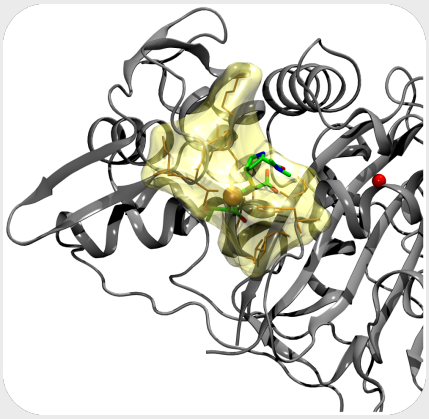

Department of Biological Sciences

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MICHAL BRYLINSKI

PhD, PharmD

EDUCATION

PharmD (2000)

Faculty of Pharmacy
Wroclaw Medical University
Wroclaw, Poland

PhD in Chemistry (2006)

Department of Chemistry
Jagiellonian University
Krakow, Poland

Department of Bioinformatics
Jagiellonian University Medical College, Krakow, Poland

Postdoc in Computational Biology (2008)

School of Biology
Georgia Institute of Technology
Atlanta, GA, USA

RESEARCH INTERESTS

- Drug discovery
- Drug repositioning
- Network pharmacology
- Structural biology
- Chemical biology
- Systems biology
- Bioinformatics
- Cheminformatics
- High-performance computing
- Heterogeneous computing

PROFESSIONAL EXPERIENCE

2018-present	**Associate Professor**, Department of Biological Sciences, Louisiana State University
2018-present	**Associate Professor**, Center for Computation & Technology, Louisiana State University
2012-2018	**Assistant Professor**, Department of Biological Sciences, Louisiana State University
2012-2018	**Assistant Professor**, Center for Computation & Technology, Louisiana State University
2011-2012	**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	**Graduate Research Assistant**, Department of Chemistry, Jagiellonian University

GRANTS

- **National Institute of General Medical Sciences:** "Combining structure-based network biology and heterogeneous computing for rational drug repositioning and polypharmacology" (**PI**; 2016-2021; **$962,055**; R35GM119524)

- **Louisiana Board of Regents:** "Network Biology approaches to systems-level functional annotation of proteins and proteomes" (**PI**; 2012-2015; **$103,802**; LQSF(2012-15)-RD-A-05)
- **LSU Council on Research:** "The utility of artificially evolved sequences in protein threading and fold recognition" (**PI**; 2012; **$5,000**; Summer Stipend Program)
- **Amazon:** "High-throughput structural bioinformatics with Amazon Web Services" (**PI**; 2012; **$25,000** in AWS credits)
- **NVIDIA:** "Accelerating the pace of protein functional annotation with graphics processors" (**PI**; 2012; donation of Tesla C2075; Academic Partnership Program)

AWARDS

- 2017 LSU Alumni Association Rising Faculty Research Award
- 2012 Ralph E. Powe Junior Faculty Enhancement Award from Oak Ridge Associated Universities

HPC ALLOCATIONS

- HPC@LSU: 28,300,000 SUs (aggregate for 2012-18)
- Louisiana Optical Network Initiative: 17,650,000 SUs (aggregate for 2012-18)
- XSEDE: 347,240 SUs (aggregate for 2013-17)

EDITOR FOR

- BMC Pharmacology and Toxicology (since 2018)
- BMC Bioinformatics (since 2016)
- Bio-Algorithms and Med-Systems (since 2011)

REVIEWER FOR

Funding: National Science Foundation (MCB), Austrian Science Fund (FWF), Czech Science Foundation (GACR), Swiss National Science Foundation (SNF)

