

## CURRICULUM VITAE

MICHAL BRYLINSKI, Ph.D.

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**EDUCATION:** M.Sc. in Pharmacy, 2000  
Faculty of Pharmacy, Wroclaw Medical University, Poland  
Ph.D. in Chemistry, 2006  
Faculty of Chemistry, Jagiellonian University, Krakow, Poland  
Department of Bioinformatics and Telemedicine, Jagiellonian University, Medical College, Krakow, Poland  
Thesis: "Late-stage folding simulation of proteins" (thesis awarded)

**RESEARCH INTERESTS:** Systems Biology, Chemical Systems Biology and Cheminformatics  
Drug discovery and design  
Ligand docking/screening  
Ligand comparative modeling  
Protein function inference  
Protein structure prediction  
Protein evolution  
High performance computing

### PROFESSIONAL EXPERIENCE:

2011-present	Senior Research Scientist, Center for the Study of Systems Biology, School of Biology, Georgia Institute of Technology
2008-2011	Research Scientist II, Center for the Study of Systems Biology, School of Biology, Georgia Institute of Technology
2006-2008	Postdoctoral Research Fellow, Center for the Study of Systems Biology, School of Biology, Georgia Institute of Technology
2004-2006	Teaching Assistant, Department of Bioinformatics and Telemedicine, Jagiellonian University, Medical College
2002-2006	Research Assistant, Faculty of Chemistry, Jagiellonian University

## MEMBERSHIP IN SCIENTIFIC SOCIETIES:

American Chemical Society

## REFEREE FOR: Bioinformatics

BMC Bioinformatics  
BMC Research Notes  
Chemistry Central Journal  
Current Opinion in Structural Biology  
Frontiers in Systems Biology  
IEEE  
Journal of Molecular Graphics and Modelling  
Journal of Molecular Modeling  
Nucleic Acids Research  
Proteins: Structure, Function, and Bioinformatics

## DEVELOPED SOFTWARE AND SERVICES:

<b><i>ActiveSite</i></b>	ligand-binding site prediction, available at <a href="http://www.bioinformatics.cm-uj.krakow.pl/activesite/">http://www.bioinformatics.cm-uj.krakow.pl/activesite/</a>
<b><i>BSR</i></b>	local refinement of ligand-binding regions in protein models, available at <a href="http://cssb.biology.gatech.edu/BSR/">http://cssb.biology.gatech.edu/BSR/</a>
<b><i>EarlyStage</i></b>	early stage intermediate structures in protein folding pathways, available at <a href="http://www.bioinformatics.cm-uj.krakow.pl/earlystage/">http://www.bioinformatics.cm-uj.krakow.pl/earlystage/</a>
<b><i>FINDSITE</i></b>	threading-based binding site prediction, protein functional inference and ligand virtual screening, available at <a href="http://cssb.biology.gatech.edu/findsite/">http://cssb.biology.gatech.edu/findsite/</a>
<b><i>FINDSITE-metal</i></b>	evolution/structure-based approach to metal binding site prediction, available at <a href="http://cssb.biology.gatech.edu/findsite-metal/">http://cssb.biology.gatech.edu/findsite-metal/</a>
<b><i>FINDSITE<sup>LHM</sup></i></b>	flexible ligand docking by homology modeling, available at <a href="http://cssb.biology.gatech.edu/findsitelhm/">http://cssb.biology.gatech.edu/findsitelhm/</a>
<b><i>Fuzzy-Oil-Drop</i></b>	hybrid, template-free model for the simulation of protein folding
<b><i>Kinome<sup>LHM</sup></i></b>	structural and functional characterization of the human kinome, available at <a href="http://cssb.biology.gatech.edu/kinomelhm/">http://cssb.biology.gatech.edu/kinomelhm/</a>
<b><i>Q-Dock<sup>LHM</sup></i></b>	low-resolution ligand docking, refinement and virtual screening
<b><i>X-React<sup>KIN</sup></i></b>	virtual cross-reactivity profiling of the human kinome, available at <a href="http://cssb.biology.gatech.edu/kinomelhm/">http://cssb.biology.gatech.edu/kinomelhm/</a>

