



# Retraction Note: Molecular docking simulation, drug-likeness assessment, and pharmacokinetic study of some cephalosporin analogues against a penicillin-binding protein of *Salmonella typhimurium*

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Retraction to: *The Journal of Antibiotics*  
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The Editor-in-chief has retracted this article because after the publication of the article, a reader noted that erroneous configurations were used for molecular docking calculations. Additionally, the publisher found that the structures presented in Table 1 are incorrect due to errors made during the publication of the article. However, PubChem CIDs displayed in Table 1 remain the same. Further investigation by the Journal found discrepancies in the structures of compounds in Table 1 (derived from PubChem) and the articles cited in PubChem [1–3]. Therefore, the molecular docking calculations presented in this manuscript do not correspond to the antibacterial activity reported in cited articles [1–3]. Additionally, these discrepancies and errors substantially affect the findings and conclusions of the article. Therefore, the Editor-in-Chief has lost confidence in the data of the article.

- The oxime structures of compounds 1–11 are *syn* in [1] and *anti* in PubChem.
- The oxime structures of compounds 12, 13, 15–21, and 23–30 are *syn* in PubChem and in Refs. [2, 3]. However,

absolute configurations of the  $\beta$ -lactam of compounds 12, 13, 15–21, and 23–30 retrieved from 3D structures (PubChem) were found to be wrong. The correct configurations should be 6*R*,7*R* because they are cephalosporin derivatives.

None of the authors have responded to any correspondence from the publisher or Editor in Chief regarding the final version of this retraction.

## References

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2. Kim SH, Son H, Nam G, Chi DY, Kim JH. Synthesis and in vitro antibacterial activity of 3-[N-methyl-N-(3-methyl-1,3-thiazolium-2-yl)amino]methyl cephalosporin derivatives. *Bioorg Med Chem Lett.* 2000;10:1143–5. [https://doi.org/10.1016/s0960-894x\(00\)00130-x](https://doi.org/10.1016/s0960-894x(00)00130-x).
3. Kim Y-Z, Lim J-C, Yeo J-H, Bang C-S, Kim W-S, Kim S-S, et al. Synthesis and antimicrobial activity of novel [(3-aminopyrimidiniumyl)thio]methyl cephalosporins. *J Med Chem.* 1994; 37:3828–33. <https://doi.org/10.1021/jm00048a018>.