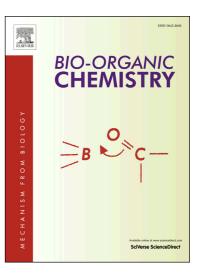
### Accepted Manuscript

Synthesis, Molecular Docking Studies of Hybrid Benzimidazole As  $\alpha$ -Glucosidase Inhibitor

Nik Khairunissa Nik Abdullah Zawawi, Muhammad Taha, Norizan Ahmat, Nor Hadiani Ismail, Abdul Wadood, Fazal Rahim

PII: DOI: Reference:	S0045-2068(16)30305-4 http://dx.doi.org/10.1016/j.bioorg.2016.12.009 YBIOO 1987
To appear in:	Bioorganic Chemistry
Received Date:	14 October 2016
Revised Date:	22 December 2016
Accepted Date:	22 December 2016



Please cite this article as: N.K. Nik Abdullah Zawawi, M. Taha, N. Ahmat, N.H. Ismail, A. Wadood, F. Rahim, Synthesis, Molecular Docking Studies of Hybrid Benzimidazole As α-Glucosidase Inhibitor, *Bioorganic Chemistry* (2016), doi: http://dx.doi.org/10.1016/j.bioorg.2016.12.009

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

### ACCEPTED MANUSCRIPT

# Synthesis, Molecular Docking Studies of Hybrid Benzimidazole As $\alpha$ -Glucosidase Inhibitor

Nik Khairunissa Nik Abdullah Zawawi<sup>a,b</sup>, Muhammad Taha<sup>\*a,b</sup>, Norizan Ahmat<sup>\*a,b</sup>, Nor Hadiani Ismail<sup>a,b</sup>, Abdul Wadood<sup>c</sup>, Fazal Rahim<sup>d</sup>

<sup>a</sup>Atta-ur-Rahman Institute for Natural Product Discovery, Universiti Teknologi MARA (UiTM), Puncak Alam Campus, 42300 Bandar Puncak Alam, Selangor D. E. Malaysia.
<sup>b</sup>Faculty of Applied Science, UiTM Shah Alam, 40450 Shah Alam, Selangor D.E. Malaysia.
<sup>c</sup>Department of Biochemistry, Abdul Wali Khan University, Mardan 23200, Pakistan
<sup>d</sup>Department of Chemistry, Hazara University, Mansehra, KPK, Pakistan

#### Abstract

Thiourea derivatives having benzimidazole **1-17** have been synthesized, characterized by <sup>1</sup>H NMR, <sup>13</sup>C NMR and EI-MS and evaluated for  $\alpha$ -glucosidase inhibition. Identification of potential  $\alpha$ -glucosidase inhibitors were done by *in vitro* screening of **17** thiourea bearing benzimidazole derivatives using Baker's yeast  $\alpha$ -glucosidase enzyme. Compounds **1-17** exhibited a varying degree of  $\alpha$ -glucosidase inhibitory activity with IC<sub>50</sub> values between 35.83±0.66 - 297.99±1.20  $\mu$ M which are more better than the standard acarbose (IC<sub>50</sub> = 774.5±1.94  $\mu$ M). Compound **10** and **14** showed significant inhibitory effects with IC<sub>50</sub> value 50.57±0.81 and 35.83±0.66  $\mu$ M, respectively better than the rest of the series. Structure activity relationships were established. Molecular docking studies were performed to understand the binding interaction of the compounds.

*Keywords:* Thiourea, Hybrid, Benzimidazole, Synthesis,  $\alpha$ -Glucosidase Inhibition, Molecular docking

E-mail: <u>taha hej@yahoo.com</u> and muhamm9000@puncakalam.uitm.edu.my, Tel: 0060193098141 (M.T.); noriz118@salam.uitm.edu.my; Tel: 03-55435590; Fax: 03-55444562 (N.A.)

<sup>\*</sup> Correspondence and reprints

Download English Version:

## https://daneshyari.com/en/article/5155243

Download Persian Version:

## https://daneshyari.com/article/5155243

Daneshyari.com