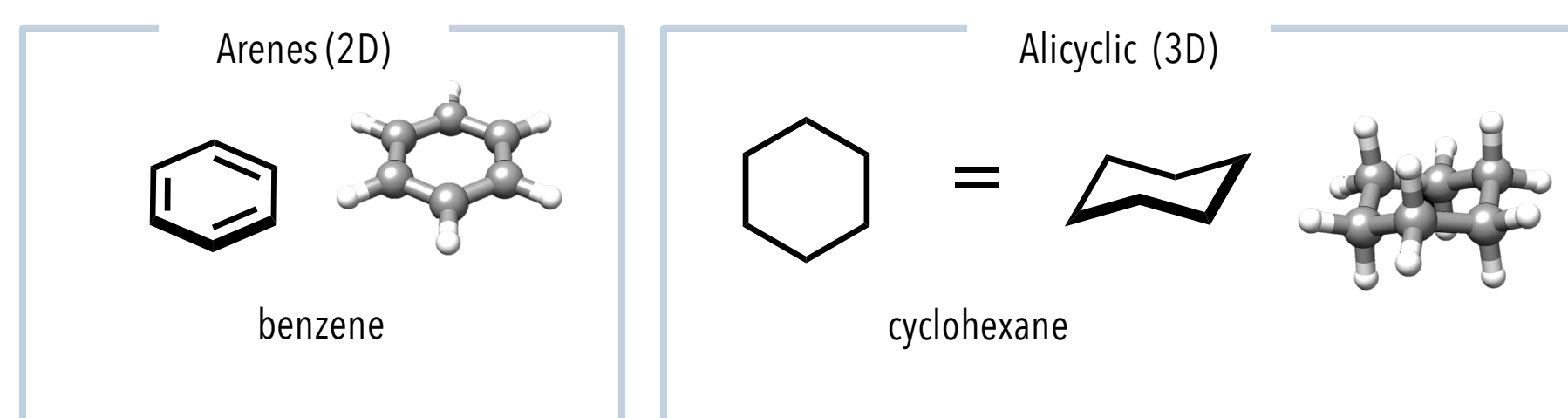


Making Molecules by Breaking Molecules: Dearomatization

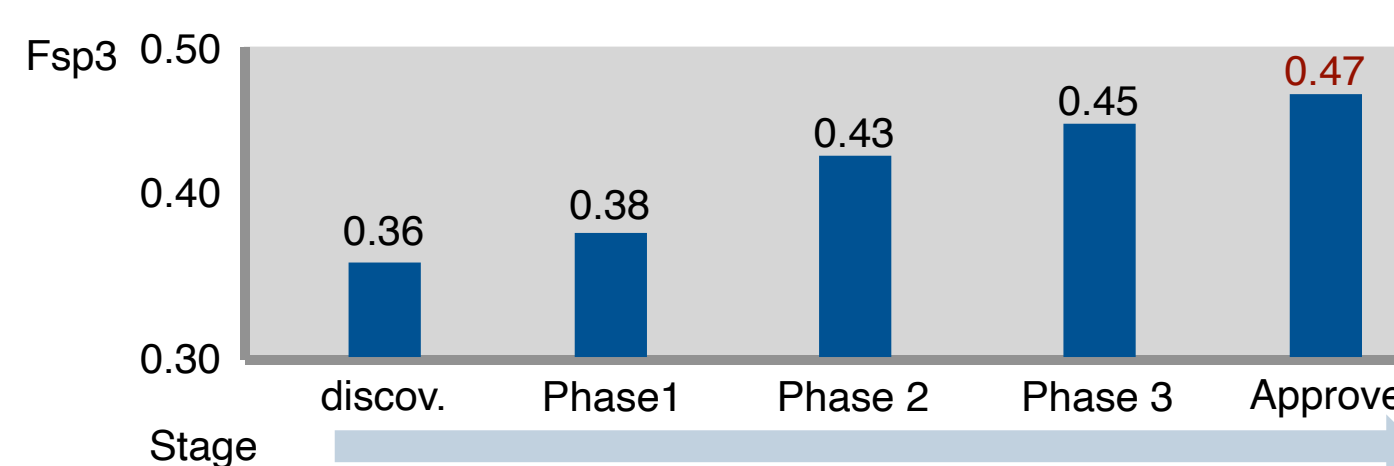
Kei Muto

Background

