

WILEY

Bucharest, Cluj and Iasi April 2014

Agenda

Introduction to Wiley / Publishing Overview
Publishing and Evaluating Research
Break

Ethics, Production and Metrics

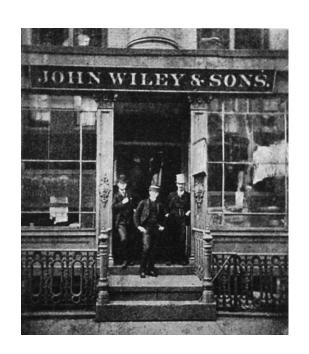
Q&A

Wiley Author Workshops

This workshop will help participants gain insight on the types of academic publications available, the processes involved in getting material published and understand the expectations editors have of authors and their work.



Leaders in quality







Evolving from being a provider of content in static form to a provider of dynamic new types of products and services

Nobel Prize Winners

Marie Curie

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Günter Grass

Woodrow Wilson

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Earl Bertrand Russell

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Linus Pauling

Mikhail Gorbachev

Milton Friedman

Akira Suzuki

Ei-ichi Negishi

Christopher A. Sims

Leymah Gbowee

Bruce A. Beutler

Jules A. Hoffman

Brian P. Schmidt

Thomas J. Sargent

Kofi Annan Nelson Mandela

Frédéric Joliot & Irène Joliot-Curie

Out of 850 Nobel Laureates, more than 460 have published with Wiley



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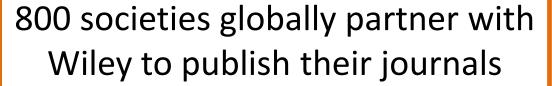




















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Architecture & Planning

Art & Applied Arts

Business, Economics, Finance & Accounting

Chemistry

Computer Science & Information Technology

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- 7 Chemistry Databases, including SpecInfo and the Encyclopedia of Reagents for Organic Syntheses (e-EROS)

Wiley Online Library

WILEY JOURNALS - KEY STATISTICS

Wiley by numbers

- 1,500 peer-reviewed journals published
- 4,000 academic libraries worldwide license our journals
- **40,000** institutions around the world purchase Wiley products every year
- **13.5 million** unique visitors visit our journals on Wiley Online Library each month

Open Access Publishing with Wiley

- 29 Open Access journals
- 1,350 Hybrid journals OnlineOpen

Wiley in 2012 JCR

1192 Wiley journals (approximately 77%) indexed in JCR.

Equivalent to 11% of all journals in JCR.

Titles indexed in 218/232 subject categories.



Wiley in 2012 JCR

Wiley journals make up the largest share of journals in 50 categories.

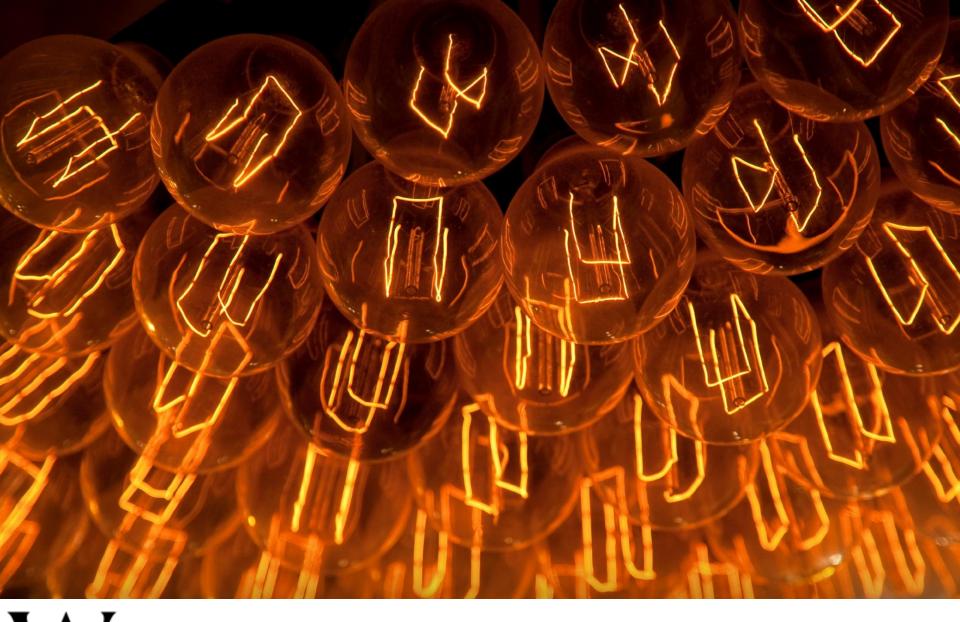
Of publishers with more than 100 journals indexed in the 2012 JCR, Wiley saw the largest proportion of titles (close to 60%) increasing in Impact Factor (IF).