Journals: 3 Biotech, AAPS Journal, Bio-Algorithms & Med-Systems, BioMed Research International, Bioinformatics, BioSystems, BMC Bioinformatics, BMC Pharmacology and Toxicology, BMC Research Notes, BMC Structural Biology, Briefings in Bioinformatics, Chemical Biology & Drug Design, Chemical Reviews, Chemistry Central Journal, Combinatorial Chemistry & High Throughput Screening, Computational Biology and Chemistry, Computers in Biology and Medicine, Current Drug Targets, Current Opinion in Structural Biology, Current Pharmaceutical Biotechnology, Database, Frontiers in Microbiology, Frontiers in Experimental Pharmacology and Drug Discovery, Future Medicinal Chemistry, IEEE Transactions on Computational Biology and Bioinformatics, IEEE Transactions on NanoBioscience, International Journal of Bioinformatics Research and Applications, Journal of Chemical Information and Modeling, Journal of Chemical Theory and Computation, Journal of Cheminformatics, Journal of Computer-Aided Molecular Design, Journal of Molecular Graphics and Modelling, Journal of Molecular Modeling, Journal of Physical Chemistry, Journal of Proteome Research, Journal of Receptors and Signal Transduction, Journal of the Royal Society Interface, Journal of Virology, Letters in Drug Design & Discovery, Methods, Nanoscale, Nucleic Acids Research, Oncotarget, PLOS Computational Biology, PLOS ONE, Proteins: Structure Function and Bioinformatics, Science, Scientific Reports, Springer Plus.

INVITED TALKS

Apr 2018	Louisiana Tech, Ruston, LA
Mar 2018	University of South Florida, Tampa, FL
Mar 2016	LSU PChem Seminar, Baton Rouge, LA
Feb 2016	Oak Ridge National Laboratory, Oak Ridge, TN
Oct 2015	MCBRC Fall Workshop, Baton Rouge, LA
Jul 2015	EPSCoR Symposium, Baton Rouge, LA
May 2015	3D Cryo-EM Workshop, Baton Rouge, LA
Apr 2015	LA-SiGMA Technical Conference, Baton Rouge, LA

Mar 2015	NanoDays, Baton Rouge, LA
Mar 2015	Pennington Biomedical Research Center, Baton Rouge, LA
Aug 2014	EPSCoR Symposium, Baton Rouge, LA
May 2014	2nd Annual Louisiana Conference on Bioinformatics, Baton Rouge, LA
Oct 2013	Computational Biology Seminar for Undergraduates, Baton Rouge, LA
Apr 2013	LA-SiGMA Technical Conference, Baton Rouge, LA
Sep 2012	LSU School of Veterinary Medicine, Baton Rouge, LA
Jun 2012	LONI HPC Users' Symposium, Baton Rouge, LA
Feb 2012	18th Annual Mardi Gras Conference on Computational Materials and Biosystems, Baton Rouge, LA

TEACHING

BIOL4001	Physical Biochemistry
BIOL4596	Biophysics of Macromolecules
BIOL7800	Computational Biology
MECH7953	Molecular Dynamics

PROFESSIONAL DEVELOPMENT

- Communication Across the Curriculum Faculty Summer Institute 2014
- HHMI/National Academies Gulf Coast Summer Institute on Undergraduate Education 2013

POSTDOCS & STUDENTS

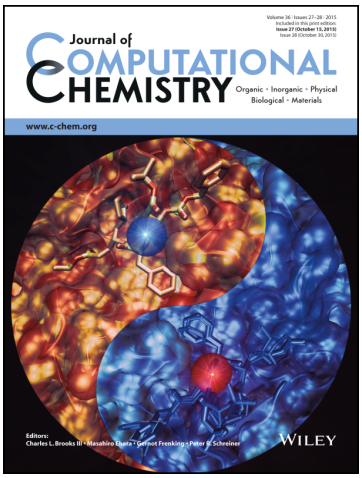
2016-present	Dr. Rajiv Gandhi Govindaraj (postdoc)
2013-present	Misagh Naderi (graduate student)
2017-present	Abd-El-Monsif Ahmed Shawky (graduate student)
2017-present	Manali Singha (graduate student)
2016-present	Omar Kana (undergraduate student)
2016-present	Jeffrey Lemoine (undergraduate student)
2016-present	Lana Thaljeh (undergraduate student)
2012-2014	Dr. Wei Feinstein (postdoc)
2012-2017	Dr. Surabhi Maheshwari (graduate student)
2013-2016	Dr. Yun Ding (graduate student)
2012-2013	Daniel Case (undergraduate student)
2012-2013	Carl Sabottke (undergraduate student)

