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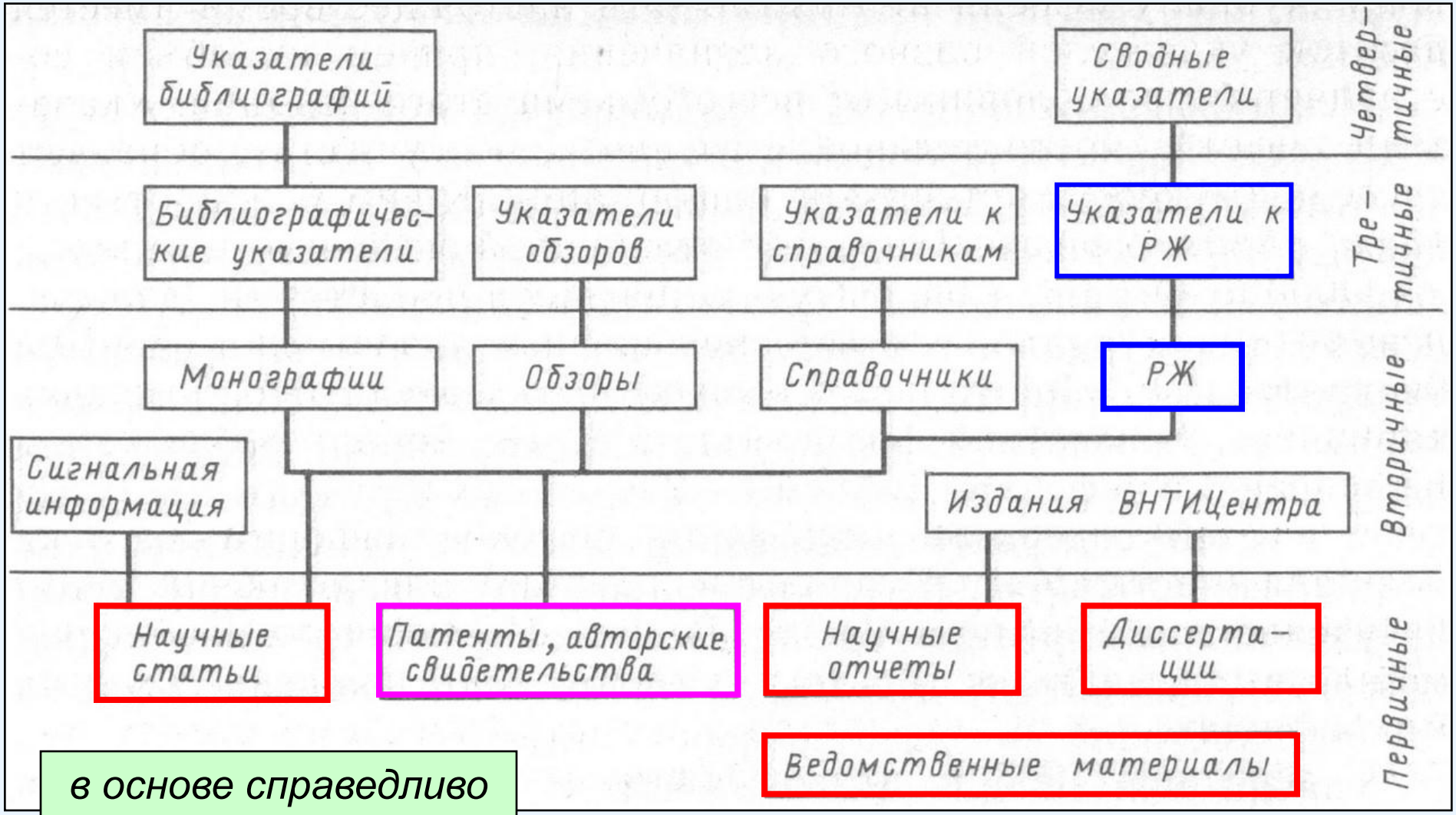

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- *В.М. Потапов, Э.К. Кочетова. Химическая информация. М., "Химия", 1988*

