

# CURRICULUM VITAE

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**EDUCATION:** M.Sc. in Chemistry, University of Warsaw, Poland, 1974  
Ph.D. in Chemistry, University of Warsaw, Poland, 1979  
Ph.D. Thesis entitled: "Computer Modeling of Radical Polymerization in Solution"  
Habilitation Thesis (1988) entitled: "Phase Transitions in Polymeric Systems. Applications of the Monte Carlo Method"

**RESEARCH:** Theoretical Chemistry. Theory of polymers and biopolymers. Phase transitions in polymeric systems. Dynamics of polymer melts and solutions. Theory of protein folding. Theory of protein structure and function. Computer simulations of complex biopolymer systems. Structural bioinformatics. Computational biology.

## PROFESSIONAL EXPERIENCE:

1998 – Head of Laboratory of Theory of Biopolymers, Department of Chemistry, University of Warsaw, Poland

2004 – 2005 Adjunct Professor, L. H. Baker Center for Bioinformatics and Biological Statistics, Iowa State University, Ames, Iowa

2002 – 2003 Professor, State University of New York at Buffalo, Center of Excellence in Bioinformatics, Buffalo, State of New York.

1999 – 2002 Professor, Donald Danforth Plant Science Center, Saint Louis, Missouri

1993 – 1999 Associate Professor of The Scripps Research Institute, Department of Molecular Biology, La Jolla, California.

1991 – 1993 Adjunct Member of The Scripps Research Institute, Department of Molecular Biology, La Jolla, California.

1990 – 1991 Visiting Research Associate, The Scripps Research Institute, Department of Molecular Biology, La Jolla, California.

1989 – 1991 Director of Computational Chemistry Laboratory, Department of Chemistry, University of Warsaw, Poland.

1985 – 1989 Visiting Associate Professor, Department of Chemistry, Washington University, St. Louis, Missouri.

1989 – Professor of Chemistry, Department of Chemistry, University of Warsaw, Poland.

1979 – 1989 Assistant Professor of Chemistry (Adiunkt), University of Warsaw, Poland.

1974 – 1979 Research Assistant, Department of Chemistry, University of Warsaw, Poland.

## HONORS AND AWARDS:

2011 – Gold Cross of Merit awarded by the President of Poland.

2009 – Prize of Foundation for Polish Science in life science and medicine.

2008 – Jan Zawidzki medal of Polish Chemical Society.

1995 – International Scholar's Award of the Howard Hughes Medical Institute (1995-2000).

1994 – Swietoslowski Award for The Best Science Done in 1984-1989, University of Warsaw, Poland.

1992 – Prize of Polish Ministry of Higher Education for Outstanding Work in Chemistry.

1990 – Prize of Polish Ministry of Higher Education for the best Habilitation Thesis.

1984 – Polish Academy of Sciences Prize for Most Outstanding Work in Chemistry.

1979 – Prize of Polish Ministry of Higher Education for the outstanding Ph.D. Thesis.

## PATENTS:

1. USA Patent No. 5265030 issued 11/23/1993 "System and method for determining three-dimensional structure of proteins" Andrzej Kolinski and Jeffrey Skolnick, inventors.
2. WO Patent (World Intellectual Property Organization) No. 1998053407, issued 12/17/1998 "Prediction of relative binding motifs of biologically active peptides and peptide mimetics" Jeffrey Skolnick, Mariusz Milik and Andrzej Kolinski, inventors.
3. USA Patent No. 5933819 issued 8/3/1999 "Prediction of relative binding motifs of biologically active peptides and peptide mimetics" Jeffrey Skolnick, Mariusz Milik and Andrzej Kolinski, inventors.
4. WO Patent No. 2000045334 issued 8/4/2000 "Protein modeling tools" Jeffrey Skolnick and Andrzej Kolinski, inventors.
5. EP Patent (European Patent Office) No. 1021771 issued 7/29/2000 "Prediction of relative binding motifs of biologically active peptides and peptide mimetics" Jeffrey Skolnick, Mariusz Milik and Andrzej Kolinski, inventors.
6. USA Patent No. 9982488 issued 10/17/2001 "Protein modeling tools" Jeffrey Skolnick and Andrzej Kolinski, inventors.
7. EP Patent No. 1163639 issued 12/17/2001 "Protein modeling tools" Jeffrey Skolnick and Andrzej Kolinski, inventors.

## PUBLICATIONS:

1. A. Orszagh, A. Kolinski, J. Les, "Komputerowa symulacja roztworu polimeru metoda Monte Carlo" (Computer Simulation of Polymer Solution by Means of the Monte Carlo Method), *Polimery* **22**:442 (1977).
2. A. Orszagh, A. Kolinski, J. Les, "Zastosowanie metody Monte Carlo do badania rozmiarow klebka makromolekularnego w roztworze" (Application of the Monte Carlo Method in Studying the Macromolecular Coil Dimensions in Solution), *Polimery* **23**:207 (1978).
3. A. Orszagh, A. Kolinski, P. Romiszowski, "Computer Modeling of Radiation-Induced in-Source Solid-State Polymerizations", *Polymer* **20**:113 (1979).
4. A. Orszagh, J. Les, A. Kolinski, "Monte Carlo Method for Statistical Thermodynamics of Polymer Chains", *Acta Physica Polonica* **A58**: 369-375 (1980).
5. A. Orszagh, A. Kolinski, "Stochastyczna symulacja rodnikowej polimeryzacji w roztworze", (Stochastic Simulation of the Free-radical Polymerization in Solution), *Polimery* **25**:124-127 (1980).
6. B. Kowalski, T. Kasprzycka-Guttman, A. Kolinski, "Molar Excess Enthalpies and Volumes of Mixtures of 2,4,6-trimethylpyridine with some Aliphatic Alcohols", *Polish J. Chem.* **54**:1995 (1980).
7. A. Orszagh, A. Kolinski, A. Sikorski, "Badanie modelu rozgalezionej makroczaścieszki metoda Monte Carlo. I. Statystyka konformacyjna", (Monte Carlo Study of Star-branched Macromolecules by Means of the Monte Carlo Method. I. Conformational Statistics), *Polimery* **26**:335-337 (1981).
8. A. Orszagh, A. Kolinski, A. Sikorski, "Badanie modelu rozgalezionej makroczaścieszki metoda Monte Carlo. II. Rozmiary klebka statystycznego", (Monte Carlo Study of Star-branched Macromolecules by Means of the Monte Carlo Method. II. Analysis of the Coil Dimensions), *Polimery* **26**:375-377 (1981).
9. A. Orszagh, A. Kolinski, J. Duda, "Monte Carlo Study of Concentrated Polymer Solutions", *Acta Physica Polonica* **A59**:839 (1981).
10. P. Romiszowski, A. Kolinski, "Monte Carlo Simulation of Radiation-Induced Solid State Polymerization", *Polymer* **23**:1226 (1982).
11. W. Pawlowski, A. Kolinski, "Water Contents and Calculation of Equilibrium Constraints in Benzene Phase on System Water - Benzene - (-OH, -COOH, -NH<sub>2</sub>, -NO<sub>2</sub>, - C<sub>1</sub>) Benzene Derivative", *Polish J. Chem.* **56**:1169-1173 (1982).
12. A. Orszagh, M. Milik, A. Kolinski, "Algorytmiczna symulacja polimeryzacji perelkowej monomerow winylowych", (Algorithmic Simulation of the Suspension Polymerization of Vinyl Monomers), *Inz. Chem. Proc.* **5**:71-80 (1984).
13. A. Kolinski, P. Romiszowski, "Monte Carlo Study of Dynamics of the Multichain Polymer System on the Tetrahedral Lattice", *J. Chem. Phys.* **79**:1523-1526 (1984).
14. A. Kolinski, "On the Entropy of the Multichain Athermal Lattice Systems", *J. Polym. Sci. Polym. Lett. Ed.* **22**:407-411 (1984).

