Publishing in the International journal: my personal experience as an author and reviewer

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November 23, 2013

Пример 1. **Рукопись статьи получает отрицательные рецензии**

Fragment-based·design,·synthesis,·biological·evaluation·and·structure–activity·relationships·of·novel·benzo/benziso[d]thiazolimino–5–aryliden–4-thiazolidinones·as·cycloxygenase/lipoxygenase·inhibitors

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Athina·Geronikaki[1],·Phaedra·Eleftheriou[2],·Dimitra·Hadjipavlou-Litina[1],·Paola·Vicini[3],·Olga·Filz[4],·Dmitry·Filimonov[4],·Vladimir·Poroikov[4·*]*¶

·AUTHOR·ADDRESS → ¶

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Пример 1. Ответ из редакции

From: Herve Galons <ejmc.els@gmail.com>
Date: 23 March 2011 13:49
Subject: Your Submission
To: geronik@pharm.auth.gr

Ms. Ref. No.: EJMECH-D-11-00416
Title: Fragment-based design, synthesis, biological evaluation and structure-activity relationships of 2-benzo/benzisothiazolimino-5-aryliden-4-thiazolidinones as cycloxygenase/lipoxygenase inhibitors
European Journal of Medicinal Chemistry

Dear Athina Geronikaki,

Reviewers' comments on your work have now been received. You will see that they are advising against publication of your work. Therefore I must reject it.

For your guidance, I append the reviewers' comments below.
Thank you for giving us the opportunity to consider your work.

Yours sincerely,

Antonio Monge-Vega
Editor
European Journal of Medicinal Chemistry

Пример 1. **Первая рецензия**

Reviewer #1: The article by Geronikaki and coworkers, "Fragment-based design ", is well written and well organized. It was easy to follow the science and appreciate what they achieved. With respect to the science, finding dual inhibitors that target COX and 5hLO is an interesting and worthwhile direction. In interplay between COX and 5hLO is well known and optimizing both of their potencies simultaneously is important. Unfortunately, the authors were un-successful in this regard for two key reasons. First, their best IC50 against LO was only 17.7 uM which is a very poor potency. The literature is replete with LO inhibitors that are not better than 10 uM. This is because weakly inhibiting LO is a rather easy job if one simply attaches a greasy tail to a polar head group, such as the fatty acid substrate is. However, the major concern for this paper much more severe than simply poor potency against LO. The major concern is the type of LO that is used in this study. The authors emphasize in the text the need for 5-LO inhibition and the lowering of leukotriene production. This is absolutely correct, and thus this reviewer was amazed to see them use soybean 15-LO as their in vitro assay. I might emphasize that the authors do not even specify the type of soybean LO they used. This is very concerning because if one looks up soybean lipoxygenase on the Sigma web site, it clearly states that this enzyme produces the 15 product of AA. So, for the authors to use this enzyme as their 5-LO model enzyme shows a significant lack of knowledge of LO biochemistry. Not only is soybean 15-LO not a 5-LO and thus a terrible model for 5-LO, but it has been shown repeatedly in the literature that it is even a terrible model for human 15-LO inhibition. So there is a dual problem, wrong isozyme, wrong species. Unfortunately, this renders all of the data with respect to LO in this paper as irrelevant since investigating the inhibition of soybean 15-LO has nothing to do with leukotriene production in humans. If the authors wish to maintain this aspect of the paper, then they need to find a source of 5-LO and test their compounds with it. Then maybe they will be able to discuss the main thrust of this paper, dual COX/LO inhibition. Until that point, this is only an exercise in finding COX inhibitors.

Пример 1. **Вторая рецензия**

Reviewer #2: **In this manuscript Geronikaki and co-workers describes fragment-based design, synthesis, biological evaluation and structure-activity relationships of 2-benzo/benzisothiazolimino-5-aryliden-4-thiazolidinones as COX/LOX inhibitors. Overall the work is interesting and generally clear, however there are some serious problem generated by the manuscript, and the authors should make efforts to improve the quality of the presentation.**

Serious questions:

1. Authors should explain the reason of using naproxen as positive control of COX inhibitor. Personally, I suggest to select celecoxib instead of naproxen bases of more similar structures of synthesized compounds with celecoxib.
2. Authors should explain the reason or consideration of linking the fragments into target molecules. Does not it just consider a convenient synthesis?
3. Authors should add docking studies in this paper in order to confirm the design and explain the biological evaluation.
4. Author should clearly point out that the balance of COX-1, COX-2, and LOX means what.
5. In Figure2, Scheme 1, and Table 2, author draw the structures of benzothiazole series and benzisothiazole series compounds with two different stereochemistry of C=N double bond. Did authors determine the configuration of C=N bond? If no, please add the experiment to confirm.

Minor questions:

1. In "Abstract" and "Text", the statement "A new statistical method was proposed "seems inaccurate, since this method has been reported by authors in JMC 2008.
2. In "Abstract", line 12, please change "cyclooxygenase-1, cyclooxygenase-2 and lipoxygenase" into "COX-1, COX-2, and LOX".
3. The number of "Keywords" is exceeded.
4. Page 6, paragraph 3, line 8: a reference (BMC 2011, 19, 2074-2083) should be added.
5. Page 11, line 6-7: number of compounds should be bold.

. . .

Пример 1. Еще одна попытка

From: Herve Galons <ejmc.els@gmail.com>
Date: 30 August 2011 10:01
Subject: Your Submission
To: geronik@pharm.auth.gr

Ms. Ref. No.: EJMECH-D-11-01214
Title: Fragment-based design, synthesis, biological evaluation and structure-activity relationships of 2-benzo/benzisothiazolimino-5-aryliden-4-thiazolidinones as cycloxygenase/lipoxygenase inhibitors
European Journal of Medicinal Chemistry

Dear Athina Geronikaki,

Reviewers have now commented on your paper. You will see that they are advising that you revise your manuscript. If you are prepared to undertake the work required, I would be pleased to reconsider my decision. Your revision will be due on Oct 29, 2011

For your guidance, reviewers' comments are appended below.

Пример 1. **Комментарии рецензентов**

Reviewer #1:

1. Author's names should be checked as they have mentioned only 8 names in graphical abstract and 10 names in the manuscript.
2. The manuscript has to be checked carefully for grammatical and typographical errors.
3. Manuscript has to be formatted to journal specific format.
4. Manuscript is elaborative (too lengthy). Authors have to reduce the Introduction, Results and discussion and other experimental parts in the manuscript.

Reviewer #3:

The manuscript is well organized, scientifically significant and related to the authors' previous publication. However, it can be published with minor changes given below;
a. The title include the docking studies as «Fragment-based design, docking, synthesis, biological evaluation and structure-activity relationships».
b. At the Abstract part:"cycloxigenase-1" has to be changed as "cycloxygenase-1" and at the first sentence "." is forgotten at the end of the sentence. The 4th and the 5th sentences can be combined to avoid the repetitions.
c. At the Keywords «bezisothiazolidinones» has to be changed as «benzisothiazolidinones».

