MICHAL BRYLINSKI

PhD, PharmD

Phone: (225) 578-2791
Email: mbrylinski@lsu.edu
Website: www.brylinski.org
ORCID: 0000-0002-6204-2869
GitHub: michal-brylinski

Department of Biological Sciences
Center for Computation and Technology
407 Choppin Hall
Louisiana State University
Baton Rouge, LA 70803

Education

2000 **Doctor of Pharmacy**

Faculty of Pharmacy, Wroclaw Medical University, Wroclaw, Poland

Thesis: Method to measure copper ion concentration in industrial electrolytes.

2006 **PhD in Chemistry**

Department of Chemistry, Jagiellonian University, Krakow, Poland

Dissertation: Late-stage folding simulations of proteins.

2008 **Postdoc in Computational Biology**

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

Focus: Computer-aided drug discovery.

Research interests

- Panomics data science
- Bioinformatics
- Cheminformatics
- Genomics
- Network pharmacology
- Structural biology
- Chemical biology
- Systems biology
- Drug discovery
- Drug repositioning
- Deep learning
- High-performance computing
- Heterogeneous computing

Work experience

2020-present **Associate Director for Machine Learning and Data Science**
Center for Computation and Technology, Louisiana State University

2018-present **Associate Professor**
Department of Biological Sciences, Louisiana State University

2018-present **Associate Professor**
Center for Computation and Technology, Louisiana State University

2012-2017 **Assistant Professor**
Department of Biological Sciences, Louisiana State University

2012-2017 **Assistant Professor**
Center for Computation and Technology, Louisiana State University

2011-2012 **Senior Research Scientist**
Center for the Study of Systems Biology, Georgia Institute of Technology

2008-2011 **Research Scientist**
Center for the Study of Systems Biology, Georgia Institute of Technology

2006-2008 **Postdoctoral Research Fellow**
Center for the Study of Systems Biology, Georgia Institute of Technology

2004-2006 **Teaching Assistant**
Department of Bioinformatics, 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

- 2020 Semifinals for the IBM Watson AI XPRIZE
- 2019 LSU Rainmaker Mid-Career Scholar Award
- 2017 LSU Alumni Association Rising Faculty Research Award
- 2012 Ralph E. Powe Junior Faculty Enhancement Award from Oak Ridge Associated Universities

Computing allocations

- **HPC@LSU:** 35,900,000 SUs (aggregate for 2012-21)
- **Louisiana Optical Network Initiative:** 19,650,000 SUs (aggregate for 2012-21)
- **XSEDE:** 347,240 SUs (aggregate for 2013-17)

Editor for

- Biomolecules (since 2019)
- Scientific Reports (since 2019)
- BMC Pharmacology and Toxicology (since 2018)
- BMC Bioinformatics (since 2016)
- Bio-Algorithms and Med-Systems (since 2011)

Reviewer for

- National Institutes of Health
- National Science Foundation
- JDRF - Type 1 Diabetes Research Funding and Advocacy
- Austrian Science Fund
- Czech Science Foundation
- Swiss National Science Foundation
- UK Biotechnology and Biological Sciences Research Council
- **Journals (59):** 3 Biotech, AAPS Journal, ASSAY and Drug Development Technologies, Bio-Algorithms & Med-Systems, BioMed Research International, Bioinformatics, BioSystems, BMC Bioinformatics, BMC Pharmacology and Toxicology, BMC Research Notes, BMC Structural Biology, Briefings in

Bioinformatics, British Journal of Pharmacology, Cancers, 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, Drug Discovery Today, Frontiers in Chemistry, Frontiers in Microbiology, Frontiers in Experimental Pharmacology and Drug Discovery, Future Medicinal Chemistry, IEEE Access, 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 Computational Chemistry, Journal of Computer-Aided Molecular Design, Journal of Molecular Biology, 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, Molecular Pharmaceutics, Nanoscale, Nature Communications, Nucleic Acids Research, Oncotarget, Peer J, PLOS Computational Biology, PLOS ONE, Proteins: Structure Function and Bioinformatics, Proteomics, Science, Scientific Reports, Springer Plus.

