Novel and simple method for the introduction of the trifluoromethoxy group into molecular compounds

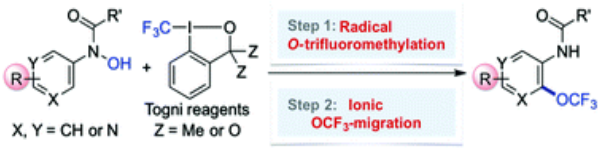
Our method of OCF_3 compound synthesis will replace older more cumbersome and expensive methods and will unlock the full potential of these compounds

Background

Among the fluorine-containing functional groups, the trifluoromethoxy group (OCF_3) is of current interest to the materials, agricultural and pharmaceutical sciences because of its unique structural and electronic properties. Many OCF_3 containing biologically active molecules show enhanced effectiveness often coupled with diminished side effects. The existing approaches for introducing OCF_3 into organic molecules require the use of highly toxic, difficult to handle and thermally unstable reagents. In addition, these transformations suffer from narrow substrate scope, poor functional group tolerance, all of which result in very expensive OCF_3-containing building blocks (e.g. $10,000/g) and hinder the exploration of OCF_3 group in the field of synthetic organic chemistry.

Technology

Dr. Ming-Yu Ngai, Assistant Professor in the Department of Chemistry at Stony Brook, has developed a new protocol which utilizes bench stable reagents, is operationally simple and amenable to gram scale and one-pot synthesis, and shows high functional group tolerance. His novel technology allows an easy trifluoromethoxylation of arenes and heteroarenes via a one-pot two-step sequence of O-trifluoromethylation of N-(hetero)aryl-N-hydroxylamine derivatives. This new technology will render the OCF_3 group as a classical group to consider in all molecular screenings from medicinal chemistry to materials science and provides an easy access to a wide range of synthetically useful ortho-OCF_3 aniline derivatives and trifluoromethoxylated heteroaromatic compounds.



Patent number/Publications:

- PCT/US2015/054958
- Hojczyk, KN. Angew Chem Int Ed Engl. 2014 Dec 22;53(52). Lee, K. Org. Biomol. Chem., Mar 2016

Advantages

- **Easy and cost effective method of producing OCF_3 compounds**
- **Gram scale synthesis**
- **High functional group tolerance**

Applications

- **Manufacturing OCF_3 substituted pharmaceuticals and agrochemicals**
- **Production and commercialization of new OCF_3 bulding blocks**
- **Molecular screening of OCF_3 containing compounds**

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