FACULTY OF 1000 BIOLOGY EVALUATIONS

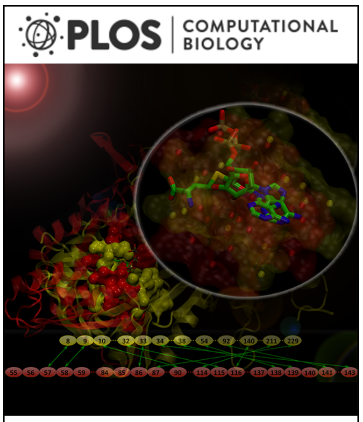
- Brylinski M and Skolnick J (2009) *PLoS Comput Biol* **5(6):** e1000405 http://f1000biology.com/article/id/1162976/evaluation (FFa: **6**)
- Skolnick J *et al*. (2009) *Proc Natl Acad Sci USA* **106(37):** 15690-5 http://f1000biology.com/article/id/2296956/evaluation (FFa: **8**)

COVERS

JCC 2015: **36(27)**



PLOS CB 2014: **10(9)**

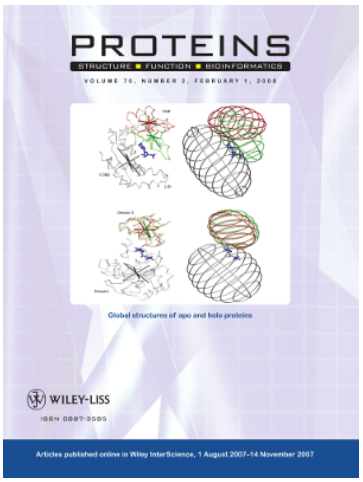


Matching drug binding pockets in protein models using sequence order-independent structure alignments

