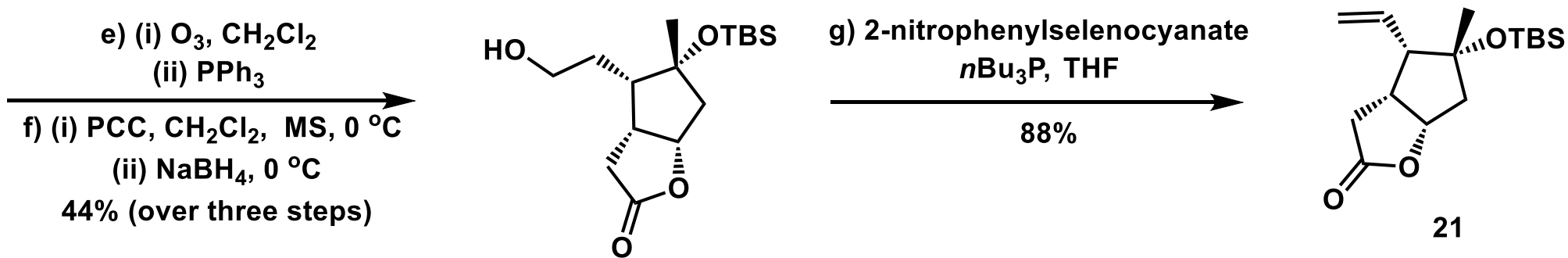
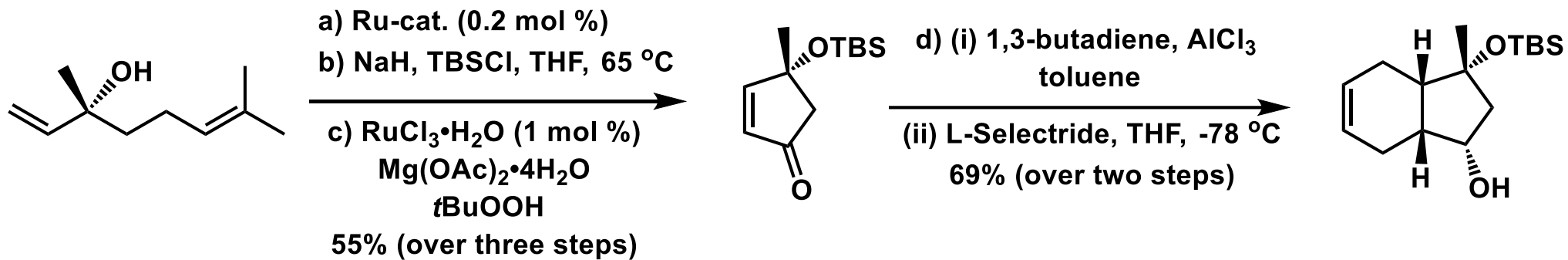
C