#1 in 25 JCR categories

Andrology * Biodiversity Conservation * Biophysics * Business, Finance * Construction & Building Technology * Dentistry, Oral Surgery & Medicine * Ecology * Education, Scientific Disciplines * Family Studies * Fisheries * Food Science & Technology * Geography, Physical * Health Care Sciences & Services * Mathematical & Computational Biology * Neuroimaging * Nuclear Science & Technology * Nursing (Science) * Oncology * Paleontology * Psychology, Educational * Public Administration * Substance Abuse * Substance Abuse (Social Science) * Transplantation * Zoology



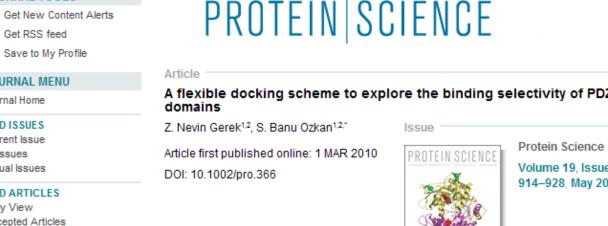


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Journal Publishing

2013

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- Current formats for online publication are limited.
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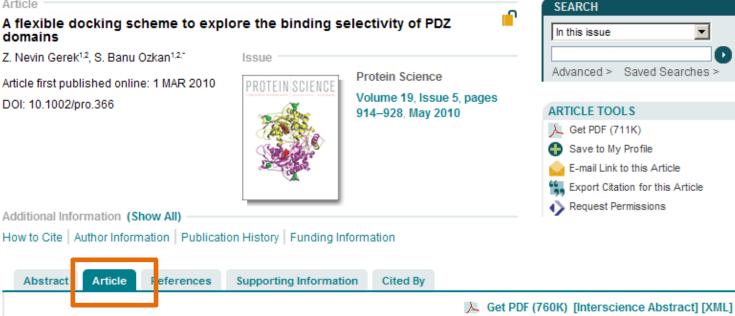
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Keywords:

protein flexibility; PDZ domain; docking; selectivity; ROSETTALIGAND

Abstract

Modeling of protein binding site flexibility in molecular docking is still a challenging problem due to the large conformational space that needs sampling. Here, we propose a flexible receptor docking scheme: A dihedral restrained replica exchange molecular dynamics (REMD), where we incorporate the normal modes obtained by the Elastic Network Model (ENM) as dihedral restraints to speed up the search towards correct binding site conformations. To our knowledge, this is the first approach that uses ENM modes to bias REMD simulations towards binding induced fluctuations in docking studies. In our docking scheme, we first obtain the deformed structures of the unbound protein as initial conformations by moving along the binding fluctuation mode, and perform REMD using the ENM modes as dihedral restraints. Then, we generate an ensemble of multiple receptor conformations (MRCs) by clustering the lowest replica trajectory. Using ROSETTALIGAND, we dock ligands to the clustered conformations to predict the binding pose and affinity. We apply this method to postsynaptic density-95/DIg/ZO-1 (PDZ) domains; whose dynamics govern their binding specificity. Our approach produces the lowest energy bound complexes with an average ligand root mean square deviation of 0.36 Å. We further test our method on (i) homologs and (ii) mutant structures of PDZ where mutations after the binding selectivity. In both cases, our approach succeeds to predict the correct pose and the affinity of binding peptides. Overall, with this approach, we generate an ensemble of MRCs that leads to predict the binding poses and specificities of a protein complex accurately.

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A flexible docking scheme to explore the binding selectivity of PDZ domains

