We have recently reported SAR data describing the pharmacological activity of a series of phenyl alkyl selenides and tellurides which catalyse the oxidation of thiols by hydrogen peroxide (H\textsubscript{2}O\textsubscript{2}). "The design of redox active thiol peroxidase mimics: dihydrolipoic acid recognition correlates with cytotoxicity and prooxidant action" B. Zadehvakili, S.M. McNeill, J.P. Fawcett, G.I. Giles (2016) [1]. This thiol peroxidase (TPx) activity is potentially useful for a number of therapeutic applications, as it can alter the outcome of oxidative stress related pathologies and modify redox signalling. This article presents data describing the molecular changes that occur to a TPx mimic upon exposure to H\textsubscript{2}O\textsubscript{2}, and then the thiol mercaptoethanol, as characterised by UV–vis spectroscopy and HPLC retention time.
How data was acquired

Jenway 6715 UV–vis spectrometer. Shimadzu LC-10AT HPLC with SPD-M10A diode array detector and Gemini C18 column (5 μm, 100 Å, 100 × 4.6 mm).

Data format

Raw.

Experimental factors

Drug solutions treated with H₂O₂ and 2-mercaptoethanol.

Experimental features

Changes to TPx mimic UV–vis spectra and HPLC retention time following oxidation and reduction. Background corrected UV–vis absorbance spectra, raw HPLC traces acquired at 270 nm after setting the channel current to zero.

Data source location

University of Otago, Dunedin, New Zealand.

Data accessibility

Data provided in article.

Value of the data

- TPx mimics display antioxidant, pro-oxidant and cytotoxic properties and are being developed as therapeutic agents. The data describe methodology to spectroscopically characterize their reactions with H₂O₂ and thiol substrates, which will be useful for future investigations into the chemical mechanism of this drug class.
- Structure-Activity Relationship (SAR) studies are currently being developed to explore the pharmacological activity of TPx mimics. The TPx mimic catalytic cycle consists of an initial oxidation step by H₂O₂, followed by reduction by a thiol to regenerate the starting mimic. The data provide information quantifying variations in TPx mimic hydrophobicity during this cycle. This parameter has never before been applied to SAR studies, and has the potential to improve our understanding of drug pharmacology.
- The data provide information on the catalytic cycle and biophysical properties of phenyl butyl telluride, a TPx mimic currently being evaluated as a prooxidant drug. This is of wide-ranging interest to researchers investigating the application of therapeutic agents to manipulate the cellular redox state.

Fig. 1. Reversibility of the TPx catalytic cycle. A: Catalytic cycle of TPx mimic T4. The reaction takes place in two steps, initially the T4 telluride is oxidised to a telluroxide by H₂O₂ [5]. The metal centre is then regenerated by reduction with a thiol [5], in this case mercaptoethanol (ME). B: Spectroscopic features characteristic of the TPx redox cycle. T4 (50 μM, black trace) reacted with H₂O₂ (1 mM) to form an oxidised intermediate (red trace). The TPx mimic was then regenerated by the addition of ME (1 mM, blue trace). The spectrum of ME alone (green trace) is shown for comparison.
1. Data

We present UV–vis spectra which characterize the initial, oxidised and regenerated forms of phenyl butyl telluride (T4). This is accompanied by HPLC data revealing a change in molecular hydrophobicity as T4 is oxidised. See Figs. 1 and 2.

1.1. Experimental design, materials and methods

1.1.1. Synthesis of phenyl butyl telluride (T4)

T4 was prepared according to an established procedure [2] and compound structure confirmed by comparison to published data [3].

1.1.2. Standardisation of H$_2$O$_2$ solutions

The concentration of a commercial H$_2$O$_2$ solution (Sigma–Aldrich, Auckland, New Zealand) was determined by UV–vis absorbance ($\varepsilon_{240} = 43.6 \text{M}^{-1}\text{cm}^{-1}$ [4]).

1.1.3. UV–vis Spectroscopy

T4 was dissolved in methanol and then diluted to 50 $\mu$M in methanol. UV–vis spectra were acquired over the wavelength range 200–400 nm with a scan rate of 4 nm/s.

1.1.4. HPLC Analysis

T4 was initially dissolved and diluted in acetonitrile to a concentration of 100 $\mu$M. A 20 $\mu$l aliquot of this solution was then injected into an HPLC system under isocratic conditions (75:25 v/v

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**Fig. 2.** Effect of oxidation on T4 hydrophobicity. A: Initial chromatogram of T4, B: chromatogram of T4 after the addition of H$_2$O$_2$ (1 mM) and incubation for 5 min, C: Superimposition of A (initial chromatogram) and B (chromatogram following addition of H$_2$O$_2$), the axis of A re-scaled for alignment.
acetonitrile:water) with a flow rate of 2.5 ml/min. Compound elution was monitored over 5 min at 270 nm.

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Appendix A. Transparency document

Transparency document associated with this article can be found in the online version at http://dx.doi.org/10.1016/j.dib.2016.05.037.

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