◆ One of the Great Stream in Organic Chemistry: Escape from Flatland



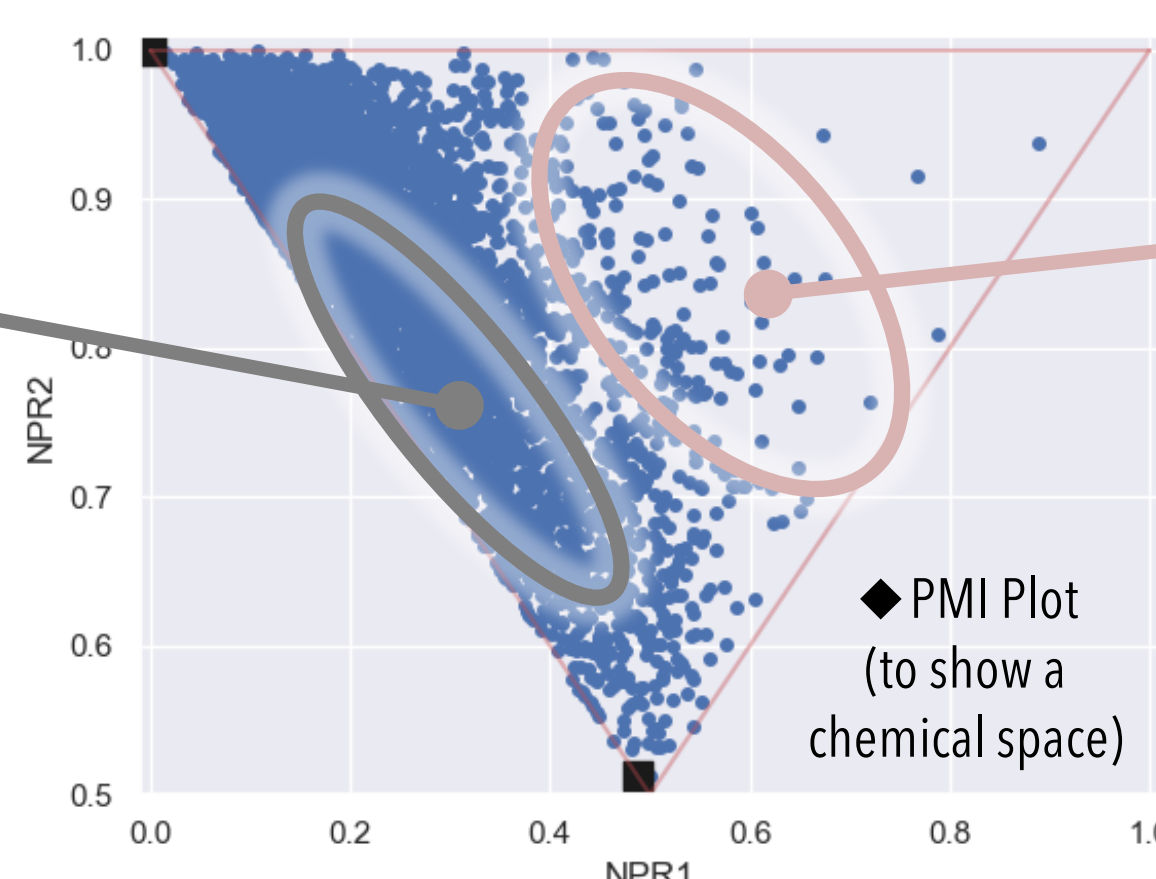
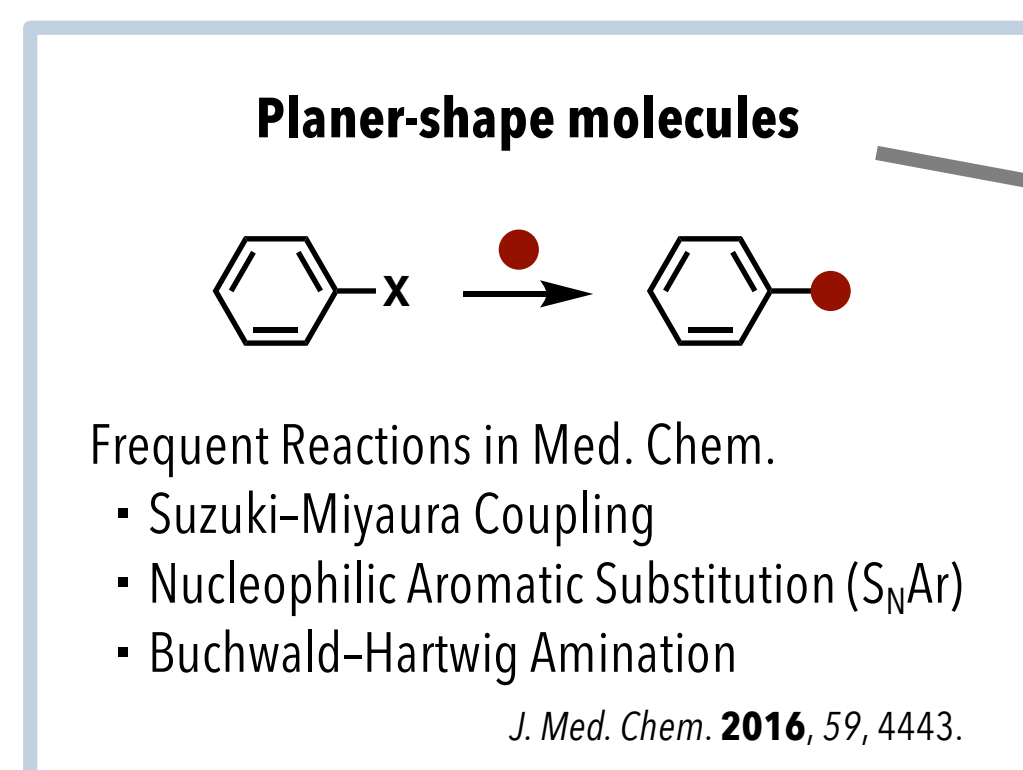
◆ Statistic Support



