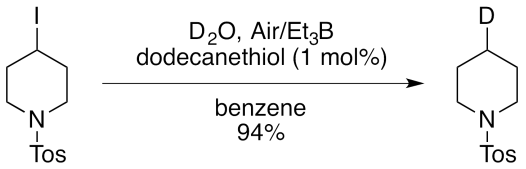
Thiol-Catalyzed Radical Deuteration of Alkyl Iodides Mediated by Triethylborane and Deuterium Oxide

V. Soulard[1], G. Villa[1], D. Vollmar[1], P. Renaud[1]*

[1]University of Bern

Preparation of organic compounds selectively labelled with deuterium atom, remains a challenging synthetic problem [1]. Radical deuteration of alkyl halides is one of the most efficient approach to perform this task. It is usually run using organotin deuterides [2] but this method has three major drawbacks: organotin deuterides are expensive, toxic [3] and led to product contamination.

We report here a method to deuterate alkyl iodides via a radical pathway with deuterated water or methanol as source of deuterium atom. Triethylborane is used to initiate and propagate the chain and dodecanethiol is used as a catalyst [4]. High deuterations and yields are obtained using this method.



[1] Maltais, F.; Jung, Y. C.; Chen, M.; Tanoury, J.; Perni, R. B.; Mani, N.; Laitinen, L.; Huang, H.; Liao, S.; Gao, H. et al. *J. Med. Chem*. **2009**, *52*, 7993.
[2] Curran, D. P.; Ramamoorthy, P. S. *Tetrahedron* **1993**, *49* (22), 4841–4858.
[3] I. J. Boyer, *Toxicology* **1989**, *55*, 253–298.
[4] B. M. Mikhailov; Y. N. Bubnov *Zh. Obshch. Khim.* **1961**, *31*, 160-166.