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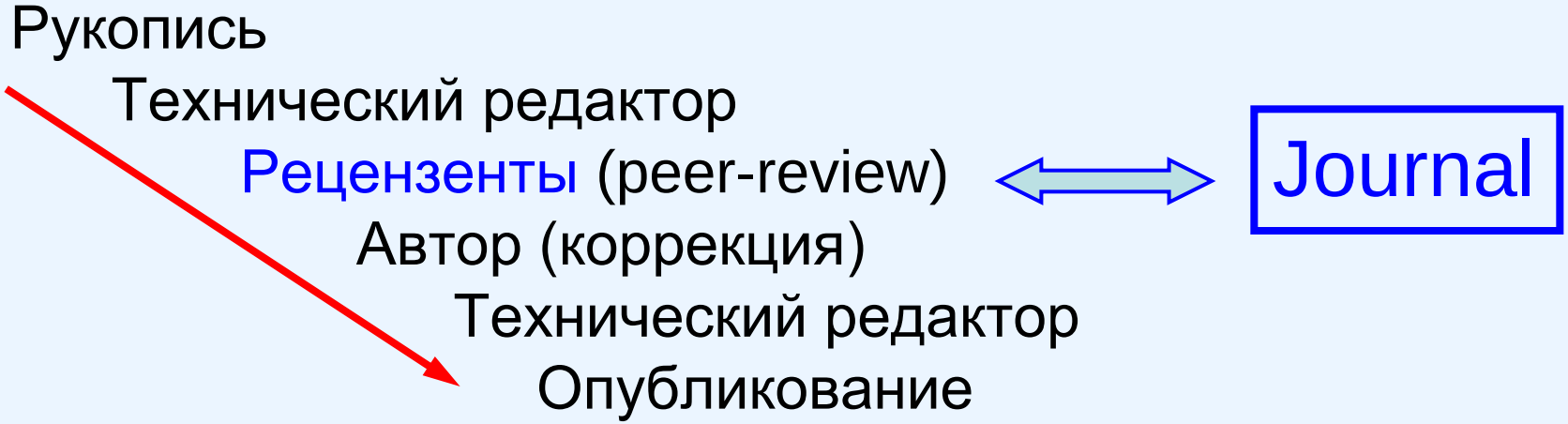

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- **Страницы** **Pages**

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  Методика эксперимента
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J. Chem. Inf. Model. **2009**, *49*, 145–152

Data Management System for Distributed Virtual Screening

Ting Zhou and Amedeo Caflisch*

Department of Biochemistry, University of Zürich, Winterthurerstrasse 190, CH-8057 Zürich, Switzerland

Received August 22, 2008

High throughput docking (HTD) using high performance computing platforms is a multidisciplinary challenge. To handle HTD data effectively and efficiently, we have developed a distributed virtual screening data management system (DVSDMS) in which the data handling and the distribution of jobs are realized by the open-source structured query language database software MySQL. The essential concept of DVSDMS is the separation of the data management from the docking and ranking applications. DVSDMS can be used to dock millions of molecules effectively, monitor the process in real time, analyze docking results promptly, and process up to 10^8 poses by energy ranking techniques. In an HTD campaign to identify kinase inhibitors a low cost Linux PC has allowed DVSDMS to efficiently assign the workload to more than 500 computing clients. Notably, in a stress test of DVSDMS that emulated a large number of clients, about 60 molecules per second were distributed to the clients for docking, which indicates that DVSDMS can run efficiently on very large compute cluster (up to about 40000 cores).

INTRODUCTION

In silico screening of large libraries of compounds is a commonly used tool in drug discovery because it efficiently identifies candidate lead compounds.[1−7] Its efficiency is due to methodological progresses and the ever increasing performance of ordinary low-cost computers. Despite these progresses, handling large libraries of compounds is still a challenge for data management in drug design and discovery. The demand for an efficient data management increases even

bookkeeping tasks associated with manual partition of jobs, data were distributed to workers as molecules were read by the master, such that the poor load balance due to the random distribution of jobs was circumvented. Furthermore, Peters and co-workers recently optimized and validated DOCK on a massively parallel system with more than 16000 processors.[14] They pointed out that as the number of processors increased, the HTC (High Throughput Computing)[15] version of the DOCK program was more efficient than the MPI version, since library docking could be run as a collection

ACKNOWLEDGMENT

We thank Armin Widmer for the continuous and extremely helpful support for the molecular modeling program Witnotp, and Philipp Schütz for useful suggestions and comments to the manuscript. This work was supported by a Swiss National Science Foundation grant to A.C. Most of the calculations were performed on the Etna and Matterhorn Beowulf cluster at the University of Zürich.

