

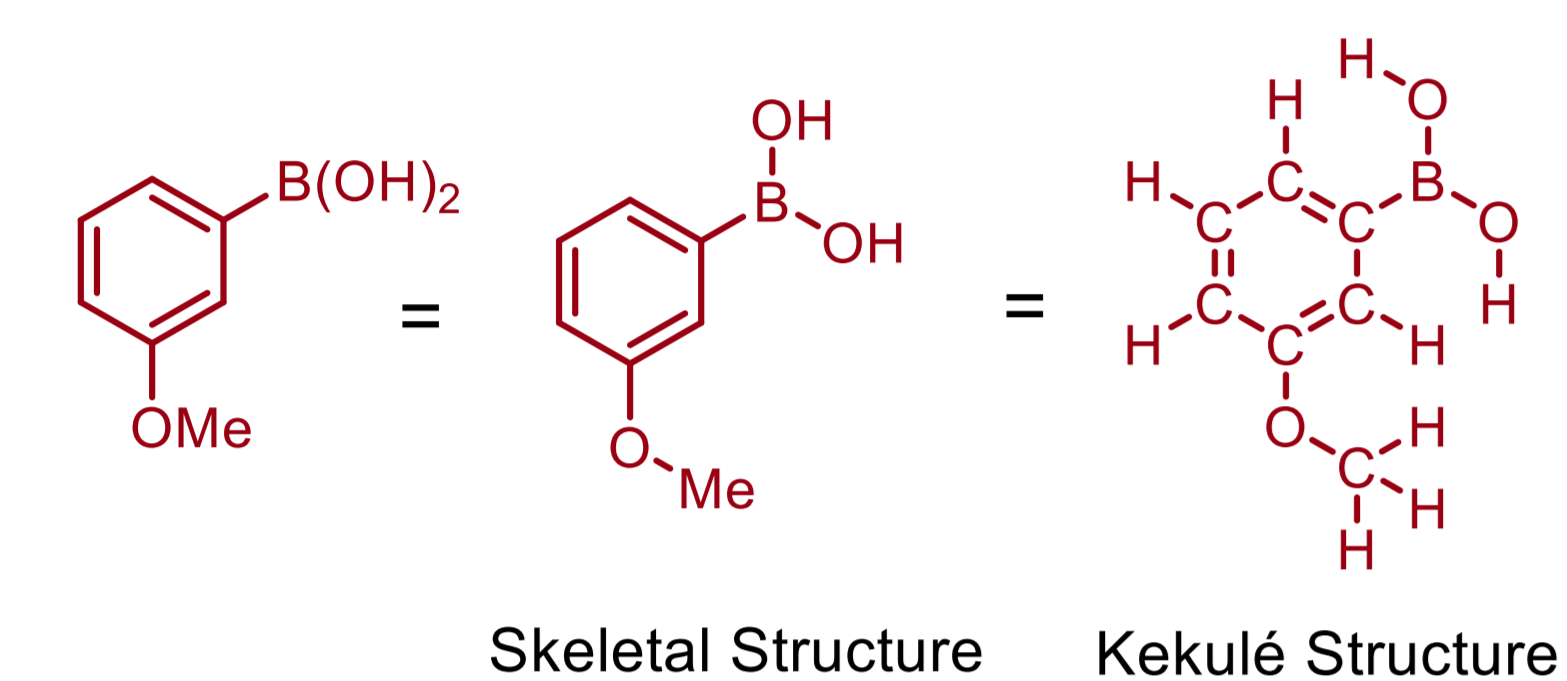
Synthesis of Boronic Esters from 3-Methoxyphenylboronic Acid for Comparison in Rh-Catalyzed Conjugate Additions

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Background

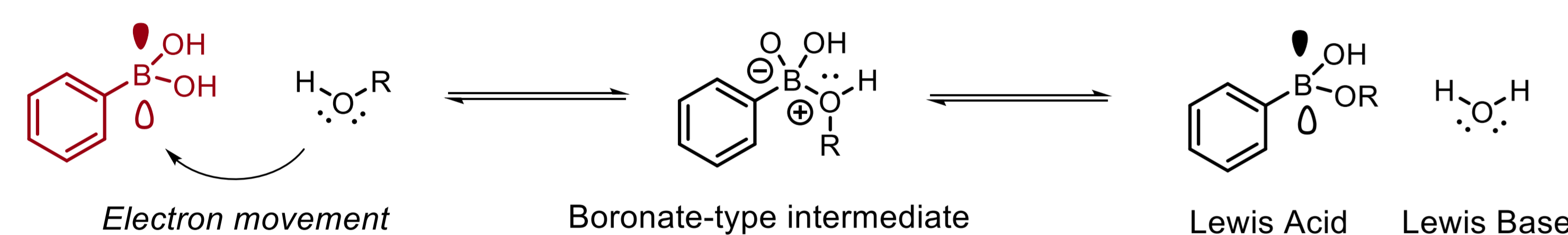
a) Understanding Skeletal Structures [1]



