# Accepted Manuscript

Title: Computational investigation of TGF-β receptor inhibitors for treatment of idiopathic pulmonary fibrosis: Field-based QSAR model and molecular dynamics simulation

Authors: Wei Li, Xue Liu, Suleiman Muhammad, JiYue Shi, YanQiu Meng, Jian Wang

PII: \$1476-9271(18)30331-1

DOI: https://doi.org/10.1016/j.compbiolchem.2018.07.002

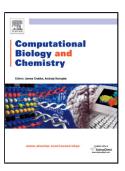
Reference: CBAC 6883

To appear in: Computational Biology and Chemistry

Received date: 10-5-2018 Revised date: 29-6-2018 Accepted date: 3-7-2018

Please cite this article as: Li W, Liu X, Muhammad S, Shi J, Meng Y, Wang J, Computational investigation of TGF-β receptor inhibitors for treatment of idiopathic pulmonary fibrosis: Field-based QSAR model and molecular dynamics simulation, *Computational Biology and Chemistry* (2018), https://doi.org/10.1016/j.compbiolchem.2018.07.002

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.



## ACCEPTED MANUSCRIPT

# Computational investigation of TGF- $\beta$ receptor inhibitors for treatment of idiopathic pulmonary fibrosis: Field-based QSAR model and molecular dynamics simulation

Wei Li [a], Xue Liu [a], Suleiman Muhammad[b], JiYue Shi[b], YanQiu Meng[a]\*, Jian Wang[b]\*

<sup>a</sup>Department of Pharmaceutical Engineering, Shenyang University of Chemical Technology, Shenyang, China.

<sup>b</sup>Key Laboratory of Structure-Based Drug Design & Discovery, Ministry of Education, Shenyang Pharmaceutical University, Shenyang 110016, China.

\* Corresponding author. Prof. Meng: E-mail address: mengyanqiu@hotmail.com; Prof. Wang: E-mail address: jianwang@syphu.edu.cn

[a] W. Li, X Liu, Y. Q. Meng

Department of Pharmaceutical Engineering,

Shenyang University of Chemical Technology

Shenyang, China

\*e-mail: mengyanqiu@hotmail.com

[b] S. Muhammad, J. Y Shi J. Wang.

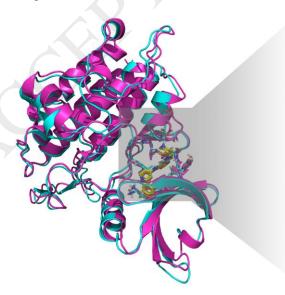
Key Laboratory of Structure-Based Drug Design & Discovery, Ministry of Education,

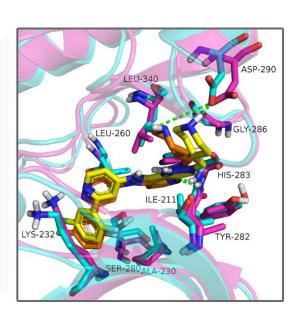
Shenyang Pharmaceutical University

Shenyang 110016, China

\*e-mail: jianwang@syphu.edu.cn

### **Graphical Abstract**





### Download English Version:

# https://daneshyari.com/en/article/6486799

Download Persian Version:

https://daneshyari.com/article/6486799

<u>Daneshyari.com</u>