15. A. Kolinski, "Some Properties of Rigid Cores with Flexible Tails-Monte Carlo Simulation of 2-dimensional Lattice Systems", *Chem. Phys. Letters* **116**:160-164 (1985).
16. A. Kolinski, J. Skolnick and R. Yaris, "Monte Carlo Dynamics of Diamond Lattice Multichain System", Proceedings of the 1985 La Jolla Workshop on Polymer Flow Interaction. *AIP Conference Proceedings*, No. **137** (Y. Rabin, ed.), 1985, 241.
17. A. Kolinski, J. Skolnick, and R. Yaris, "On the Short Time Dynamics of Dense Polymeric Systems and the Origin of the Glass Transition: A Model System", *J. Chem. Phys.* **84**:1922-1931 (1986).
18. A. Kolinski, J. Skolnick and R. Yaris, "Monte Carlo Study of Local Orientational Order in a Semiflexible Polymer Melt Model", *Macromolecules* **19**:2550-2560 (1986).
19. A. Kolinski, J. Skolnick and R. Yaris, "Order-Disorder Transitions in Tetrahedral Lattice Polymer Systems", *Macromolecules* **19**:2560-2567 (1986).
20. A. Kolinski, J. Skolnick and R. Yaris, "Monte Carlo Simulations on an Equilibrium Globular Protein Folding Model", *Proc. Natl. Acad. Sci., USA* **83**:7267-7271 (1986).
21. A. Kolinski, J. Skolnick and R. Yaris, "The Collapse Transition of Semiflexible Polymers. A Monte Carlo Simulation of a Model System". *J. Chem. Phys.* **85**:3585-3597 (1986).
22. A. Kolinski, J. Skolnick and R. Yaris, "Dynamic Monte Carlo Study of the Conformational Properties of Long Flexible Polymers", *Macromolecules* **20**:438-440 (1987).
23. A. Kolinski, J. Skolnick and R. Yaris, "Does Reptation Describe the Dynamics of Entangled Polymer Systems? A Model Simulation", *J. Chem. Phys.* **86**:1567-1585 (1987).
24. A. Kolinski, J. Skolnick and R. Yaris, "Monte Carlo Studies on the Long Time Dynamic Properties of Dense Cubic Lattice Multichain Systems. I. The Homopolymeric Melt", *J. Chem. Phys.* **86**:7164-7174 (1987).
25. A. Kolinski, J. Skolnick and R. Yaris, "Monte Carlo Studies on the Long Time Dynamic Properties of Dense Cubic Lattice Multichain Systems. II. Probe Polymer in a Matrix of Different Degrees of Polymerization", *J. Chem. Phys.* **86**:7174-7180 (1987).
26. A. Kolinski, J. Skolnick and R. Yaris, "Monte Carlo Studies on Equilibrium Globular Protein Folding. I. homopolymeric Lattice Models of  $\beta$ -Barrel Proteins", *Biopolymers* **26**:937 (1987).
27. J. Skolnick, A. Kolinski and R. Yaris, "Monte Carlo Studies of the Long Time Dynamic Properties of Dense Polymer Systems. The Failure of the Reptation Model", *Accts. Chem. Research* **20**:350-356 (1987).
28. J. Skolnick, R. Yaris and A. Kolinski, "Phenomenological Theory of the Dynamics of Polymer Melts. I. Analytic Treatment of Self Diffusion", *J. Chem. Phys.* **88**:1407-1417 (1988).
29. J. Skolnick, A. Kolinski and R. Yaris, "Monte Carlo Simulations of the Folding of  $\beta$ -Barrel Globular Proteins", *Proc. Natl. Acad. Sci. USA* **85**:5057-5061 (1988).
30. J. Skolnick, R. Yaris, and A. Kolinski, "Phenomenological Theory of Polymer Melt Dynamics", *Int. J. Mod. Phys.* **3**, No. 1, 33-64 (1989).
31. J. Skolnick, A. Kolinski and R. Yaris, "Monte Carlo Studies on Equilibrium Globular Protein Folding. II.  $\beta$ -Barrel Globular Protein Models", *Biopolymers* **28**, 1059-1095 (1989).
32. J. Skolnick, A. Kolinski and R. Yaris, "Dynamic Monte Carlo study stranded Greek Key Globular Protein", *Proc. Natl. Acad. Sci. USA* **86**:1229-1233 (1989).
33. J. Skolnick, A. Kolinski, A. Sikorski and R. Yaris, "Dynamic Monte Carlo Simulation of a Melt of Ring Polymers", *Polymer Preprints* **30**: 70-73 (1989).
34. A. Kolinski, K. Kurcinski, A. Orszagh, "Combinatorial Entropy of Dense Systems of n-mers. The Effect of Shape Studied by Monte Carlo Method", *Acta. Phys. Polonica* **75**:879-890 (1989).
35. J. Skolnick and A. Kolinski, "Computer Simulations of Globular Protein Folding and Tertiary Structure", *Annual. Rev. Phys. Chem.* **40**: 207-235 (1989).
36. J. Skolnick and A. Kolinski, "Dynamics of Dense Polymer Systems: Computer Simulations and Analytic Theories", *Advances in Chemical Physics* **77**:223-278 (1990).
37. J. Skolnick, A. Kolinski and A. Sikorski, "Dynamic Monte Carlo Simulations of Globular Protein Folding, Structure and Dynamics", *Comments on Mol. and Cell. Biol.* **6**:223-247 (1990).
38. J. Skolnick and A. Kolinski, "Dynamic Monte Carlo Simulations of Globular Protein Folding/Unfolding Pathways. I. Six Member, Greek Key  $\beta$ -Barrels", *J. Mol. Biol.* **212**:787-817 (1990).
39. J. Skolnick, A. Kolinski and A. Sikorski, "Dynamic Monte Carlo Globular Protein Folding and Structure", *Chemical Design Automation News* **5**, No. 3, 1-20 (1990).
40. M. Milik, A. Kolinski and J. Skolnick, "Monte Carlo Dynamics of a Dense System of Chain Molecules Constrained to Lie Near an Interface. A Simplified Membrane Model", *J. Chem. Phys.* **93**:(6) 4440-4446 (1990).
41. J. Skolnick and A. Kolinski, "Simulations of the Folding of a Globular Protein", *Science* **250**:1121-1125 (1990).