Supporting Information Available: Docking details, and the estimation of the maximum amount of molecules distributed per seconds for the MPI version of dock. This material is available free of charge via the Internet at http://pubs.acs.org.

REFERENCES AND NOTES

(1) Vangrevelinghe, E.; Zimmermann, K.; Schoepfer, J.; Portmann, R.; Fabbro, D.; Furet, P. Discovery of a Potent and Selective Protein Kinase CK2 Inhibitor by High-Throughput Docking. *J. Med. Chem.* **2003**, *46*, 2656–2662.

(2) Jorgensen, W. L. The Many Roles of Computation in Drug Discovery. *Science* **2004**, *303*, 1813–1818.

(3) Desai, P. V.; Patny, A.; Gut, J.; Rosenthal, P. J.; Tekwani, B.; Srivastava, A.; Avery, M. Identification of Novel Parasitic Cysteine Protease Inhibitors by Use of Virtual Screening. 2. The Available

(18) Brooks, B. R.; Bru
Swaminathan, S.; Ka
lecular Energy, Minimization
Chem. **1983**, *4*, 187–217.

(19) Stewart, J. J. P. Optimization o
I. Method. *J. Comput. Chem.*

(20) Huang, D.; Caflisch, A. Effic
Using Continuum Electrostat
5791–5797.

(21) Zhou, T.; Huang, D.; Caflisch
for Predicting Binding Free E
4288.

(22) Charifson, P. S.; Corkery, J
Consensus scoring: A Method
Docking Databases of Three
J. Med. Chem. **1999**, *42*, 510

(23) Clark, R. D.; Strizhev, A.; Le
Consensus Scoring for Ligan
Modell. **2002**, *20*, 281–295.

(24) Gohlke, H.; Klebe, G. Statis
Applied to Protein-ligand Bin
231–235.

(25) Irwin, J. J.; Shoichet, B. K. Z
Available Compounds for V
2005, *45*, 177–182.

(26) Momany, F. A.; Rone, R. V
ta(R)3.2/Charmm(R) Force-F
900.

(27) *SQLAlchemy*, 0.4.6; Michael

(28) LaCour, J.; Haus, D.; Menten
(accessed 31, Oct, 2008).

(29) MySQL::MySQL 5.1 Refere
http://dev.mysql.com/doc/ref

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Ting Zhou, Amedeo Caflisch
Journal of Chemical Information and Modeling **2009** *49* (1), 145-152

Zhou, T.; Huang, D.; Caflisch, A. Is Quantum Mechanics Necessary for Predicting Binding Free Energy. *J. Med. Chem.* **2008**, *51*, 4280–4288.

- Краткое. *Пример:*

Zhou T. et al. J. Med.Chem, 51, 4280 (2008)