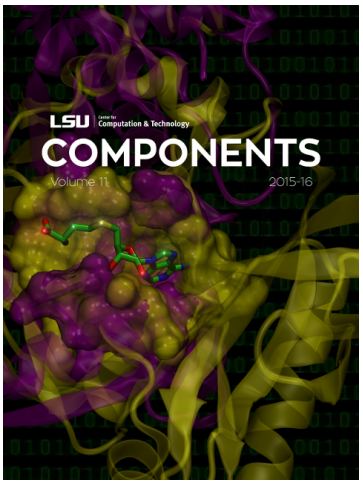
PCCP 2011: **13(38)**

JCIM 2010: **50(10)**

Proteins 2007: **70(2)**



Components 2016: **11**



Components 2012: **8**

PUBLICATIONS

81. Pu L, Naderi M, Liu T, Wu HC, Mukhopadhyay S, Brylinski M (2018) *e*ToxPred: A machine learning-based approach to estimate the toxicity of drug candidates. Submitted.
80. Naderi M, Lemoine JM, Govindaraj RG, Kana OZ, Feinstein WP, Brylinski M. (2018) Binding site matching in rational drug design: Algorithms and applications. Submitted.
79. Naderi M, Brylinski M. (2018) *e*Model-BDB: A database of comparative structure models of drug-target interactions from the Binding Database. Submitted.
78. Rider P, Coghill L, Naderi M, Brylinski M, Brown JM, Kousoulas KG. (2018) Evolutionary analysis and structure prediction identify functionally important domains and residues in a protein critical for alphaherpesvirus pathogenesis. Submitted.
77. Brylinski M, Naderi M, Govindaraj RG, Lemoine J. (2018) *e*Repo-ORP: Exploring the opportunity space to combat orphan diseases with existing drugs. *J Mol Biol*. In press.
76. Govindaraj RG, Naderi M, Singha M, Lemoine J, Brylinski M. (2018) Large-scale computational drug repositioning to find treatments for rare diseases. *NPJ Syst Biol Appl* **4**: 13.
75. Govindaraj RG, Brylinski M. (2018) Comparative assessment of strategies to identify similar ligand-binding pockets in proteins. *BMC Bioinformatics* **19**: 91.
74. Brylinski M. (2018) Aromatic interactions at the ligand-protein interface: Implications for the development of docking scoring functions. *Chem Biol Drug Des* **91**: 380-390.
73. Maheshwari S, Brylinski M. (2017) Across-proteome modeling of dimer structures for the bottom-up assembly of protein-protein interaction networks. *BMC Bioinformatics* **18**: 257.
72. Liu T, Naderi M, Alvin C, Mukhopadhyay S, Brylinski M. (2017) Break down in order to build up: Decomposing small molecules for fragment-based drug design with *e*MolFrag. *J Chem Inf Model* **57**: 627-631.
71. Brylinski M. (2017) Local alignment of ligand binding sites in proteins for polypharmacology and drug repositioning. *Methods Mol Biol* **1611**: 109-122.
70. Rider P, Naderi M, Bergeron S, Chouljenko VN, Brylinski M, Kousoulas KG. (2017) Cysteines and N-glycosylation sites conserved among all alphaherpesviruses regulate membrane fusion in herpes simplex virus type-1 infection. *J Virol* **91**: e00873-17.

69. Chouljenko D, Jambunathan N, Chouljenko VN, Naderi M, Brylinski M, Kousoulas KG. (2016) Herpes simplex virus type 1 UL37 protein tyrosine residues conserved among all alphaherpesviruses are required for interactions with glycoprotein K (gK), cytoplasmic virion envelopment, and infectious virus production. *J Virol* **90**: 10351-10361.
68. Ding Y, Fang Y, Moreno J, Ramanujam R, Jarrell M, Brylinski M. (2016) Assessing the similarity of ligand binding conformations with the Contact Mode Score. *Comput Biol Chem* **64**: 403-413.
67. Mummadisetti MP, Frankel LK, Bellamy HD, Sallans L, Goettert JS, Brylinski M, Limbach PA, Bricker TM. (2016) Use of protein crosslinking and radiolytic labeling to elucidate the structure of PsbO within higher plant photosystem II. *Biochemistry* **55**: 3204-3213.
66. Fang Y, Ding Y, Feinstein WP, Koppelman DM, Moreno J, Jarrell M, Ramanujam J, Brylinski M. (2016) GeauxDock: Accelerating structure-based virtual screening with heterogeneous computing. *PLoS ONE* **11**: e0158898.
65. Feinstein WP, Brylinski M. (2016) Many-core devices in computer-aided drug discovery. *Curr Drug Targets* **17**: 1595-1609.
64. Naderi M, Alvin C, Mukhopadhyay S, Brylinski M. (2016) A graph-based approach to construct target-focused libraries for virtual screening. *J Cheminform* **8**: 14.
63. Jambunathan N, Subramanian R, Charles AS, Saied AA, Naderi M, Brylinski M, Chouljenko VN, Kousoulas KG. (2016) The amino terminus of herpes simplex virus type-1 glycoprotein K (gK) is required for virus entry into neuronal axoplasm. *J Virol* **90**: 2230-2239.
62. Wang C, Hu G, Wang K, Brylinski M, Xie L, Kurgan L. (2016) PDID: Database of molecular-level putative protein-drug interactions in the structural human proteome. *Bioinformatics* **32**: 579-586.
61. Maheshwari S, Brylinski M. (2016) Template-based identification of protein-protein interfaces using *e*FindSite^{PPI}. *Methods* **93**: 64-71.
60. Maheshwari S, Brylinski M. (2015) Predicted binding site information improves model ranking in protein docking using experimental and computer-generated target structures. *BMC Struct Biol* **15**: 23.
59. Ding Y, Fang Y, Feinstein WP, Ramanujam J, Koppelman DM, Moreno J, Brylinski M, Jarrell M. (2015) GeauxDock: A novel approach for mixed-resolution ligand docking using a descriptor-based force field. *J Comput Chem* **36**: 2013-2026.
58. Feinstein WP, Brylinski M. (2015) Many-core accelerated structural bioinformatics for drug discovery. *High Performance Parallelism Pearls* **2**: 55-72.