Пример 1. **Статья опубликована**

Contents lists available at SciVerse ScienceDirect

European Journal of Medicinal Chemistry

journal homepage: http://www.elsevier.com/locate/ejmech

Original article

Fragment-based design, docking, synthesis, biological evaluation and structure–activity relationships of 2-benzo/benzisothiazolimino-5-aryliden-4-thiazolidinones as cycloxygenase/lipoxygenase inhibitors

Phaedra Eleftheriou [b], Athina Geronikaki [a,*], Dimitra Hadjipavlou-Litina [a], Paola Vicini [c], Olga Filz [d,**], Dmitry Filimonov [d], Vladimir Poroikov [d], Shailendra S. Chaudhaery [e], Kuldeep K. Roy [e], Anil K. Saxena [e]

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[b] Department of Medical Laboratory Studies, School of Health and Medical Care, Alexander Technological Education Institute of Thessaloniki, Thessaloniki 57400, Greece
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Keywords:
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Inflammation
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Benzo/benzisothiazolidinones
Fragment-based drug design

ABSTRACT

Balanced modulation of several targets is one of the current strategies for the treatment of multi-factorial diseases. Based on the knowledge of inflammation mechanisms, it was inferred that the balanced inhibition of cyclooxygenase-1/cyclooxygenase-2/lipoxygenase might be a promising approach for treatment of such a multifactorial disease state as inflammation. Detection of fragments responsible for interaction with enzyme's binding site provides the basis for designing new molecules with increased affinity and selectivity. A new chemoinformatics approach was proposed and applied to create a fragment library that was used to design novel inhibitors of cycloxygenase-1/cycloxygenase-2/lipoxygenase enzymes. Potential binding sites were elucidated by docking. Synthesis of novel compounds, and the *in vitro*/*in vivo* biological testing confirmed the results of computational studies. The benzothiazolyl moiety was proved to be of great significance for developing more potent inhibitors.

Пример 2. Как повысить качество журнала в котором может быть опубликована статья?

Some Scientific Journals	SJR (2010)	IF (2010)
Cell	9.428	32.406
Pharmacological Reviews	2.279	23.857
Trends in Pharmacological Sciences	1.284	10.254
Drug Discovery Today	0.599	7.290
Journal of Medicinal Chemistry	0.451	5.207
Current Pharmaceutical Design	0.341	4.774
Current Medicinal Chemistry	0.393	4.630
Journal of Chemical Information and Modeling	0.297	3.822
Journal of Computer-Aided Molecular Design	0.255	3.522
European Journal of Medicinal Chemistry	0.164	3.193
Bioorganic and Medicinal Chemistry	0.194	3.108
Phytomedicine	0.133	2.837
SAR and QSAR in Environmental Research	0.104	1.560

Пример 2. Первый вариант: “Top-Down”

Some Scientific Journals	SJR (2010)	IF (2010)
Cell	9.428	32.406
Pharmacological Reviews	2.279	23.857
Trends in Pharmacological Sciences	1.284	10.254
Drug Discovery Today	0.599	7.290
Journal of Medicinal Chemistry	0.451	5.207
Current Pharmaceutical Design	0.341	4.774
Current Medicinal Chemistry	0.393	4.630
Journal of Chemical Information and Modeling	0.297	3.822
Journal of Computer-Aided Molecular Design	0.255	3.522
European Journal of Medicinal Chemistry	0.164	3.193
Bioorganic and Medicinal Chemistry	0.194	3.108
Phytomedicine	0.133	2.837
SAR and QSAR in Environmental Research	0.104	1.560

Пример 2. Второй вариант: “Bottom-Up”

Some Scientific Journals	SJR (2010)	IF (2010)
Cell	9.428	32.406
Pharmacological Reviews	2.279	23.857
Trends in Pharmacological Sciences	1.284	10.254
Drug Discovery Today	0.599	7.290
Journal of Medicinal Chemistry	0.451	5.207
Current Pharmaceutical Design	0.341	4.774
Current Medicinal Chemistry	0.393	4.630
Journal of Chemical Information and Modeling	0.297	3.822
Journal of Computer-Aided Molecular Design	0.255	3.522
European Journal of Medicinal Chemistry	0.164	3.193
Bioorganic and Medicinal Chemistry	0.194	3.108
Phytomedicine	0.133	2.837
SAR and QSAR in Environmental Research	0.104	1.560

Пример 2. **Реальный пример**

Some Scientific Journals	SJR (2010)	IF (2010)
Cell	9.428	32.406
Pharmacological Reviews	2.279	23.857
Trends in Pharmacological Sciences	1.284	10.254
Drug Discovery Today	0.599	7.290
Journal of Medicinal Chemistry	0.451	5.207
Current Pharmaceutical Design	0.341	4.774
Current Medicinal Chemistry	0.393	4.630
Journal of Chemical Information and Modeling	0.297	3.822
Journal of Computer-Aided Molecular Design	0.255	3.522
European Journal of Medicinal Chemistry	0.164	3.193
Bioorganic and Medicinal Chemistry	0.194	3.108
Phytomedicine	0.133	2.837
SAR and QSAR in Environmental Research	0.104	1.560

Пример 2. **Статья опубликована.**

Current Medicinal Chemistry, 2003, *10*, 225-233

Prediction of Biological Activity Spectra for Substances: Evaluation on the Diverse Sets of Drug-Like Structures

A.V. Stepanchikova*, A.A. Lagunin, D.A. Filimonov and V.V. Poroikov

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Abstract: The concept of Biological Activity Spectrum served as a basis for developing PASS (Prediction of Activity Spectra for Substances) software product. PASS predicts simultaneously more than 780 pharmacological effects and biochemical mechanisms based on the structural formula of a substance. It may be used for finding new targets (mechanisms) for known pharmaceuticals and for searching new biologically active substances. PASS prediction ability was evaluated by activity spectra prediction for 63 substances that are presented in the Molecule of the Month section of Prous Science (http://www.prous.com), belong to different chemical classes and reveal various types of biological activity. Mean accuracy of prediction turned out to be about 90%; therefore, it is reasonable to use PASS for finding and optimizing new lead compounds. A web-site with a new internet version of PASS is introduced into practice in December 2001 (http://www.ibmh.msk.su/PASS). On the site, one can find a detailed description of the PASS approach as well as some examples of its applications, and estimate the quality of prediction by submitting structures of substances with known activities.

Пример 3. Как отвечать на трудные вопросы рецензентов

Получены результаты:

Вторичные метаболиты бактерий обладают различными видами биологической активности, которые традиционно выявляют на основе случайного скрининга. Основываясь на информации о путях биосинтеза можно предсказать in silico структуру макролидов, поскольку биосинтез осуществляется поликетидсинтазами по модульному принципу (каждая поликетидсинтаза добавляет определенный фрагмент в структуру синтезируемой молекулы). Поскольку экспериментально с использованием генной инженерии исследовать все возможные варианты нельзя из-за их разнообразия, мы разработали компьютерную программу BioGenerator, которая генерирует виртуальные библиотеки структур макролидов на основе всевозможных комбинаций поликетидсинтаз. На основе компьютерного прогноза биологической активности можно отобрать в этих библиотеках структуры веществ, которые потенциально обладают требуемыми свойствами. Возможность использования такого подхода продемонстрирована на примере библиотек аналогов эритромицина и макролактина, информация о которых была нами собрана из литературы. Предложены новые структуры макролидов с требуемыми свойствами и определены пути их биосинтеза, что позволяет направленно выполнять соответствующие генно-инженерные модификации.