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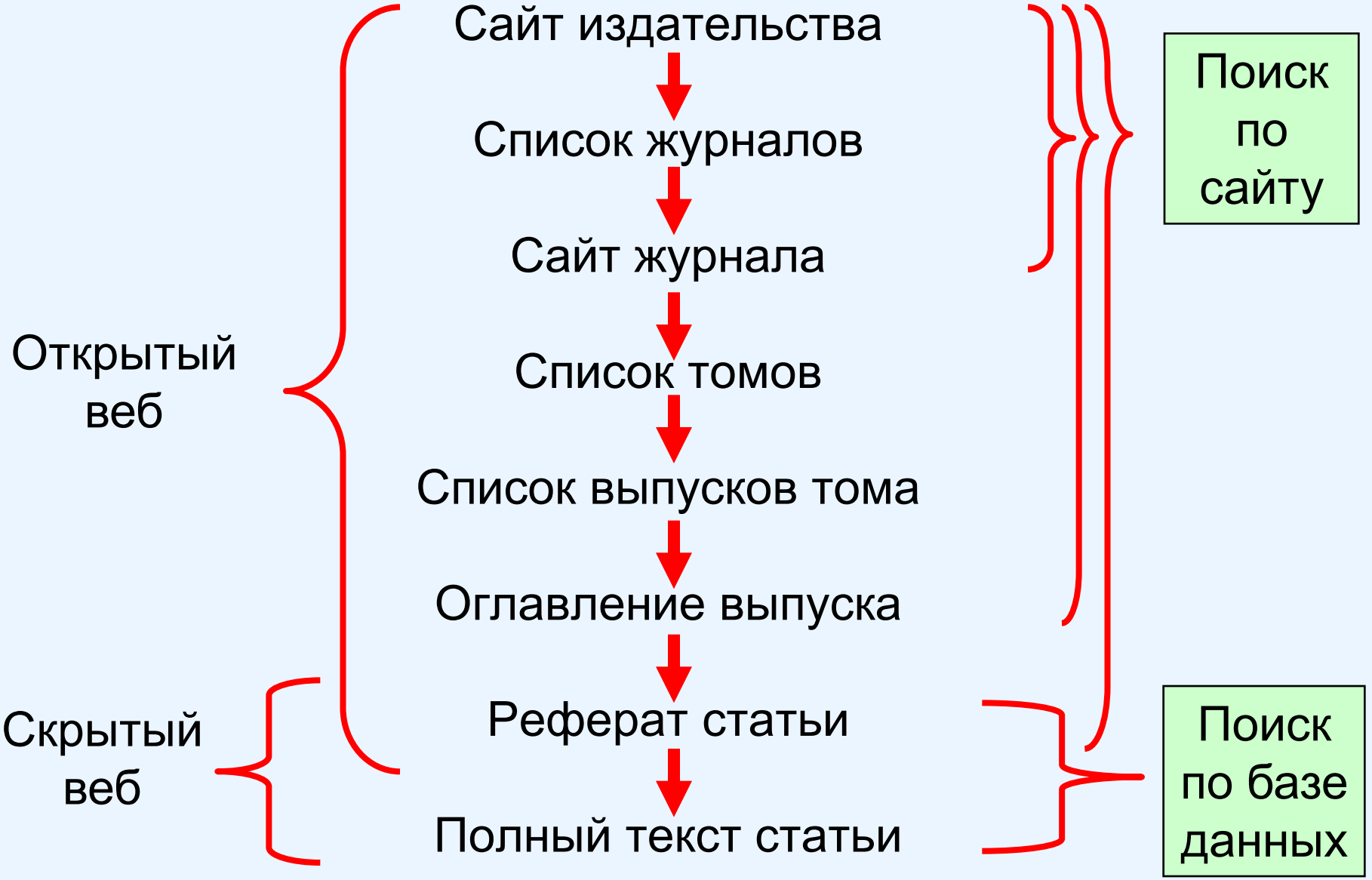