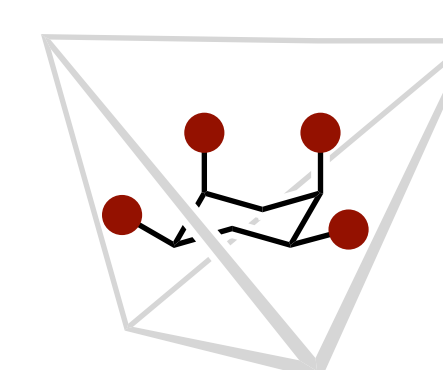
Molecules with a 3D structure is Highly Valuable in Medicinal Chemistry.

J. Med. Chem. **2009**, 52, 6752.

◆ Limited Chemical Space



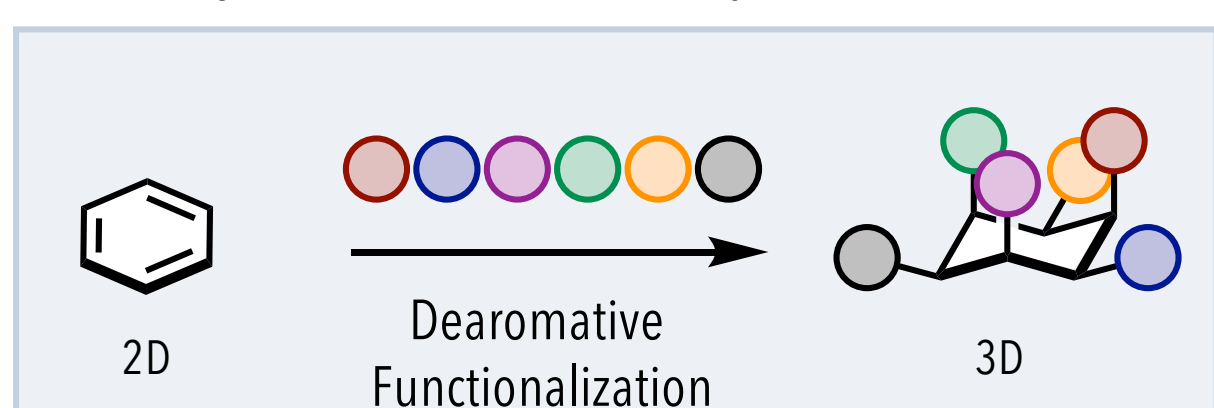
3D-shape molecules



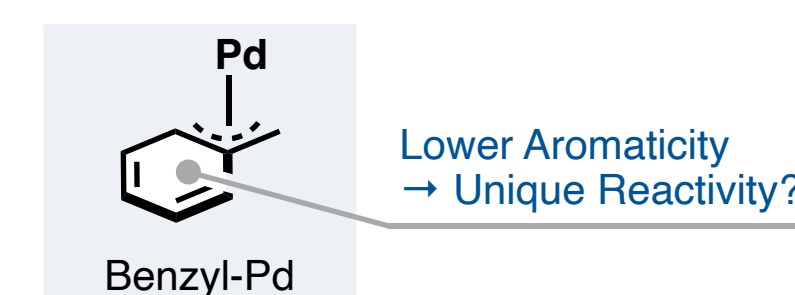