42. A. Kolinski, M. Milik and J. Skolnick, "Static and Dynamic Properties of a New Lattice Model of Polypeptide Chains", *J. Chem. Phys.* **94**: 3978-3985 (1991).
43. J. Skolnick and A. Kolinski, "Dynamic Monte Carlo Simulations of a New Lattice Model of Globular Protein Folding, Structure, and Dynamics", *J. Mol. Biol.* **221**:499-531 (1991).
44. Y. K. Levine, A. Kolinski and J. Skolnick, "Monte Carlo Dynamics Study of Motions in CIS-Unsaturated Hydrocarbon Chains", *J. Chem. Phys.* **95**: 3826-3834 (1991).
45. A. Kolinski, M. Vieth and A. Sikorski, "Collapse Transition of Semiflexible Polymers in 2-dimensional Systems", *Acta. Phys. Polonica* **79**:601-612 (1991).
46. M. Vieth and A. Kolinski, "Prediction of Protein Secondary Structure by an Enhanced Neural Network", *Acta. Biochim. Polonica* **38**:335-351 (1991).
47. A. Godzik, J. Skolnick and A. Kolinski, "Simulations of the Folding Pathway of TIM-type  $\alpha/\beta$  Barrel Proteins", *Proc. Natl. Acad. Sci. USA* **89**:2692 (1992).
48. M. Milik, J. Skolnick and A. Kolinski, "Monte Carlo Studies of an Idealized Model of a Lipid - Water System", *J. Phys. Chem.* **96**:4015-4022 (1992).
49. A. Godzik, J. Skolnick and A. Kolinski, "A Topology Fingerprint Approach to the Inverse Protein Folding Problem", *J. Mol. Biol.* **227**:227-238 (1992).
50. A. Rey, A. Kolinski, J. Skolnick and Y. Levine, "Effect of Double Bonds on the Dynamics of Hydrocarbon Chains", *J. Chem. Phys.* **97**:1240-1249 (1992).
51. A. Kolinski and J. Skolnick, "Discretized Model of Proteins. I. Monte Carlo Study of Cooperativity in Homopolypeptides", *J. Chem. Phys.* **97**:9412-9426 (1992).
52. M. Vieth, A. Kolinski, J. Skolnick and A. Sikorski, "Prediction of Protein Secondary Structure by neural Networks: Encoding Short and Long Range Patterns of Amino Acid Packing", *Acta Biochim. Polonica* **39**, 39-392 (1992).
53. A. Kolinski and J. Skolnick, "Comment on Local Knot Model of Entangled Polymer Chains", *J. Phys. Chem.* **97**:3450 (1993).
54. A. Kolinski, A. Godzik and J. Skolnick, "A General Method for the Prediction of the Three Dimensional Structure and Folding Pathway of Globular Proteins. Application to Designed Helical Proteins", *J. Chem. Phys.* **98**:7420-7433 (1993).
55. J. Skolnick, A. Kolinski, A. Godzik, "From Independent Modules to Molten Globules: Observations on the Nature of Protein Folding Intermediates", *Proc. Natl. Acad. Sci. USA* **90**:2099-2100 (1993).
56. Y. K. Levine, A. Kolinski and J. Skolnick, "A Lattice Dynamics Study of a Langmuir Monolayer of Monounsaturated Fatty Acids", *J. Chem. Phys.* **98**:7581-7587 (1993).
57. J. Skolnick, A. Kolinski, C. L. Brooks, III, A. Godzik and A. Rey, "A Method for Prediction of Protein Structure from Sequence", *Current Biology* **3**:414-423 (1993).
58. A. Godzik, A. Kolinski and J. Skolnick, "Lattice Representations of Globular Proteins: How good are they?", *J. Comput. Chem.* **14**:1194-1202 (1993).
59. A. Godzik, A. Kolinski and J. Skolnick, "De Novo and Inverse Folding Predictions of Protein Structure and Dynamics", *J. Computer Aided Molecular Design* **7**:397-438 (1993).
60. A. Godzik, J. Skolnick and A. Kolinski, "Regularities in Interaction Patterns of Globular Proteins", *Protein Engng.* **6**:801-810 (1993).
61. A. Kolinski and J. Skolnick, "Monte Carlo Simulations of Protein Folding. I. Lattice Model and Interaction Scheme", *Proteins* **18**:338-352 (1994).
62. A. Kolinski and J. Skolnick, "Monte Carlo Simulations of Protein Folding. II. Application to Protein A, ROP and Crambin", *Proteins* **18**:353-366 (1994).
63. M. Vieth, A. Kolinski, C. L. Brooks, III, and J. Skolnick, "Prediction of the Folding Pathways and Structure of the GCN4 Leucine Zipper", *J. Mol. Biol.* **237**:361-367 (1994).
64. J. Skolnick and A. Kolinski, "De Novo Prediction of Protein Tertiary Structure", *Polymer Preprints* **35**:82-83 (1994).
65. A. Sikorski, A. Kolinski and J. Skolnick, "Dynamics of Star Branched Polymers in a Matrix of Linear Chains - A Monte Carlo Study", *Macromolecular Theory and Simulations* **3**: 715-729 (1994).
66. M. Milik, A. Kolinski, J. Skolnick, "A Neural Network System for Protein Structure Evaluation" *Protein Engng.* **8**:225-236 (1995)
67. M. Vieth, A. Kolinski and J. Skolnick, "A Simple Technique To Estimate Partition Functions and Equilibrium Constants From Monte Carlo Simulations", *J. Chem. Phys.* **102**:6189-6193, (1995).