NIH study sections

- 2023/05 ZRG1 BBBT-M (80) A, Topics in Biomedical Research
- 2022/10 ZRG1 BST-N (55) R, Biomedical Data Repositories and Knowledgebases
- 2022/05 ZRG1 BST-M (80) A, Topics in Bioengineering
- 2021/10 ZRG1 VH-A (90) S, Artificial Intelligence for Multimodal Data Modeling and Bioinformatics Center
- 2021/05 ZRG1 BST-F (80) A, Bioengineering Sciences and Technologies
- 2020/05 ZRG1 BST-F (80) A, Bioengineering Sciences and Technologies
- 2019/05 ZRG1 BST-F (80) A, Bioengineering Sciences and Technologies
- 2019/01 MSFD, Macromolecular Structure and Function D
- 2018/10 ZRG1 BCMB-G (02) M, Computational Structural Biology

NSF panels

- 2019/05 Infrastructure Innovation for Biological Research
- 2019/05 Cyberinfrastructure for Biological Research

Resource allocation committees

2019-present Chair, HPC Resources Allocation Committee
High-Performance Computing, Louisiana State University

2012-present Member, LONI Resource Allocation Committee
Louisiana Optical Network Infrastructure

Invited talks

Apr 2019 Lawrence Berkeley National Lab, Berkeley, CA

Mar 2019 MCBIOS19, Birmingham, AL

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

BIOL1800	Bytes & Molecules (undergraduate)
BIOL4001	Physical Biochemistry (undergraduate)
BIOL4596	Biophysics (undergraduate)
BIOL7800	Computational Biology (graduate)
MECH7953	Molecular Dynamics (graduate, team taught)
MEDP7121	Radiobiology (graduate, team taught)

Lab members

2019-present	Dr. Limeng Pu (researcher)
2022-present	Aashutosh Ghimire (graduate student)
2021-present	Mengmeng Liu (graduate student)
2022-present	Xialong Ni (graduate student)
2021-present	Gopal Srivastava (graduate student)
2012-2014	Dr. Wei Feinstein (postdoc)
2016-2018	Dr. Rajiv Gandhi Govindaraj (postdoc)
2019-2021	Dr. Noha Osman (postdoc)
2013-2016	Dr. Yun Ding (graduate student)
2012-2017	Dr. Surabhi Maheshwari (graduate student)
2013-2018	Dr. Misagh Naderi (graduate student)
2018-2019	Dr. Limeng Pu (graduate student)
2019-2020	Mahmoud Dondeti (graduate student)
2020-2020	Prasanga Neupane (graduate student)
2019-2021	Guannan Liu (graduate student)
2017-2020	Abd-El-Monsif Ahmed Shawky (graduate student)
2018-2022	Dr. Wentao Shi (graduate student)
2017-2022	Dr. Manali Singha (graduate student)
2019-2020	Ahmed Tohamy (graduate student)
2018-2019	Shuangyan Yang (graduate student)
2012-2013	Daniel Case (undergraduate student)
2016-2018	Omar Kana (undergraduate student)

2016-2019	Jeffrey Lemoine (undergraduate student)
2016-2017	Ainsley Rothschild (undergraduate student)
2012-2013	Carl Sabottke (undergraduate student)
2016-2019	Lana Thaljeh (undergraduate student)

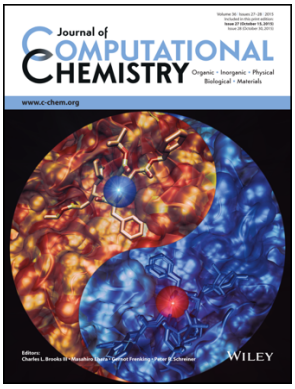
Software and databases

ACCase	Database of amino-oxazole complexes with bacterial biotin carboxylase isoforms
Bionoi	Conversion of biomolecules to Voronoi diagrams
BionoiNet	Classification of ligand-binding pockets with convolutional neural network
CMS/xCMS	Contact-based similarity measure for ligand binding conformations
DeepDrug3D	Classification of ligand-binding pockets with a 3D convolutional neural network
***e*Aromatic**	Analysis of aromatic interactions in protein-ligand complexes
***e*BoxSize**	Optimal box size for ligand docking and virtual screening
***e*FindSite**	Ligand binding site prediction and virtual screening
***e*FindSite^{PPI}**	Prediction of protein binding sites, residues, and interactions
***e*MatchSite**	Sequence order-independent alignment of ligand binding sites
***e*Model-BDB**	Database of comparative models of drug-target interactions from the BindingDB
***e*MolFrag**	Decomposing small molecules for fragment-based drug design
***e*Rank^{PPI}**	Dimer model ranking with machine learning
***e*Repo-ORP**	Large-scale computational drug repositioning to find treatments for rare diseases
***e*SimDock**	Similarity-based ligand docking and binding affinity prediction
***e*Synth**	Graph-based approach to construct target-focused libraries for virtual screening
***e*Thread**	Template-based protein structure prediction with meta-threading
***e*ToxPred**	Machine learning-based approach to estimate the toxicity of drug candidates
***e*Volver**	Optimization of synthetic protein sequences to stabilize the respective structures
FINDSITE	Combined evolution/structure-based approach to protein function prediction
FINDSITE^{LHM}	Threading-based approach to ligand homology modeling
FINDSITE-metal	Metal binding site prediction with evolutionary information and machine learning
GeauxDock	Mixed-resolution ligand docking using a descriptor-based force field
GraphDTI	A deep learning predictor of drug-target interactions from heterogeneous data
GraphGR	A graph neural network to predict the effect of drugs on the cancer cell growth
GraphSite	Ligand-binding site classification with deep graph learning

