

# Accepted Manuscript

Design, synthesis, and structure-activity-relationship of a novel series of CXCR4 antagonists

Zhanhui Li, Yujie Wang, Chunyan Fu, Xu Wang, Jun Jun Wang, Yi Zhang, Dongping Zhou, Yuan Zhao, Lusong Luo, Haikuo Ma, Wenfeng Lu, Jiyue Zheng, Xiaohu Zhang



PII: S0223-5234(18)30172-7

DOI: [10.1016/j.ejmech.2018.02.042](https://doi.org/10.1016/j.ejmech.2018.02.042)

Reference: EJMECH 10219

To appear in: *European Journal of Medicinal Chemistry*

Received Date: 20 December 2017

Revised Date: 7 February 2018

Accepted Date: 12 February 2018

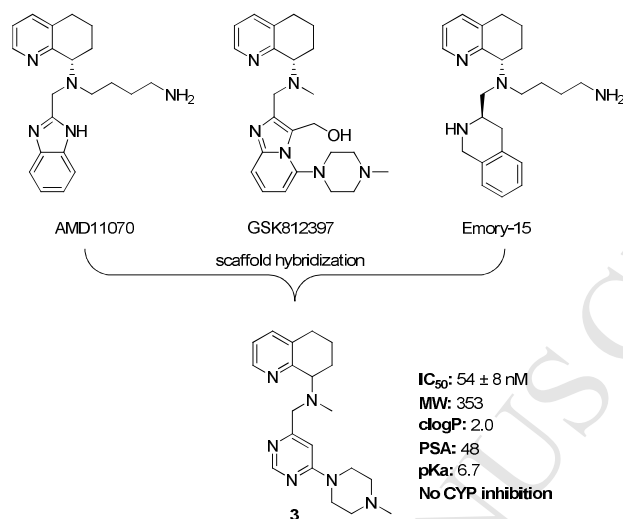
Please cite this article as: Z. Li, Y. Wang, C. Fu, X. Wang, J.J. Wang, Y. Zhang, D. Zhou, Y. Zhao, L. Luo, H. Ma, W. Lu, J. Zheng, X. Zhang, Design, synthesis, and structure-activity-relationship of a novel series of CXCR4 antagonists, *European Journal of Medicinal Chemistry* (2018), doi: 10.1016/j.ejmech.2018.02.042.

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.

## Graphical Abstract

## Design, Synthesis, and Structure-Activity-Relationship of a Novel Series of CXCR4 Antagonists

Zhanhui Li, Yujie Wang, Chunyan Fu, Xu Wang, Jun Jun Wang, Yi Zhang, Dongping Zhou, Yuan Zhao, Lusong Luo, Haikuo Ma, Wenfeng Lu, Jiyue Zheng, and Xiaohu Zhang



A novel series of CXCR4 antagonists was developed by a scaffold hybridization strategy. The most promising lead of this series, compound **3**, binds potently with CXCR4 receptor ( $IC_{50} = 54$  nM) and inhibits CXCL12 induced cytosolic calcium increase ( $IC_{50} = 2.3$  nM). Furthermore, compound **3** possesses good physicochemical properties (MW 353, clogP 2.0, PSA 48, pKa 6.7), exhibits minimal CYP isozyme and hERG inhibition.

Download English Version:

<https://daneshyari.com/en/article/7796652>

Download Persian Version:

<https://daneshyari.com/article/7796652>

[Daneshyari.com](https://daneshyari.com)