Пример 3. **Появилась конкурирующая публикация**

J|A|C|S
ARTICLES
Published on Web 06/16/2005

J. Am. Chem. Soc., 2005, *127* (27), pp 9930-9938
DOI: 10.1021/ja051586y
Publication Date (Web): June 16, 2005

Theoretical Considerations and Computational Analysis of the Complexity in Polyketide Synthesis Pathways

Joanna González-Lergier, Linda J. Broadbelt,* and Vassily Hatzimanikatis*

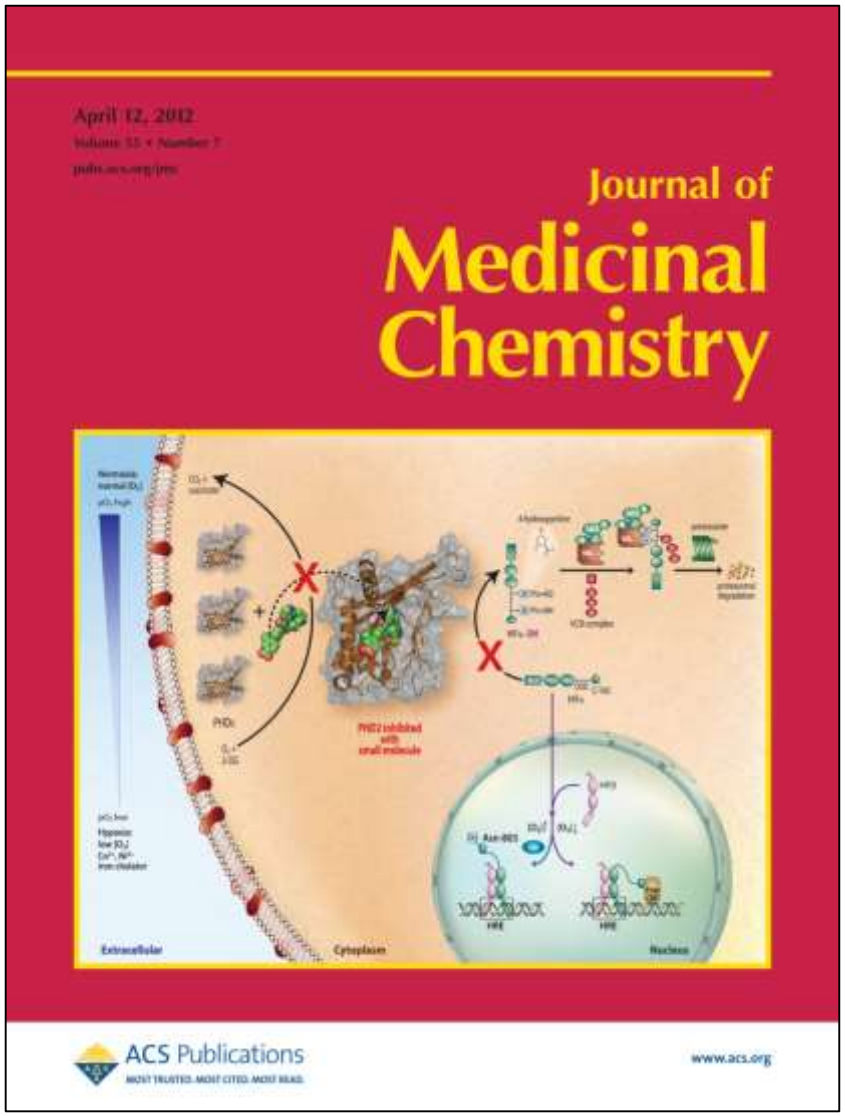
Contribution from the Department of Chemical and Biological Engineering, Northwestern University, Evanston, Illinois 60208

Received March 11, 2005; E-mail: vassily@northwestern.edu

Abstract: The emergence of antimicrobial resistance has led to an increase in research directed toward the engineering of novel polyketides. To date, less than 10 000 polyketide structures have been discovered experimentally; however, the theoretical analysis of polyketide biosynthesis performed suggests that over a billion possible structures can be synthesized. Polyketide synthesis, which involves the formation of a linear chain and its subsequent cyclization, is catalyzed by an enzyme complex called polyketide synthase (PKS). There are a number of variables in the linear chain synthesis controlled by the PKS: the number, identity, stereochemistry and sequence of the monomer units used in the elongation steps, and the degree of reduction that occurs after each of the condensation reactions. The theoretical analysis performed demonstrates that changes in these variables lead to the formation of different polyketide linear chains and, consequently, a high diversity of polyketide structures. The complexity in the number of possible structures led to the implementation of this system in BNICE, a computational framework that generates all possible biochemical pathways using a given set of enzyme reaction rules. This formulation allowed the analysis of the evolution of diversity in the synthesis mechanism and the construction of the pathway architecture of polyketide biosynthesis. It is expected that, after future implementation of the cyclization reactions, this framework can be used to identify all possible polyketides and their corresponding synthesis pathways. Consequently, this formulation would prove useful in guiding experimental approaches to engineer novel polyketides, a number of which will likely have medicinal properties.

JACS IF (2010) = 9.023

Пример 3. **Нужно публиковать в не менее авторитетном журнале!**



JMC IF (2010) = 5.207

Пример 3. Рецензия была положительная, но …

… в ней отмечалось, что результаты компьютерных расчетов не проверены в непосредственных экспериментах.

Рекомендовалось осуществить такого рода экспериментальную проверку компьютерных прогнозов и направить в печать новый вариант рукописи, дополнив ее соответствующими экспериментальными данными.

Пример 3. Как добиться принятия статьи в печать, не проводя дополнительных экспериментов ?

Пример 3. Что делать?

1. **Исследовать, были ли в последние годы в Journal of Medicinal Chemistry публикации, в которых результаты компьютерного моделирования проверялись не в непосредственных экспериментах, а на основе ретроспективного анализа опубликованных литературных данных и составить список соответствующих публикаций.**
2. **Объяснить редактору , что проведение генно-инженерных экспериментов займет 1-2 года и при этом будет получено 2-3 вещества из класса макролидов. Результаты биологического тестирования этих веществ (положительные или отрицательные) не будут статистически значимыми с точки зрения валидации предложенных нами расчетных методов.**
3. **Объяснить редактору , что в этих условиях единственным вариантом валидации предложенных нами методов является ретроспективный анализ достаточно больших выборок, собранных из литературы (и привести список такого рода публикаций в Journal of Medicinal Chemistry в последние годы).**

Пример 3. **Письмо в редакцию (15.12.2005)**

Dear Professor Krogsgaard-Larsen,

We are very much grateful to you and to the rewires for very careful consideration of our manuscript JM051035I entitled "Rational Design of Macrolides by Virtual Screening…". The comments help us to improve the manuscript substantially.

The main point described by reviewer 3 that is also reflected in your accompanying letter is the experimental validation of computer predictions. We agree that in general such approach provides the most objective estimates (see e.g. our publication Geronikaki et al. Design of new cognition enhancers: from computer prediction to synthesis and biological evaluation. *J. Med. Chem.* 2004, *47*(11), 2870-2876.). However, such approach is not well applicable in the case of this manuscript because most of computer predictions should be validated on statistically reasonable samples. When we are going to design a new bacteria producing biologically active compounds with the desirable properties only one or a few strains can be really created by genetic engineering, and it may take several years. On this basis only one or few predictions can be checked experimentally. This is not enough for statistically significant conclusions. That is why we used a validation based on experimental data about thousands macrolides taken from literature. It is necessary to stress that such kind of validation is widely used in practice (see e.g. Oloff et al. Application of Validated QSAR Models of D1 Dopaminergic Antagonists for Database Mining J. Med. Chem.; (Article); 2005; 48(23); 7322-7332.; Xiao et al. Antitumor Agents. Modeling of pipodophyllotoxin Derivatives Using Variable Selection *k* Nearest Neighbor QSAR Method.J. Med. Chem., 2002 *Vol. 45, No. 11* 2309; Sutherland et al. A Comparison of Methods for Modeling Quantitative Structure-Activity Relationships J. Med. Chem., 2004, *47,* 5541-5554; Ducki et al. J. Quantitative Structure-Activity Relationship (5D-QSAR) Study of Combretastatin-like Analogues as Inhibitors of Tubulin Assembly. J. Med. Chem., 2005; *2005, Vol. 48, No. 2* 465, etc.). We do hope that you will take in to account the arguments given above.