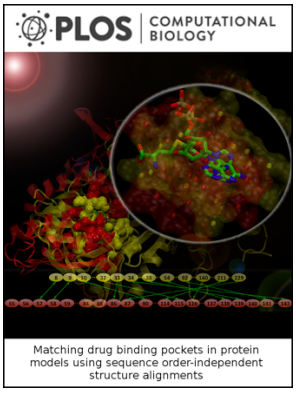
Ixodes	Late-stage folding simulator of proteins
Q-Dock	Low-resolution flexible ligand docking with pocket-specific threading restraints
Q-Dock^{LHM}	Low-resolution refinement for ligand comparative modeling
SPInka	Structure predictability index for protein sequences
TOUGH-C1	Dataset to evaluate algorithms for binding site classification
TOUGH-D1	Dataset to evaluate algorithms for ligand docking
TOUGH-M1	Dataset to evaluate algorithms for binding site matching
X-React^{KIN}	Cross-reactivity virtual profiling of the human kinome

Covers

JCC 2015: **36(27)**



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



PCCP 2011: **13(38)**

JCIM 2010: **50(10)**

Proteins 2007: **70(2)**

Components 2016: **11**

Components 2012: **8**

Publications

96. Singha M, Pu L, Stanfield BA, Uche IK, Rider PJF, Kousoulas KG, Ramanujam J, Brylinski M. (2022) Artificial intelligence to guide precision anticancer therapy with multitargeted kinase inhibitors. *BMC Cancer* 22:1211.
95. Shi W, Singha M, Pu L, Ramanujam J, Brylinski M. (2022) GraphSite: Ligand-binding site classification with deep graph learning. *Biomolecules* 12:1053.
94. Pu L, Singha M, Ramanujam J, Brylinski M. (2022) CancerOmicsNet: A multi-omics network-based approach to anti-cancer drug profiling. *Oncotarget* 13: 695-706.
93. Pu L, Singha M, Wu HC, Busch C, Ramanujam J, Brylinski M. (2022) An integrated network representation of multiple cancer-specific data for graph-based machine learning. *NPJ Syst Biol Appl* 8: 14.
92. Shi W, Singha M, Srivastava G, Pu L, Ramanujam J, Brylinski M. (2022) Pocket2Drug: An encoder-decoder deep neural network for the target-based drug design. *Front Pharmacol* 13: 837715.
91. Osman N, Shawky AE, Brylinski M. (2022) Exploring the effects of genetic variation on gene regulation in cancer in the context of 3D genome structure. *BMC Genom Data* 23: 13.
90. Bess A, Berglind F, Mukhopadhyay S, Brylinski M, Griggs N, Cho T, Galliano C, Wasan KM. (2022) Artificial intelligence for the discovery of novel antimicrobial agents for emerging infectious diseases. *Drug Discov Today* 27: 1099-1107.
89. Liu G, Singha M, Pu L, Neupane P, Feinstein J, Wu HC, Ramanujam J, Brylinski M. (2021) GraphDTI: A robust deep learning predictor of drug-target interactions from multiple heterogeneous data. *J Cheminform* 13: 58.
88. Feinstein J, Shi W, Ramanujam J, Brylinski M. (2020) Bionoi: A Voronoi diagram-based representation of ligand-binding sites in proteins for machine learning applications. *Methods Mol Biol* 2266: 299-312.
87. Shi W, Lemoine JM, Shawky MA, Singha M, Pu L, Yang S, Ramanujam J, Brylinski M. (2020) BionoiNet: Ligand-binding site classification with off-the-shelf deep neural network. *Bioinformatics* 36: 3077-3083.
86. Thaljeh LF, Rothschild JA, Naderi M, Coghill LM, Brown JM, Brylinski M. (2019) Hinge region in DNA packaging terminase pUL15 of herpes simplex virus: A potential allosteric target for antiviral drugs. *Biomolecules* 9: 603.
85. Rider P, Coghill L, Naderi M, Brown JM, Brylinski M, Kousoulas KG. (2019) Identification and visualization of functionally important domains and residues in herpes simplex virus glycoprotein K (gK) using a combination of phylogenetics and protein modeling. *Sci Rep* 9: 14625.
84. Kana OZ, Brylinski M. (2019) Elucidating the druggability of the human proteome with *e*FindSite. *J Comput Aided Mol Des* 33: 509-519.
83. Pu L, Naderi M, Liu T, Wu HC, Mukhopadhyay S, Brylinski M. (2019) *e*ToxPred: A machine learning-based approach to estimate the toxicity of drug candidates. *BMC Pharmacol Toxicol* 20: 2.
82. Pu L, Govindaraj RG, Wu HC, Brylinski M. (2019) DeepDrug3D: Classification of ligand-binding pockets in proteins with a convolutional neural network. *PLoS Comput Biol* 15: e1006718.
81. Wang C, Brylinski M, Kurgan L. (2019) PDID: database of experimental and putative drug targets in human proteome. *In silico drug design: Repurposing techniques and methodologies* 827-847.