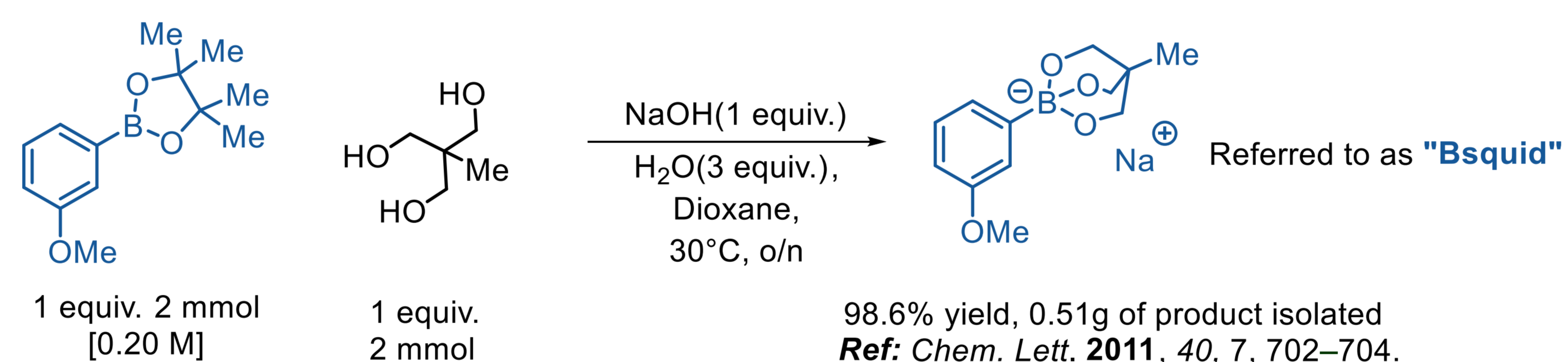
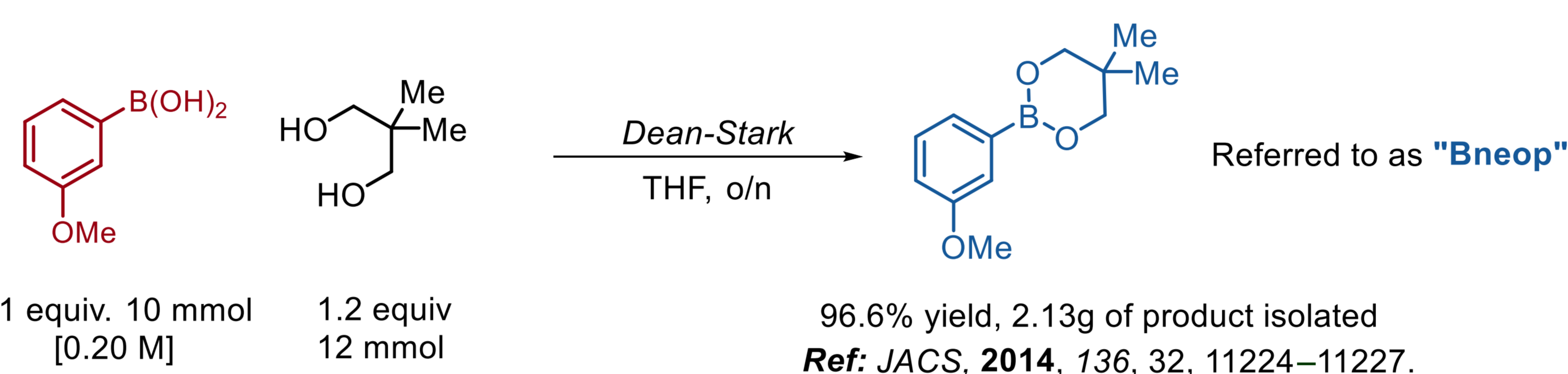
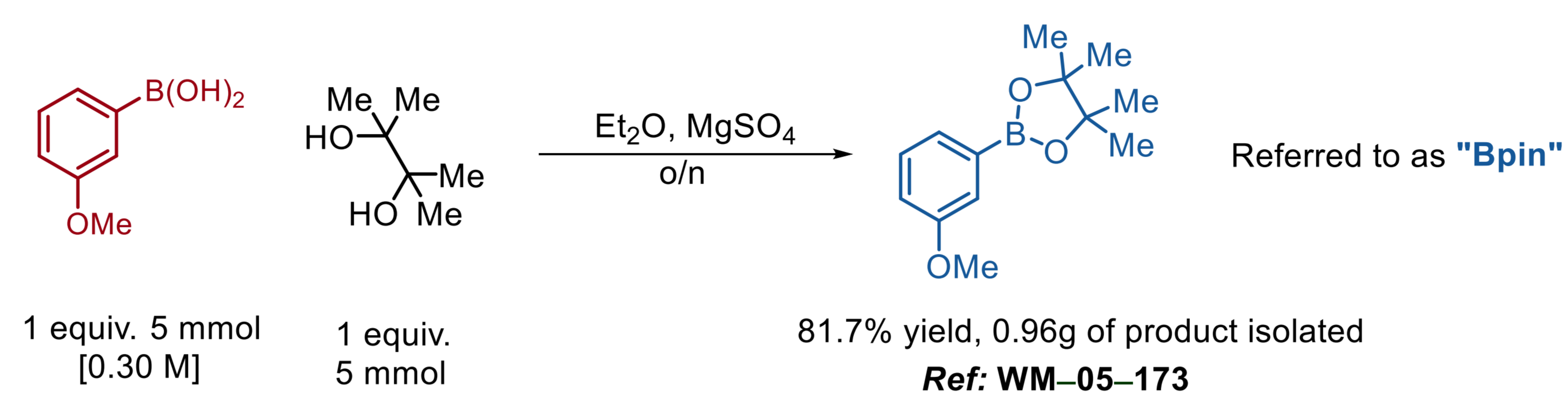
- 3-Methoxyphenylboronic acid illustrated as a Skeletal structure and Kekulé structure.

