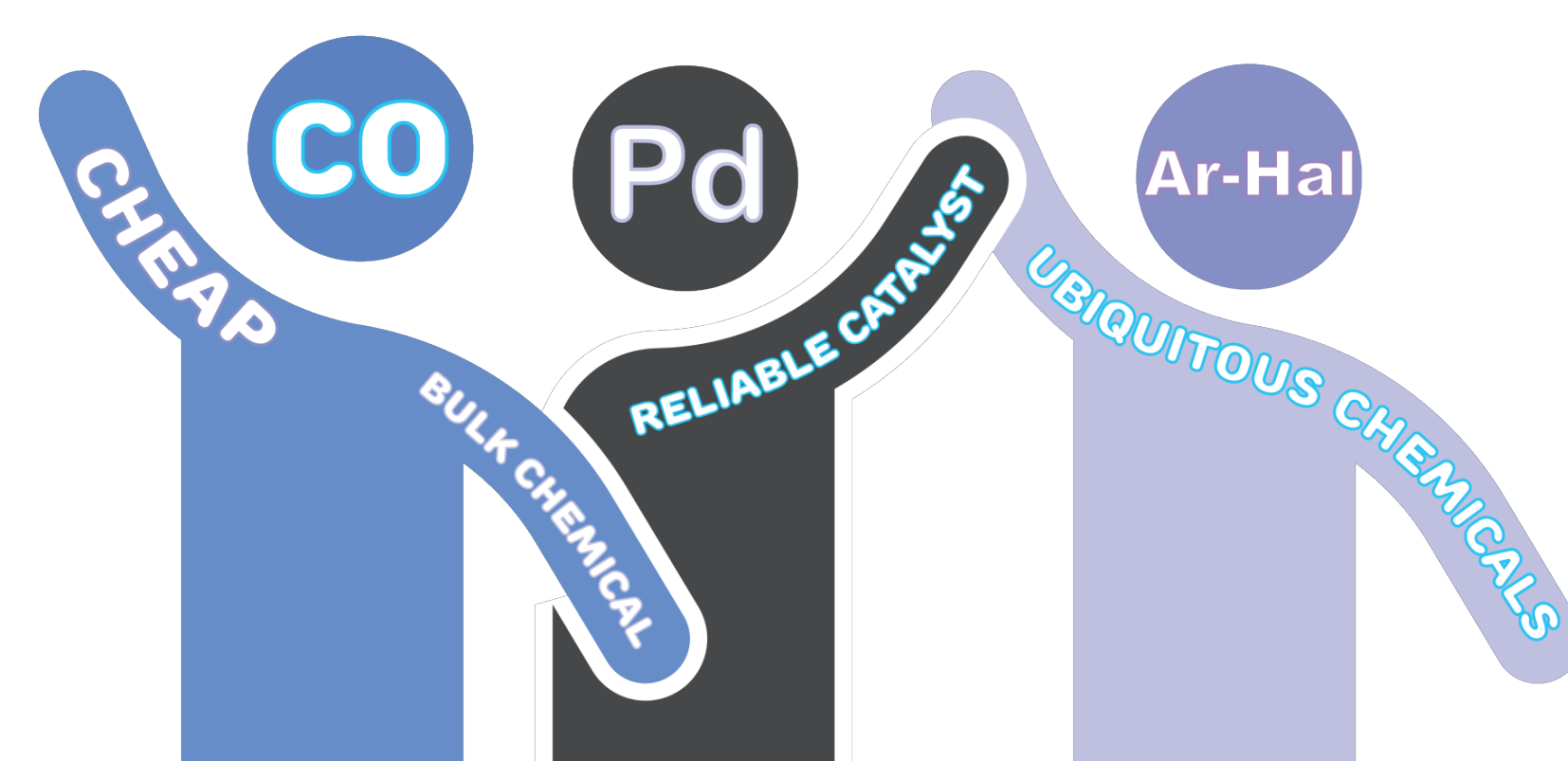


Selective Pd-Catalyzed Carbonylation of Polyhalogenated (Hetero)Arenes: A Role of Temperature and Electronic Effects of Substituents



Vadym Dudko, Maksym Nechayev, Rostyslav Skoropad, Dmytro Leha, Serhiy Ryabukhin, Dmytro Volochnyuk