68. J. Skolnick, M. Vieth, A. Kolinski, and C. Brooks III, "De Novo Simulations of the Folding of GCN4 and Its Mutants", *Modeling of Biomolecular Structures and Mechanisms* **8**:95-98, A. Pullman, et al (Eds), Kluwer Acad. Netherlands (1995).
69. M. Vieth, A. Kolinski, C. L. Brooks, III, and J. Skolnick, "Prediction of the quaternary structure of coiled coils. Application to mutants of the GCN4 Leucine Zipper", *J. Mol. Biol.* **251**: 448-467 (1995).
70. A. Godzik, A. Kolinski, and J. Skolnick, "Are proteins ideal mixtures of amino acids? Analysis of energy parameter sets", *Protein Sci.* **4**: 2107-2117 (1995).
71. A. Kolinski, M. Milik, J. Rycombel, and J. Skolnick, "A reduced model of short range interactions in polypeptide chains", *J. Chem. Phys.* **103**: 4312-4323 (1995).
72. A. Kolinski, W. Galazka, and J. Skolnick, "Computer Design Of Idealized  $\beta$ -Motifs", *J. Chem. Phys.* **103**: 10286-10297 (1995).
73. M. Vieth, A. Kolinski, C. L. Brooks, III, and J. Skolnick, "Prediction of the quaternary structure of the GCN4 Leucine Zipper and its Mutants", in: *Proceedings of the International Conference on Molecular and Structural Biology*, A.J. Kungl, P.J. Andrew and H. Schreiber, Eds., pp:156-163 (1995)
74. A. Olszewski, A. Kolinski and J. Skolnick, "Does a backwardly read protein sequence have a unique native state?", *Protein Engng.* **9**:5-14 (1996).
75. M. Vieth, A. Kolinski, C. L. Brooks III, and J. Skolnick, "A hierarchical approach to the prediction of the quaternary structure of GCN4 and its mutants", *DIMACS* **23**:233-236 (1996).
76. A. Kolinski, J. Skolnick and A. Godzik, "An algorithm for prediction of structural elements in small proteins", *Proceeding of I-st Pacific Symposium on Biocomputing*. L. Hunter and T. E. Klein, Eds. World Scientific Pub. 1996 pp:446-460
77. M. Vieth, A. Kolinski, C. L. Brooks, III and J. Skolnick, "Prediction of quaternary structure of coiled coils: GCN4 leucine zipper and its mutants", *Proceeding of I-st Pacific Symposium on Biocomputing*. L. Hunter and T. E. Klein, Eds. World Scientific Pub. 1996 pp:653-662
78. M. Vieth, A. Kolinski and J. Skolnick, "Method for predicting the state of association of discretized protein models. Application to leucine zippers", *Biochemistry* **35**:955-967 (1996)
79. K. Olszewski, A. Kolinski, and J. Skolnick, "Folding simulations and computer redesign of Protein A three-helix bundle motifs" *Proteins* **25**:286-299 (1996).
80. A. Kolinski, W. Galazka and J. Skolnick, "On the origin of the cooperativity of protein folding. Implications from model simulations.", *Proteins* **26**:271-287 (1996)
81. A. Kolinski and J. Skolnick, "*Lattice models of protein folding. Dynamics and thermodynamics*", Austin, TX, Chapman & Hall. 1996.
82. J. Skolnick and A. Kolinski, "Monte Carlo Lattice Dynamics and the Prediction of Protein Folds.", *Computer Simulations of Biomolecular Systems. Theoretical and Experimental Applications*, Edited by W. F. van Gunsteren, P.K. Weiner and A. J. Wilkinson, ESCOM Science Publ., Leideb, The Netherlands, pp:395-429 (1997)
83. A. Kolinski, J. Skolnick, A. Godzik and W-P. Hu, "A method for the prediction of surface "U"-turns and transglobular connections in small proteins.", *Proteins* **27**:290-308, 1997.
84. M. Milik, A. Kolinski and J. Skolnick, "An algorithm for rapid reconstruction of protein backbone from alpha carbon coordinates", *J. Comput. Chem.* **18**:80-85 (1997)
85. J. Skolnick, A. Kolinski and A. R. Ortiz, "MONSSTER: A method for folding globular proteins with a small number of distance restrains", *J. Mol. Biol.* **265**:217-241 (1997)
86. A. R. Ortiz, W-P. Hu, A. Kolinski and J. Skolnick, "Method for low resolution prediction of small protein tertiary structure", *Proceeding of II-nd Pacific Symposium on Biocomputing*. R. B. Altman, A. K. Dunker, L. Hunter and T. E. Klein Eds. World Scientific Pub. 1997, pp: 316-327
87. J. Skolnick, L. Jaroszewski, A. Kolinski and A. Godzik, "Derivation and testing of pair potential for protein folding. When is the quasicheical approximation correct?" *Protein Sci.* **6**:676-688 (1997)
88. A. Kolinski and J. Skolnick, "Determinants of secondary structure of polypeptide chains: interplay between short range and burial interactions", *J. Chem. Phys.* **107**:953-964 (1997)
89. A. Kolinski and P. Madziar, "Collapse transitions in protein-like lattice polymers. The effect of sequence patterns", *Biopolymers* **42**:537-548 (1997)
90. A. Kolinski and J. Skolnick, "High coordination model of protein structure, dynamics and thermodynamics", *Acta Biochim. Polonica* **44**:389-422 (1997)
91. W-P. Hu, A. Kolinski and J. Skolnick, "Improved method for prediction of protein backbone "U"-turn positions and major secondary structures between "U"-turns. *Proteins* **29**:443-460 (1997)