Our response on the other reviewers comments are provided below.

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Пример 3. Ответ из редакции (25.01.2006)

Dear Dr. Poroikov:

We are pleased to inform you that your manuscript entitled "Rational Design of Macrolides by Virtual Screening of Combinatorial Libraries Generated Through In Silico Manipulation of Polyketide Synthases" (manuscript ID jm051035i) has been accepted for publication in Journal of Medicinal Chemistry. Your manuscript has been forwarded to the ACS Publications office.

You will be contacted in the near future by the ACS Journal Publishing Staff regarding the page proofs for your manuscript. Your paper will be published on the Web approximately 48 hours after you approve your page proofs. In view of this fast publication time it is important to review your page proofs carefully. Once a manuscript appears on the web it is published. Any change after that point must be considered additions / corrections.

Kind regards,
Povl Krogsgaard-Larsen
European Editor, Journal of Medicinal Chemistry
jmc@dfuni.dk

Пример 3. **Статья опубликована.**

J. Med. Chem. **2006,** *49,* 2077−2087

Rational Design of Macrolides by Virtual Screening of Combinatorial Libraries Generated through in Silico Manipulation of Polyketide Synthases

Sergey B. Zotchev,[†] Alla V. Stepanchikova,[‡] Anastasia P. Sergeyko,[‡] Boris N. Sobolev,[‡] Dmitrii A. Filimonov,[‡] and Vladimir V. Poroikov*[,‡]

Department of Biotechnology, Norwegian University of Science and Technology, Trondheim, Norway and Institute of Biomedical Chemistry of Russian Academy of Medical Science, Moscow, Russia

Received October 14, 2005

Bacterial secondary metabolites display diverse biological activities, thus having potential as pharmacological agents. Although most of these compounds are discovered by random screening, it is possible to predict and re-design their structures based on the information on their biosynthetic pathways. Biosynthesis of macrolides, governed by modular polyketide synthases (PKS), obeys certain rules, which can be simulated in silico. PKS mode of action theoretically allows for a huge number of macrolides to be produced upon combinatorial manipulation. Since engineering of all possible PKS variants is practically unfeasible, we created Biogenerator software, which simulates manipulation of PKS and generates virtual libraries of macrolides. These libraries can be screened by computer-aided prediction of biological activities, as exemplified by analysis of erythromycin and macrolactin libraries. This approach allows rational selection of macrolides with desired biological activities and provides instructions regarding the composition of the PKS gene clusters necessary for microbial production of such molecules.

Пример 4. «Патентовать нельзя публиковать»

НООТРОПНОЕ ДЕЙСТВИЕ НЕКОТОРЫХ АНТИГИПЕРТЕНЗИВНЫХ ПРЕПАРАТОВ: КОМПЬЮТЕРНЫЙ ПРОГНОЗ И ЭКСПЕРИМЕНТАЛЬНОЕ ТЕСТИРОВАНИЕ

Крыжановский С.А., Салимов Р.М.,
Лагунин А.А., Филимонов Д.А., Глориозова Т.А., Поройков В.В.

Реферат

На основе прогнозируемых с помощью компьютерной программы PASS спектров биологической активности было отобрано несколько антигипертензивных препаратов из группы ингибиторов АПФ для экспериментальной оценки ноотропной активности. Эксперименты проведены на мышах по тесту спонтанной ориентации (поведения патрулирования) в крестообразном лабиринте. В результате проведенных экспериментов обнаружено, что периндоприл в дозе 1 мг/кг, а квинаприл и моноприл в дозе 10 мг/кг вызывают улучшение показателей поведения патрулирования лабиринта. Данный эффект имеет сходство с эффектами эталонных ноотропных препаратов пирацетам и меклофеноксат (в дозах 300 и 120 мг/кг соответственно). Обнаруженное нами ноотропное действие некоторых ингибиторов АПФ, скорее всего, не связано с их антигипертензивным эффектом, поскольку ноотропное действие имело место лишь при относительно малых дозах периндоприла, квинаприла и моноприла и исчезало при дальнейшем увеличении дозы. Выявление ноотропных свойств у широко применяемых в медицинской практике антигипертензивных препаратов открывает возможности для их новых клинических применений с учетом соответствующих индивидуальных особенностей пациентов.

Рукопись была подготовлена для публикации в 2005 году.

Пример 4. «Патентовать нельзя публиковать»

И положена в ящик стола. Мы ждали, что фирма, с которой было подписано соглашение о конфиденциальности, запатентует найденные нами новые свойства препаратов, разрешенных к медицинскому применению: 2005, 2006, 2007, 2008, 2009, 2010, 2011 . . .

Пример 4. Были подготовлены материалы для патентной заявки…

… однако, финансовая ситуация компании, которая планировала патентование, резко ухудшились.

И, в конце концов, компания исчезла совсем.

Пример 4. Было решено опубликовать результаты как можно скорее, поскольку они «пролежали в ящике» почти 7 лет.

ISSN 0023-1134
Ежемесячный научно-технический и производственный журнал
Основан в январе 1967 г.
12 выпусков в год, 1/8 (60×90), 56 стр.

В журнале освещаются молекулярно-биологические проблемы создания лекарственных средств, методы синтеза и технология производства новых лекарственных препаратов, а также экологические и экономические проблемы, связанные с поиском и производством лекарственных средств и фармацевтических препаратов.
Территория распространения журнала (на русском языке): Россия, страны СНГ и Балтии, Китай, Германия, Франция, Австрия, Нидерланды, Бельгия, Польша, Венгрия, Чехия, Болгария.
ХФЖ реферируется международными реферативными журналами *Chemical Abstracts*, *Chemical Titles*, *Current Abstracts*, *International Abstracts of Biological Sciences*, *Biological Abstracts* и информационным бюро *Excerpta Medica*.
На английском языке журнал распространяется по подписке издательством Springer под названием "Pharmaceutical Chemistry Journal".

http://chem.folium.ru/index.htm

Пример 4. **Статья была принята к публикации и опубликована за полгода.**

С. А. Крыжановский[1], *Р. М. Салимов*[1], *А. А. Лагунин*[2], *Д. А. Филимонов*[2], *Т. А. Глориозова*[2], *В. В. Поройков*[2]

НООТРОПНОЕ ДЕЙСТВИЕ НЕКОТОРЫХ АНТИГИПЕРТЕНЗИВНЫХ ПРЕПАРАТОВ: КОМПЬЮТЕРНЫЙ ПРОГНОЗ И ЭКСПЕРИМЕНТАЛЬНОЕ ТЕСТИРОВАНИЕ

[1] Учреждение Российской академии медицинских наук Научно-исследовательский институт фармакологии имени В. В. Закусова РАМН, Москва, Россия;
[2] Учреждение Российской академии медицинских наук Научно-исследовательский институт биомедицинской химии им. В. Н. Ореховича РАМН, Москва, Погодинская ул., Россия

