

Accepted Manuscript

Preparation, anticholinesterase activity and molecular docking of new lupane derivatives

María Julia Castro, Victoria Richmond, Carmen Romero, Marta S. Maier, Ana Estévez-Braun, Ángel G. Ravelo, María Belén Faraoni, Ana Paula Murray

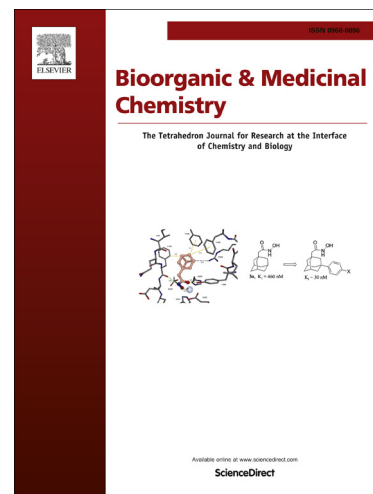
PII: S0968-0896(14)00315-0
DOI: <http://dx.doi.org/10.1016/j.bmc.2014.04.050>
Reference: BMC 11545

To appear in: *Bioorganic & Medicinal Chemistry*

Received Date: 12 March 2014
Revised Date: 16 April 2014
Accepted Date: 25 April 2014

Please cite this article as: Castro, M.J., Richmond, V., Romero, C., Maier, M.S., Estévez-Braun, A., Ravelo, Á., Faraoni, M.B., Murray, A.P., Preparation, anticholinesterase activity and molecular docking of new lupane derivatives, *Bioorganic & Medicinal Chemistry* (2014), doi: <http://dx.doi.org/10.1016/j.bmc.2014.04.050>

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.



Preparation, anticholinesterase activity and molecular docking of new lupane derivatives

María Julia Castro^a, Victoria Richmond^b, Carmen Romero^c, Marta S. Maier^b, Ana Estévez-Braun^c, Ángel G. Ravelo^c, María Belén Faraoni^a, Ana Paula Murray^{a,*}

^a *INQUISUR-CONICET, Departamento de Química, Universidad Nacional del Sur, Av. Alem 1253, B8000CPB, Bahía Blanca, Argentina*

^b *UMYMFOR (CONICET-UBA) and Departamento de Química Orgánica, Facultad de Ciencias Exactas y Naturales, Universidad de Buenos Aires, Ciudad Universitaria, Pabellón 2, 1428 Buenos Aires, Argentina*

^c *Instituto Universitario de Bio-Organica (CIBICAN), Av. Astrofísico Francisco Sánchez 2, 38206, Departamento de Química Orgánica, Universidad de La Laguna, Tenerife, Spain*

* Corresponding author. Tel.: +54 291 4595101.

E-mail address *apmurray@uns.edu.ar*

ABSTRACT

A set of twenty one lupane derivatives (**2-22**) was prepared from the natural triterpenoid calenduladiol (**1**) by transformations on the hydroxyl groups at C-3 and C-16, and also on the isopropenyl moiety. The derivatives were tested for their inhibitory activity against acetylcholinesterase (AChE) and butyrylcholinesterase (BChE) and some structure-activity relationships were outlined with the aid of enzyme kinetic studies and docking modelization. The most active compound resulted to be 3,16,30-trioxolup-20(29)-ene (**22**), with an IC₅₀ value of 21.5 μM for butyrylcholinesterase, which revealed a selective inhibitor profile towards this enzyme.

Keywords: Alzheimer's disease; cholinesterase inhibitors; lupane derivatives; triterpenoids; molecular modelling

Download English Version:

<https://daneshyari.com/en/article/10584774>

Download Persian Version:

<https://daneshyari.com/article/10584774>

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