

**Poster Presentation (PP-73)**  
**Inter-Disciplinary Explorations in Chemistry (I-DEC 2018)**

**A Simple Substitution on Thyroid Hormones Remarkably Alters the Regioselectivity of Deiodination by a Deiodinase Mimic**

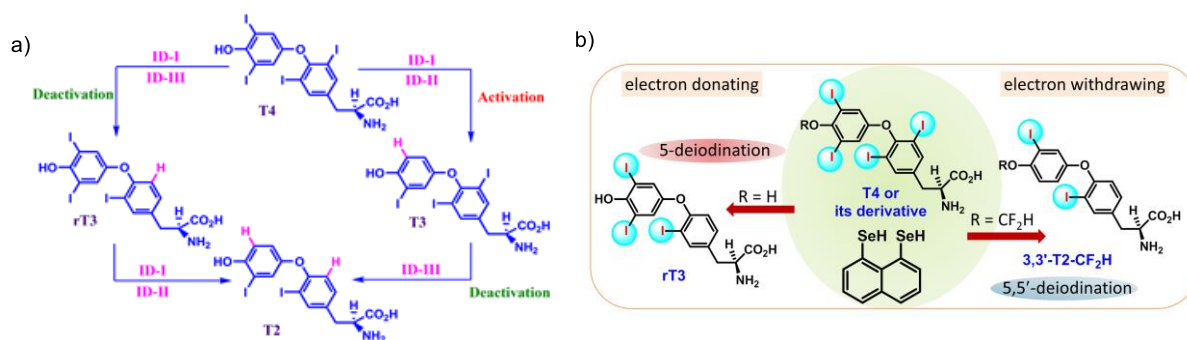
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Thyroid hormones play important roles for growth, development and regulation of energy metabolism in the human body. Thyroid gland mainly produced prohormone T4 (3,3',5,5'-tetraiodothyronine), whereas the biologically active form T3 (3,5,3'-triiodothyronine) is produced from the outer ring (5'-) deiodination of T4 by iodothyronine deiodinase enzyme, which contains a selenocysteine in the active site. Three different forms of iodothyronine deiodinase enzymes are present in human (ID-I, ID-II, ID-III). ID-I mediates both 5'- and 5-deiodinations of T4 to produce T3 and rT3, respectively. In contrast, the other two enzymes, ID-II and ID-III are selective to 5'- and 5-deiodination to produce T3 and rT3, respectively (Scheme 1a).



**Figure1:** a) The regioselective deiodination of thyroid hormones catalysed by three isoforms of iodothyronine deiodinase. b) Regioselective deiodination of thyroxine by deiodinase mimic.

Our group has reported that the naphthyl-based compound bearing peri-substituted thiol/selenol groups shows inner ring (5-) deiodination<sup>1,2</sup>. Mechanistic investigations revealed that a cooperative halogen bond and chalcogen bond is responsible for specific inner ring deiodination<sup>3</sup>. In this context, we will show that the regioselectivity of deiodination can be changed dramatically by altering the electronic properties of the iodine atoms through substitution at the 4'-OH of T4 under physiological conditions (Scheme 1b). In this poster, it will be discussed that the –OH group of T4 can act as both hydrogen bond acceptor and donor, which may play a key role in the regioselectivity of the deiodination reaction.

**References and Notes:**

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