92. A. Sikorski, A. Kolinski and J. Skolnick, "Computer simulations of *de novo* designed helical proteins, *Biophysical J.* **75**:92-105 (1998)
93. A. R. Ortiz, A. Kolinski and J. Skolnick, "Tertiary structure prediction of the KIX domain CPB using Monte Carlo simulations driven by restraints derived from multiple sequence alignments", *Proteins* **30**:287-294 (1998)
94. A. Kolinski and J. Skolnick, "Assembly of protein structure from sparse experimental data: An efficient Monte Carlo model", *Proteins* **32**:475-494 (1998)
95. A. R. Ortiz, A. Kolinski and J. Skolnick, "Combined multiple sequence reduced protein model approach to predict the tertiary structure of small proteins", *Proceedings of the Pacific Symposium on Biocomputing '98*, R. B. Altman, A. K. Dunker, L. Hunter and T. E. Klein Eds. World Scientific Pub. 1998, pp: 377-388
96. A. Kolinski, P. Rotkiewicz and J. Skolnick, "Application of high coordination lattice model in protein structure prediction", *Proceedings of HRCL Workshop on Monte Carlo Approach to Biopolymers and Protein Folding*, P. Grassberger, G. T. Barkema and W. Nadler, Eds., World Scientific, Singapore/London, 1998, pp: 100-130.
97. A. Kolinski, J. Skolnick and W. Galazka, "Monte Carlo study of the thermodynamics and kinetics of reduced protein models. Application to small helical,  $\beta$ , and  $\alpha/\beta$  proteins", *J. Chem. Phys.* **108**:2608-2617 (1998)
98. A. Kolinski, L. Jaroszewski, P. Rotkiewicz and J. Skolnick, "An efficient Monte Carlo model of protein chains. Modeling the short-range correlations between side group centers of mass", *J. Phys. Chem.* **102**:4628-4637 (1998)
99. A. R. Ortiz, A. Kolinski and J. Skolnick, "Fold assembly of small proteins using Monte Carlo simulations driven by restraints derived from multiple sequence alignments", *J. Mol. Biol.* **277**:419-448 (1998)
100. A. R. Ortiz, A. Kolinski and J. Skolnick, "Nativelike topology assembly of small proteins using predicted restraints in Monte Carlo folding simulations", *Proc. Natl. Acad. Sci. USA* **95**:1020-1025 (1998)
101. M. Vieth, J. Hirst, A. Kolinski and C. L. Brooks III, "Assessing energy functions for flexible docking", *J. Comput. Chem.* **19**:1612-1622 (1998)
102. A. Kolinski, "Struktura, dynamika i termodynamika bialek globularnych. Siatkowe modele Monte Carlo" ("Structure, dynamics and thermodynamics of globular proteins. Lattice Monte Carlo models") *Polimery* **43**(6):341-350 (1998)
103. A. Kolinski, A. Godzik and J. Skolnick, "Contact map", in: *Encyclopedia of Molecular Biology*, T. Creighton Ed. John Wiley and Sons, New York 1999. pp: 567-571
104. J. Skolnick, A. Kolinski and A. R. Ortiz, "Reduced protein models and their applications to the protein folding problem", *Journal of Biomolecular Structure and Dynamics* **16**:381-396 (1998)
105. J. Skolnick and A. Kolinski, "Monte Carlo approaches to the protein folding problem", Monte Carlo Methods in Chemical Physics. D. Ferguson, J. I. Siepmann and D. G. Truhlar, Eds., *Advances in Chemical Physics*, John Wiley and Sons, Volume 105, pp. 203-242 (1999)
106. J. Skolnick and A. Kolinski, "Protein Modeling" in: *Encyclopedia of Computational Chemistry*. P. V. Schleyer, N. L. Allinger, T. Clark, J. Gasteiger, P. A. Kollman, H. F. Schaefer III and P. R. Shreiner Eds., John Wiley and Sons Publ., Chichester, U.K. 1998, Vol 3. pp: 2200-2211
107. J. Skolnick, A. Kolinski and D. Mohanty, "De novo predictions of the quaternary structure of leucine zippers and other coiled coils" *International Journal of Quantum Chemistry* **75**:165-176 (1999)
108. J. Skolnick, A. Kolinski and A. R. Ortiz, "Application of reduced models to protein structure prediction" in: *Computational Molecular Biology: Theoretical and Computational Chemistry Book Series 8*, J. Leszczynski Ed., Elsevier, Amsterdam 1999. pp: 397-440
109. D. Mohanty, A. Kolinski, J. Skolnick, "De novo simulation of the folding thermodynamics of the GCN4 leucine zipper" *Biophysical J.* **77**:54-69 (1999)
110. D. Mohanty, B. Dominy, A. Kolinski, C. L. Brooks III and J. Skolnick, "Correlation between knowledge-based and detailed atomic potentials. Application to the GCN4 leucine zipper" *Proteins* **35**:447-452 (1999)
111. J. Skolnick, J. Fetrow, A. R. Ortiz and A. Kolinski, "The role of computational biology in the genomic revolution" in: *Impact of Advances in Computing and Communications Technologies on Chemical Sciences and Technology, Proceedings of the National Research Council*, National Academy Press, Washington, D.C. (1999) pp: 44-61
112. A. R. Ortiz, A. Kolinski, P. Rotkiewicz, B. Ilkowski and J. Skolnick, "Ab initio folding of proteins using restraints derived from evolutionary information", *Proteins* **37**, *Suppl. 3*:177-185 (1999)
113. A. Kolinski, P. Rotkiewicz, B. Ilkowski and J. Skolnick, "A method for the improvement of threading-based protein models", *Proteins* **37**:592-610 (1999)
114. A. Kolinski, B. Ilkowski and J. Skolnick, "Folding dynamics and thermodynamics of  $\beta$ -hairpin assembly: Insight from various simulation techniques" *Biophys. J.* **77**:2942-2952 (1999)