80. Naderi M, Lemoine JM, Govindaraj RG, Kana OZ, Feinstein WP, Brylinski M. (2019) Binding site matching in rational drug design: Algorithms and applications. *Brief Bioinform* 20: 2167-2184.

79. Gadzala M, Dulak D, Kalinowska B, Baster Z, Brylinski M, Konieczny L, Banach M, Roterman I. (2018) The aqueous environment as an active participant in the protein folding process. *J Mol Graph Model* 87: 227-239.

78. Naderi M, Brylinski M. (2018) *e*Model-BDB: A database of comparative structure models of drug-target interactions from the Binding Database. *GigaScience* 7: 1-9.

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* 430: 2266-2273.

76. Govindaraj RG, Brylinski M. (2018) Comparative assessment of strategies to identify similar ligand-binding pockets in proteins. *BMC Bioinformatics* 19: 91.

75. 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.

74. 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.

73. 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.

72. 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.

71. 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.

70. Brylinski M. (2017) Local alignment of ligand binding sites in proteins for polypharmacology and drug repositioning. *Methods Mol Biol* 1611: 109-122.

69. 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.

68. 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.

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. Maheshwari S, Brylinski M. (2016) Template-based identification of protein-protein interfaces using *e*FindSite^{PPI}. *Methods* 93: 64-71.

65. Feinstein WP, Brylinski M. (2016) Many-core devices in computer-aided drug discovery. *Curr Drug Targets* 17: 1595-1609.

64. 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.

63. 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.

62. 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.

61. 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.

60. 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. **Cover article**.

59. Maheshwari S, Brylinski M. (2015) Predicting protein interface residues using easily accessible on-line resources. *Brief Bioinform* 16: 1025-1034.

58. 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.

57. 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.

56. 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.

55. 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**.

54. 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.

53. Feinstein WP, Brylinski M. (2015) Accelerated structural bioinformatics for drug discovery. *High Performance Parallelism Pearls* 2: 55-72.

52. Brylinski M. (2014) *e*MatchSite: Sequence order-independent structure alignments of ligand binding pockets in protein models. *PLoS Comput Biol* 10: e1003829. **Cover article**.

51. 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.

50. 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.

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. 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.

47. Brylinski M. (2013) Non-linear scoring functions for similarity-based ligand docking and binding affinity prediction. *J Chem Inf Model* 53: 3097-3112.

46. Brylinski M. (2013) The utility of artificially evolved sequences in protein threading and fold recognition. *J Theor Biol* 328: 77-88.

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) Exploring the "dark matter" of a mammalian proteome by protein structure and function modeling. *Proteome Sci* 11: 47.
42. Brylinski M. (2013) Unleashing the power of meta-threading for evolution/structure-based function inference of proteins. *Front Genet* 4: 118.
41. 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.
40. 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.
39. 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.
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.