Erratum to: Computational analysis of the binding ability of heterocyclic and conformationally constrained epibatidine analogs in the neuronal nicotinic acetylcholine receptor

Elena Soriano · José Marco-Contelles ·
Inés Colmena · Luis Gandía

Published online: 19 November 2009
© Springer Science+Business Media B.V. 2009

Erratum to: Mol Divers DOI 10.1007/s11030-009-9161-9

The crystallographic structure of epibatidine–AChBP complex cited in the electronic supplementary material of the original publication (pdb code 2BYQ) was reported by Hansen et al. [1].

This crystallographic structure, which supports our docking results, was the first to orient epibatidine in a cation pi pocket and define atomic interactions between the ligand and bound conformation. Accordingly, this reference should have been cited in the text.

Reference

1. Hansen SB, Sulzenbacher G, Huxford T, Marchot P, Taylor P, Bourne Y (2005) Structures of Aplysia AChBP complexes with agonists and antagonists reveal distinctive binding interfaces and conformations. *EMBO J* 24:3635–3646. doi:[10.1038/sj.emboj.7600828](https://doi.org/10.1038/sj.emboj.7600828)

The online version of the original article can be found under doi:[10.1007/s11030-009-9161-9](https://doi.org/10.1007/s11030-009-9161-9).

E. Soriano (✉) · J. Marco-Contelles
Laboratorio de Radicales Libres y Química Computacional
(LRL/QC), IQOG (CSIC), C/Juan de la Cierva 3, 28006 Madrid,
Spain
e-mail: esoriano@iqog.csic.es

I. Colmena · L. Gandía
Instituto Teófilo Hernando de I+D del Medicamento, Departamento
de Farmacología, Facultad de Medicina, Universidad Autónoma de
Madrid, C/ Arzobispo Morcillo, 4, 28029 Madrid, Spain