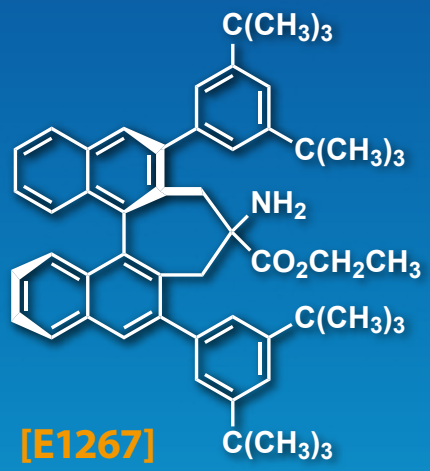
Chiral Amine Catalyzing Enantioselective Fluorination of α-Branched Aldehydes

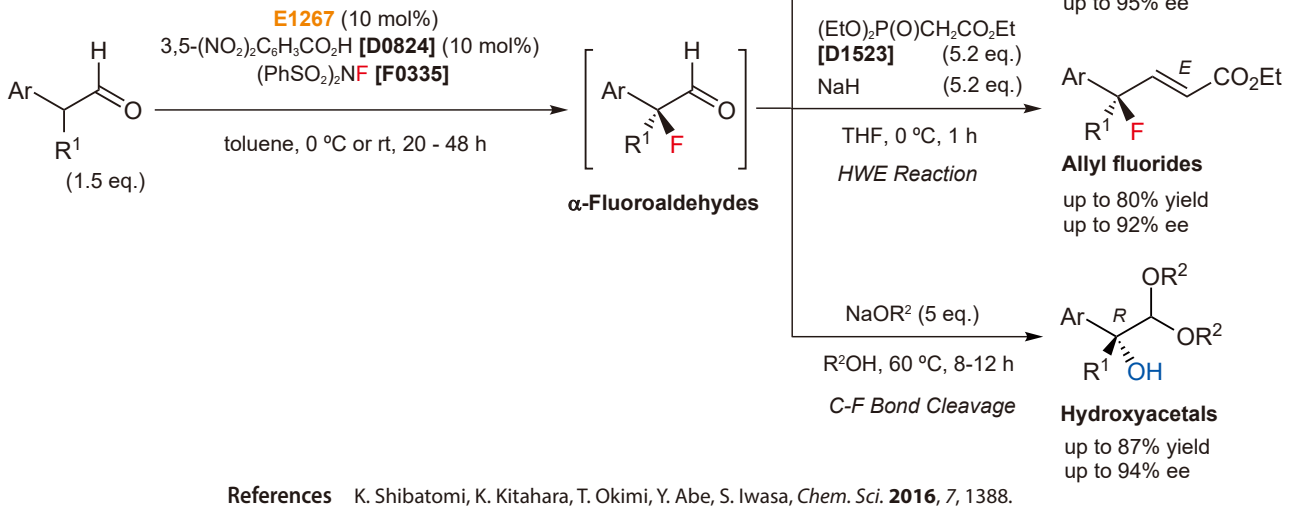


[E1267]

Advantages

- Catalyze the asymmetric fluorination of α-branched aldehydes using *N*-fluorobenzenesulfonimide (NFSI) as a fluorine source.
- The generated chiral tertiary fluorides can be converted into various optically-active compounds.

Application



References K. Shibatomi, K. Kitahara, T. Okimi, Y. Abe, S. Iwasa, *Chem. Sci.* **2016**, *7*, 1388.

Ethyl (11b*R*)-4-Amino-2,6-bis(3,5-di-*tert*-butylphenyl)-4,5-dihydro-3*H*-cyclohepta-[1,2-*a*:7,6-*a*']dinaphthalene-4-carboxylate 50mg [E1267]

This product was produced by collaboration with Assoc. Prof. Kazutaka Shibatomi, Toyohashi University of Technology.

Related Products

3,5-Dinitrobenzoic Acid	25g / 500g [D0824]
***N*-Fluorobenzenesulfonimide (= NFSI)**	5g / 25g [F0335]
Sodium Borohydride	25g / 100g / 500g [S0480]
Triethyl Phosphonoacetate	25g / 100g / 500g [D1523]

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Introduction of the Researcher

Shibatomi Laboratory

Department of Environmental and Life Sciences, Toyohashi University of Technology

The members of the Shibatomi laboratory with Assoc. Prof. Kazutaka Shibatomi on the far left

Research Description

The Shibatomi group aims to develop the new synthetic methods of organic molecules, especially focusing on design and synthesis of novel chiral catalysts and their application to the asymmetric reactions. The Shibatomi group is also developing the efficient synthetic method for chiral pharmaceutical and agricultural compounds with the above-mentioned chiral catalysis. Recently, the Shibatomi group found highly enantioselective halogenation of carbonyl compounds and applied this method for the synthesis of a GPR119 agonist which is a potential drug for type 2 diabetes.

Experimental Procedure (synthesis of 2-fluoroalcohol; Ar=Ph, R^1=CH_3)

To a solution of **E1267** (20 mg, 0.026 mmol, 10 mol%) in toluene (0.54 mL) is added 3,5-dinitrobenzoic acid (5.5 mg, 0.026 mmol, 10 mol%), 2-phenylpropionaldehyde (52 mg, 0.39 mmol, 1.5 eq.), and *N*-fluorobenzenesulfonimide (NFSI) (0.26 mmol, 82 mg, 1 eq.) at 0 °C. The reaction mixture is stirred at 0 °C for 48 h, then poured into CH_3OH/CH_2Cl_2 (1:4, 1.3 mL) at 0 °C. To this solution, $NaBH_4$ (1.6 mmol, 6 eq.) is added, and the mixture is stirred at room temperature for 1 h. The reaction is quenched with saturated aq. NH_4Cl, and the mixture is extracted with Et_2O. The organic layer is dried over Na_2SO_4, and concentrated. The residue is purified by silica gel chromatography (eluent: hexane/ethyl acetate = 3/1) to give (*S*)-2-fluoro-2-phenylpropan-1-ol (34.5 mg, 86% yield based on NFSI, 95% ee) as a white solid.

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