b) Lewis Acid and Base Chemistry [2]

- The atom boron, widely utilized in the pharmaceutical industry, is a well-known Lewis acid. Lewis acids are compounds which contain vacant orbitals that have the ability to accept an electron pair from Lewis bases resulting in the formation of new bonds.



Starting Material Synthesis



Catalysis and Results

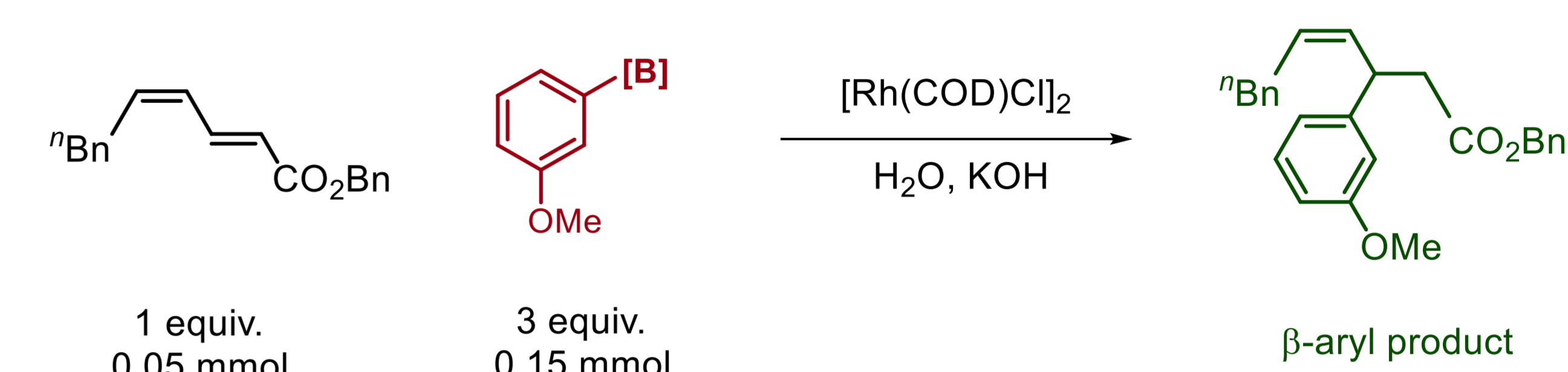
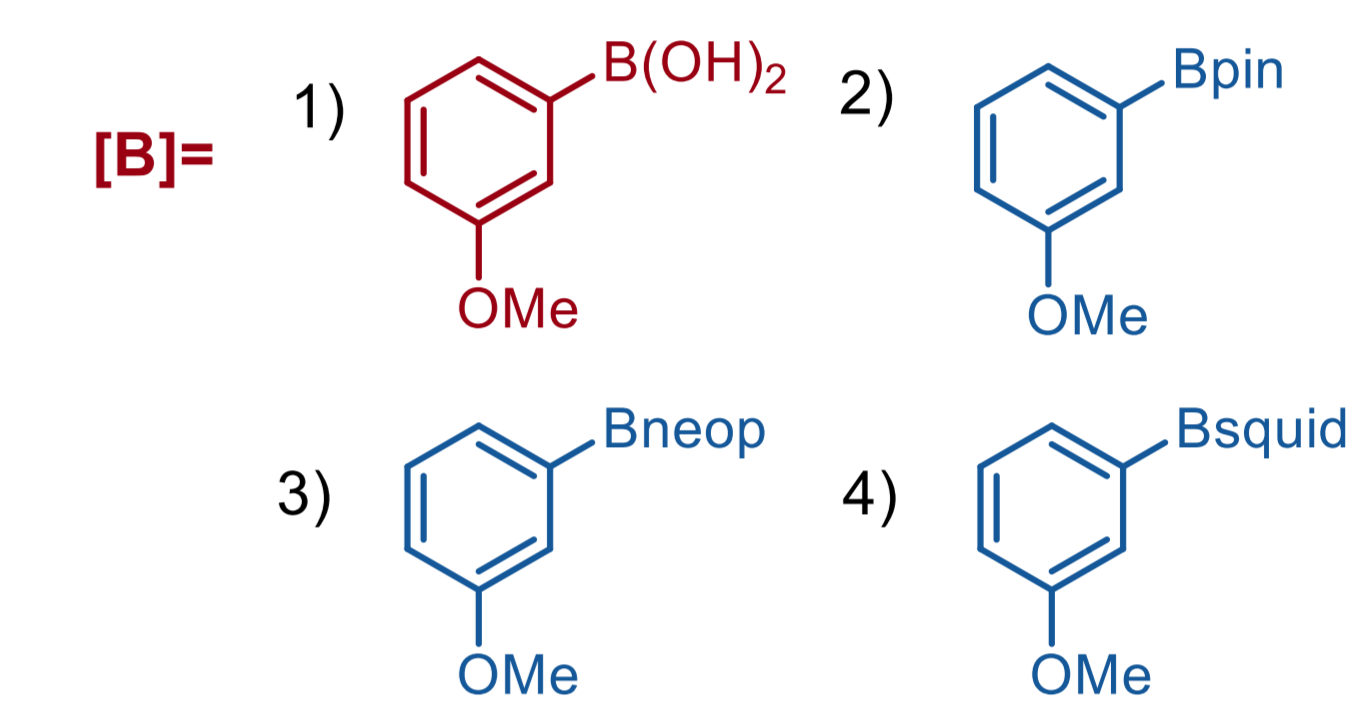


Figure 4. An instrument used for NMR (Nuclear Magnetic Resonance) spectroscopy to identify molecules and assess their purity. Results presented on the right were obtained from the NMR instrument.

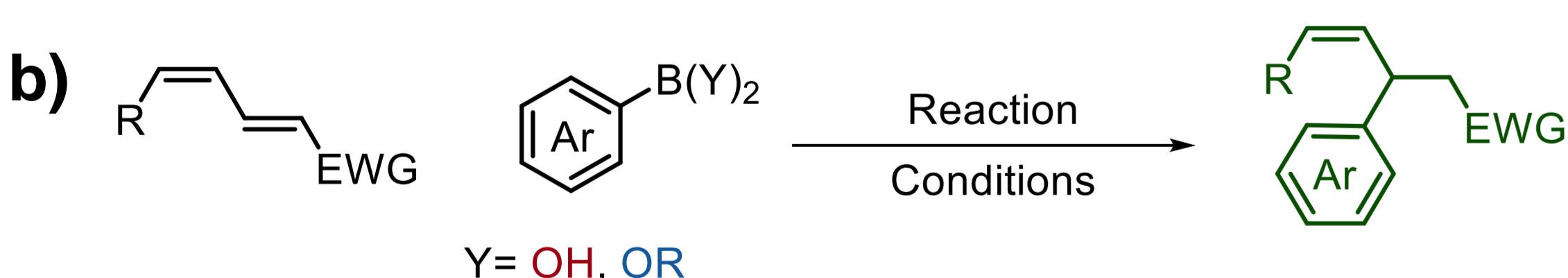
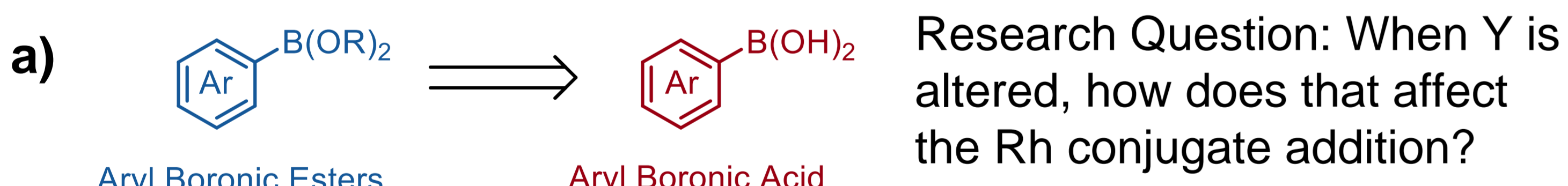


