Design and synthesis of indole derivatives for the inhibition of G6PD and detailed in silico studies

Sinan BAYINDIR
Department of Chemistry,
Faculty of Sciences and Arts,
Bingöl University, Bingöl, 12000, Turkey
sbayindir@bingol.edu.tr

Adnan AYNA
Department of Chemistry,
Faculty of Sciences and Arts
Bingöl University, Bingöl, 12000, Turkey
aayna@bingol.edu.tr

Yusuf Temel
Department Of Health Services,
Vocational Schools,
Bingöl University, Bingöl, 12000, Turkey
ytemel@bingol.edu.tr

***Abstract*—** Glucose-6-phosphate dehydrogenase (G6PD) is an enzyme participates in the pentose phosphate pathway, a metabolic pathway that supplies reducing energy to cells (such as erythrocytes). G6PD reduces NADP+ to NADPH while oxidizing glucose-6-phosphate [1]. In last decade, the role of G6PD in apoptosis and the efficacy to anti-cancer therapy has been reported which makes it a promising target for cancer treatment. The aim of the work described in this study was to synthesise potent inhibitors of G6PD and investigate their effects on the enzyme along with in silico molecular docking studies. Among two derivatives tested we found that the compounds 1 and 2 inhibited the activity with an IC50 of 3.39 and 3.89 µM respectively. In silico docking studies of 1 and 2 were also carried out to understand binding mechanism in detail.

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

References

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