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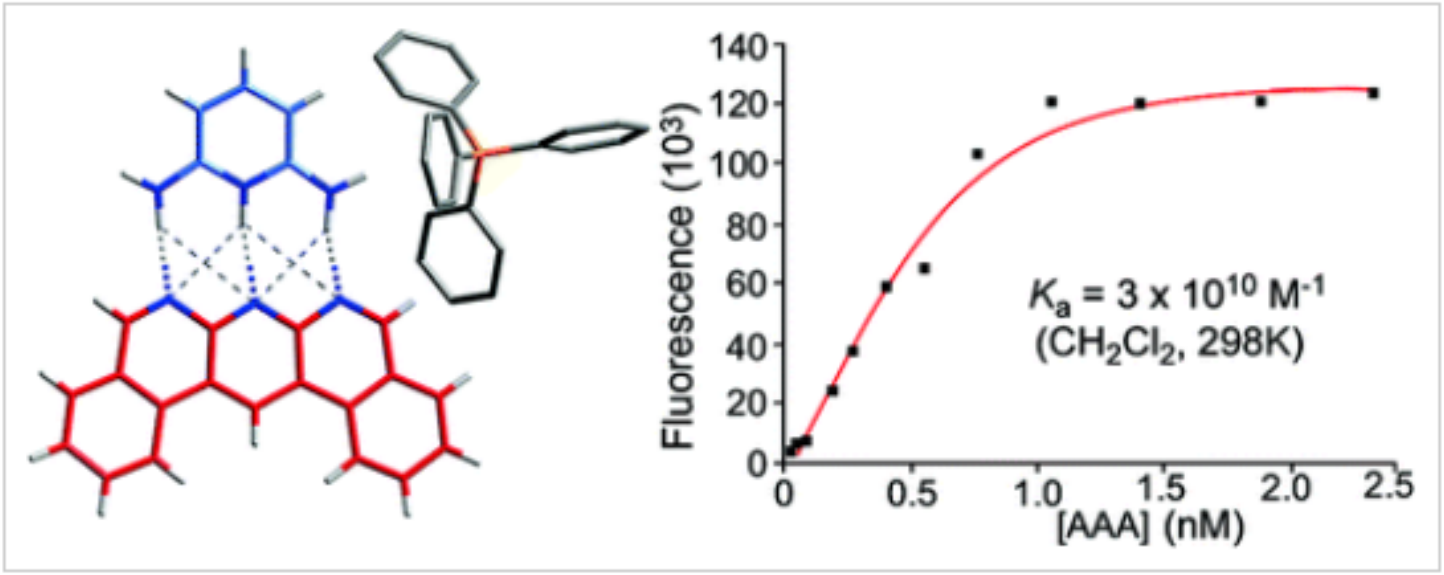
Barry A. Blight, Amaya Camara-Campos, Smilja Djurdjevic, Martin Kaller, David A. Leigh, Fiona M. McMillan, Hamish McNab and Alexandra M. Z. Slawin

Articles ASAP (As Soon As Publishable)
Publication Date (Web): September 11, 2009 (Article)
DOI: 10.1021/ja906061v



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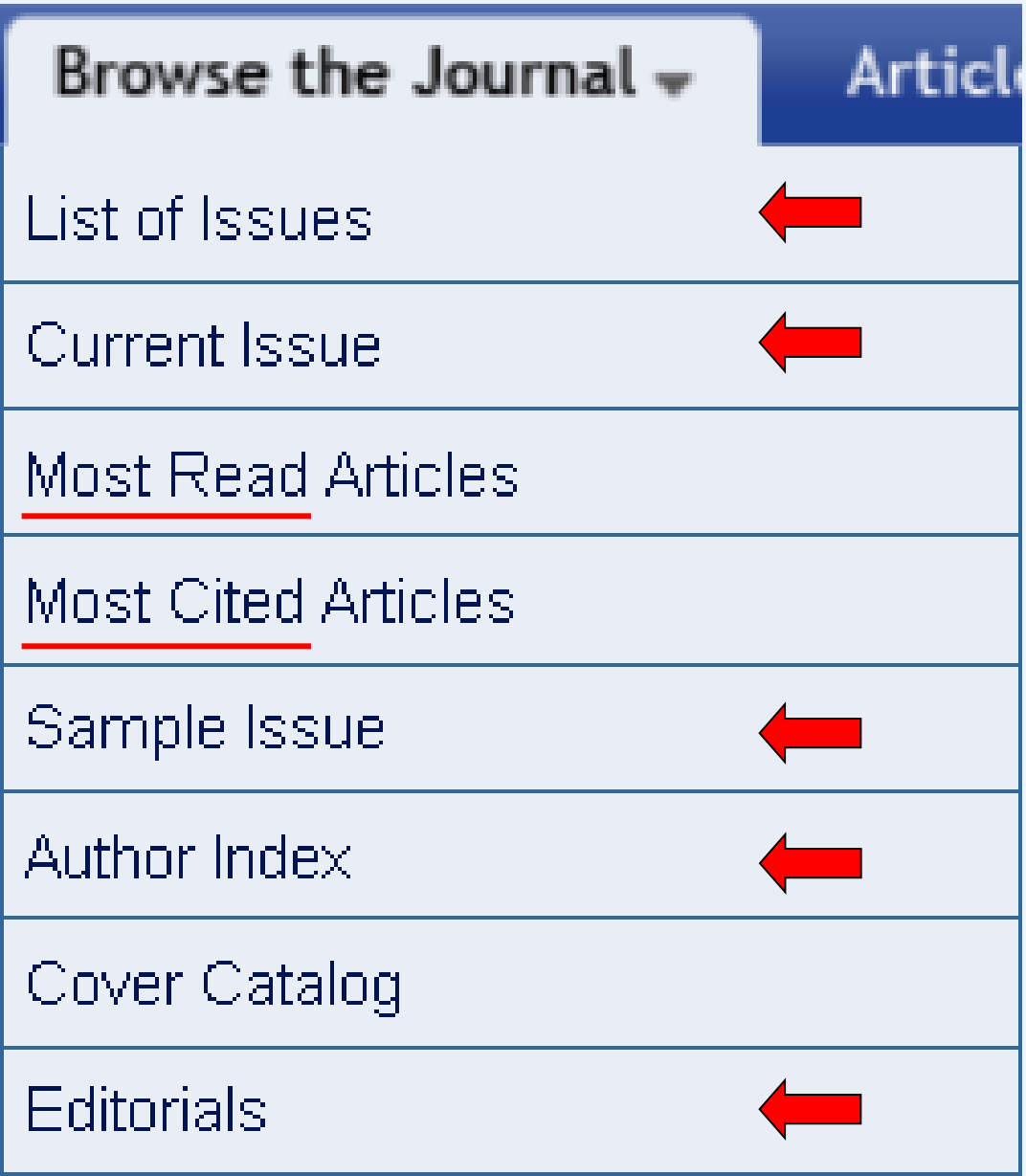

