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June 29, 2010

Two-thirds of Wiley-Blackwell's Journal Portfolio now has an Impact Factor

Hoboken, N.J.

Wiley-Blackwell, the scientific, technical, medical, and scholarly business of John Wiley & Sons, Inc., today announced that **two thirds of its journals (67% and 1,013 titles) have an Impact Factor** according to the Thomson ISI® 2009 Journal Citation Reports (JCR). This is a higher proportion of the list than any other major journals publisher. Of these ranked titles, **nearly a quarter are in the top ten of their subject category (332 titles) whilst two thirds are in the top half of their category.**

Wiley-Blackwell has **36 number 1 rankings (from 33 titles**, with *Econometrica* top of three, and *Worldviews on Evidence-Based Nursing* top of two categories respectively), the joint highest number of top ranked titles as a proportion of the list. **The Wiley-Blackwell journal *CA-A Cancer Journal for Clinicians* remains in first place overall with an Impact Factor of 87.925.**

51 new titles were added to Wiley-Blackwell's listing in the JCR for 2009 with 4 titles re-listed.

Wiley-Blackwell's average Impact Factor saw a 5.3% rise last year. **This year, the company's average was 2.1, compared to 2.0 last year.** This is in the context of an overall 1.7% reduction in average Impact Factor between JCR 2008 and 2009.

Overall, Wiley-Blackwell published 11.2% of the journals, 11.3 % of the articles, and received 11.1% of the citations.

"We are delighted with the Impact Factor results this year", said Steve Miron, Senior Vice President, Wiley-Blackwell. "They reflect the hard work of our external Editors, society partners and Wiley colleagues to continually drive the quality of the journals that we publish and to ensure they meet the needs of authors and researchers alike".

Impact factors are a metric that reflect the frequency that peer-reviewed journals are cited by researchers, making them an important tool for evaluating a journal's quality.

Within the 2009 Journal Citation Report were a number of key changes in the rankings for individual titles.

Highlights in Chemistry and Physical Sciences:

Angewandte Chemie, a journal of the German Chemical Society published under the Wiley-VCH brand, has further increased its Impact Factor to 11.829, strengthening its position as the leading chemistry journal publishing primary research and review articles.

ChemSusChem, also from Wiley-VCH and co-owned and supported by ChemPubSoc Europe (an association of 16 European Chemical Societies), received an impressive first Impact Factor of 4.767.

Biofuels, *Bioproducts*, *Biorefining - Biofpr*, published on behalf of the Society for Chemical Industry, increased its Impact Factor by over 68% to 4.885 and now ranks 2nd after just two years.

There are four number one ranked journals in physical sciences, including *Mass Spectrometry Reviews* for the 11th consecutive year and *Advanced Synthesis and Catalysis* for its 7th year.

Highlights in Life Sciences:

Within Life Sciences we have achieved 9 number one rankings. 4 journals retain their number one rankings - *Aging Cell* in the Geriatrics and Gerontology category, *Global Ecology and Biogeography* in Physical Geography, *Human Brain Mapping* in the Neuroimaging category and *Journal of Avian Biology* in Ornithology.

5 journals rise to number one ranking – *Fish and Fisheries* in the Fisheries category, *Global Change Biology* in the Biodiversity Conservation category, *Journal of Comparative Neurology* has risen to number one in Zoology and *Molecular Nutrition and Food Research* is now number one in the Food Science and Technology category. *Evolutionary Anthropology* is ranked first in the Anthropology category.

Recently launched journals that achieved an Impact Factor for the first time include *Evolutionary Applications* – 4.744 and is ranked 9th in the Evolutionary Biology category, and *Insect Conservation and Diversity* which also receives its first Impact Factor of 2.828 and is ranked 4th in the Entomology category. *Autism Research* gets its first Impact Factor of 1.375 and *Ecohydrology*, which launched in 2008, gains its first Impact Factor at 1.719.

FEMS Microbiology Reviews Impact Factor rose from 7.963 to 9.783 and is ranked 6/94 in the Microbiology category and for the sixth consecutive year *Ecology Letters* increased its Impact Factor to 10.318 and remains the highest ranking primary research journal in Ecology

Highlights in Social Sciences & Humanities:

Wiley-Blackwell's consistent leadership in social science is demonstrated through our publishing more titles listed in the Social Science JCR than any other publisher.

11 of our journals were ranked number one within their subject category – these included *Child Development* (ranked number one for the fifth consecutive year), *Econometrica*, *Industrial Relations* and *Journal of Computer-Mediated Communication*.

75 of our journals are ranked in the top ten of their respective SSCI categories.

