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Affinity of Benzimidazole derivatives towards Alpha-Glucosidase and Galectin-3: *In-Silico* comparative preliminary study

Mohd Hadzrul Hisham Bin Abdul Manaf
Universiti Teknologi MARA (UiTM), Malaysia

Alpha Glucosidase (AG), a digestive enzyme for polysaccharides (complex sugar) in the small intestine. In treatment of diabetes mellitus, AG inhibitor is used to control postprandial (after meal) hyperglycaemia (high blood glucose). Although postprandial blood glucose maintenance is available, the treatment of the etiology (cause) of diabetes mellitus which is insulin resistance is still unavailable. Recent finding shows the involvement of a protein known as Galectin-3 (Gal-3), a cellular signalling protein, in causing insulin resistance and the inhibition of Gal-3 able to reverse insulin resistance. Although both AG and Gal-3 are distinguishable by its origin and function, however both exhibit high affinity towards polysaccharides. Previous studies (*in-vitro* and *in silico*) on benzimidazoles derivatives have shown potent inhibition towards AG; however the same effect on Gal-3 is not yet available. In this study, the affinities of AG and Gal-3 were examined through docking simulation (Autodock 4.2) towards inhibiting compound. Inhibiting both AG and Gal-3 can provide a synergistic effect in treating diabetes mellitus. The results shows benzimidazole derivatives are biologically active towards both AG and Gal-3. However the pattern of inhibition is nonreciprocal towards AG and Gal-3. The binding energy (kcal/mol) is inversed in the compound ranking. This due to the distribution of hydrogen donating accepting group in both of the proteins are inversed with each other. The distribution of hydrogen accepting and donating group with each of the protein amino acids scaffold resulting in inverse pattern for inhibition of the benzimidazole derivatives.

hadzrul_hisham86@yahoo.com

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