




# Errata

## Correction to “Identification of Novel Scaffolds with Dual Role as Antiepileptic and Anti-Breast Cancer”

Shailima Rampogu, Ayoung Baek, Rohit Bavi ,  
Minky Son, Guang Ping Cao, Raj Kumar , Chanin Park,  
Amir Zeb, Rabia Mukhtar Rana,  
Seok Ju Park, and Keun Woo Lee 

THE authors of “Identification of Novel Scaffolds with Dual Role as Antiepileptic and Anti-Breast Cancer” which appeared in the September/October issue of this journal [1] would like to provide updated Figs. 3b, 8, and 9.

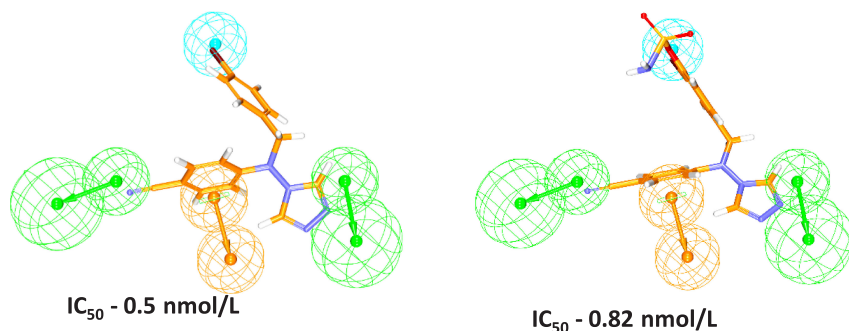


Fig. 3B. Represents the mapping of best pharmacophore model Hypo1 to the most active compounds in training set used as reference compounds.

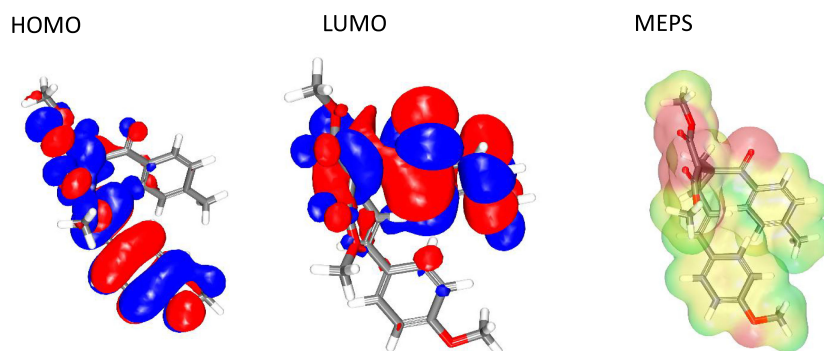


Fig. 9. Molecular electrostatic potential (MEP) map of the Hit3.

- S. Rampogu, A. Baek, R. Bavi, M. Son, G. P. Cao, R. Kumar, C. Park, A. Zeb, R. M. Rana, and W. Lee are with the Division of Applied Life Science (BK21 Plus Program), Systems and Synthetic Agrobiotech Center (SSAC), Plant Molecular Biology and Biotechnology Research Center (PMBBRC), Research Institute of Natural Science (RINS), Gyeongsang National University (GNU)501 Jinju-daero, Jinju 52828, Republic of Korea.  
E-mail: {shailima.rampogu, rohitsbavi, rajkumar250287, chaninpark0806, zebamir85, rabia.mukhtar.rana}@gmail.com, {ayoung, minky, kwlee}@gnu.ac.kr, tsao@bio.gnu.ac.kr.
- S. J. Park is with the Department of Internal Medicine, College of Medicine, Busan Paik Hospital, Inje University, Gimhae, Republic of Korea.  
E-mail: psigenesis@hanmail.net.

(Corresponding author: Keun Woo Lee.)

Digital Object Identifier no. 10.1109/TCBB.2019.2953011

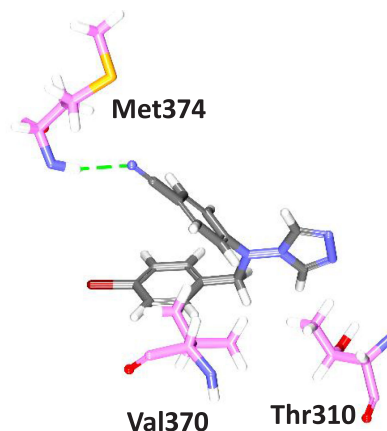


Fig. 8. An update to molecular docking result of reference compound with  $IC_{50}$  0.5 nmol/L which demonstrated a Gold fitness score of 48.25. Both the reference compounds have displayed a similar pattern of binding mode and pharmacophore alignment. Compound with  $IC_{50}$  0.82 nmol/L was used as reference for molecular dynamics simulation, binding free energy and molecular docking studies.

## REFERENCES

- [1] S. Rampogu *et al.*, “Identification of novel scaffolds with dual role as antiepileptic and anti-breast cancer,” *IEEE/ACM Trans. Comput. Biol. Bioinf.*, vol. 16, no. 5, pp. 1663–1674, Sep./Oct. 2019.