115. J. Skolnick, A. Kolinski and A. R. Ortiz, "Derivation of protein specific pair potentials based on weak sequence fragment similarity" *Proteins* **38**:3-16 (2000)
116. A. Sikorski, A. Kolinski and J. Skolnick, "Computer simulations of the properties of the  $\alpha 2$ ,  $\alpha 2C$ , and  $\alpha 2D$  de novo designed helical proteins" *Proteins* **38**:17-28 (2000)
117. A. Kolinski, P. Rotkiewicz, B. Ilkowski and J. Skolnick, "Protein folding: Flexible lattice models", *Progress of Theoretical Physics Suppl. (Kyoto)*, **138**:292-300 (2000)
118. J. Skolnick, J. Fetrow and A. Kolinski, "Structural genomics and its importance for gene function analysis", *Nature Biotechnology*, **18**:283-287 (2000)
119. B. Ilkowski, J. Skolnick and A. Kolinski, " Helix -coil and beta sheet - coil transitions in a simplified protein model", *Macromol. Theory Simul.*, **9**:523-533 (2000)
120. C. Simmerling, M. Lee, A. R. Ortiz, A. Kolinski, J. Skolnick and P. A. Kollman, "Combining MONSSTER and LES/PME to predict protein structure from amino acid sequence: Application to the small protein CMTI-1", *J.American.Chem.Soc.* **122**:8392-8402 (2000)
121. D. Gront, A. Kolinski and J. Skolnick, "Comparison of three Monte Carlo conformational search strategies for protein-like polymer models: Identification of low energy structures and folding thermodynamics", *J. Chem. Phys.* **113**:5065-5071 (2000).
122. M. Feig, P. Rotkiewicz, A. Kolinski, J. Skolnick and C. L. Brooks, III, "Accurate reconstruction of all-atom protein representation from side chain based low resolution models", *Proteins* **41**:86-97 (2000)
123. A. Sikorski, A. Kolinski and J. Skolnick, "Monte Carlo Simulation of Designed Helical Proteins", *Acta Poloniae Pharmaceutica –Drug Research Suppl.* **57**:119-121, (2000)
124. A. Kolinski, P. Rotkiewicz and J. Skolnick, "Structure of proteins: New approach to molecular modeling", *Polish J. Chem.* **75**:587-599 (2001)
125. D. Gront, A. Kolinski and J. Skolnick, "A new combination of Replica Exchange Monte Carlo and histogram analysis for protein folding and thermodynamics", *J. Chem. Phys.* **115**:1569-1574 (2001)
126. A. Kolinski, M. Betancourt, D. Kihara, P. Rotkiewicz and J. Skolnick, "Generalized comparative modeling (GENECOMP): A combination of sequence comparison, threading, lattice and off-lattice modeling for protein structure prediction and refinement", *Proteins* **44**:133-149 (2001)
127. P. Rotkiewicz, W. Sicinska, A. Kolinski and H. F. DeLuca, "Model of three-dimensional structure of vitamin D receptor and its binding mechanism with  $1\alpha$ , 25-dihydroxivitamin D", *Proteins* **44**:188-199 (2001)
128. J. Skolnick, A. Kolinski, Daisuke Kihara, Marcos Betancourt, Piotr Rotkiewicz and Michal Boniecki, "Ab initio Protein Structure Prediction via a Combination of Threading, Lattice Folding , Clustering, and Structure Refinement", *Proteins* **45**, Suppl. S5 CASP4 , 149-156 (2001)
129. D. Kihara, H. Lu, A. Kolinski and J. Skolnick, "TOUCHSTONE: An Ab initio Protein Structure Prediction Method that Uses Threading-Based Tertiary Restraints", *Proc. Natl. Acad. Sci., USA* **98**:10125-10130 (2001)
130. J. M. Bujnicki, P. Rotkiewicz, A. Kolinski and L. Rychlewski, "Three-dimensional fold prediction and ab initio modeling of the I-TevI homing endonuclease catalytic domain, a GIY-YIG superfamily member", *Protein Engng.* **14**:717-721 (2001)
131. J. Skolnick and A. Kolinski, "Computational Studies of Protein Folding", *Computing in Science and Engineering* **3**:40-49 (2001)
132. D. Kihara, Y. Zhang, A. Kolinski and J. Skolnick, "Ab initio protein structure prediction on a genomic scale: Application to the Mycoplasma Genitalium Genome", *Proc. Natl. Acad. Sci., USA* **99**:5993-5998 (2002).
133. J. Skolnick and A. Kolinski, "A unified approach to the prediction of protein structure and function", *Adv. Chem. Phys.* **120**:131-192 (2002)
134. R. R. Sicinski, A. Kolinski, P. Rotkiewicz, W. Sicinska, J. M. Prahl, C. M. Smith and H. F. De Luca, "2-Ethyl and 2-Ethylidene Analogs of  $1\alpha$ , 25-Dihydroxy-19-norvitamin D<sub>3</sub>: Synthesis, Conformational Analysis, Biological Activities, and Docking to the Modeled rVDR Ligand Binding Domain", *J. Medicinal Chem.*, **45**:3366-3380 (2002)
135. A. Sikorski, A. Kolinski and J. Skolnick, "Computer simulation of protein folding with a small number of distance restraints", *Acta Biochim. Polonica* **49**:683-692 (2002)
136. J. Fetrow, A. Giammona, A. Kolinski and J. Skolnick, "The protein folding problem, biophysical enigma", *Curr. Pharma. Biotech.* **3**:329-347 (2002)
137. J. Vinals, A. Kolinski and J. Skolnick, "Numerical study of the entropy loss of dimerization of the GCN4 leucine zipper", *Biophys. J.* **83**:2801-2811 (2002)
138. A. Kolinski, D. Gront, P. Pokarowski and J. Skolnick, "A simple lattice model that exhibits a protein-like cooperative all-or-none folding transition", *Biopolymers* **69**:399-405 (2003)