## SOFTWARE MANUALS: FINDSITE

FINDSITE-metal  
FINDSITE<sup>LHM</sup>

## PROFESSIONAL ACTIVITIES:

- 2002 Annual Meeting of The Interdisciplinary Centre for Mathematical and Computational Modelling, Bialowieza, Poland
- 2003 3<sup>rd</sup> International Summer School on Computational Biology, Warsaw, Poland
- 2003 5<sup>th</sup> European Symposium of The Protein Society, Florence, Italy
- 2004 CASP6, Cracow.pl group member
- 2005 6<sup>th</sup> European Symposium of The Protein Society, Barcelona, Spain
- 2006 Integrated Biosystems Institute, Georgia Institute of Technology, poster
- 2008 CASP8, TASSER/SiteHunter group member
- 2008 GPCR Dock, The Scripps Research Institute, La Jolla
- 2008 Frontiers in Multi-Scale Systems Biology, Atlanta
- 2010 Integrated Biosystems Institute, Georgia Institute of Technology, poster
- 2010 CASP9, TASSER/SiteHunter group member
- 2010 GPCR Dock, The Scripps Research Institute, La Jolla
- 2010 Systems Biology of Complex Traits Workshop, Atlanta
- 2011 Cancer Systems Biology Workshop, Atlanta
- 2011 AFP/CAFA Program Committee member

## TEACHING EXPERIENCE:

Computer laboratory courses in:

Computational Chemistry and Biochemistry for students of medicine

Biostatistics for students of medicine

Informatics for students of medicine

Bioinformatics for students of applied informatics, mathematics, chemistry and medical physics

## FACULTY OF 1000 BIOLOGY EVALUATIONS:

Brylinski M & Skolnick J (2009) *PLoS Comput Biol* **5(6)** :e1000405

<http://f1000biology.com/article/id/1162976/evaluation> (FFa: **6**)

Skolnick J *et al.* (2009) *Proc Natl Acad Sci USA* **106(37)** :15690-5

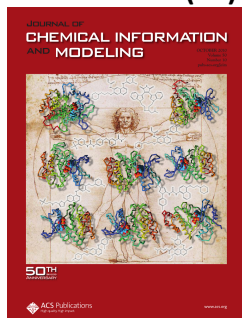
<http://f1000biology.com/article/id/2296956/evaluation> (FFa: **8**)

## JOURNAL COVERS:

*Proteins* 2007:**70**(2)



*JCIM* 2010:**50**(10)



## PUBLICATIONS:

38. Brylinski M, Gao M, Skolnick J. (2011) Why not consider a spherical protein? Implications of backbone hydrogen bonding for protein structure and function. *Phys Chem Chem Phys*, in press. **Cover article**.
37. Brylinski M, Lee SY, Zhou H, Skolnick J. (2011) The utility of geometrical and chemical restraint information extracted from predicted ligand binding sites in protein structure refinement. *J Struct Biol* **173**: 558-569.
36. Brylinski M, Skolnick J. (2011) FINDSITE-metal: Integrating evolutionary information and machine learning for structure-based metal binding site prediction at the proteome level. *Proteins* **79**: 735-751.
35. Brylinski M, Skolnick J. (2010) Cross-reactivity virtual profiling of the human kinome by X-React<sup>KIN</sup> – a Chemical Systems Biology approach. *Mol Pharm* **7**: 2324-2333.
34. Brylinski M, Skolnick J. (2010) Comprehensive structural and functional characterization of the human kinome by protein structure modeling and ligand virtual screening. *J Chem Inf Model* **50**: 1839-1854. **Cover article**.
33. Pandit SB, Brylinski M, Zhou H, Gao M, Arakaki AK, Skolnick J. (2010) PSiFR: an integrated resource for prediction of protein structure and function. *Bioinformatics* **26**: 687-688.
32. Brylinski M, Skolnick J. (2010) Q-Dock(LHM): Low-resolution refinement for ligand comparative modeling. *J Comput Chem* **31**: 1093-1105.
31. Brylinski M, Skolnick J. (2010) Comparison of structure-based and threading-based approaches to protein functional annotation. *Proteins* **78**: 118-134.
30. Skolnick J, Arakaki AK, Lee SY, Brylinski M. (2009) The continuity of protein structure space is an intrinsic property of proteins. *Proc Natl Acad Sci USA* **106**: 15690-15695.
29. Brylinski M, Skolnick J. (2009) FINDSITE(LHM): a threading-based approach to ligand homology modeling. *PLoS Comput Biol* **5**: e1000405.
28. Skolnick J, Brylinski M. (2009) FINDSITE: a combined evolution/structure-based approach to protein function prediction. *Brief Bioinform* **10**: 378-91.

