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Reaction of hypotaurine or taurine with superoxide produces the organic peroxysulfonic acid peroxytaurine

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## Abstract

Hypotaurine and taurine are amino acid derivatives and abundant molecules in many eukaryotes. The biological reaction in which hypotaurine is converted to taurine remains poorly understood. Here, hypotaurine and taurine were observed to react with superoxide anion *in vitro* to form the novel molecule peroxytaurine. In contrast, hypotaurine reacts with hydrogen peroxide to form taurine, but taurine does not react with hydrogen peroxide *in vitro*. Mass and NMR spectrometry as well as FTIR and Raman spectroscopy support the molecular characterization of peroxytaurine. Gravimetric and spectroscopy experiments suggest a stoichiometry of two superoxides reacting with one hypotaurine or taurine. The newly identified molecule is a semi-stable, organic peroxysulfonic acid that may be an intermediate metabolite in taurine synthesis.

## Keywords

Hypotaurine, taurine, peroxide, superoxide, mass spectrometry, FTIR, HPLC, Raman

## Introduction

Taurine is one of the most abundant, free, amino acid-derived molecules in the cells of humans and other eukaryotes. A derivative of cysteine, taurine (2-aminoethanesulfonic acid) comprises up to 0.1% of the body weight of humans (1). It has been implicated in a number of biological processes, such as regulation of osmolarity, calcium modulation, membrane stabilization, reproduction, pathogen immunity, function of the central nervous system, and neonatal development (1,2). Its concentration has been measured between 1–50 mM in liver, retina, leukocytes, neutrophils, the central nervous system, skeletal and cardiac muscles, and semen (1,3). Only a few biological roles for taurine are currently well understood, such as in bile acid production (1).

Along with its biological roles being poorly understood, taurine as a molecule is often mischaracterized in the scientific literature. First, it is widely called an amino acid, though it lacks the carboxylic acid that would permit that designation. Second, it is referred to as an antioxidant and has been tested for antioxidant properties in a number of studies (4,5). According to one study, taurine does not react readily with superoxide, hydrogen peroxide, or hydroxyl radical (5), which are some of the molecules collectively called Reactive Oxygen Species (ROS). Taurine does react with hypochlorous acid to become taurine chloramine (5), but with a rate constant 100-fold less than for the reaction of glutathione with hypochlorous acid (6). The taurine chloramine reaction is relevant in activated neutrophils that produce hypochlorous acid, but taurine chloramine is itself a reactive oxidizing agent (5).

Taurine is derived from the metabolic pathways of cysteine degradation and pantothenate synthesis. Cysteine is enzymatically oxidized to cysteinesulfinic acid (7), which is then enzymatically

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