На основе прогнозируемых с помощью компьютерной программы PASS спектров биологической активности было отобрано несколько антигипертензивных препаратов из группы ингибиторов АПФ для экспериментальной оценки ноотропной активности. Эксперименты проведены на мышах по тесту спонтанной ориентации (поведения патрулирования) в крестообразном лабиринте. В результате проведенных экспериментов обнаружено, что периндоприл в дозе 1 мг/кг, а квинаприл и моноприл в дозе 10 мг/кг вызывают улучшение показателей поведения патрулирования лабиринта. Данный эффект имеет сходство с эффектами эталонных ноотропных препаратов пирацетам и меклофеноксата (в дозах 300 и 120 мг/кг соответственно). Обнаруженное нами ноотропное действие некоторых ингибиторов АПФ, скорее всего не связано с их антигипертензивным эффектом, поскольку ноотропное действие имело место лишь при относительно малых дозах периндоприла, квинаприла и моноприла и исчезало при дальнейшем увеличении дозы. Выявление ноотропных свойств у широко применяемых в медицинской практике антигипертензивных препаратов открывает возможности для их новых клинических применений с учетом соответствующих индивидуальных особенностей пациентов.

Ключевые слова: репозиционирование лекарств, компьютерное прогнозирование, PASS, антигипертензивные препараты, ноотропное действие

В химико-фармацевтической науке нередки ситуации, когда лекарственное средство, первоначально создаваемое с целью терапии определенной патологии, впоследствии находило медицинское применение в плане лечения других нозологических единиц. Пожалуй, одним из относительно свежих примеров такого рода является Виагра (силденафил) — ингибитор фосфодиэстеразы 5, который в 1992 г. тестировался фирмой Пфайзер в клинике как антиангинальное средство, а в настоящее время широко применяется как препарат для лечения эректильной дисфункции [1]. Другие примеры такого рода препаратов "двойного назначения" приведены в табл. 1.

До последнего времени новые свойства обнаруживались у известных препаратов случайным образом в ходе углубленного доклинического тестирования или клинических испытаний. В работах [2, 3] предложен так называемый SOSA-подход (SOSA: Selective Optimization of Side Action), который предполагает усиление "побочного действия" и ослабление "основного эффекта" путем направленной модификации структуры известных препаратов, что, с учетом уже накопленных данных по фармакодинамике и фармакокинетике известного класса лекарственных средств, создает основы для их рационального дизайна.

Нами было предложено использовать компьютерное прогнозирование спектров биологической активности веществ для определения их наиболее вероятных видов биологической активности [4 – 6]. В результате компьютерного прогноза биологической активности для 200 наиболее продаваемых в США препаратов было показано, что даже для таких, казалось бы, детально исследованных лекарственных средств прогнозируются новые эффекты, которые могут стать основой для их нового медицинского применения [7]. В частности, для некоторых ингибиторов ангиотензин-превращающего фермента (АПФ) с достаточно высокой вероятностью предсказывалось наличие ноотропного действия.

Целью настоящей работы явилось компьютерное прогнозирование спектров биологической активности ряда антигипертензивных препаратов — ингибиторов АПФ и тестирование их ноотропной активности в эксперименте на лабораторных животных.

Экспериментальная часть

Компьютерное прогнозирование биологической активности. Компьютерный прогноз спектров биологической активности веществ был выполнен с использованием программы PASS (актуальная на момент выполнения расчета версия 1.917[1]), которая позволяла оценить вероятности наличия/отсутствия около 2000 фармакологических эффектов, механизмов действия (ингибиторы и активаторы ферментов, агонисты и антагонисты рецепторов и др.), побочных эффектов и специфической токсичности. Химическая структура

[1] В настоящее время актуальная версия PASS 10.1 – детали см. на веб-сайте: http://pharmaexpert.ru/passonline

Pharmaceutical Chemistry Journal, Vol. 45, No. 10, January, 2012 (Russian Original Vol. 45, No. 10, September, 2011)

NOOTROPIC ACTION OF SOME ANTIHYPERTENSIVE DRUGS: COMPUTER PREDICTING AND EXPERIMENTAL TESTING

S. A. Kryzhanovskii,[1] R. M. Salimov,[1] A. A. Lagunin,[2] D. A. Filimonov,[2] T. A. Gloriozova,[2] and V. V. Poroikov[2]

Translated from Khimiko-Farmatsevticheskii Zhurnal, Vol. 45, No. 10, pp. 25 – 31, October, 2011.

Original article submitted October 1, 2011.

Several antihypertensive drugs belonging to the group of ACE inhibitors have been selected for testing their nootropic activity based on a computer-aided prediction of their biological activity spectra using the PASS computer program package. Experiments were conducted on mice by the spontaneous orientation test (patrolling behavior) in a cross-maze. It was found that perindopril at a dose of 1 mg/kg in addition to quinapril and monopril at a dose of 10 mg/kg improved the patrolling behavior in the cross-maze test. This effect is similar to the effects of the standard nootropic drugs piracetam and meclofenoxate (at doses of 300 and 120 mg/kg, respectively). The observed nootropic effect of some ACE inhibitors is likely to be unrelated to their antihypertensive effect since the nootropic action took place only at relatively low doses of perindopril, quinapril, and monopril and was not observed with further increase of the dose. The identification of nootropic action of antihypertensive drugs that are commonly used in clinical practice leads to their new clinical applications with allowance for the relevant idiosyncrasies of patients.

Key words: drug repurposing, computer-aided prediction of activity (PASS), antihypertensive drugs, nootropic action.

Situations where a drug that was initially created for therapy of a certain disease finds medical application for treatment of other clinical indications are well known in chemical and pharmaceutical science. Perhaps one of the relatively recent examples of this is Viagra (sildenafil), a phosphodiesterase 5 inhibitor that was tested clinically in 1992 by Pfizer as an antianginal agent and is currently widely used as a drug for treating erectile dysfunction [1]. Table 1 presents other examples of this type of "dual purpose" drugs.

Until recently new properties were observed for known drugs in a random manner during expanded preclinical testing or clinical trials. The so-called SOSA-approach (Selective Optimization of Side Action) that proposes strengthening of a side action and weakening of the principal effect by directed modification of the structures of known drugs was reported [2, 3]. This forms a basis for their rational design considering already accumulated data on the pharmacodynamics and pharmacokinetics of a known class of drugs.

We proposed using computer-aided prediction of biological activity spectra of compounds in order to determine their most probable types of biological activity [4 – 6]. Computer-aided prediction of the biological activity for the 200 most prescribed drugs in the USA showed that new effects that could become the basis for new medical applications were predicted even for seemingly thoroughly investigated drugs [7]. In particular, nootropic activity was predicted with rather high probability for several angiotensin-converting enzyme (ACE) inhibitors.

The goal of the present work was computer-aided prediction of the biological activity spectra of several antihypertensive drugs, ACE inhibitors, and testing of their nootropic activity in experiments on laboratory animals.

EXPERIMENTAL PART

Computer-aided prediction of biological activity. Computer-aided prediction of biological activity spectra of com-

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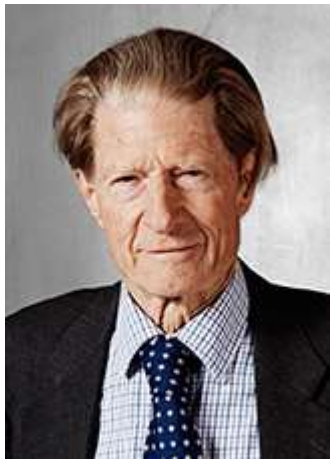
November 23, 2013

What is common between these people?