24 journals have received their first Impact Factor with *Developing World Bioethics* entering the Ethics category at number seven.

In 18 categories we publish the most journals in the category confirming our exceptional market presence in anthropology, business - finance, demography, economics, family studies, geography, gerontology, health policy & services, history of social sciences, law, management, nursing, planning and development, psychology (developmental and social), public, environmental & occupational health, public administration and social sciences – mathematical methods.

Highlights in Health Sciences: (I)

291 Wiley-Blackwell health science journals received an Impact Factor in 2009 with an average of 2.62, 26 journals increased their score by 0.5 or more and 24 titles received their first Impact Factor. In addition 30 titles achieved an Impact Factor of 5 or more, with 9 titles ranked number 1 in their category and a further 50 in the top 10.

The journal *CA – A Cancer Journal for Clinicians*, published on behalf of The American Cancer Society, was awarded an Impact Factor of 87.925 - the highest Impact Factor among all medical titles. In the Oncology category, Wiley is now the third leading Publisher with 17 titles.

The Wiley EBM portfolio continues to gain strength, with *Worldviews on Evidence-Based Nursing*, an official journal of the Honor Society of Nursing, Sigma Theta Tau International, claiming the number 1 spot of 72 journals in the Nursing (science) category with an impact factor of 1.944, an increase from 1.294 in 2008. The *Cochrane Database of Systematic Reviews* climbed to 5.653, moving up the rankings for the 2nd year, since its inclusion in the Journal Citation Reports in 2007, to 11th place in Medicine, General & Internal.

Highlights in Health Sciences: (II)

From our Nursing portfolio, in addition to *Worldviews on Evidence-Based Nursing* now being ranked number 1, *Birth* is now ranked as the number 2 journal with an impact factor of 1.919. *BJOG*'s Impact Factor has increased to 3.437, while *Ultrasound in Obstetrics & Gynecology* now has an Impact Factor of 3.154. *American Journal of Transplantation*, published on behalf of the American Society of Transplantation (AST) and the American Society of Transplant Surgeons (ASTS) received a 2009 Impact Factor of 6.433, maintaining its status as the number 1 ranked journal in Transplantation. *Hepatology*, published on behalf of The American Association of the Study of the Liver, is the highest ranking hepatology journal and second in the gastroenterology and hepatology category, with an Impact Factor of 10.840.

The journal *Allergy*, published on behalf of The European Academy of Allergy and Clinical Immunology, was awarded an Impact Factor of 6.380, ranking it number 2 in the category for the fifth year. In dentistry, Wiley-Blackwell has 11 titles ranked in the top 20. *Journal of Clinical Periodontology* and *Periodontology 2000* are ranked as number 1 and 4 respectively.

In veterinary sciences 14 of our titles saw a rise in impact factor, notably *Journal of Veterinary Internal Medicine* increasing from 1.885 to 2.168 and now ranking in the top 10 at number 8. *Zoonoses and Public Health*'s impact factor leapt from 1.333 to 1.912.

Highlights in Health Sciences: (III)

Addiction and *Addiction Biology* keep their number 1 ranking in the categories of Substance Abuse (Social Science) and Substance Abuse respectively and *Alcoholism's* Impact Factor has increased to 3.392. *Bipolar Disorders*, published by Wiley-Blackwell on behalf of the International Society for Bipolar Disorders, jumped up 13 places in the Psychiatry category with an increased Impact Factor of 5.502.

The journals of the BPS (British Pharmacological Society) received increased Impact Factors, with *BJP (British Journal of Pharmacology)* increasing to 5.204, confirming it as the highest ranked general pharmacology research journal. The *Journal of Pathology's* 2009 Impact Factor of 6.466 places it number 2 in the Pathology category. *Brain Pathology* has also seen its Impact Factor rise for the 2nd year running, rising to 5.903.



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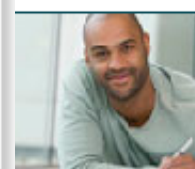
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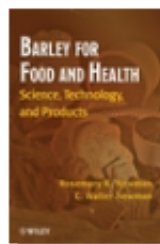
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Anytime a user enters a term in one of the Wiley Online Library search boxes, the system performs automatic stemming of the term(s) eliminating the need for users to manually type several common variations of the search term. The chart below summarizes the common expansions the system will automatically find for English language terms. In addition, for our German language journals and books, German specific stemming rules are applied.

