

Accepted Manuscript

Docking model of the nicotinic acetylcholine receptor and nitromethylene neonicotinoid derivatives with a longer chiral substituent and their biological activities

Hikaru Nagaoka, Hisashi Nishiwaki, Takuya Kubo, Miki Akamatsu, Satoshi Yamauchi, Yoshihiro Shuto

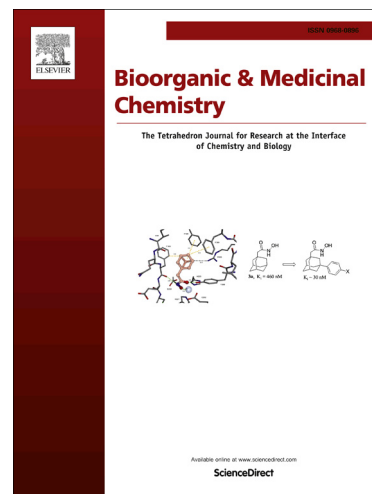
PII: S0968-0896(14)00916-X
DOI: <http://dx.doi.org/10.1016/j.bmc.2014.12.058>
Reference: BMC 11990

To appear in: *Bioorganic & Medicinal Chemistry*

Received Date: 23 October 2014
Revised Date: 8 December 2014
Accepted Date: 24 December 2014

Please cite this article as: Nagaoka, H., Nishiwaki, H., Kubo, T., Akamatsu, M., Yamauchi, S., Shuto, Y., Docking model of the nicotinic acetylcholine receptor and nitromethylene neonicotinoid derivatives with a longer chiral substituent and their biological activities, *Bioorganic & Medicinal Chemistry* (2015), doi: <http://dx.doi.org/10.1016/j.bmc.2014.12.058>

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.



1

2

3 Docking model of the nicotinic acetylcholine receptor and nitromethylene neonicotinoid
4 derivatives with a longer chiral substituent and their biological activities

5

6 Hikaru Nagaoka,[†] Hisashi Nishiwaki,^{*†} Takuya Kubo,[†] Miki Akamatsu,[‡] Satoshi
7 Yamauchi,[†] Yoshihiro Shuto[†]

8

9 [†] Faculty of Agriculture, Ehime University, 3-5-7 Tarumi, Matsuyama, Ehime 790-8566,
10 Japan

11 [‡] Graduate School of Agriculture, Kyoto University, Kita-Shirakawa, Sakyo-Ku, Kyoto
12 606-8502, Japan

13

14 * To whom correspondence should be addressed.

15 Tel: +81-89-946-9973, Fax: +81-89-977-4364

16 E-mail: nishiwaki.hisashi.mg@ehime-u.ac.jp

17

18 **Keywords**

19 Nitromethylene neonicotinoids; QSAR; docking model; *Musca domestica*; nicotinic
20 acetylcholine receptor

21

22 **Abbreviations**

23 Ac, *Aplysia californica*; CH-IMI, nitromethylene analogue of imidacloprid; IMI,

24 imidacloprid; LBD, ligand-binding domain; Ls, *Lymnaea stagnalis*; nAChR, nicotinic

25 acetylcholine receptor; NIA, propargyl propyl phenylphosphonate (Niagara 16388); QSAR,

26 quantitative structure-activity relationship; SAR, structure-activity relationship

Download English Version:

<https://daneshyari.com/en/article/10583307>

Download Persian Version:

<https://daneshyari.com/article/10583307>

[Daneshyari.com](https://daneshyari.com)