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Corrigendum

Corrigendum to "Integrated structure-based activity prediction model of benzothiadiazines on various genotypes of HCV NS5b polymerase (1a, 1b and 4) and its application in the discovery of new derivatives" [Bioorg. Med. Chem. 20(7) (2012) 2455–2478]

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1. **In page 2455, we placed the citation for reference 13 (Barreca, Iraci et al. 2011) incorrectly so the paragraph was corrected as shown below while highlighting the citation in italics**.

Recently, several direct acting antiviral agents have been identified (DAAs). They are mainly directed towards specific proteins involved in Hepatitis C replication like NS3-4A protease, NS3 helicase, NS5b and NS5a polymerase. Those agents are collectively known as 'specifically targeted antiviral therapy for HCV' (STAT-C)[3–5] and are object of intense research these days.[6,7]

Of specific concern in this study is the HCV-NS5b polymerase enzyme. This enzyme has no mammalian counterpart and so it is expected that inhibition of the enzyme will not cause target-related side effects.[8–11]

Up to now, five allosteric binding sites of NS5B polymerase have been identified: two thumb sites (thumb I and II) which are located in the thumb domain and three palm sites (palm I, II and III) which are closer to the active site in the palm domain.[12] According to these sites, we will refer to the inhibitors *using conventions adopted from Barreca et al.*[13]: palm site I NNIs (PSI-NNIs), palm site II NNIs (PSII NNIs),palm site III NNIs (PSIII-NNIs), thumb site I NNIs (TSI-NNIs) and thumb site II NNIs (TSII-NNIs). Out of these different allosteric sites and their corresponding inhibitors, we focused this study on palm I site and in particular on benzothiadiazines as one of the main palm I-NNI (non-nucleoside inhibitors) (see Figures S1 and S2 in the Supplementary data and see full account on the different allosteric sites in Section 1.1 HCV general information).

2. **In Section (1.1 HCV general information) in the Supplementary data which refers to the aforementioned corrected part of the introduction, the citation for the reference (Barreca, Iraci et al. 2011) was not correctly placed.** *Therefore, the file of the Supplementary data was revised and a corrected version of it is attached* **where the following paragraphs were modified as following:**

- The caption of Figure S2 should be: different allosteric sites of NS5b polymerase inhibitors and representative inhibitor for each site. *This figure was adapted from Barreca et al. using Accelrys Discovery studio 3.5 and Pose view instead of pymol and chemsketch.*
- The paragraph entitled **Types of NS5b polymerase inhibitors** should be: The inhibitors can be classified into nucleoside and non-nucleoside inhibitors. The latter can be categorized as shown in the flowchart below. *This categorization is adopted from Barreca et al.*

Supplementary data

Supplementary data associated with this article can be found, in the online version, at http://dx.doi.org/10.1016/j.bmc.2013.07.001.

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