

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

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Cuiping Li,^{a†} Youxun Liu,^{a†} Yun Fu,^a Tengfei Huang,^{a,b} Lixia Kang,^c and Changzheng Li^{a,b}

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Supplementary material

1. Growth inhibition of DpdtC correlated to H₂O₂ content

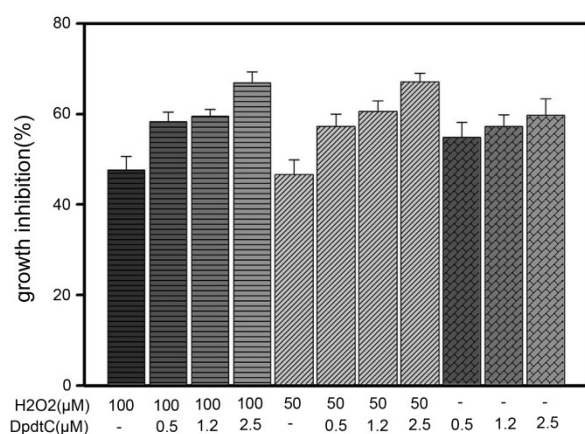


Fig. S1 Growth inhibition of DpdtC in the presence of varying concentration of H₂O₂.

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

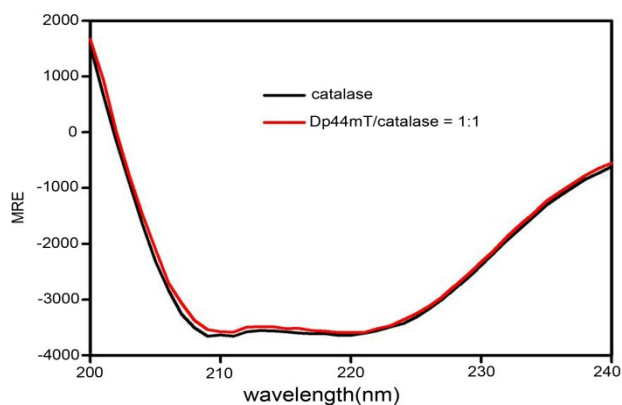


Fig.2 The CD spectra of catalase in the absence or presence of DpdtC

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

^a Department of Molecular Biology & Biochemistry, Xinxiang Medical University, Xinxiang, Henan, P. R. China, 453003;

^b Henan Collaborative Innovation Center of Molecular Diagnostics and Laboratory Medicine, Xinxiang 453003, Henan, China.

^c Clinical Laboratory, the third affiliated hospital of Xinxiang Medical University, Xinxiang, Henan, P. R. China, 453003.

† These authors contributed equally to this work

* changzhenl@yahoo.com; Tel.: +86-373-383-1739

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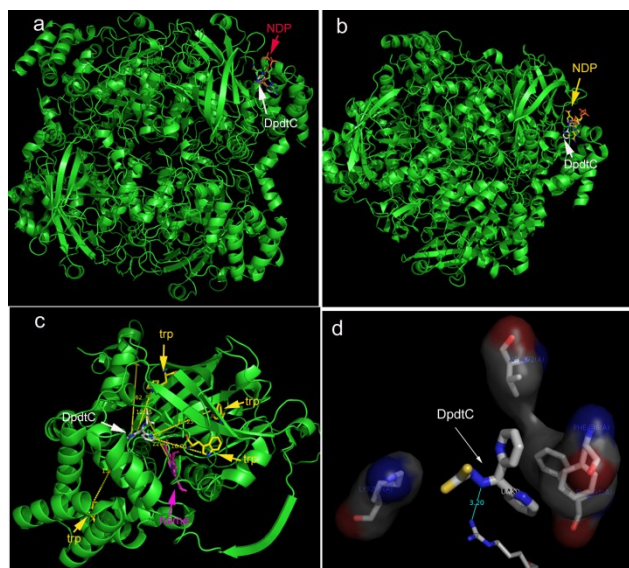


Fig. S3 Molecular docking study. (a) DpdtC was located on catalase from beef liver at NDP binding site; (b) DpdtC was located on human catalase at NDP binding site; (c) distance between DpdtC and Trps in catalase; (d) density map of amino acids of catalase around DpdtC.

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

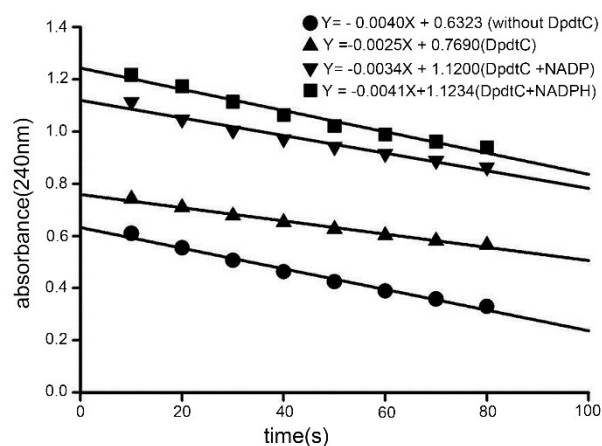


Fig. S4 The effect of NADP(H) on catalase activity in the presence or absence of DpdtC. The conditions as indicated in the figure. The rate was the slope of the regression line. Condition: 0.1 μ M for NADP(H), 9.2 nM for catalase, 8 μ M for DpdtC, the others were same as in dynamic assay.

5. FTIR spectra revealed there was no obvious interaction of sulphide with neighbouring amino acids except pyridine^{1,2}

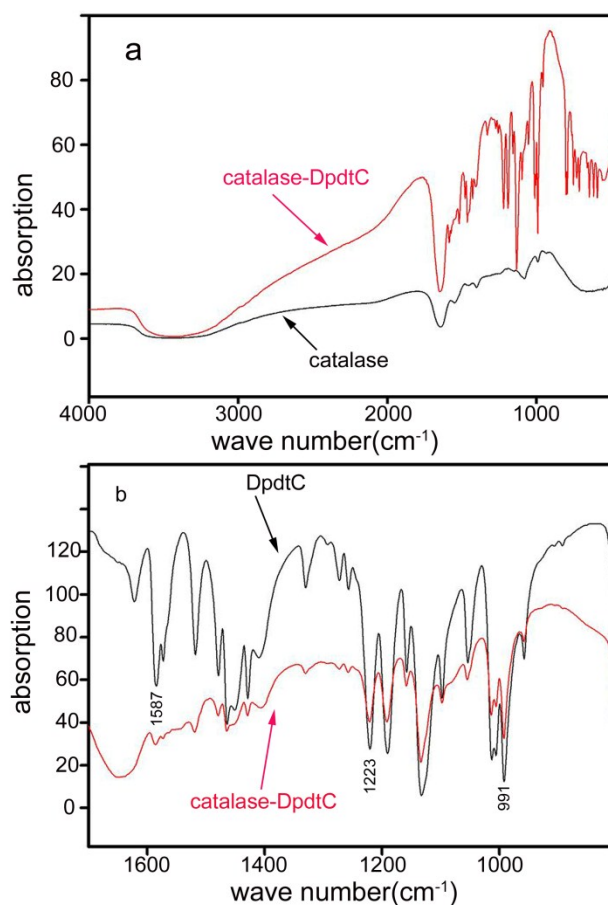


Fig. S5 FTIR of catalase in the absence or presence of DpdtC. (a) comparison of catalase and with catalase-DpdtC; (b) comparison of DpdtC with catalase-DpdtC.

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