James E. Rothman	Randy W. Schekman	Thomas C. Südhof	Sir John B. Gurdon	Shinya Yamanaka
h-Index: 106	16	134	75	44

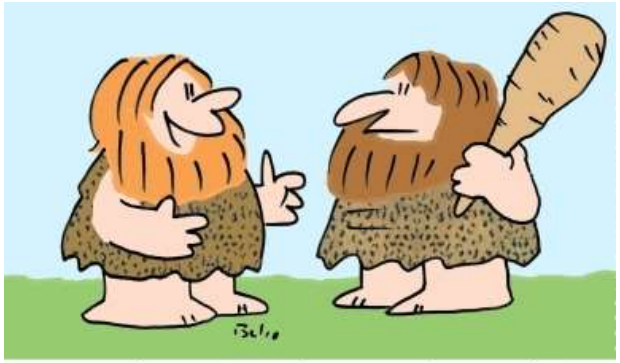
The Nobel Prize in Physiology or Medicine 2013 was awarded jointly to James E. Rothman, Randy W. Schekman and Thomas C. Südhof *"for their discoveries of machinery regulating vesicle traffic, a major transport system in our cells"*.

The Nobel Prize in Physiology or Medicine 2012 was awarded jointly to Sir John B. Gurdon and Shinya Yamanaka *"for the discovery that mature cells can be reprogrammed to become pluripotent".*

All they published their articles in English in peer-reviewed journals.

November 23, 2013

Нередко авторам статей приходится также быть рецензентами рукописей других авторов.



«Рецензенты имеют право не только говорить людям в глаза, что они дураки, но даже доказывать им это».

Г. К. Литхтенберг

«Поступайте по отношению к другим так, как вы хотели бы, чтобы другие поступали по отношению к вам».

«Золотое правило нравственности»

Рукопись поступила на рецензию

Journal of Proteomics
Manuscript Draft

Manuscript Number: JPROT-D-11-00065

Title: From In Silico Target Prediction to Multi-Target Drug Design: Current Databases, Methods and Applications

Article Type: SI: Pharmacoproteomics and Toxicoprot.

Section/Category: Review Article

Keywords: Target prediction; polypharmacology; mode of action; target fishing; in silico; off targets

Abstract: Given the tremendous growth of bioactivity databases, the use of computational tools to predict protein targets of small molecules has been gaining importance in recent years. Applications span a wide range, from the designed polypharmacology of compounds to mode-of-action analysis. In this review, we firstly survey databases that can be used for ligand-based protein target prediction and which have grown tremendously in size in the past. We furthermore outline methods for target prediction that exist, both based on the knowledge of bioactivities from the ligand side, as well as methods that can be applied in situations when a protein structure is known. Applications of successful in silico target identification attempts are discussed in detail, which were based partly or in whole on computational target predictions in the first instance. This includes the authors' own experience using target prediction tools, in this case considering phenotypic antibacterial screens and the analysis of high-throughput screening data. Finally, we will conclude with the prospective application of databases to not only predict, retrospectively, the protein targets of a small molecule, but also how to design ligands with desired polypharmacology in a prospective manner.

November 23, 2013

Comments on the paper "From In Silico Target Prediction to Multi-Target Drug Design: Current Databases, Methods and Applications"

The paper presents an overview of currently available databases and software, which provides the options for prediction of drug-like molecules' interaction with many pharmacological targets (polypharmacology assessment). Such prediction is very important due to the necessity both to obtain/design pharmaceutical agents with multi-target action that lead to additive/synergistic useful pharmacotherapeutic effect and to avoid adverse/toxic effects in compounds under study.

Based on the stated above, this paper could be recommended for publication in the Journal of Proteomics. However, some principal works performed in this field are missed in the manuscript, which should be corrected to present more completely the background and the existing opportunities. Also, there are some other comments on the manuscript, which are presented below.

Page 4, line 44: It seems better to give a reference on the original work of Paul Ehrlich, not on the secondary publication(s).

Page 4, lines 44-46: "Key-and-lock" concept in enzymology was introduced by Emil Fisher in 1984, and the appropriate reference is also desirable.

November 23, 2013

Page 4, lines 49-51: When the authors present some publications about multi-target pharmaceutical agents, it is worse not to mention one of the first publications in this field: Wermuth C. Multitargeted drugs: the end of the "one-target-one disease philosophy? *Drug Disc. Today*, 2004, *9*, 826-827. In this paper for the first time it was stressed that "…the preparation of dual- or multiple-ligands on an almost rational basis is now conceivable and it can be expected that many of these molecules will yield drugs of superior clinical value compared to monotarget formulations". In another paper published in the same year (Wermuth C.G. Selective optimization of side activities: another way for drug discovery. J Med Chem. 2004 Mar 11;47(6):1303-14) Camille Wermuth proposed to use a knowledge about multi-target action of drugs for rational design of new pharmaceutical agents with the required action.

Page 7, lines 115-116: Of course, it is not possible to require from the authors to present a complete picture of all publicly and commercially available bioactivity databases. However, since the authors mentioned the existence of both types of databases, it seems necessary to give a few examples of the most important commercially available databases, and make some comparison between the public and commercially available sources.

Page 7, lines 127-128: This is too strong statement. If the authors know which computational tools for integration of information are already prepared within each pharmaceutical company?

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. . .

Page 23, line 504: Once again about chemical similarity (see also the comments above). Chemically similar compounds may be or may not be similar in biological activity (Y. Martin, 2002). Therefore, all examples of successful application of this method are just particular cases. No transferability could be expected. In any particular case the researcher can be either lucky or not.

Page 23, lines 516-518: The emphasis of the paper [89] cited here is not prediction of bioactivity for St John's Wort, but great potential of computational methods in prediction of multi-target bioactivity spectra for complex mixtures of phytoconstituents and other natural products.

Page 29, line 651: Misprint, it should be "zinc", not "cinc".

Page 34-36: It is necessary to consider the dynamic behavior of biological networks, not the static picture (see, for instance, Przytycka T.M. and Kim Y-A. *BMC Biology*, 2010, 8:48). However, this approach is rather difficult and is often ignored. If the authors have some ideas how to overcome these difficulties?

Page 37, line 843: How the authors computed the "minimum synergistic combinations of targets"? Which criteria were used to discriminate between the additive and synergistic effects?

Ответы рецензентам

*Detailed Response to Reviewers

Dear Editor, please note the changes made to our manuscript, based on careful consideration of the points by the referees, as follows:

Reviewers' comments:

Reviewer #1: The paper presents an overview of currently available databases and software, which provides the options for prediction of drug-like molecules' interaction with many pharmacological targets (polypharmacology assessment). Such prediction is very important due to the necessity both to obtain/design pharmaceutical agents with multi-target action that lead to additive/synergistic useful pharmacotherapeutic effect and to avoid adverse/toxic effects in compounds under study.

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> The authors thank the referee for appreciating the importance of the topic of this review.

. . .

Статья опубликована.