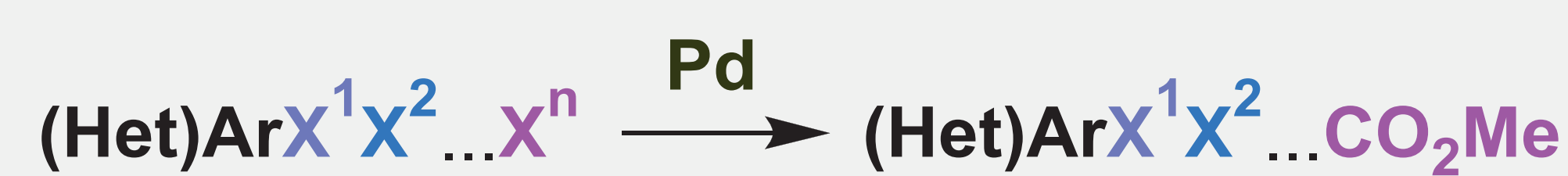
Background & Overview of the Project



RCONu

- carbonyl compounds exist widely in natural products, agrochemicals, medicals, advanced materials, etc.
- impressive progress has been achieved during the past decades in Pd-supported carbonylation from 1974
- polyhalogenated arenes are easily accessible compounds
- CO is a unique, nearly unlimited, and the cheapest C1 source

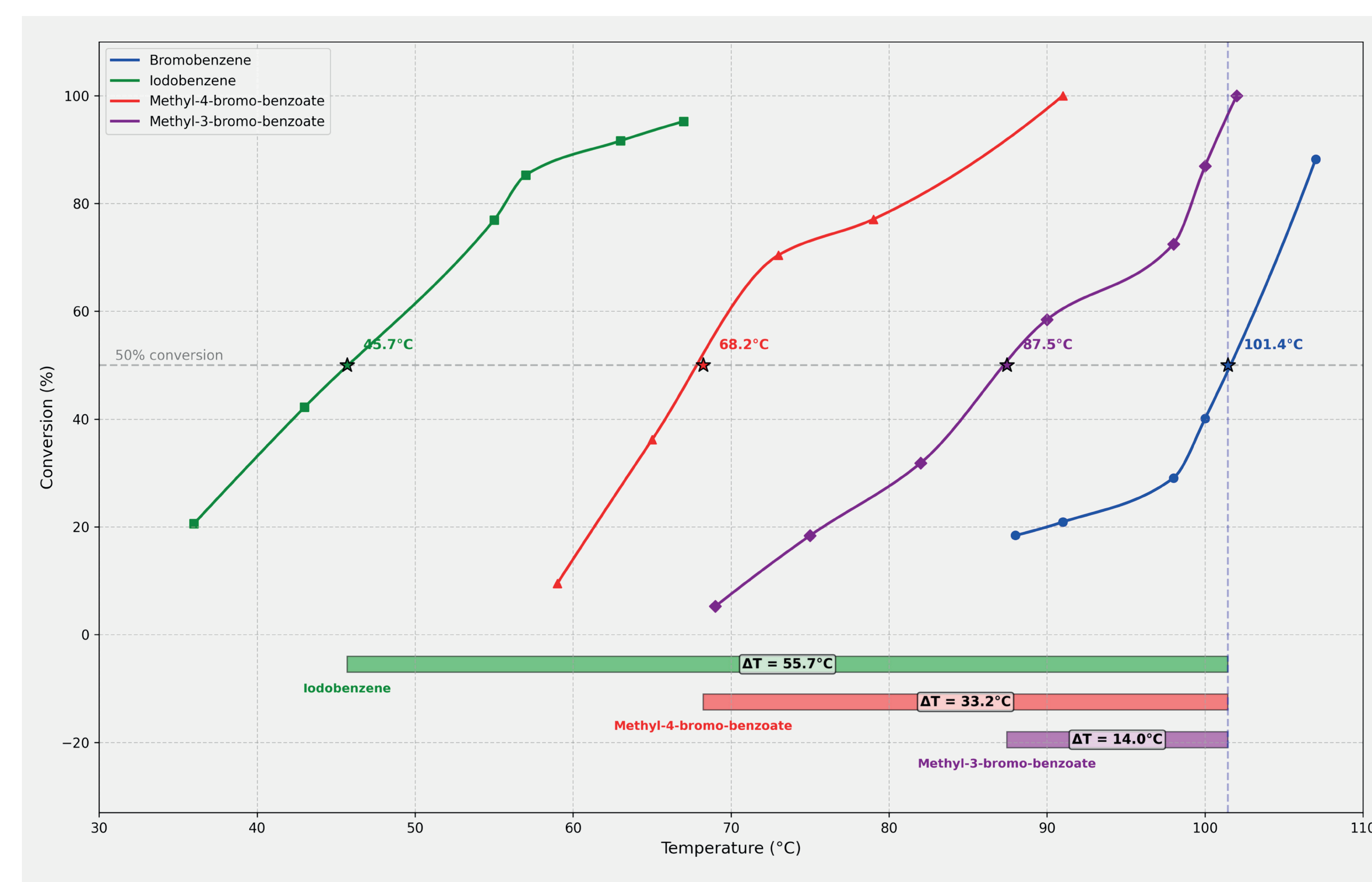
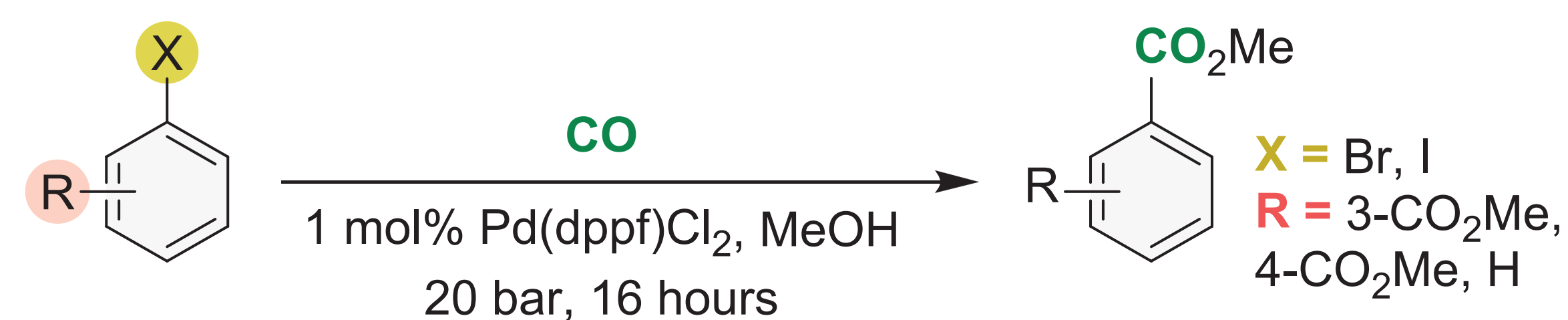
THIS WORK