57. Maheshwari S, Brylinski M. (2015) Predicting protein interface residues using easily accessible on-line resources. *Brief Bioinform* **16**: 1025-1034.
56. Feinstein WP, Brylinski M. (2015) Calculating an optimal box size for ligand docking and virtual screening against experimental and predicted binding pockets. *J Cheminform* **7**: 18. **Highly accessed.**
55. Feinstein WP, Moreno J, Jarrell M, Brylinski M. (2015) Accelerating the pace of protein functional annotation with Intel Xeon Phi coprocessors. *IEEE Trans Nanobioscience* **14**: 429-439.
54. Brylinski M. (2015) Is the growth rate of Protein Data Bank sufficient to solve the protein structure prediction problem using template-based modeling? *Bio Algorithms Med Syst* **11**: 1-7.
53. Maheshwari S, Brylinski M. (2015) Prediction of protein-protein interaction sites from weakly homologous template structures using meta-threading and machine learning. *J Mol Recognit* **28**: 35-48.
52. Mummadisetti MP, Frankel LK, Bellamy HD, Sallans L, Goettert JS, Brylinski M, Limbach PA, Bricker TM. (2014) Use of protein cross-linking and radiolytic footprinting to elucidate PsbP and PsbQ interactions within higher plant Photosystem II. *Proc Natl Acad Sci USA* **111**: 16178-16183.
51. Brylinski M. (2014) *e*MatchSite: Sequence order-independent structure alignments of ligand binding pockets in protein models. *PLoS Comput Biol* **10**: e1003829. **Cover article**.
50. Ragothaman A, Boddu SC, Kim N, Feinstein WP, Brylinski M, Jha S, Kim J. (2014) Developing *e*Thread pipeline using SAGA-Pilot abstraction for large-scale structural bioinformatics. *Biomed Res Int* **2014**: 348725.
49. Brylinski M, Waldrop GL. (2014) Computational redesign of bacterial biotin carboxylase inhibitors using structure-based virtual screening of combinatorial libraries. *Molecules* **19**: 4021-4045.
48. Feinstein WP, Brylinski M. (2014) *e*FindSite: Enhanced fingerprint-based virtual screening against predicted ligand binding sites in protein models. *Mol Inform* **33**: 135-150.
47. Brylinski M. (2013) Exploring the “dark matter” of a mammalian proteome by protein structure and function modeling. *Proteome Sci* **11**: 47.
46. Brylinski M. (2013) Non-linear scoring functions for similarity-based ligand docking and binding affinity prediction. *J Chem Inf Model* **53**: 3097-3112.

45. Brylinski M. (2013) *e*Volver: an optimization engine for evolving protein sequences to stabilize the respective structures. *BMC Res Notes* **6**: 303.
44. Brylinski M, Feinstein WP. (2013) *e*FindSite: Improved prediction of ligand binding sites in protein models using meta-threading, machine learning and auxiliary ligands. *J Comput Aided Mol Des* **27**: 551-567.
43. Brylinski M. (2013) Unleashing the power of meta-threading for evolution/structure-based function inference of proteins. *Front Genet* **4**: 118.
42. Brylinski M. (2013) The utility of artificially evolved sequences in protein threading and fold recognition. *J Theor Biol* **328**: 77-88.
41. Brylinski M, Lingam D. (2012) *e*Thread: A highly optimized machine learning-based approach to meta-threading and the modeling of protein tertiary structures. *PLoS ONE* **7**: e50200.
40. Brylinski M, Feinstein WP. (2012) Setting up a meta-threading pipeline for high-throughput structural bioinformatics: *e*Thread software distribution, walkthrough and resource profiling. *J Comput Sci Syst Biol* **6**: 001-010.
39. Skolnick J, Zhou H, Brylinski M. (2012) Further evidence for the likely completeness of the library of solved single domain protein structures. *J Phys Chem B* **116**: 6654-6664.
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* **13**: 17044-17055. **Cover article**.
37. 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.
36. 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.
35. 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**.
34. 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.