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1 Introduction

Jump to a section

Protein kinases have become major class of druggable targets in the pharmaceutical industry and a number of low molecular mass inhibitors are in the clinic now. (1, 2) The role of the stress-

1. Noble, M. E.; Endicott, J. A.; Johnson, L. N.Protein kinase inhibitors: Insights into drug design from structure *Science* **2004** 303 1800 1805 [CrossRef], [PubMed], [ChemPort]

Иллюстрации: встроенные, внешние.

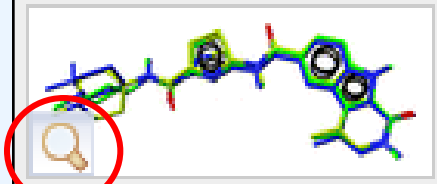

Figure 5. Superimposition of pharmacophore models (HypoA and HypoB) and the binding conformation of high active compound **67**. The HypoA conformation is in yellow; the HypoB conformation is in green, and binding conformation is in blue.

Сохранение на диск внешних иллюстраций – **отдельная операция**

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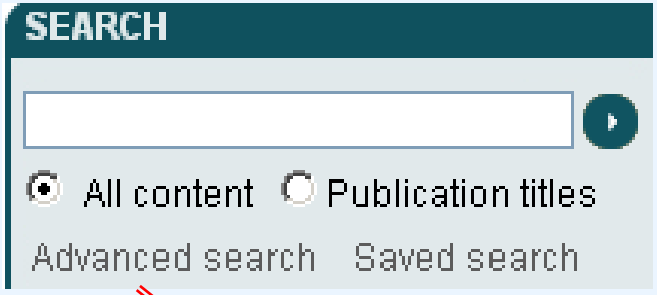