(R)-Linalool







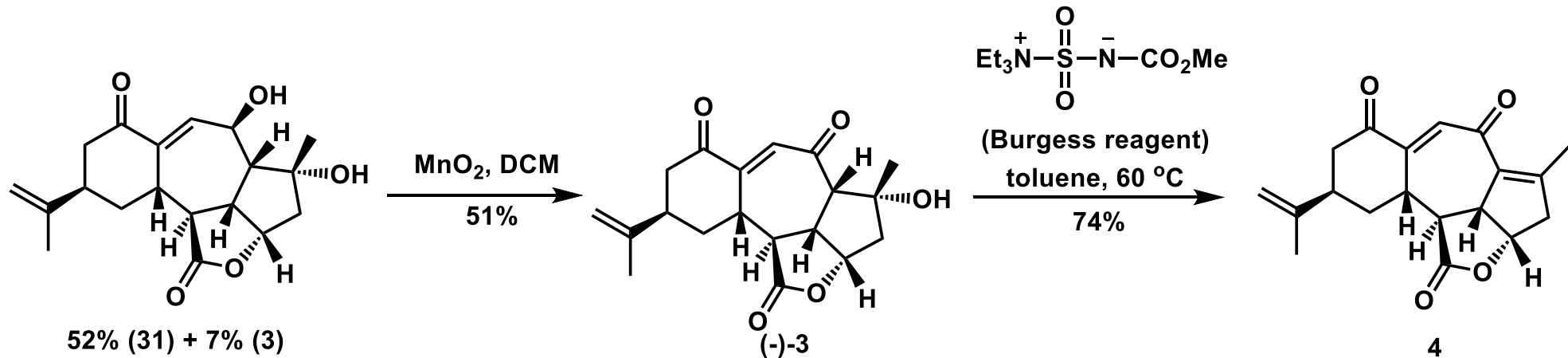
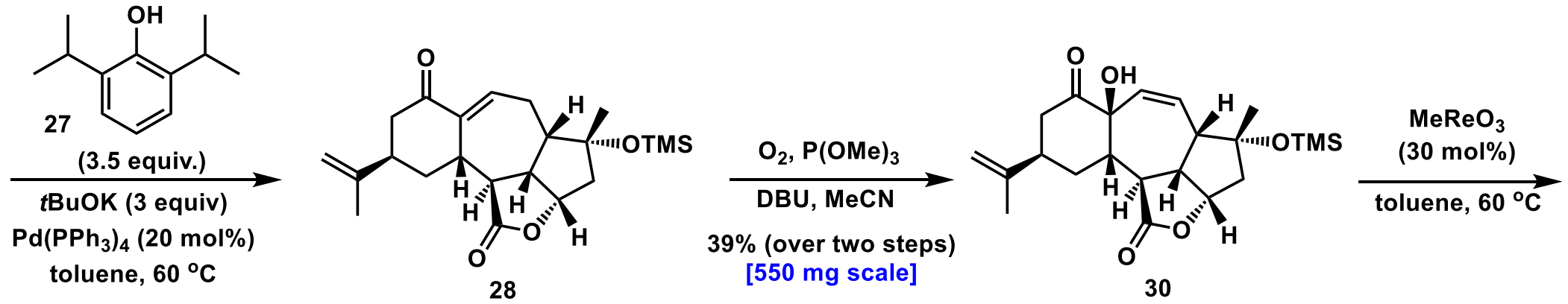
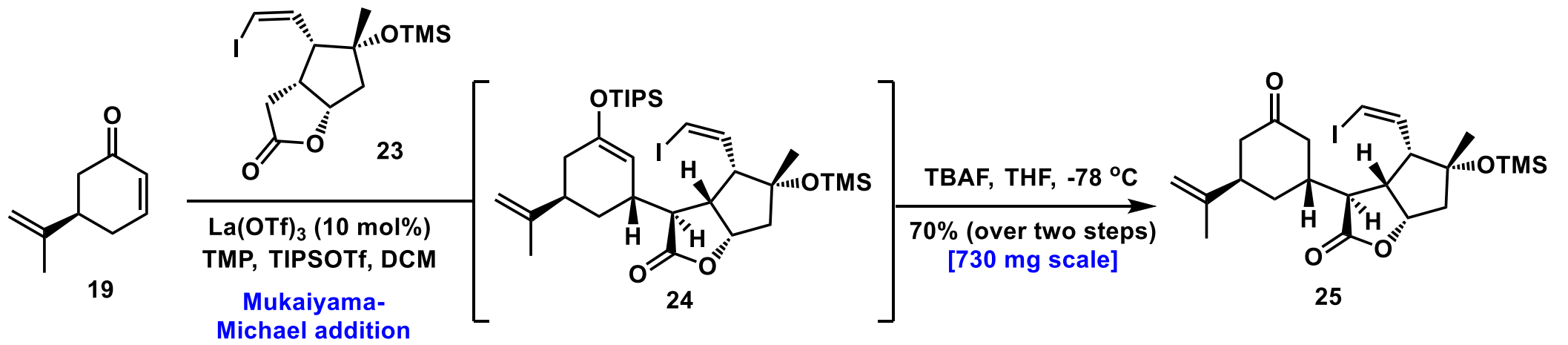
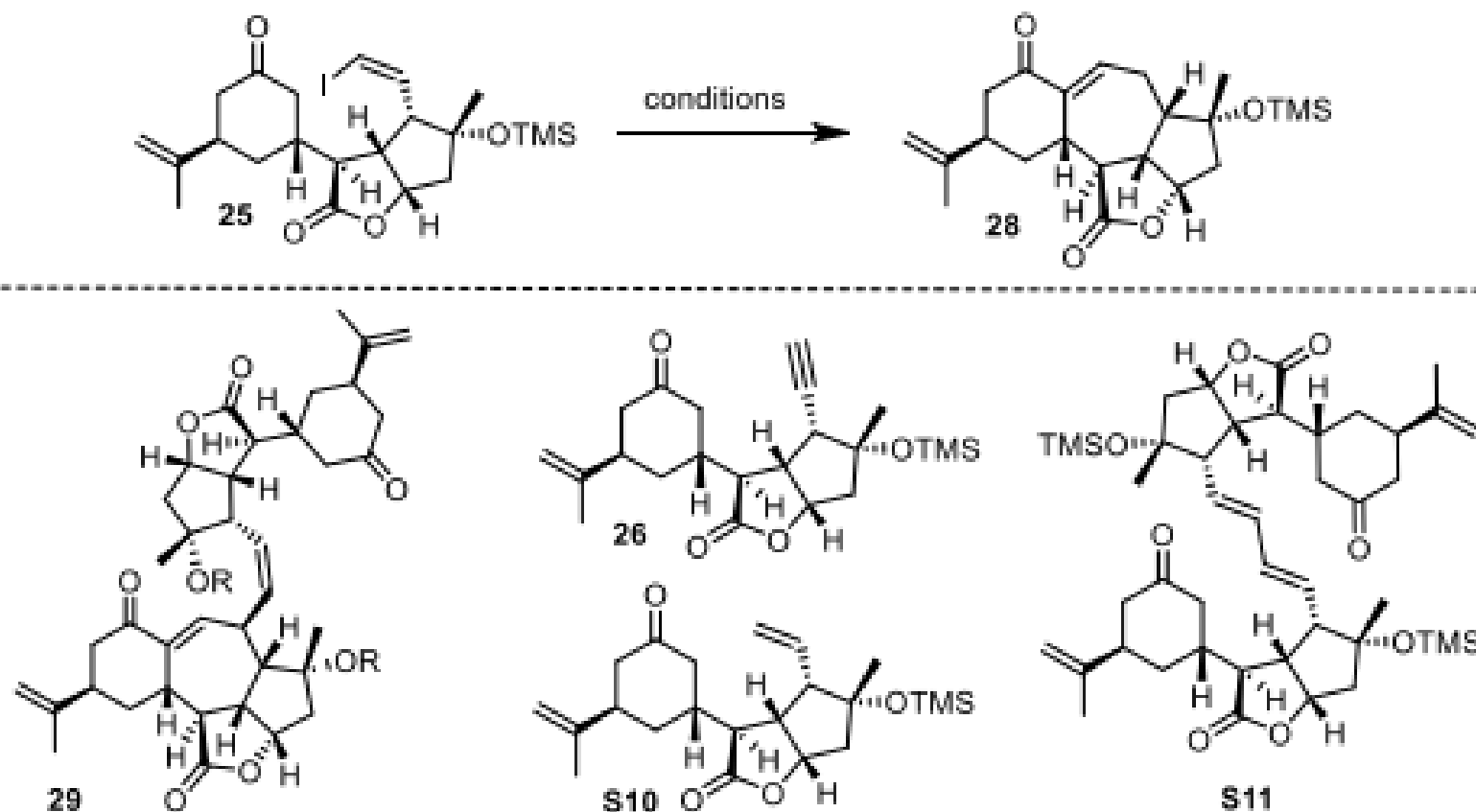