33. Brylinski M, Skolnick J. (2010) Comparison of structure-based and threading-based approaches to protein functional annotation. *Proteins* **78**: 118-134.
32. Brylinski M, Skolnick J. (2010) Cross-reactivity virtual profiling of the human kinome by X-React^{KIN} - a Chemical Systems Biology approach. *Mol Pharm* **7**: 2324-2333.
31. Brylinski M, Skolnick J. (2010) Q-Dock(LHM): Low-resolution refinement for ligand comparative modeling. *J Comput Chem* **31**: 1093-1105.
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**: 378-391.
27. Skolnick J, Brylinski M. (2009) Novel computational approaches to drug discovery. *Proceedings of the International Conference of the Quantum Bio-Informatics III*: 327-336.
26. 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.
25. Roterman I, Brylinski M, Konieczny L. (2009) Active site recognition in silico. *Structure-function relation in proteins*: 105-127.
24. Roterman I, Konieczny L, Brylinski M. (2009) Folding process in the presence of specific ligand. *Structure-function relation in proteins*: 129-148.
23. Roterman I, Konieczny L, Brylinski M. (2009) Late-stage folding intermediate in silico model. *Structure-function relation in proteins*: 79-103.
22. Brylinski M, Konieczny L, Kononowicz A, Roterman I. (2008) Conservative secondary structure motifs already present in early-stage folding (in silico) as found in serpines family. *J Theor Biol* **251**: 275-285.
21. Brylinski M, Skolnick J. (2008) Q-Dock: Low-resolution flexible ligand docking with pocket-specific threading restraints. *J Comput Chem* **29**: 1574-1588.

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, 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.
17. 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.
16. Roterman I, Brylinski M, Konieczny L, Jurkowski W. (2007) Early-stage protein folding - In silico model. *Recent Advances in Structural Bioinformatics*: 69-104.
15. 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.
14. Brylinski M, Konieczny L, Roterman I. (2006) Hydrophobic collapse in (in silico) protein folding. *Comput Biol Chem* **30**: 255-267.
13. 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.
12. 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.
11. Brylinski M, Konieczny L, Roterman I. (2006) Hydrophobic collapse in late-stage folding (in silico) of bovine pancreatic trypsin inhibitor. *Biochimie* **88**: 1229-1239.
10. 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.
9. Konieczny L, Brylinski M, Roterman I. (2006) Gauss-function-Based model of hydrophobicity density in proteins. *In Silico Biol* **6**: 15-22.
8. Brylinski M, Konieczny L, Roterman I. (2006) Ligation site in proteins recognized in silico. *Bioinformation* **1**: 127-129.

7. Brylinski M, Kochanczyk M, Konieczny L, Roterman I. (2006) Sequence-structure-function relation characterized in silico. *In Silico Biol* **6**: 589-600.
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. Brylinski M, Jurkowski W, Konieczny L, Roterman I. (2004) Limited conformational space for early-stage protein folding simulation. *Bioinformatics* **20**: 199-205.
2. Jurkowski W, Brylinski M, Konieczny L, Wisniowski Z, Roterman I. (2004) Conformational subspace in simulation of early-stage protein folding. *Proteins* **55**: 115-127.
1. Brylinski M, Jurkowski W, Konieczny L, Roterman I. (2004) Limitation of conformational space for proteins - early stage folding simulation of human α and β hemoglobin chains. *TASK Quarterly* **8**: 413-422.