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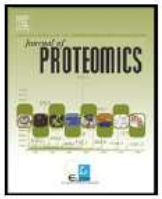

Review

From *in silico* target prediction to multi-target drug design: Current databases, methods and applications

Alexios Koutsoukas[a], *Benjamin Simms*[b], *Johannes Kirchmair*[a], *Peter J. Bond*[a], *Alan V. Whitmore*[c,d], *Steven Zimmer*[c], *Malcolm P. Young*[c,e], *Jeremy L. Jenkins*[b], *Meir Glick*[b], *Robert C. Glen*[a,*], *Andreas Bender*[a,*]

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ABSTRACT

Given the tremendous growth of bioactivity databases, the use of computational tools to predict protein targets of small molecules has been gaining importance in recent years. Applications span a wide range, from the 'designed polypharmacology' of compounds to mode-of-action analysis. In this review, we firstly survey databases that can be used for ligand-based target prediction and which have grown tremendously in size in the past. We furthermore outline methods for target prediction that exist, both based on the knowledge of bioactivities from the ligand side and methods that can be applied in situations when a protein structure is known. Applications of successful *in silico* target identification attempts are discussed in detail, which were based partly or in whole on computational target predictions in the first instance. This includes the authors' own experience using target prediction tools, in this case considering phenotypic antibacterial screens and the analysis of high-throughput screening data. Finally, we will conclude with the prospective application of databases to not only predict, retrospectively, the protein targets of a small molecule, but also how to design ligands with desired polypharmacology in a prospective manner.

Ситуация, когда бескомпромиссность – лучшее решение.

3D-QSAR Study of Synthetic Furanones as Inhibitors of Quorum Sensing by Using CoMFA and CoMSIA Approach

Ping-Hua Sun[a], Zhao-Qi Yang[a], Mao-Kang Li[a], Wei-Min Chen[a,*], Qian Liu[a], and Xin-Sheng Yao[a,b,*]

[a]Faculty of Pharmacy, Jinan University, Guangzhou 510 632, China

[b]Institute of Traditional Chinese Medicine and Natural products, Jinan University, Guangzhou 510 632, China

The chemical signals such as *N*-acylhomoserine lactones (AHLs) controlling quorum sensing (QS) processes have attracted growing interest in the development of non-native ligands that can intercept these signals and emerged as a possible target pathway for the design of novel antimicrobial compounds. Twenty six synthetic furanones with variable inhibition of QS were selected to develop models to establish the 3D-QSAR using two types of molecular field analysis techniques: comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA). The statistical results showed that the 3D-QSAR models derived from CoMFA were superior to those generated from CoMSIA. The optimal CoMFA model exhibited good cross-validated q^2 and conventional r^2 values at 0.639 and 0.992. The external test sets (r^2_{pred}) value of 0.56 further confirmed the predictive capacity of the resultant CoMFA models. A set of 3D contour plots drawn based on the CoMFA models reveal modifications of substituents at C2, C3 and C5 of the furanone which my be useful to improve the activity of the inhibitors of QS. Results showed that both the steric and electrostatic factors should appropriately be taken into account in future rational design and development of more active QS inhibitors for the design of a novel antimicrobial lead compound.

Keywords: 3D-QSAR; CoMFA; CoMSIA; Quorum-Sensing; Furanones

November 23, 2013

Фрагмент моей рецензии

SAR and QSAR in Environmental Research

Referee's Report on the paper of Ping-Hua Sun, Zhao-Qi Yang, Mao-Kang Chen, Qian Liu, and Xin-Sheng Yao "3D-QSAR Study of Synthetic Furanone of Quorum Sensing by Using CoMFA and CoMSIA Approach".

Referee no. 08-110

1.	Is this paper suitable for publication:	
	a) in its present form?	No
	b) if minor changes were made?	No
2.	Could this paper be suitable for publication if a major revision were made?	No
3.	If a major revision is required, would you wish to see the paper again after resubmission?	No
4.	Is this paper unsuitable for publication:	
	a) because of lack of originality?	Yes
	b) because of demonstrable errors?	Yes
	c) because the subject matter is of insufficient interest?	Yes/No
	d) because the subject matter is not appropriate to this journal?	No

Обоснование

The paper does not correspond to the requirements and level of the SAR and QSAR in Environmental Research:

<u>Because of the lack of novelty.</u> The paper with very close content has been published recently in the Letters in Drug Design and Discovery, *5*: 449-453 (2008): Sun P-H. et al. "3D-QSAR analysis of N-phenylacetonoyl-L-homoserine lactones as inhibitors of bacterial quorum sensing via CoMFA approach". No reference on this earlier paper is given, no difference between two papers is explained in this paper.

<u>Because of the lack of quality.</u> The paper presents the results of work made at the "student's level". It might be useful for some training in learning of CoMFA and CoMSIA methods, however the techniques used and the results obtained are not suitable for publication.

<u>Conclusions.</u> The paper should be rejected despite the rather interesting topic concerning the quorum sensing regulation and inhibition.

Ответ китайского редактора китайскому автору (середина XIX века)

"Преславный брат солнца и луны, раб твой распростерт у твоих ног. Я целую землю перед тобой и молю мне разрешить жить и говорить. Твоя уважаемая рукопись удостоила нас своего просвещенного лицезрения, и мы с восторгом прочли ее. Клянусь останками моих предков, я никогда не читал ничего столь возвышенного! Со страхом и трепетом отсылаю ее назад. Если бы я дерзнул напечатать это сокровище, то император повелел бы, чтобы оно навсегда служило образцом и чтобы я никогда не смел напечатать ничего, что было бы ниже его. При моей литературной неопытности, я знаю что такие перлы попадаются раз в 10 тысяч лет, и поэтому я возвращаю его тебе. Молю тебя, прости меня.

Склоняюсь к твоим ногам.

Слуга твоего слуги, редактор".

Если редактор попытается «накрутить» импакт-фактор журнала?

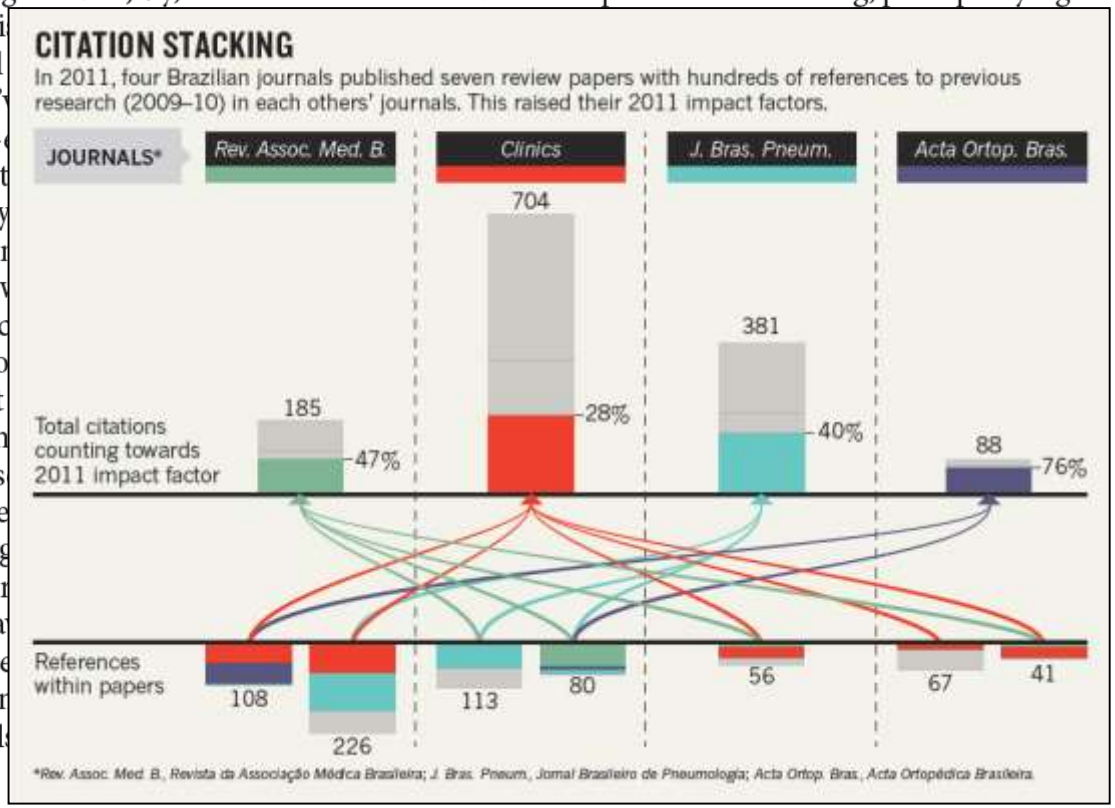
Brazilian citation scheme outed

Thomson Reuters suspends journals from its rankings for 'citation stacking'.