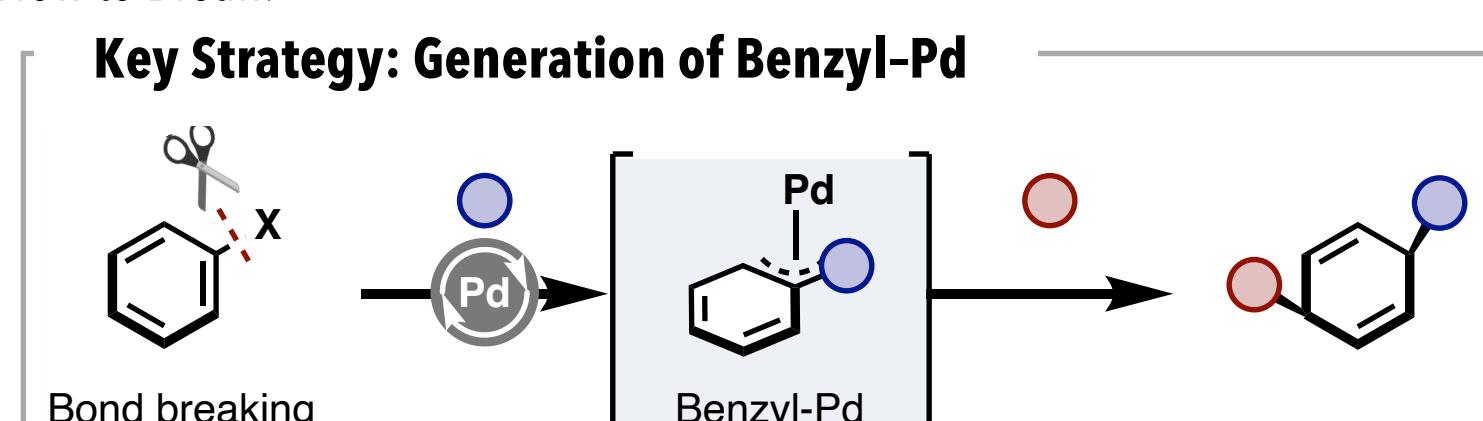
× Lack of Reliable Methodologies
Usually not Easy to Synthesize in Med. Chem.

Our Approach

◆ Breaking Arenes (2D) to Make Alicyclic Molecules (3D)

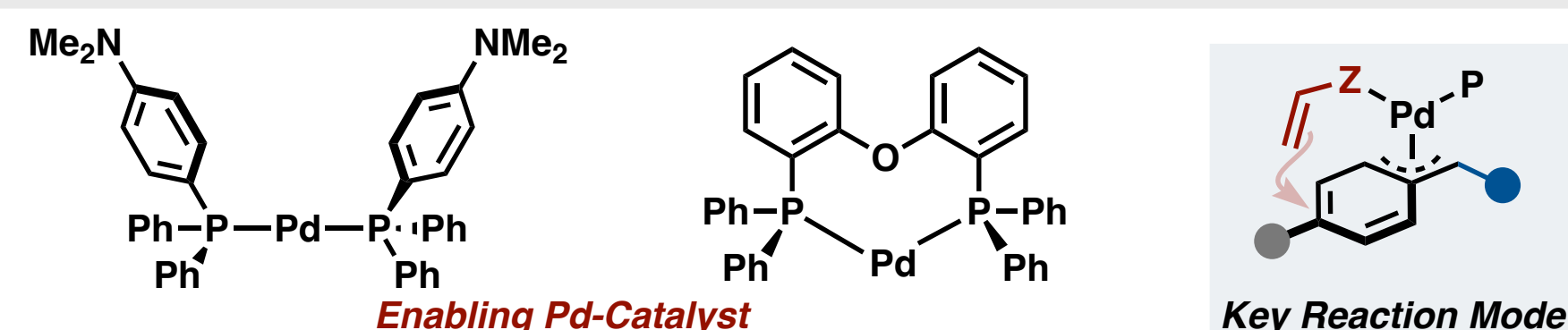
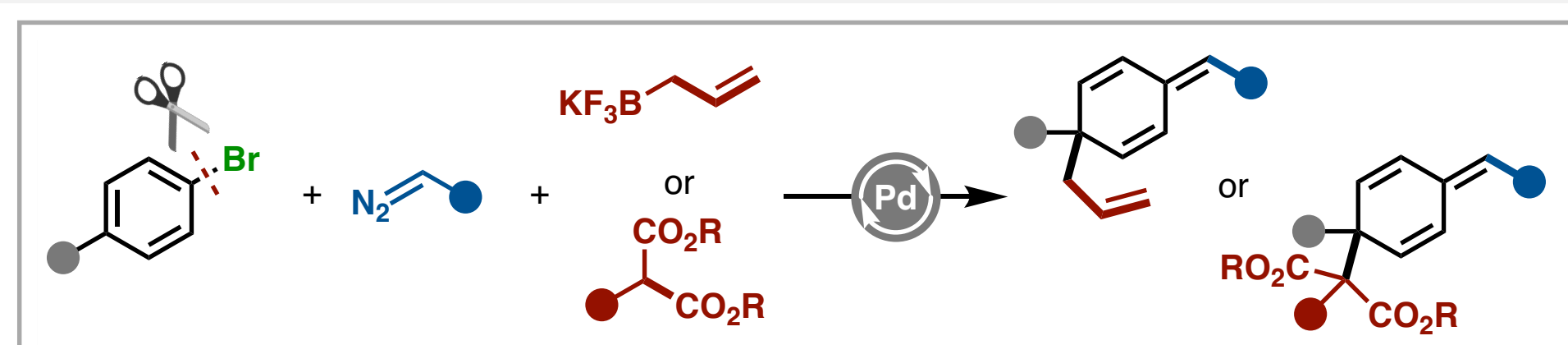


