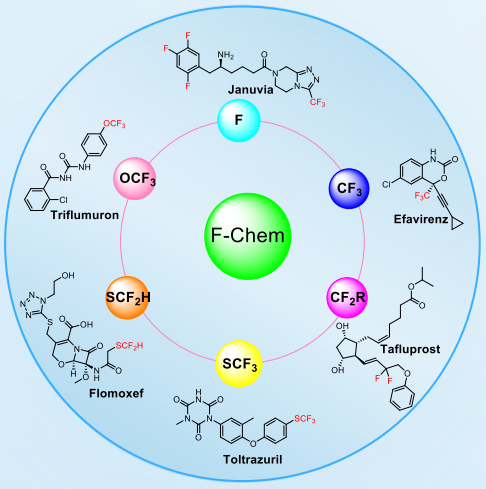
WuXi AppTec

Research Chemistry Services

Fluorine Chemistry Platform

- Founded in 2012, we have a professional and experienced team specializing in fluorine chemistry
- Our collection contains most reagents used for introducing fluorine-containing groups into small molecules
- Developed and established the application of SF_4 in Flow Chemistry

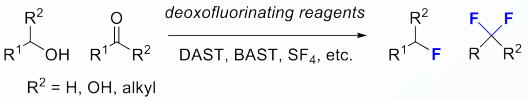
Capability of Fluorine Chemistry Platform



- Condition Screening & Optimization
- Scalable Procedure
- Late-stage Functionalization
- F-containing Building Blocks

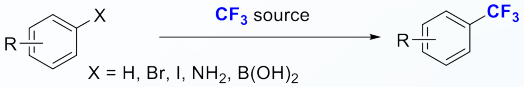
Well-Developed Condition Optimization System

Deoxyfluorinatioan (F)



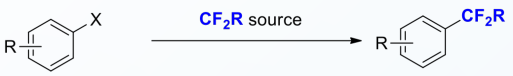
R^2 = H, OH, alkyl

Trifluoromethylation (CF_3)



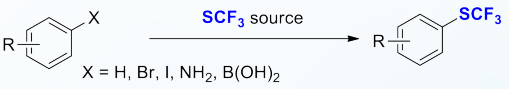
X = H, Br, I, NH_2, $B(OH)_2$

Difluoroalkylation (CF_2R)



X = H, Br, I, NH_2, $B(OH)_2$, R = H, COOEt, Br

Trifluoromethylthiolation (SCF_3)



X = H, Br, I, NH_2, $B(OH)_2$

OCF_3, N-CF_3, SF_5, etc.

15+ years experience

10K+ fluorinated BBs

66%+ internal success rate

20+ reaction types

<48 h from request to proposal

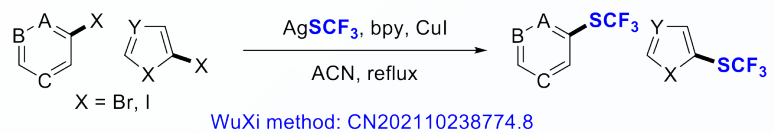
mg to kg scale

Contact us

https://rcs.wuxiapptec.com

chemistry_service@wuxiapptec.com

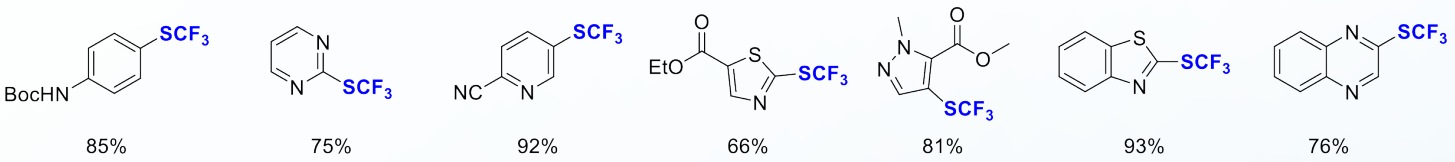
Improved Trifluoromethylthiolation by Fluorine Chemistry Platform



WuXi method: CN202110238774.8

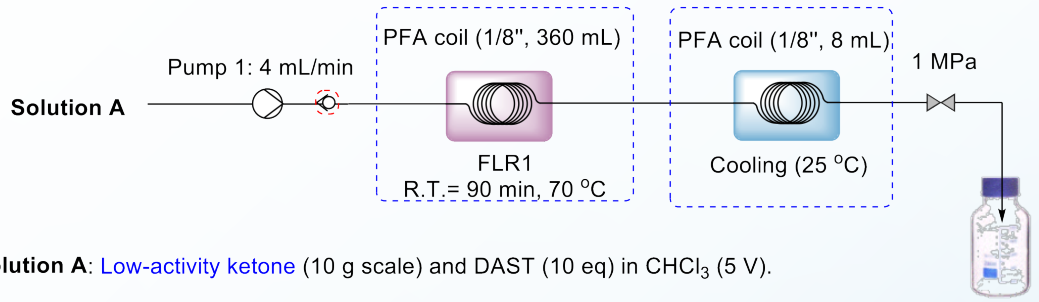
- Broad substrate scope
- Good functional group tolerance
- Good to excellent yield
- Commercially available reagents

Selected examples



85% 75% 92% 66% 81% 93% 76%

Cross-Platform Cooperation: Fluorine + Flow-Chemistry

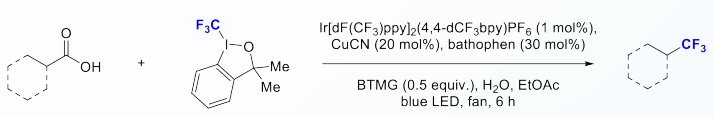


Solution A: Low-activity ketone (10 g scale) and DAST (10 eq) in $CHCl_3$ (5 V).

- Higher yield & safer operation for sterically hindered ketones

Cross-Platform Cooperation: Fluorine + Photo-Chemistry

Decarboxylative Trifluoromethylation

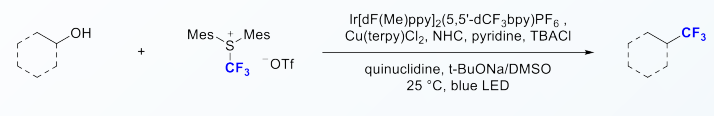


Carboxylic acids — Togni's Reagent I

J. Am. Chem. Soc. **2018**, *140*, 6522−6526

- Highly efficient: no need for pre-activated substrates
- Excellent functional group compatibility: heterocycles, olefins, alcohols, and strained ring systems

Deoxytrifluoromethylation of Alcohols



Alcohols — Mes-Umemoto Reagent

J. Am. Chem. Soc. **2022**, *144*, 11961−11968

- Large substrate scope: primary, secondary, and tertiary alcohols
- Late-stage functionalization, such as sugars, nucleosides and complex drug-like molecules