Table S5. Studies on ring closure by palladium catalyzed intramolecular alkenylation; the reactions were performed at a concentration of 10 mM, unless stated otherwise



Entry	Conditions	Results ^[a]
1	Pd(PPh ₃) ₄ 0.2 eq, PhOH 1.7 eq, tBuOK 1.5 eq, toluene, 65 °C, 2 h	28 (20%)
2	Pd(PPh ₃) ₄ 0.2 eq, PhOH 3.5 eq, tBuOK 3.0 eq, toluene, 65 °C, 2 h	28 (30%)
3	Pd ₂ (dba) ₃ 0.2 eq, SPhos 0.6 eq, PhOH 3.5 eq, tBuOK 3 eq, toluene, 65 °C, 2 h	28 (30%)

4	Pd(PPh ₃) ₄ 0.2 eq, tBuOK 3.0 eq toluene, 65 °C, 1.5 h	26 and S10
5	Pd(PPh ₃) ₄ 0.2 eq, PhOH 3.5 eq, tBuOK 3 eq, THF, 60 °C, 20 h	26 and S10
6	Pd(PPh ₃) ₄ 0.2 eq, tBuOK 3.0 eq, THF, RT, 5 min	unidentified product
7	Pd(PPh ₃) ₄ 0.2 eq, Cs ₂ CO ₃ 3.0 eq, toluene, 65 °C, 2.5 h	S11
8	PdCl ₂ (PPh ₃) ₂ 0.2 eq, Cs ₂ CO ₃ 3.0 eq, TEA 3.0 eq, toluene, 90 °C, 24 h	S10 and S11
9	Pd(PPh ₃) ₄ 0.2 eq, tBuONa 3.0 eq, dioxane, 60 °C, 20 h	S10 and S11
10	PdCl ₂ dppf 0.2 eq, K ₂ CO ₃ 3.0 eq, MeOH, 60 °C, 2 h	S10 and S11
11	Pd(OAc) ₂ 0.05 eq, PPh ₃ 0.3 eq, TBAB 1 eq, K ₂ CO ₃ 4.0 eq, DMF:H ₂ O (10:1), 90 °C, 20 h	S10 and S11
12	Pd(PPh ₃) ₄ 0.2 eq, 2,6- dimethylphenol 3.5 eq, tBuOK 3.0 eq, toluene, 65 °C, 70 min	28 (21%), 29 (32%)
13	Pd(PPh ₃) ₄ 0.2 eq, 2,6- diisopropylphenol 3.5 eq, tBuOK 3.0 eq, toluene, 65 °C, 70 min	28 (46%), 29 (13%)
14	Pd(PPh ₃) ₄ 0.2 eq, 2,6-di-tert-butylphenol 3.5 eq, tBuOK 3.0 eq, toluene, 65 °C, 70 min	28 (7%), 29 (4%)
15	Pd(PPh ₃) ₄ 0.2 eq, 2,6- diisopropylphenol 3.5 eq, tBuOK 3.0 eq, toluene, 60 °C, 70 min,	28 (57%), 29 (29%)

c = 2 mM