◆ How to Break?



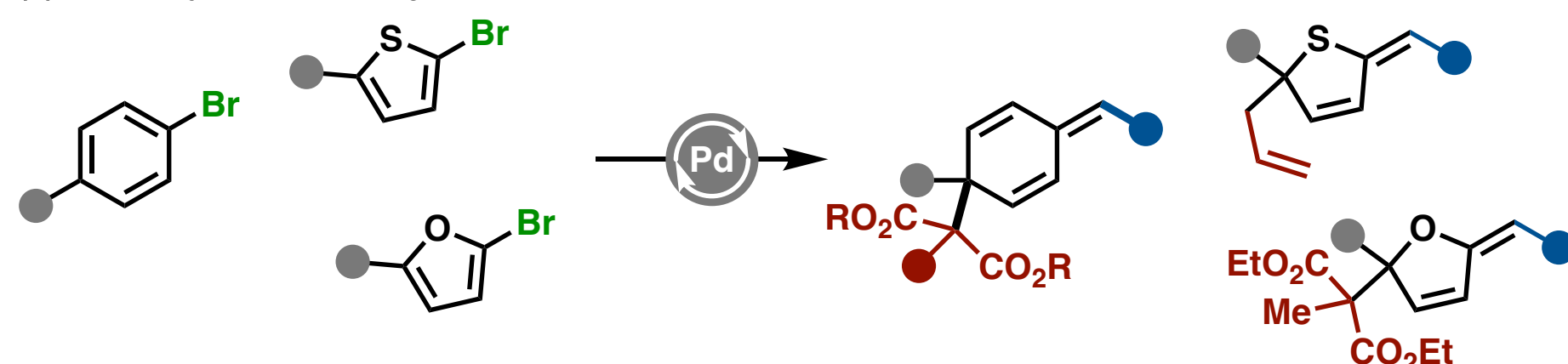
Yamamoto, Y. et al. *J. Am. Chem. Soc.* **2001**, 123, 759.

