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ARTICLE

## The Antiproliferative Activity of Di-2-pyridylketone Dithiocarbamate Partly Attributed to Catalase Inhibition: Detailed the Interaction by Spectroscopic Methods

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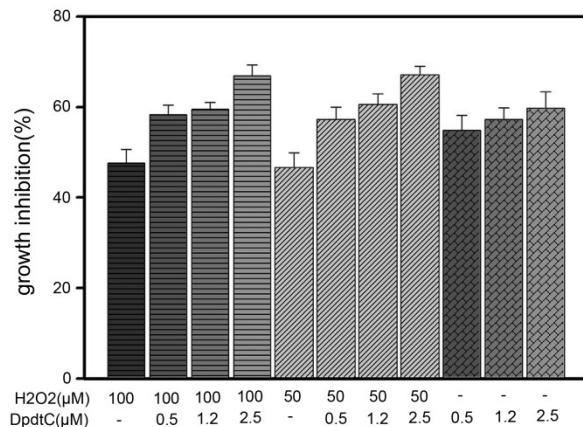
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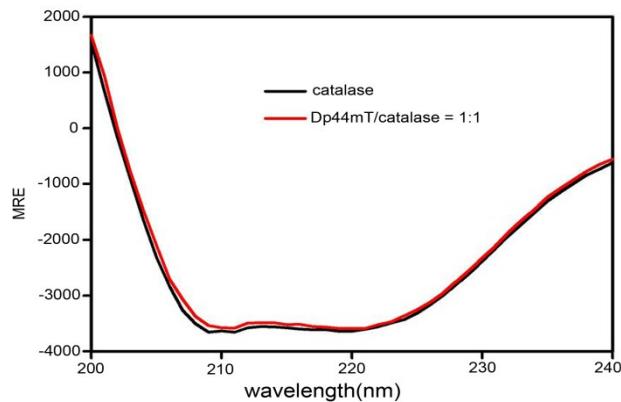
### Supplementary material

#### 1. Growth inhibition of DpdtC correlated to H<sub>2</sub>O<sub>2</sub> content



**Fig. S1** Growth inhibition of DpdtC in the presence of varying concentration of H<sub>2</sub>O<sub>2</sub>.

#### 2. No obvious Interaction of Dp44mT with catalase revealed by CD spectra



**Fig.2** The CD spectra of catalase in the absence or presence of DpdtC

#### 3. DpdtC can be randomly docked into catalase both from human and beef liver

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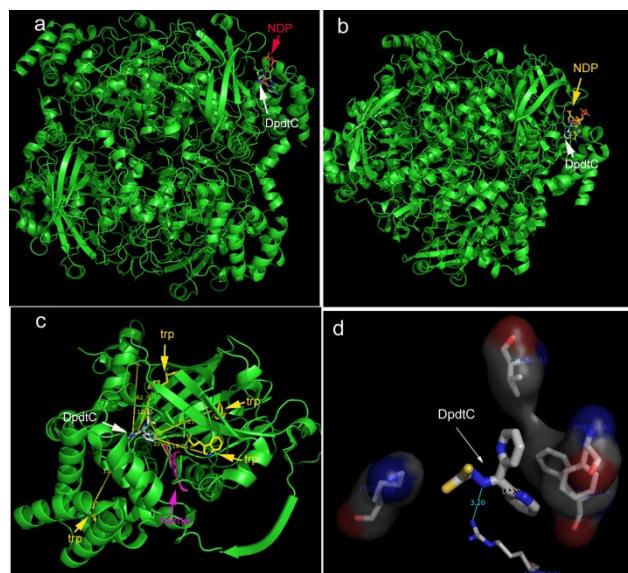
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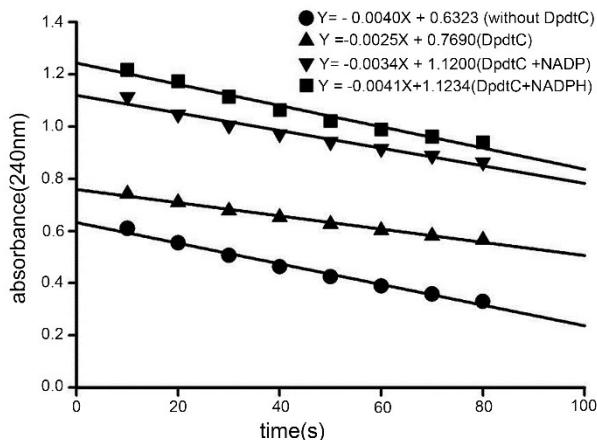
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Electronic Supplementary Information (ESI) available: [details of any supplementary information available should be included here]. See DOI: 10.1039/x0xx00000x