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2. COMMON BRITISH vs. AMERICAN ENGLISH SPELLING VARIANTS

Search **TUMOR**

Search **CENTER**

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3. NON-STANDARD PLURAL VARIANTS

Search **MOUSE**

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Singular	MOUSE
Plural	MICE

4. COMMON IRREGULAR VERBS

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 Article first published online : 18 NOV 2008, DOI : 10.1002/acp.1534
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The effect of long-term training on police officers' use of open and closed questions in field investigative interviews of children (FIIC)
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 Volume 3, Issue 3, October 2006, Pages: 165–181, Trond Myklebust and Roald A. Bjørklund
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A modified cognitive interview procedure for frontline police investigators
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 Volume 23, Issue 5, July 2009, Pages: 698–716, Coral Dando, Rachel Wilcock, Rebecca Milne and Lucy Henry
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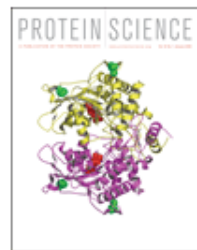
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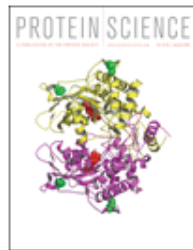
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Review



A synergistic approach to protein crystallization: Combination of a fixed-arm carrier with surface entropy reduction (pages 901–913)

Andrea F. Moon, Geoffrey A. Mueller, Xuejun Zhong and Lars C. Pedersen

Article first published online: 1 MAR 2010 | DOI: 10.1002/pro.368

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A flexible docking scheme to explore the binding selectivity of PDZ domains (pages 914–928)

Z. Nevin Gerek and S. Banu Ozkan

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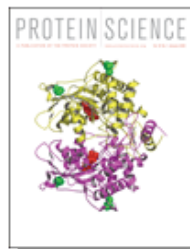
A flexible docking scheme to explore the binding selectivity of PDZ domains

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

Article first published online: 1 MAR 2010

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Abstract

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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 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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8

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presented random snapshots. Principal component analysis (PCA) were also performed to generate the multiple receptor conformations (to bind in nature). Thus, the crucial ingredient in generating MRCs is to mimic nature and sample binding induced conformations using smart sampling strategies. Recently, Abagyan and collaborators²⁹ were able to incorporate the multiple receptor conformational ensemble in a single docking simulation and reduce the sampling time with their approach.

In this present study, we come up with a novel sampling strategy by combining the ENM with replica exchange molecular dynamics (REMD)³⁰ to generate “binding induced” MRCs. Clustering molecular dynamics snapshots^{8–13} and generating conformations by perturbing the conformation along normal modes^{18, 19, 24, 31–33} have been separately applied to incorporate the receptor flexibility in

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

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

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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

of the P+1 loop, located in the C-terminus of the activation segment, and the following helix α EF (Fig. 2). The interface is stabilized by a salt bridge between Glu196 in helix α EF of one monomer and Arg279, located between helices α I and α J, in the other monomer, as well as van der Waals contacts between several hydrophobic residues from helix α EF of one monomer and the hydrophobic pocket located between helices α G and α F of the partner monomer. The activation segment, which commonly is 20–30 residues in length and contains one or several phosphorylation sites, is a critical structural element for regulation of kinase activity.¹² Electron density is not clearly defined in either study for the phosphorylation site, Thr185, or the C-terminal part of the activation loop. The partially disordered activation segment suggests that the OSR1 kinase domain structures represent an inactive conformation, because a correctly positioned activation segment is required for ATP binding.

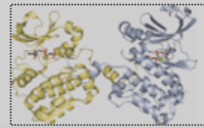


Figure 1. The kinase domain of oxidative stress responsive 1 (OSR1) forms a domain-swapped dimer. Each monomer binds one molecule of Mg-AMP-PNP. The two monomers from the coordinate file PDB 3DAK are depicted in blue and yellow, respectively; the AMP-PNP molecules are shown as CPK-colored bonds; and the Mg^{2+} ions are shown as green spheres. An [interactive view](#) is available in the electronic version of the article. [Interactive View](#)