Achievement 1: Dearomative Three Component Reaction

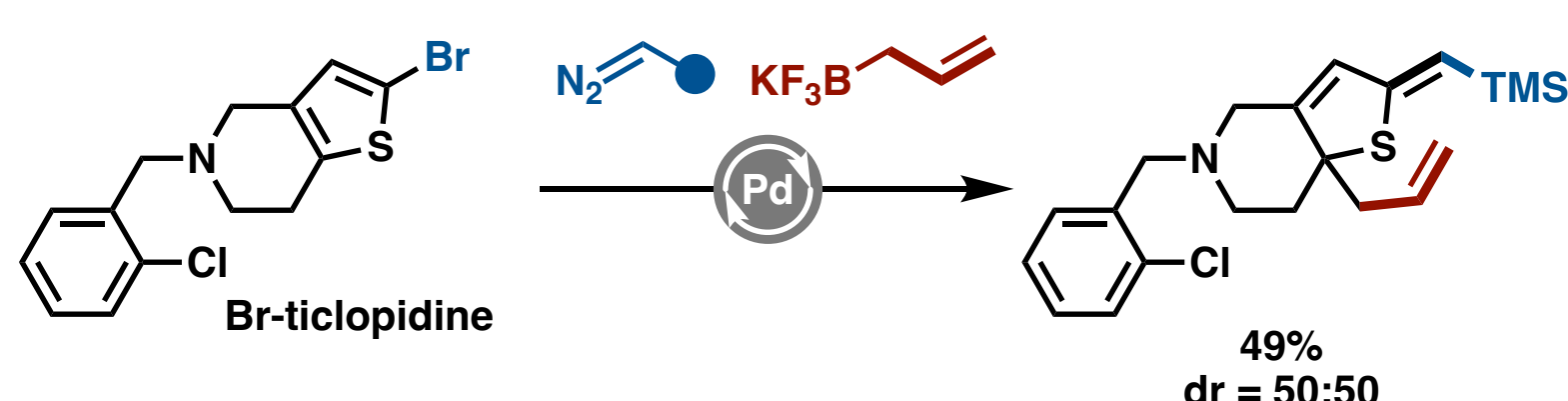


ACS Catal. **2019**, 9, 8991.. *Chem. Sci.* **2020**, 11, 8779. *Asian J. Org. Chem.* **2023**, Just Accepted.