139. P. Pokarowski, A. Kolinski and J. Skolnick, "A minimal physically realistic protein-like lattice model: Designing an energy landscape that ensures all-or-none folding to a unique native state", *Biophys. J.* **84**:1518-1526 (2003)
140. W. Li, Y. Zhang, D. Kihara, Y. J. Huang, D. Zheng, G. T. Montelione, A. Kolinski and J. Skolnick, "TOUCHSTONEX: protein structure prediction using sparse NMR data", *Proteins* **53**:290-306 (2003)
141. T. Haliloglu, A. Kolinski and J. Skolnick, "Use of NMR residual dipolar coupling (RDCs) as restraints in ab initio protein structure prediction", *Biopolymers* **70**:548-562 (2003)
142. Y. Zhang, A. Kolinski and J. Skolnick, "TOUCHSTONE II: A new approach to ab initio protein structure prediction", *Biophys. J.* **85**:1145-1164 (2003)
143. J. Skolnick, Y. Zhang, A. K. Arakaki, A. Kolinski, M. Boniecki, A. Szylagyi and D. Kihara, "TOUCHSTONE: A unified approach to protein structure prediction", *Proteins: Structure, Function and Genetics, CASP5 Supplement, S6* **56**:469-479 (2003)
144. A. Kolinski, P. Klein, P. Romiszowski and J. Skolnick, "Unfolding of globular proteins: Monte Carlo dynamics of a realistic reduced model", *Biophys. J.* **85**:3271-3278 (2003)
145. M. Boniecki, P. Rotkiewicz, J. Skolnick and A. Kolinski, "Protein fragment reconstruction using various modeling techniques", *J. Comput. Aided Mol. Design* **17**:725-737 (2003)
146. A. Kolinski and J. Skolnick, "Reduced models of proteins and their applications", *Polymer* **45**:511-524 (2004)
147. A. Kolinski, "Protein modeling and structure prediction with a reduced representation", *Acta Biochimica Polonica* **51**:349-371 (2004)
148. E. Bolesta, A. Kowalczyk, A. Wierzbicki, P. Rotkiewicz, B. Bambach, I. Horwacik, A. Kolinski, H. Rokita, M. Brecher, S. Ferrone and D. Kozbor, "DNA vaccine expressing the mimotope of GD2 Ganglioside induces protective GD2 cross-reactive antibody responses", *Cancer Research*, **65**:3410-3418 (2005)
149. P. Pokarowski, A. Kloczkowski, R. L. Jernigan, N. S. Kothari, M. Pokarowska and A. Kolinski, "Inferring ideal amino acid interaction forms from statistical protein contact potentials" *Proteins* **59**:49-57 (2005)
150. D. Gront and A. Kolinski, "A new approach to prediction of short range conformational propensities in proteins" *Bioinformatics* **21**:981-987 (2005)
151. D. Gront and A. Kolinski, "HCPM – program for hierarchical clustering of protein models", *Bioinformatics*, **21**:3179-3180 (2005)
152. P. Pokarowski, K. Droste and A. Kolinski, "A minimal protein-like lattice model: an alpha-helix motif", *J. Chem. Phys.* **122**:214915 (2005)
153. E. Malolepsza, M. Boniecki, A. Kolinski and L. Piela, "Theoretical model of prion propagation: a misfolded protein induces misfolding", *Proc. Natl. Acad. Sci. USA* **102**:7835-7840 (2005)
154. D. Plewczynska and A. Kolinski, "Protein folding with a reduced model and inaccurate short-range restraints", *Macromol. Theory Simul.*, **14**:444-451 (2005)
155. D. Ekonomiuk, M. Kielbasinski and A. Kolinski, "Protein modeling with a reduced representation: statistical potentials and protein folding mechanism", *Acta Biochimica Polonica* **52**:741-748 (2005)
156. D. Gront, U. H. E. Hansmann and A. Kolinski, "Exploring protein energy landscapes with hierarchical clustering", *Int. J. Quantum Chemistry* **105**:826-830 (2005)
157. A. Kolinski and J. M. Bujnicki, "Generalized protein structure prediction based on combination of fold-recognition with de novo folding and evaluation of models", *Proteins* **61**(S7):84-90 (2005)
158. D. Gront, A. Kolinski and U. H. E. Hansmann, "Protein structure prediction by tempering spatial constraints", *J. Comput. Aided Mol. Design* **19**(8):603-608 (2005)
159. J. Skolnick, Y. Zhang and A. Kolinski, "Ab initio modeling", in: *Structural Genomics and High Throughput Structural Biology*, A. Edwards, M. Norin and M. Sundstorm, Eds., CRC/Taylor & Francis, Boca Raton, FL, Chapter VIII, pp 137-162, 2006
160. S. Kmiecik, M. Kurcinski, A. Rutkowska, D. Gront and A. Kolinski, "Denatured proteins and early folding intermediates simulated in a reduced conformational space", *Acta Biochimica Polonica*, **53**:131-143 (2006)
161. D. Gront & A. Kolinski, "BioShell - a package of tools for structural biology computations", *Bioinformatics* **22**:621-622 (2006)
162. J. M. Bujnicki, K. Ginalski, A. Kolinski and Jan Kosinski, "Odgadywanie struktur zycia", („Discovering structures of life"), *Swiat Nauki (World of Science – Polish edition of Scientific American)* **174**(2):38-47 (2006)
163. D. Gront, S. Kmiecik & A. Kolinski, "High throughput method for protein structure prediction", in: *Publication Series of the John von Neumann Institute for Computing (NIC), NIC Series, Volume 34, NIC Workshop 2006: From Computational Biophysics to System Biology*, J. Meinke, O. Zimmermann, S. Mohanty & U.H.E. Hansmann, Eds., pp:79-82, 2006
164. A. Kolinski, D. Gront, S.Kmiecik, M. Kurcinski & D. Latek, "Modeling protein structure, dynamics and thermodynamics with reduced representation of conformational space", in: *Publication Series of the John von*