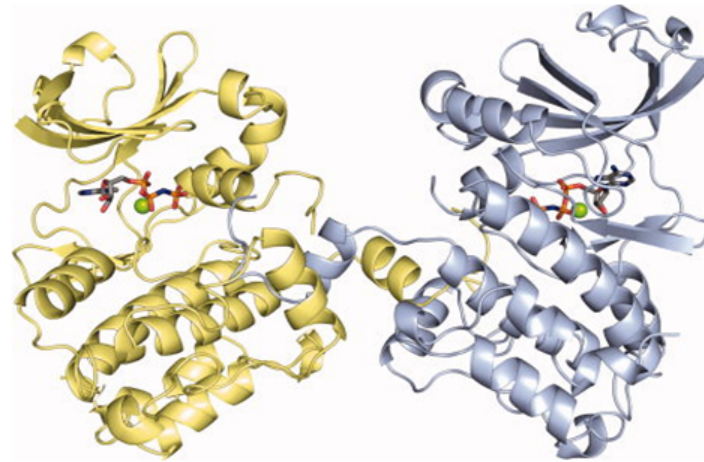


Figure 1. The kinase domain of oxidative stress responsive 1 (OSR1) forms a domain-swapped dimer. Each monomer binds one molecule of Mg-AMP-PNP. The two monomers from the coordinate file PDB 3DAK are depicted in blue and yellow, respectively; the AMP-PNP molecules are shown as CPK-colored bonds; and the Mg^{2+} ions are shown as green spheres. An [interactive view](#) is available in the electronic version of the article. [Interactive View](#)

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in Arg279 of one monomer
interaction between Lys148 of
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with residues in α EF of the
an inactive kinase, including
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placed from the core of the molecule. This
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Thr catalytic triad. These observations imply
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Lee *et al.* did not identify any key differences in the amino acid sequences between homologous domain-swapped and non-swapped kinases. Swapped domains often do not share similarity in sizes and sequences, based on the currently available high-resolution structures.¹⁹ Owing to the relatively small differences in free energy of monomers and oligomers, many domain-swapped oligomers show low-affinity and are only observed in crystals.²⁰ Indeed, OSR1 kinase domain is monomeric in solution.^{5, 6} In contrast, the previously identified domain-swapped kinase domains of SLK, LOK, and DAPK3 form stable dimers in solution.⁴ Biochemical data for these kinases strongly support the involvement of dimers in the autophosphorylation reaction. However, the functional relevance of dimerization cannot be judged solely from the affinity in aqueous solution and coimmunoprecipitation experiments indicate that both the kinase domain alone and the full-length OSR1 are capable of forming oligomers in cells.¹⁰

Intrinsic conformational plasticity is critical for structural transitions between active and inactive states of protein kinases, and biophysical evidence suggests that conformational dynamics may be coupled to catalysis.^{21–24} Results from NMR spectroscopy and molecular dynamics simulations have linked conformational flexibility to domain swapping in other protein molecules.^{25, 26} Therefore, domain swapping may be a consequence of the intrinsic conformational flexibility of kinase domains. The impact of domain swapping on the autophosphorylation reaction, if indeed they are coupled, remains to be fully elucidated, and additional structural and biochemical data are required to clarify the functional role



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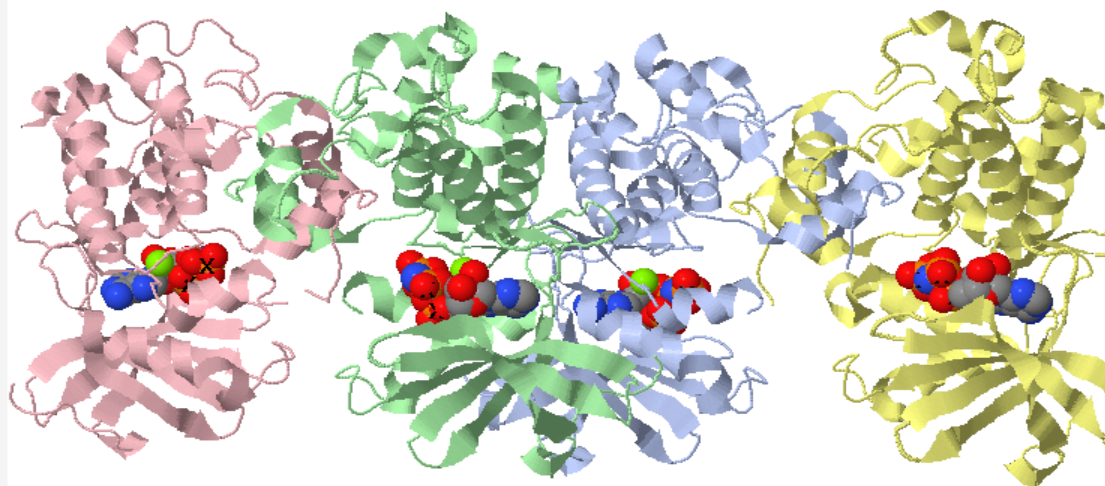
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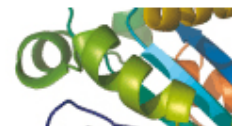
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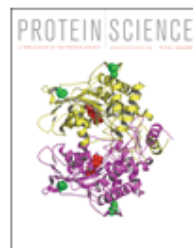
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