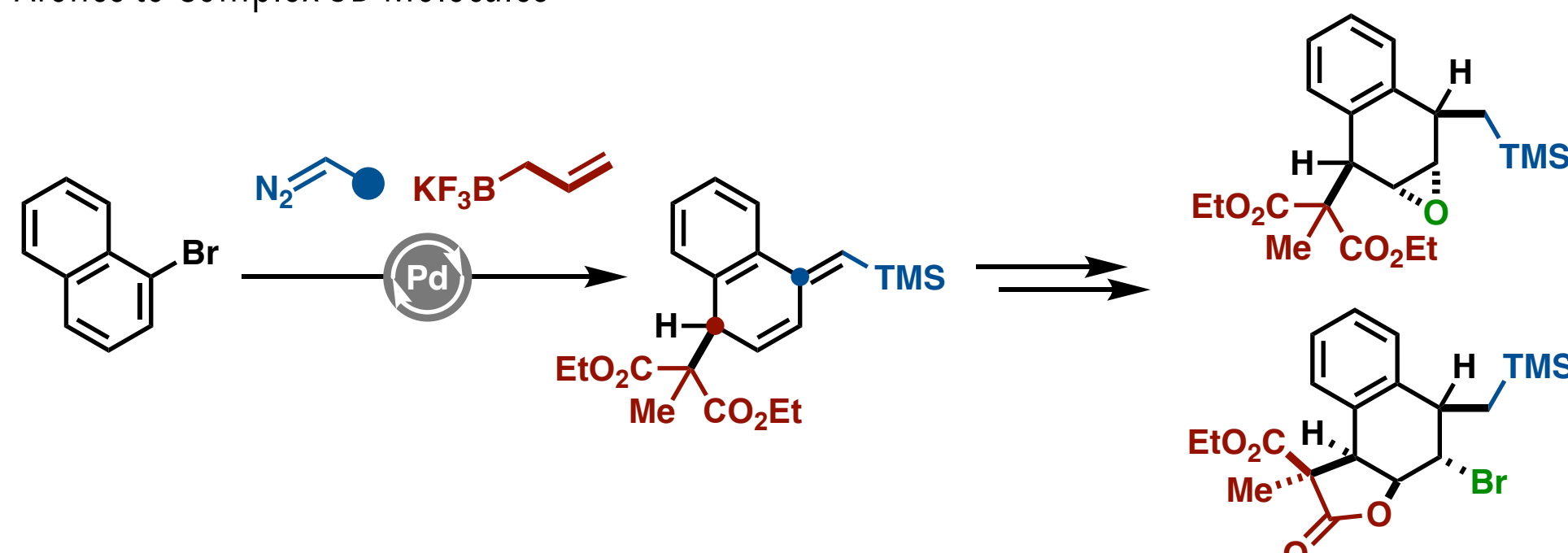
Applicability: Broad Range of Arenes



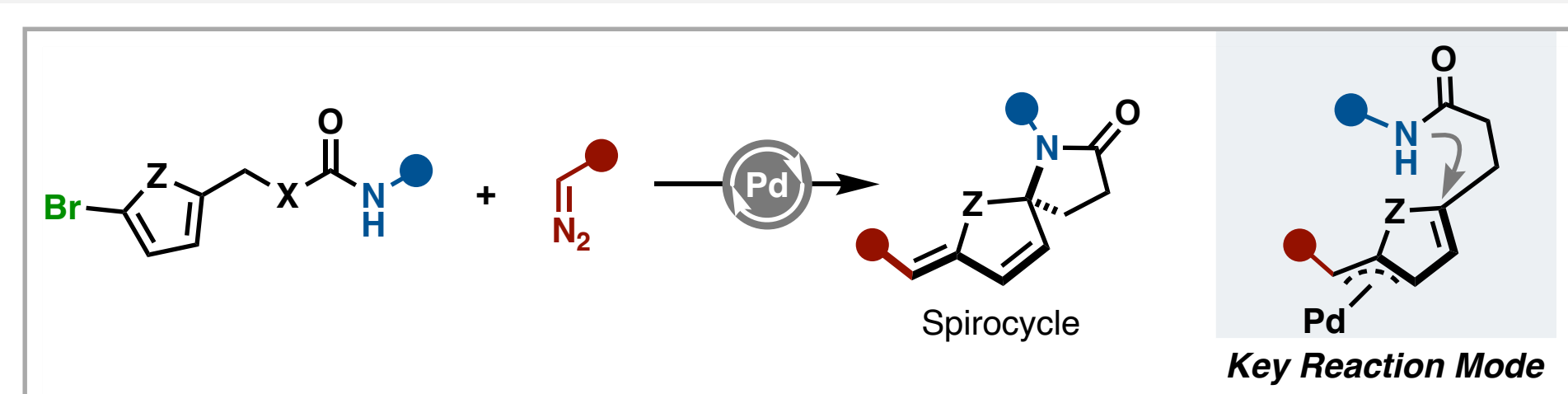
Late-stage Transformation of Drug Molecules