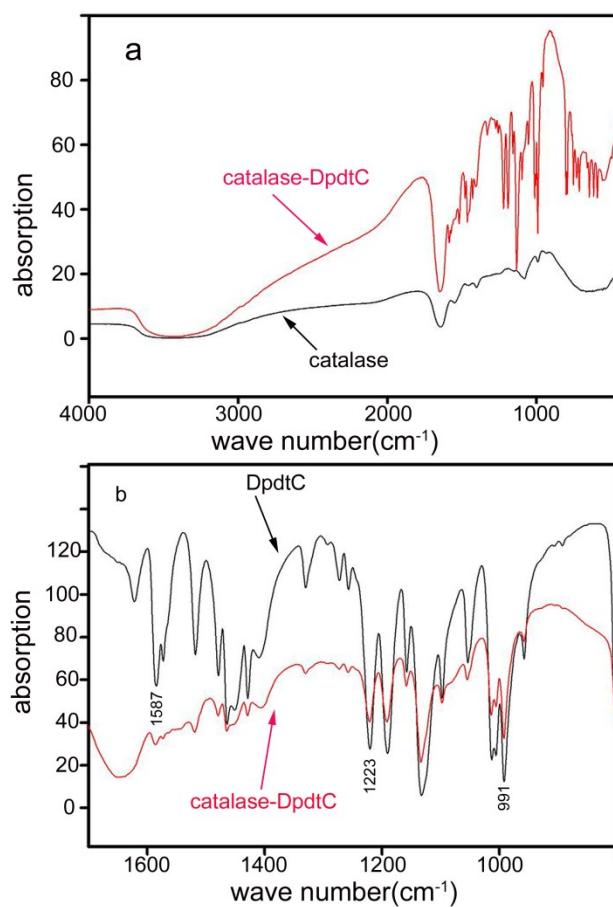
**Fig. S3** Molecular docking study. (a) DpdtC was located on catalase from beef liver at NDP binding site; (b) DpdtC was located on human catalase at NDP binding site; (c) distance between DpdtC and Trps in catalase; (d) density map of amino acids of catalase around DpdtC.

#### 4. NADP(H) rescued the catalase inhibition induced by DpdtC



**Fig. S4** The effect of NADP(H) on catalase activity in the presence or absence of DpdtC. The conditions as indicated in the figure. The rate was the slope of the regression line. Condition: 0.1  $\mu$ M for NADP(H), 9.2 nM for catalase, 8  $\mu$ M for DpdtC, the others were same as in dynamic assay.

#### 5. FTIR spectra revealed there was no obvious interaction of sulphide with neighbouring amino acids except pyridine<sup>1,2</sup>



**Fig. S5** FTIR of catalase in the absence or presence of DpdtC. (a) comparison of catalase and with catalase-DpdtC; (b) comparison of DpdtC with catalase-DpdtC.

1. M. Katcka and T. Urbanski, *Bulletin de l'Académie polonaise des sciences. Série des sciences chimiques*, 1964, **XII**, 615-621.
2. H. Nabipour, S. Ghannamay, S. Ashuri and Z. S. Aghbolagh, *Org. Chem. J.* 2010, **2**, 75-80.