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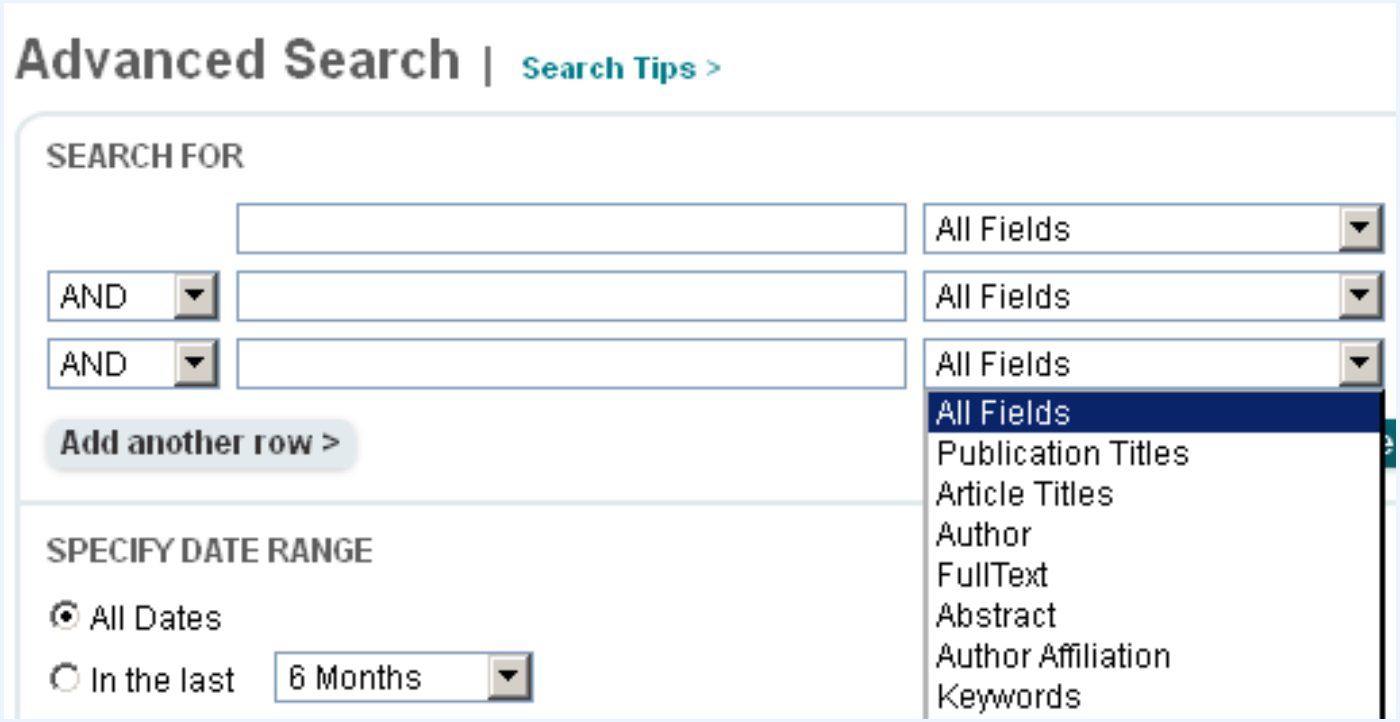

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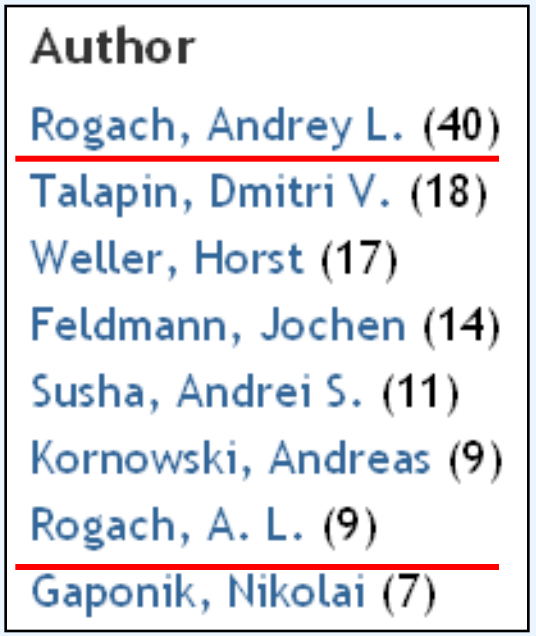

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г	g, h		ц	ts, c
е	e, ie, ye		ш	sh, s
и	i, y		ы	y, i
й	y, i, j		ю	u, iu, yu
х	kh, h		я	ya, ia, a

Пример: Рахманько

Rakhman'ko, Rahman'ko,

Rakhmanko, Rahmanko

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Журнал органической химии	0,513