To investigate and establish the methodological foundations of Pd-catalyzed carbonylation of polyhalogenated arenes

Synthetic strategies toward spiro-a-prolines

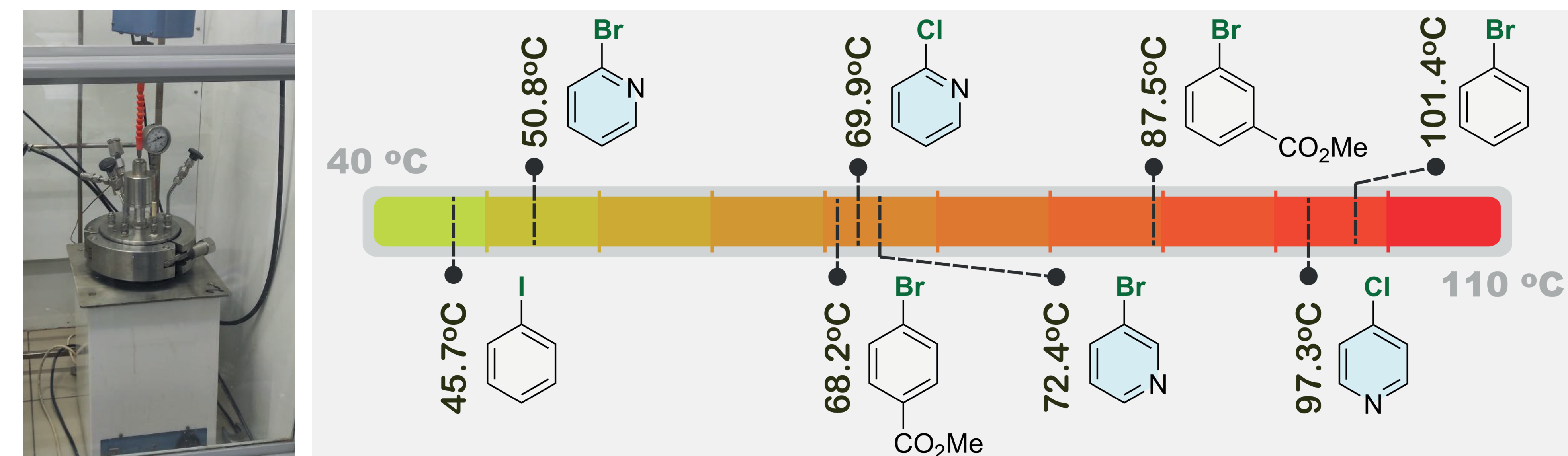
TEMPERATURE-DEPENDENT CONVERSION PROFILES OF HALOGENATED BENZENES



USEFUL NOTES LEARNED FROM THE GRAPH

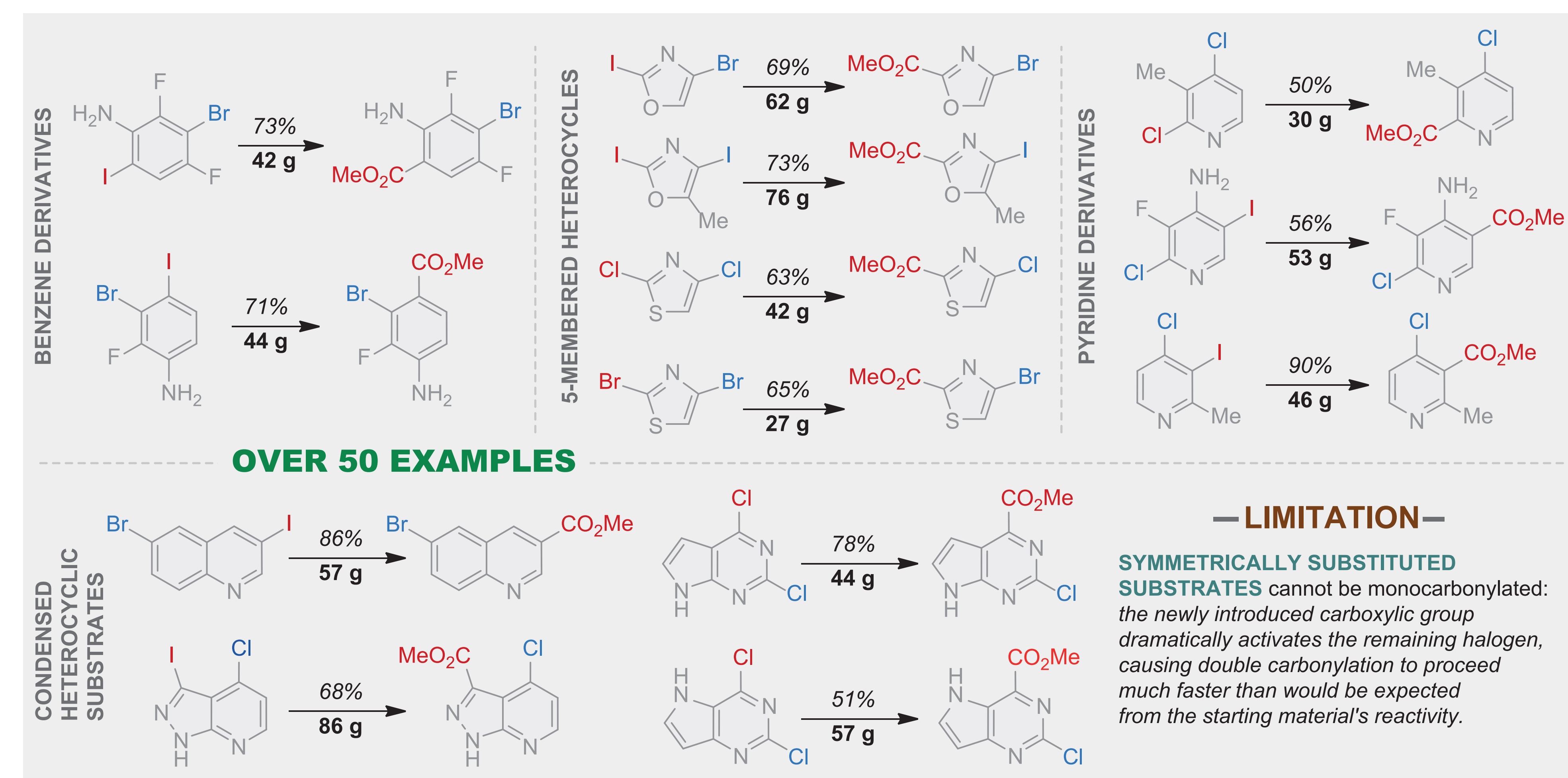
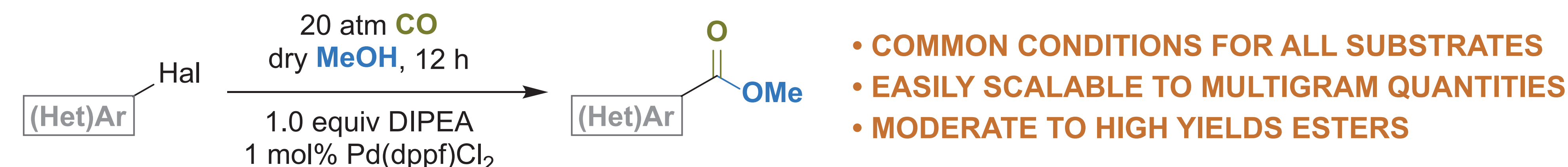
- the introduction of an EWG group significantly enhances the reactivity of C-Br bonds
- the positional effect is particularly noteworthy (para-substitution is more active than meta-substitution)
- the reactivity of the C-I bond is higher than that of the C-Br bond

REACTIVITY HIERARCHY BASED ON THE 50% CONVERSION TEMPERATURES



- the introduction of an N-atom into the aromatic ring dramatically enhances halogen reactivity, with the effect being highly position-dependent

Experimentally confirmed reactivity patterns



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