- Neumann Institute for Computing (NIC), NIC Series, Volume 34, NIC Workshop 2006: From Computational Biophysics to System Biology*, J. Meinke, O. Zimmermann, S. Mohanty & U.H.E. Hansmann, Eds., pp:21-28, 2006
165. M. Hoffmann, K. Eitner, M. von Grotthuss, L. Rychlewski, E. Banachowicz, T. Grabarkiewicz, T. Szkoda & A. Kolinski, "Three dimensional model of severe acute respiratory syndrome coronavirus helicase ATPase catalytic domain and molecular design of severe acute respiratory syndrome coronavirus helicase inhibitors.", *J. Comput. Aided Mol. Design* **20(5)**:305-319 (2006)
  166. D. Gront, M. Kurcinski & A. Kolinski, "Clustering as a supporting tool for structural drug design", *Acta Pol. Pharm.-Drug Research* **63(5)**:436-438 (2006)
  167. A. Kloczkowski & A. Kolinski, "Theoretical models and simulations of polymer chains" in: *Physical Properties of Polymers Handbook*, J. E. Mark, Ed., Springer-Verlag, New York, 2006, pp: 67-82
  168. D. Gront & A. Kolinski, "Efficient scheme for optimization of parallel tempering Monte Carlo method", *J. Phys.: Condens. Matter* **19(3)** #036225 (2007)
  169. D. Gront, S. Kmiecik & A. Kolinski, "Backbone building from quadrilaterals. A fast and accurate algorithm for protein backbone reconstruction from alpha carbon coordinates", *J. Comput. Chem.* **28(9)**:1593-1597 (2007)
  170. D. Latek, D. Ekonomiuk & A. Kolinski, "Protein structure prediction: combining de novo modeling with sparse experimental data", *J. Comput. Chem.* **28(10)**:1668-76 (2007)
  171. M. Kurcinski & A. Kolinski, "Hierarchical modeling of protein interactions", *J. Mol. Modeling* **13(6-7)**:691-698 (2007)
  172. A. Kolinski, "Wieloskalowe modelowanie molekularne białek", *Miesięcznik Politechniki Warszawskiej*, („Mutiscale molecular modeling of proteins"), *Technical University of Warsaw Monthly* **2007(2)**:1-6 (2007)
  173. M. Kurcinski & A. Kolinski, "Steps towards flexible docking: Modeling of three-dimensional structures of the nuclear receptors bound with peptide ligands mimicking co-activators' sequences", *J. Steroid Biochem. and Mol. Biol.* **103**:357-360 (2007)
  174. D. Gront & A. Kolinski, "T-pile – a package for thermodynamic calculation for biomolecules", *Bioinformatics* **23**:1840-1942 (2007)
  175. P. Pokarowski, A. Kloczkowski, S. Nowakowski, M. Pokarowska, R. L. Jernigan & A. Kolinski, "Ideal amino acid exchange forms for approximating substitution matrices" *Proteins*, **69**:379-393 (2007)
  176. S. Kmiecik & A. Kolinski, "Characterization of protein folding pathways by reduced-space modeling", *Proc. Natl. Acad. Sci. USA* **104(30)**:12330-12335 (2007)
  177. S. Kmiecik, D. Gront & A. Kolinski, "Towards high-resolution structure prediction. Fast refinement of reduced models with all-atom force field", *BMC Structural Biology* **7**:43 (2007)
  178. E. M. Ibryashkina, Zakharova M.V., Bogdanova E.S., Den'mukhamedov M.M., Melnik B.S., Kolinski A., Gront D., Feder M., Solonin A.S., Bujnicki J.M., "Type II restriction endonuclease R.Eco29KI is a member of the GIY-YIG nuclease superfamily", *BMC Structural Biology* **7**:48 (2007)
  179. A. Kolinski & D. Gront, "Comparative modeling without implicit sequence alignments", *Bioinformatics* **23(19)**:2522-2527 (2007)
  180. A. Rutkowska & A. Kolinski, "Why proteins divide into domains? Insights from lattice model simulations", *Biomacromolecules* **8**:3519-3524 (2007)
  181. S. Kmiecik & A. Kolinski, "Folding pathway of the B1 domain of protein G explored by a multiscale modeling", *Biophys. J.* **94(3)**:726-736 (2008)
  182. S. Kawashima, P. Pokarowski, M. Pokarowska, A. Kolinski, T. Katayama, M. Kanehisa, "AAindex: Amino Acid index database, progress report 2008", *Nucleic Acid Res.* **36**:D202-D205 (2008)
  183. T. Z. Sen, M. Kloster, A. Kloczkowski, A. Kolinski, J. M. Bujnicki & R. L. Jernigan, "Predicting the structure and functional mechanism of the outer membrane transporter and signal transducer FecA", *Biophys. J.* **94**:2482-2491 (2008)
  184. L. Knizewski, K. Steczkiewicz, K. Kuchta, L. Wyrwicz, D. Plewczynski, A. Kolinski, L. Rychlewski & K. Ginalski, "Uncharacterized DUF1574 *Leptospira* proteins are SGNH hydrolases", *Cell Cycle* **7(4)**:542-544 (2008)
  185. D. Gront & A. Kolinski, "Utility library for structural bioinformatics", *Bioinformatics* **24(4)**:584-585 (2008)
  186. D. Gront, D. Latek, M. Kurcinski & A. Kolinski, "Wieloskalowe modelowanie białek" ("Multiscale protein modeling") in: *Na pograniczu chemii i biologii (At the Treshold of Chemistry and Biology)*, H. Korniak, J. Barciszewski, Eds. Vol. 17 pp:239-256 (2008)
  187. D. Latek & A. Kolinski, "Contact prediction in protein modeling. Scoring, folding and refinement of coarse-grained models", *BMC Structural Biology* **8**:36 (2008)

188. S. Kmiecik, M. Jamroz, A. Zwolinska, P. Gniewek & A. Kolinski, "Designing an automated pipeline for protein structure prediction", in: *Publication Series of the John von Neumann Institute for Computing (NIC), NIC Series, Volume 40, NIC Workshop 2008: From Computational Biophysics to System Biology*, U.H.E. Hansmann, J. Meinke, S. Mohanty, W. Nadler & O. Zimmermann, Eds., pp:105-107, 2008
189. D. Gront & A. Kolinski, "Fast and accurate method for predicting short-range constraints in protein models" *J. Comput. Aided Mol. Design* **20**:783-788 (2008)
190. D. Gront, D. Latek, M. Kurcinski & A. Kolinski, "Template-free predictions of three-dimensional protein structures: From first principles to knowledge-based potentials." in: *Prediction of Protein Structures, Functions, and Interactions*, J. M. Bujnicki, Ed., John Wiley & Sons, Chichester, UK, 2008, pp:117-142
191. A. Kloczkowski, R. L. Jernigan, Z. Wu, G. Song, L. Yang, A. Kolinski & P. Pokarowski, "Distance matrix-based approach to protein structure prediction", *J. Struct. and Funct. Genomics* **10**:67-81 (2009)
192. M. Jamroz & A. Kolinski, "Modeling of loops in proteins: a multi-method approach", *BMC Structural Biology* **10**:5 (2010)
193. S. Trojanowski, A. Rutkowska & A. Kolinski, "TRACER. A new approach to comparative modeling that combines threading with free-space conformational sampling", *Acta Biochimica Polonica* **57**:125-133 (2010)
194. M. Kurcinski & A. Kolinski, "Theoretical study of molecular mechanism of binding TRAP220 coactivator to Retinoid X Receptor alpha, activated by 9-cis retinoic acid", *J. Steroid Biochem. and Mol. Biol.* **121**:124-129 (2010)
195. P. Gniewek & A. Kolinski, "Coarse-grained Monte Carlo simulations of mucus: structure, dynamics and thermodynamics", *Biophys. J.* **99**:3507-3516 (2010)
196. S. Saraswathi, R. L. Jernigan, A. Kloczkowski & A. Kolinski, "Protein secondary structure prediction using knowledge-based potentials", in: *Proceedings of the International Conference on Fuzzy Computation and 2<sup>nd</sup> International Conference on Neural Computation*, pp: 370-375 (2010)
197. A. Kolinski, "Preface" in: *Multiscale Approaches to Protein Modeling*, A. Kolinski, Ed., Springer, New York, 2011
198. A. Kolinski, "Lattice polymers and protein models" in: *Multiscale Approaches to Protein Modeling*, A. Kolinski, Ed., Springer, New York, pp: 1-20, 2011
199. M. Kurcinski, M. Jamroz & A. Kolinski, "Multiscale protein and peptide docking" in: *Multiscale Approaches to Protein Modeling*, A. Kolinski, Ed., Springer, New York, pp: 21-34, 2011
200. S. Kmiecik, M. Jamroz & A. Kolinski, "Multiscale approach to protein folding dynamics" in: *Multiscale Approaches to Protein Modeling*, A. Kolinski, Ed., Springer, New York, pp: 281-294, 2011
201. D. Latek & A. Kolinski, "CABS-NMR – de novo tool for rapid global fold determination from chemical shifts, residual dipolar couplings and sparse methyl-methyl NOEs", *J. Comput. Chem.* **32**:536-544 (2011)
202. P. