Investigation the effects of hetero aromatic compounds on rat erythrocyte 6PGD and in silico molecular docking experiments

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***Abstract*—** The pentose phosphate pathway (PPP) is an anabolic pathway that utilizes glucose to generate molecular building blocks of nucleic acids and reducing equivalents in the form of NADPH through 6-phosphogluconolactone dehydrogenase (6PGD). Recently, it was reported that 6PGD is implicated in cancer disease which makes designing 6PGD inhibitors in cancer treatment a necessity [1-3]. Herein we reported the synthesis of 3,3'-bisindole derivatives and studied their effects on the corresponding enzyme. The studies demonstrated that o bisindole derivative 1 inhibited the activity of 6PGD with an IC50 of 115.8 µM, while the activity was increased in the presence of 2. In silico docking studies were also performed to clarify the mechanism of inhibition/activation.

Keywords—component; *Glucose-6-phosphate dehydrogenase (G6PD) indole, indole derivatives, in silico docking*

References

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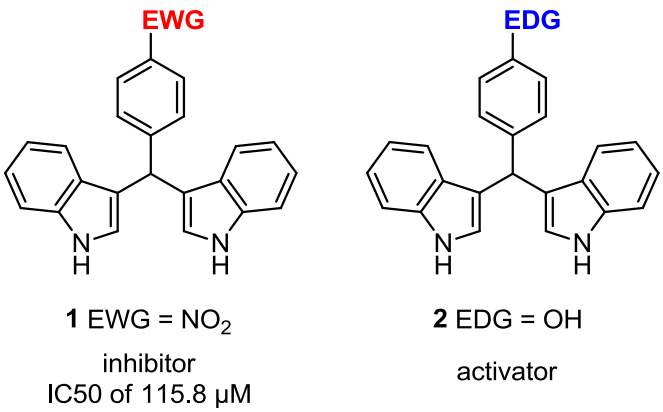

1 EWG = NO_2
inhibitor
IC50 of 115.8 µM

2 EDG = OH
activator