



[Skip to content](#)



- [Librarians](#)
- [Authors & Editors](#)
- [Societies](#)

- [Register](#)
- [Sign in](#)
- [Mobile](#)

-  [Browse](#)
- [Products](#)
- [Open access](#)
- [Shortlist](#)
-  [Cart](#)

The online platform for Taylor & Francis Group content

Cookies Notification

This site uses cookies. By continuing to browse the site you are agreeing to our use of cookies. [Find out more.](#)

Search <input type="text"/>
Search Advanced and citation search <input checked="" type="radio"/> Within current journal <input type="radio"/> Entire site

[Home](#) > [List of Issues](#) > [Latest articles](#) > Investigation on critical structural motifs of ligands for triggering glucocorticoid receptor nuclear migration through molecular docking simulations

Browse journal

[View all volumes and issues](#)

[Current issue](#)

[Latest articles](#)

[Most read articles](#)

[Most cited articles](#)

[Open access articles](#)

[Submit](#)

[Instructions for authors](#)

[Submit online](#)

[Subscribe](#)

[About this journal](#)

[Aims & scope](#)

[Journal information](#)

[Editorial board](#)

[Abstracting & indexing](#)

[News & offers](#)

**Journal of Biomolecular Structure
and Dynamics**

Select Language | ▼

[Translator disclaimer](#)



Original Articles

Investigation on critical structural motifs of ligands for triggering glucocorticoid receptor nuclear migration through molecular docking simulations

[PreviewFull text HTML](#)

[PDF](#)

[Supplemental](#)

[Access options](#)

DOI:

10.1080/07391102.2015.1074113

[Ya-Lin Liu^a](#), [Soonmin Jang^b](#), [Shih-Min Wang^c](#), [Chiu-Hao Chen^d](#) & [Feng-Yin Li^{a*}](#)

[Publishing models and article dates explained](#)

- Received: 9 Aug 2015
- Accepted: 15 Jul 2015
- Accepted author version posted online: 22 Jul 2015
- Published online: 14 Aug 2015

[Alert me](#)

- [New content email alert](#)
- [New content RSS feed](#)
- [Citation email alert](#)
- [Citation RSS feed](#)

Abstract

The glucocorticoid receptor (GR), a transcription factor regulating gene expression in a ligand-dependent fashion, is known for flexibility in adapting various ligands with their structures ranging from steroid to non-steroid. However, in our previous study, GR shows a stringent discrimination against a set of steroid ligands with highly similar structures for triggering its nuclear migration. In order to resolve this puzzle, we employed molecular docking simulations to investigate the origin of this structural discrimination. By analyzing the docking orientations and the related ligand–GR interaction patterns, we found that the hydrophilicity mismatch between the docking ligand and the GR ligand-binding site is the main cause combined with the steric hindrance and structural rigidity of these steroid ligands. Furthermore, we utilized this knowledge to rationalize how the structure–binding interaction of non-steroid ligands triggers GR nuclear migration with their structures available in Protein Data Bank.

- [Full text HTML](#)
- [PDF](#)
- [Supplemental](#)

Keywords

- [glucocorticoid receptor](#),
- [molecular docking simulation](#),
- [solvent-exposed hydrophobic groove](#),
- [nuclear migration](#)

Related articles

[View all related articles](#)

-

- [Add to shortlist](#)
- [Link](#)

Permalink

<http://dx.doi.org/10.1080/07391102.2015.1074113>

- [Download Citation](#)
- Recommend to:
 - [A friend](#)

- [Information](#)
- [Full text](#)
- [Figures & Tables](#)
- [References](#)
- [Supplemental](#)
- [Citations](#)
- [Reprints & permissions](#)

Details

- **Citation information:** [PubMed](#)
- **Received:** 9 Aug 2015
- **Accepted:** 15 Jul 2015
- **Accepted author version posted online:** 22 Jul 2015
- **Published online:** 14 Aug 2015



Author affiliations

- ^a Department of Chemistry, National Chung Hsing University, Taichung, Taiwan
- ^b Department of Chemistry, Sejong University, Seoul 143-747, Korea
- ^c Institute of Nuclear Energy Research, Lungtan, Taoyuan, Taiwan
- ^d General Education Center, Wenzao Ursuline University of Languages, Kaohsiung, Taiwan

Journal news

- [Authors can publish interactive 3D models with their papers using Proteopedia](#)
- **2014 Impact Factor: 2.919**

Latest two full volumes
FREE to you for 14 days

Article metrics

- **Views: 71**
- **Citations**
[CrossRef \(10\)](#)
-

[Article metrics information](#)

Users also read

- [Novel glucocorticoid receptor agonists in the](#)



Librarians

- [Librarians' area](#)
- [Pricing](#)
- Institutional account
- Access entitlements
- Co-branding
- IP ranges
- Link resolver preferences
- Usage reports

Authors & Editors

- [Book authors](#)
- [Journal authors](#)
- [Reference work authors](#)
- [Editors](#)

Societies

- [Current partners](#)
- [Publish with us](#)

Help & Information

- [Help](#)
- [FAQs](#)
- [Contact us](#)
- [Press releases](#)
- [Commercial services](#)

Taylor & Francis Group

-  Taylor & Francis
Taylor & Francis Group
-  Routledge
Taylor & Francis Group
-  Psychology Press
Taylor & Francis Group
-  CRC Press
Taylor & Francis Group
-  Garland Science
Taylor & Francis Group

- [Privacy Policy & Cookies](#)
- [Terms & Conditions](#)
- [Accessibility](#)

Powered by [Atypon® Literatum](#)

© [Informa UK Limited, an Informa Group Company](#)