

Aerobic oxidation of phosphines to phosphine oxides promoted by cofactor flavin derivatives

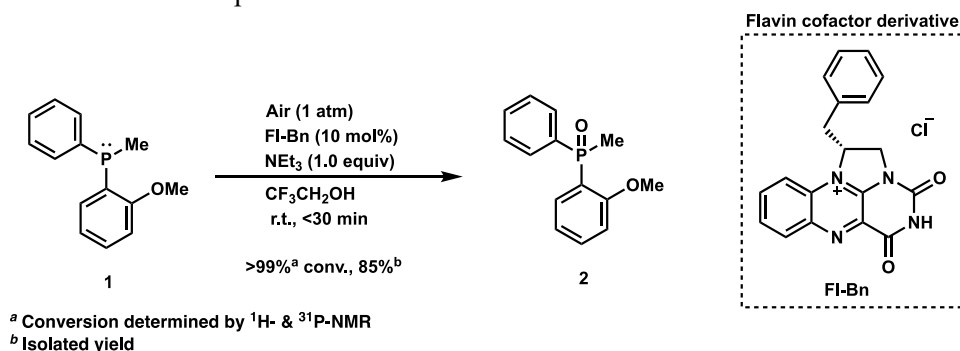
(Department of Chemistry and Biochemistry, Global Center for Science and Engineering, School of Advanced Science and Engineering, Waseda University) ○Rui-Qi Zhu, Zi-Ying Jin, Kana Yamamoto

Keywords: *Organocatalyst; Biomimetic catalyst; Flavin coenzyme; Green Chemistry; Aerobic oxidation*

Phosphine oxides have played multiple roles in organic chemistry, as ligands in metal catalysts, as reagents, as modifiers of pharmaceuticals, and as supramolecules. The simplest methods to obtain these compounds are by direct oxygenation of phosphines. Numerous methods and oxidants have been developed for this purpose, however, not many of them are catalytic, and with a broad substrate applicability.

We have been interested in use of cofactor flavin derivatives to promote oxidative transformations, and have found that phosphorous compounds can be smoothly oxidized under air in the presence of these catalysts.^{1,2} Under the optimized conditions, phosphine **1** was smoothly oxidized to its oxide in the presence of flavin derivative **FI-Bn** (02 equiv) in acetonitrile under air after 24h. However, the reaction was case sensitive and its mechanism was unclear. Herein, we present new findings of the reaction that enable much faster and reliable results.

After further screening of solvents and additives, we found that alcoholic solvents, in particular use of trifluoroethanol promoted the reaction to completion within half an hour under otherwise identical conditions. The reaction completed even with 1 mol% of the catalyst in 24 h. In addition, we found a new role of amine additive, which may be acting as radical inhibitor, suppressing side reactions. Our mechanistic investigation and the working mechanism, as well as more comprehensive studies on substrate scope and limitation will also be disclosed in this poster.



- 1) ○Eika Sarga, Ziying Jin, Masahiro Kobayashi, Kana Yamamoto, 101th JCS meeting, 2021 (online).
- 2) ○ Ziying Jin, Kana Yamamoto, 101th JCS meeting, 2021 (online).