27. Skolnick J, Brylinski M, Lee SY. (2009) Reply to Zimmerman et al: The space of single domain protein structures is continuous and highly connected. *Proc Natl Acad Sci USA* **106**: E138.
26. Skolnick J, Brylinski M. (2009) Novel computational approaches to drug discovery. *Proceedings of the International Conference of the Quantum Bio-Informatics III*: 327-336.
25. Roterman I, Konieczny L, Brylinski M. (2009) Late-stage folding intermediate in silico model. *Structure-function relation in proteins*: 79-103.
24. Roterman I, Brylinski M, Konieczny L. (2009) Active site recognition in silico. *Structure-function relation in proteins*: 105-127.
23. Roterman I, Konieczny L, Brylinski M. (2009) Folding process in the presence of specific ligand. *Structure-function relation in proteins*: 129-148.
22. Brylinski M, Skolnick J. (2008) Q-Dock: Low-resolution flexible ligand docking with pocket-specific threading restraints. *J Comput Chem* **29**: 1574-1588.
21. Brylinski M, Konieczny L, Kononowicz A, Roterman I. (2008) Conservative secondary structure motifs already present in early-stage folding (in silico) as found in serpins family. *J Theor Biol* **251**: 275-285.
20. Brylinski M, Skolnick J. (2008) A threading-based method (FINDSITE) for ligand-binding site prediction and functional annotation. *Proc Natl Acad Sci USA* **105**: 129-134.
19. Brylinski M, Skolnick J. (2007) What is the relationship between the global structures of apo and holo proteins? *Proteins* **70**: 363-377. **Cover article.**
18. Brylinski M, Konieczny L, Roterman I. (2007) Is the protein folding an aim-oriented process? Human haemoglobin as example. *Int J Bioinf Res App* **3**: 234-260.
17. Brylinski M, Prymula K, Jurkowski W, Kochanczyk M, Stawowczyk E, Konieczny L, Roterman I. (2007) Prediction of functional sites based on the fuzzy oil drop model. *PLoS Comput Biol* **3**: e94.
16. Brylinski M, Kochanczyk M, Broniatowska E, Roterman I. (2007) Localization of ligand binding site in proteins identified in silico. *J Mol Model* **13**: 665-675.
15. Roterman I, Brylinski M, Konieczny L, Jurkowski W. (2007) Early-stage protein folding - In silico model. *Recent Advances in Structural Bioinformatics*: 69-104.
14. Brylinski M, Konieczny L, Roterman I. (2006) Ligation site in proteins recognized in silico. *Bioinformation* **1**: 127-129.
13. Brylinski M, Kochanczyk M, Konieczny L, Roterman I. (2006) Sequence-structure-function relation characterized in silico. *In Silico Biol* **6**: 589-600.
12. Brylinski M, Konieczny L, Roterman I. (2006) Hydrophobic collapse in (in silico) protein folding. *Comput Biol Chem* **30**: 255-267.
11. Dabrowska J, Brylinski M. (2006) Stereoselectivity of 8-OH-DPAT toward the serotonin 5-HT1A receptor: biochemical and molecular modeling study. *Biochem Pharmacol* **72**: 498-511.
10. Konieczny L, Brylinski M, Roterman I. (2006) Gauss-function-Based model of hydrophobicity density in proteins. *In Silico Biol* **6**: 15-22.

9. Meus J, Brylinski M, Piwowar M, Piwowar P, Wisniowski Z, Stefaniak J, Konieczny L, Surowka G, Roterman I. (2006) A tabular approach to the sequence-to-structure relation in proteins (tetrapeptide representation) for de novo protein design. *Med Sci Monit* **12**: BR208-214.
8. Brylinski M, Konieczny L, Roterman I. (2006) Hydrophobic collapse in late-stage folding (in silico) of bovine pancreatic trypsin inhibitor. *Biochimie* **88**: 1229-1239.
7. Brylinski M, Konieczny L, Roterman I. (2006) Fuzzy-oil-drop hydrophobic force field - a model to represent late-stage folding (in silico) of lysozyme. *J Biomol Struct Dyn* **23**: 519-528.
6. Brylinski M, Konieczny L, Czerwonko P, Jurkowski W, Roterman I. (2005) Early-stage folding in proteins (in silico) sequence-to-structure relation. *J Biomed Biotechnol* **2**: 65-79.
5. Brylinski M, Konieczny L, Roterman I. (2005) SPI - structure predictability index for protein sequences. *In Silico Biol* **5**: 227-237.
4. Jurkowski W, Brylinski M, Konieczny L, Roterman I. (2004) Lysozyme folded in silico according to the limited conformational sub-space. *J Biomol Struct Dyn* **22**: 149-158.
3. Jurkowski W, Brylinski M, Konieczny L, Wisniowski Z, Roterman I. (2004) Conformational subspace in simulation of early-stage protein folding. *Proteins* **55**: 115-127.
2. Brylinski M, Jurkowski W, Konieczny L, Roterman I. (2004) Limited conformational space for early-stage protein folding simulation. *Bioinformatics* **20**: 199-205.
1. Brylinski M, Jurkowski W, Konieczny L, Roterman I. (2004) Limitation of conformational space for proteins - early stage folding simulation of human  $\alpha$  and  $\beta$  hemoglobin chains. *TASK Quarterly* **8**: 413-422.