

Molecular docking study on anticancer activity of phycocyanobilin

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Abstract: Phycocyanobilin (PCB) has been well known as a blue tetrapyrrole chromophore of C-phycocyanin with proven anticancer activity [1]; however, its mode of action has not been clearly defined. In the current study, PCB was docked with different receptor proteins that regulate cell proliferation and apoptosis including cyclin-dependent protein kinase 2 (CDK-2), CDK-6, DNA topoisomerases I (topo I) and topo II using autodock 4.2 simulation software. The docking results showed that PCB demonstrated better binding energies to CDK-2 and DNA topo I than the known CDK-2 and DNA topo I inhibitors (-11.26 and -11.90 kcal/mol, respectively). Further *in silico* analysis showed key hydrogen bonds and hydrophobic interactions between PCB and targets. Docking results of PCB and CDK-2 revealed forming three H-bonds with residues Gln 85, Leu 83 and Lys 83 at a distance of 3.07, 2.63 and 3.12 Å, respectively. On the other hand, PCB formed two key H-bonds with active site of DNA topo I with residues Arg 364 and Lys 751 at a distance of 2.75 and 2.67 Å, respectively. Combination of our computational results with *in vitro* experimental data can help us to achieve better understanding of anticancer mechanism of PCB in a short time.

Keywords: Docking study; Anticancer; Phycocyanobilin

References

[1] R. Konickova, K. Vankova and *et al.* Anti-cancer effects of blue-green alga *Spirulina platensis*, a natural source of bilirubin-like tetrapyrrolic compounds, *Ann Hepatol.*, 13 (2014) 273-283.