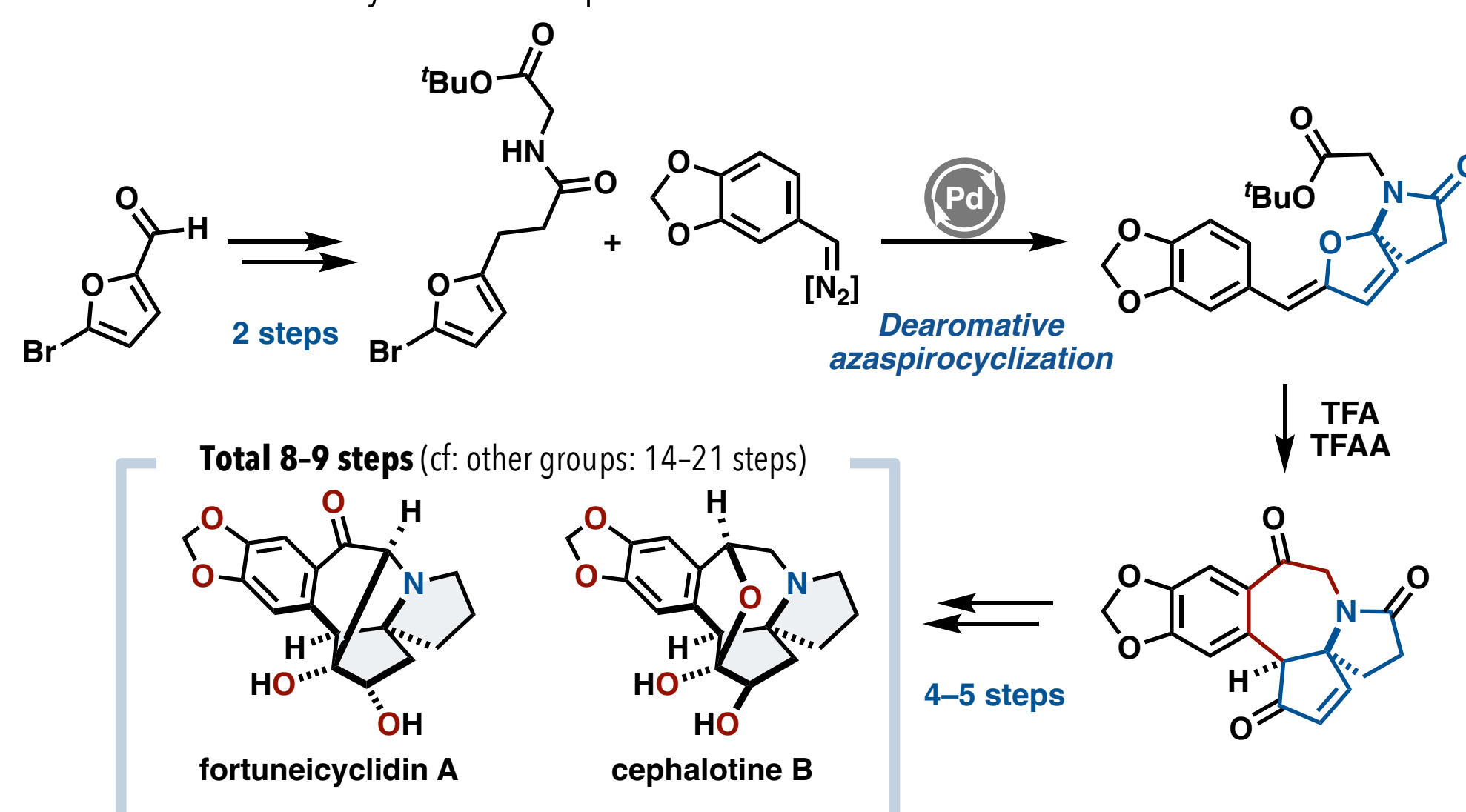
Arenes to Complex 3D Molecules



Achievement 2: Dearomative Spirocyclization

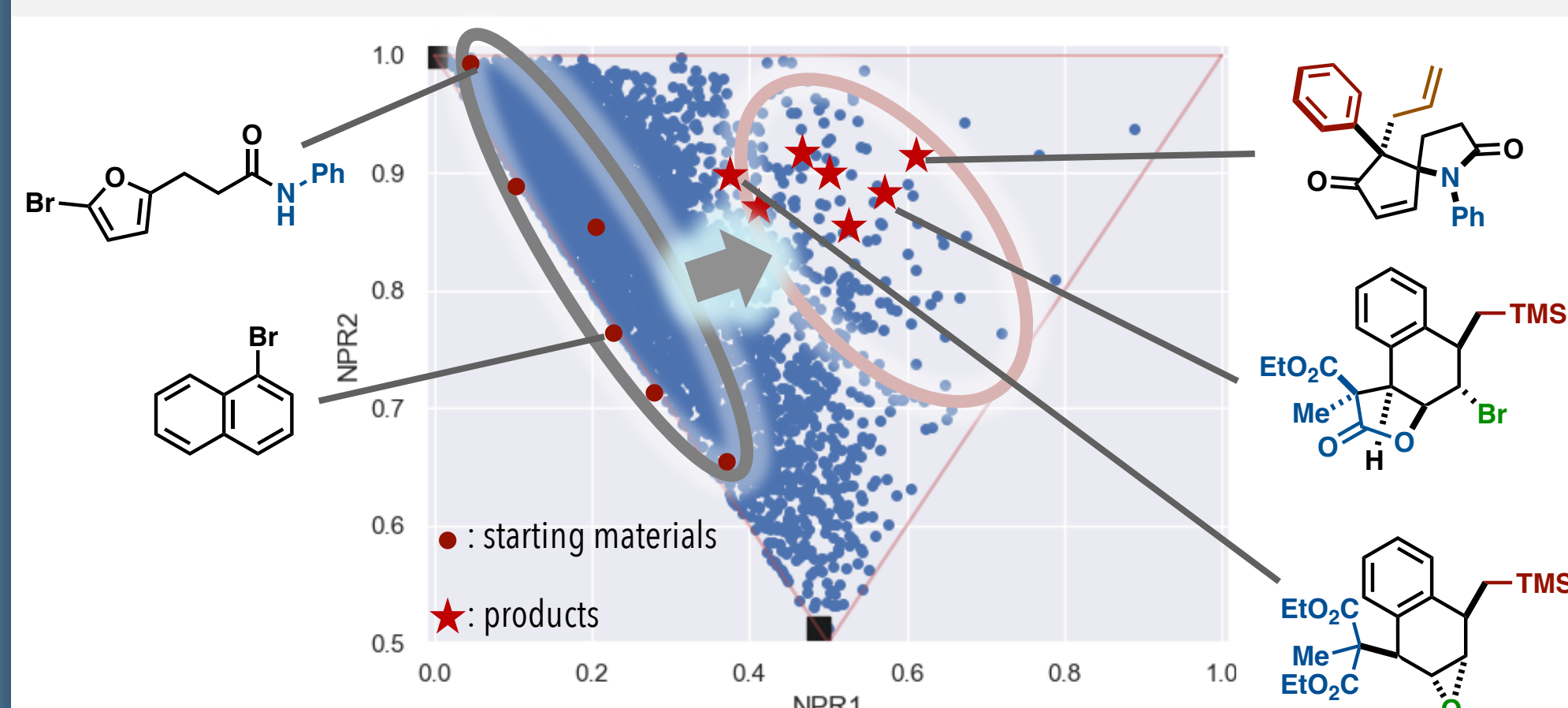


Powerful Method to Synthesize Complex Natural Products



ACS Catal. **2021**, 11, 10429. *Chem. Eur. J.* **2023**, early view.

Summary: Our Methods Clearly Opened A New Chemical Space



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