Results:

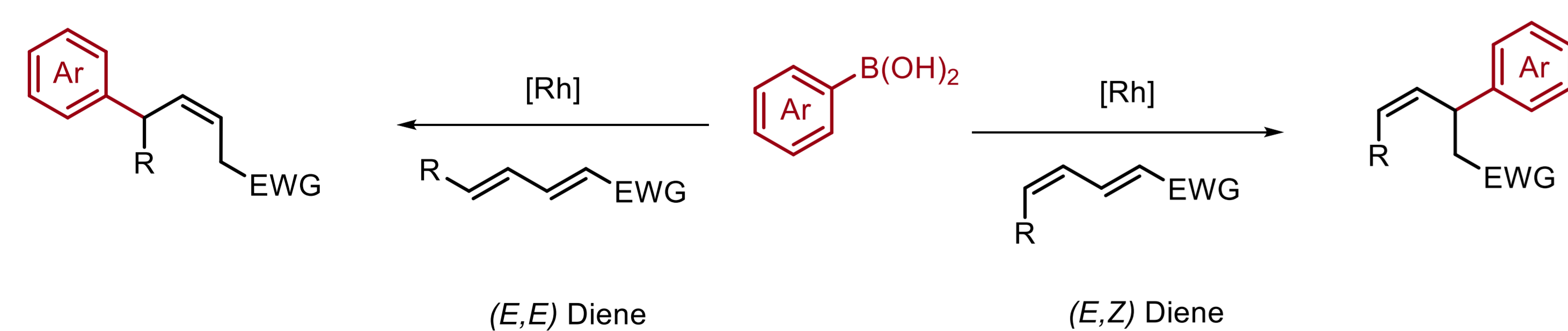
- 1) 96% yield, 100% conv.
- 2) 87% yield, 98% conv.
- 3) 87% yield, 93% conv.
- 4) 0% yield, 100% conv.
- 4*) 51% yield, 58% conv.

*Bsquid reaction ran again without base(KOH) and at 0°C

Objective: Starting Material Synthesis^[a] and Application^[b]



Rh-Conjugate Addition



Ref: JACS, 2021, 143, 28, 10770-10777.

Ref: Org. Lett. 2005, 7, 25, 5629-5632.

Ref: JACS, 2010, 132, 23, 7872-7873.

Lab Methods



Figure 1. Samples obtained from silica column chromatography using the Biotage automated flash chromatography instrument.



Figure 2. Reaction setup employing the use of a Dean-Stark trap, a piece of glassware designed for removal of water.



Figure 3. Aqueous Workup being done for removal of aqueous soluble substances, for instance water, present in an organic solution.

Conclusions

- Successfully acquired β -aryl products from reagents 1, 2, 3 and 4 through Rh-catalyzed conjugate additions.
- Catalysis appeared the fastest with reagents 1, slowest with 2 and 3 and, surprisingly, proceeded without the addition of base with 4.
- Synthesized complex boronic esters can be utilized by others for current and future lab research projects.
- Procedures and methods could potentially be applied in the pharmaceutical industry.

Acknowledgements

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- Lastly, I would like to thank the University of Alberta, Canada Summer Jobs and the WISEST team for providing me with this amazing opportunity and for their guidance throughout the program.

References:

[1] McMurry J. Structure and Bonding. In *Organic Chemistry*, 8th ed.; Brooks/Cole, Cengage Learning, 2011; pp 1-33.

[2] McMurry J. Polar Covalent Bonds; Acids and Bases. In *Organic Chemistry*, 8th ed.; Brooks/Cole, Cengage Learning, 2011; pp 34-73.

Dr. Lundgren

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