BY RICHARD VAN NOORDEN

Mauricio Rocha-e-Silva thought that he had spotted an easy way to raise the profiles of Brazilian journals. From 2009, he and several other editors published articles containing hundreds of references to papers in each others' journals — in order, he says, to elevate the journals' impact factors.

Because each article avoided citing papers published by its own journal, the agreement flew under the radar of analyses that spot extremes in self-citation — until 19 June, when the pattern was discovered. Thomson Reuters, the firm that calculates and publishes the impact factor, revealed that it had designed a program to spot concentrated bursts of citations from one journal to another, a practice that it has dubbed 'citation stacking'. Four Brazilian journals were among 14 to have their impact factors suspended for a year for such stacking. And in July, Rocha-e-Silva was fired from hi journal "We' Rocha- tors of t lared by additio others v they esc Edito impact citation Thoms on exce red-flag familiar nals ha elsewhe searchin journals be responsible for stacking, perhaps trying to



November 23, 2013

Заключительный реальный пример (http://scientific.ru)

28.04.2012 Никстем

Ищу партнёра, имеющего опыт публикаций научных статей в престижных зарубежных научных журналах. Соавторство в фундаментальных научных открытиях гарантируются. Статья уже готовая, но на русском языке.

29.04.2012 ЕЛ

1. **Выбираете журнал, подходящий для Вашей работы.**
2. **Внимательно просматриваете несколько статей по сходной тематике.**
3. **Доводите Вашу статью до нужной кондиции в соответствии с правилами для авторов - структура резюме, объем и содержание введения (не забудьте про новые ссылки и желательно про ссылки на выбранный журнал), оформляете рисунки по правилам данного журнала, в обсуждении отражаете важность полученных Вами результатов в контексте мировой литературы, оформляете список литературы.**
4. **Переводите на англ. яз., снабдив переводчика парой статей на англ. яз. по данной теме, желательно из выбранного журнала.**

Заключительный реальный пример (продолжение)

5. Отправляете текст в одну из фирм "English to English", есть, например, в «Nature».

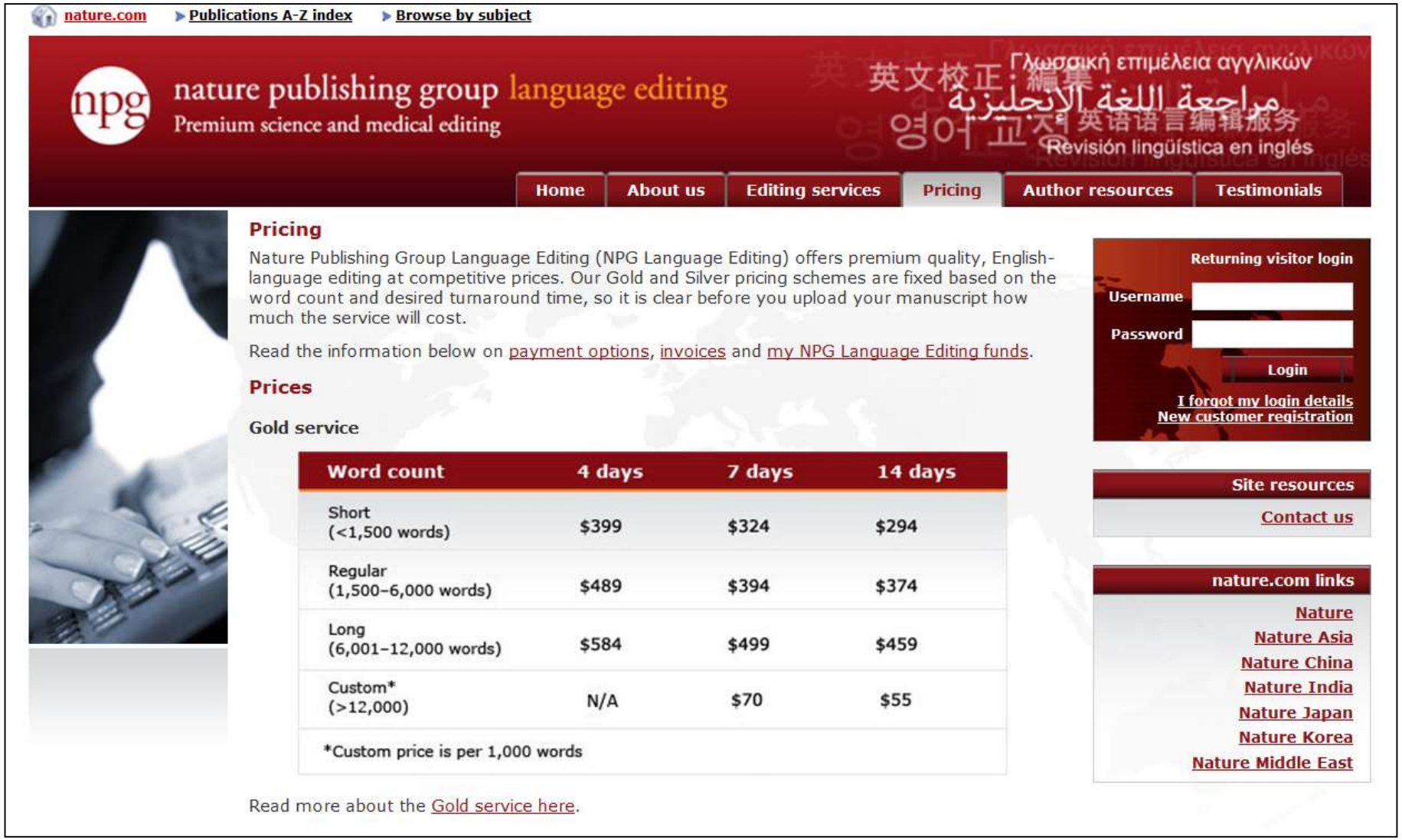
6. Проверяете, правильно ли переведены специальные термины.

7. Отправляете в журнал, приложив письмо, что английский Вашей статьи отредактирован - особенно действует, если это фирма при «Nature».

8. Если отразили, выбираете другой журнал и все повторяете.

9. Если приняли с замечаниями, методично отвечаете пункт за пунктом на все высказанные замечания, часть можно оспаривать. Отправляете снова.

Редакции могут помочь улучшить англоязычный вариант рукописи



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О пользе международного научного сотрудничества

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«Дорога начинается с первого шага».

November 23, 2013