Z. Nevin Gerek^{1,2} and S. Banu Ozkan^{1,2}*

94.1%

Center for Biological Physics, Arizona State University, Tempe, Arizona

Received 20 August 2009; Revised 16 December 2009; Accepted 8 February 2010

DOI: 10.1002/pro.366

Published online 1 March 2010 proteinscience.org

Abstract: Modeling of protein binding site flexibility in molecular docking is still a challenging problem due to the large conformational space that needs sampling. Here, we propose a flexible receptor docking scheme: A dihedral restrained replica exchange molecular dynamics (REMD), where we incorporate the normal modes obtained by the Elastic Network Model (ENM) as dihedral restraints to speed up the search towards correct binding site conformations. To our knowledge, this is the first approach that uses ENM modes to bias REMD simulations towards binding induced fluctuations in docking studies. In our docking scheme, we first obtain the deformed structures of the unbound protein as initial conformations by moving along the binding fluctuation mode, and perform REMD using the ENM modes as dihedral restraints. Then, we generate an ensemble of multiple receptor conformations (MRCs) by clustering the lowest replica trajectory. Using Rosettaligand, we dock ligands to the clustered conformations to predict the binding pose and affinity. We apply this method to postsynaptic density-95/Dlg/ZO-1 (PDZ) domains; whose dynamics govern their binding specificity. Our approach produces the lowest energy bound complexes with an average ligand root mean square deviation of 0.36 Å. We further test our method on (i) homologs and (ii) mutant structures of PDZ where mutations alter the binding selectivity. In both cases, our approach succeeds to predict the correct pose and the affinity of





²Department of Physics, Arizona State University, Tempe, Arizona

User Behaviour



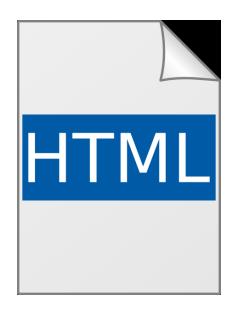
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American Journal of Medical Genetics Part A

Research Article

Fractures in Children With Neurofibromatosis Type 1 From Two NF Clinics

Jaya K. George-Abraham Lisa J. Martin Heidi J. Kalkwarf Margaret B. Rieley David A. Stevenson David H. Viskochil Robert J. Hopkin Austin M. Stevens Heather Hanson Dr. Elizabeth K. Schorry

First published: 25 March 2013 Full publication history

DOI: 10.1002/ajmg.a.35541



Volume 161, Issue 5 May 2013

Cincinnati Children's Hospital Medical Center, 3333 Burnet Avenue, MLC 4006, Cincinnati, OH 45229.

Abstract

Neurofibromatosis type 1 (NF1) is an autosomal dominant genetic disorder with osseous abnormalities occurring in up to one-third of patients. Several studies have documented osteopenia in both children and adults with NF1; however, the significance of lower bone mineral density (BMD) in relationship to fracture incidence is not well elucidated in NF1, particularly in children. We undertook a retrospective study to determine prevalence and location of fractures in children and adolescents with NF1, ages 5-20 years, using a standardized questionnaire. We surveyed 256 individuals with NF1 from two multidisciplinary NF centers and 178 controls without NF1 of similar ages and sex. Participants with known long bone dysplasia (LBD) were analyzed separately. Data collected included numbers and location of fractures, dietary calcium intake, and physical activity levels. There was no difference in prevalence of ever having a fracture between the NF1 group without LBD (22%) and the control group (25%); median number of fractures also



Wiley in Romania





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- Universitatea Alexandru Ioan Cuza
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Published Papers in Wiley Journals

Table to show the number of unique papers published by Romanian authors and academics in Wiley Journals

Year	Total unique papers *
2009	202
2010	233
2011	232
2012	223 (Jan to October)
Total	890

^{*} includes articles, reviews and proceeding papers





Feedback from Romanian Market

1. What type of content are academics using in Romania?

Product	% of academics using each product
Full text journals	80%
Databases	75%
E-books, Encyclopaedias and E-dictionaries	40%
Patent databases	25%
Other	6%

Based on feedback from academics as featured in the ANELIS survey, http://www.anelis.ro/images/stories/seis.pdf (p. 25)



Feedback from Romanian Market

2. Informational requirements* from Romanian academics:

- -Need for broad area of interest
- -The need for a vast spectre of information from numerous sources
- -High interest in scientific fields related to their subject area
- -The absence of linguistic barriers



^{*} Source: Acces national electronic la literatura stiintifica de cercetare, ANELIS, http://www.anelis.ro/images/stories/seis.pdf (p. 25)

Demand for Wiley content in Romania

- 89% of institutions surveyed¹ wanted access to Wiley Online Library
- The number of articles accessed tripled from 2009 to 2011

Year	Total usage (downloads)
2009	55,180 *
2010	162,293 *
2011	171,864 *
2012	57,820 **

¹ Source: ANELIS survey of 47 Romanian institutions, Acces national electronic la literatura stiintifica de cercetare, ANELIS, http://www.anelis.ro/images/stories/seis.pdf (p. 10)



^{*} Source: ANELIS, http://www.anelis.ro/index.php?option=com_content&view=article&id=81&Itemid=2

^{**} Source: Wiley Online Library usage statistics for ANELIS institutions

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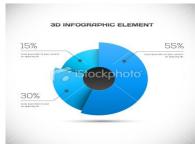


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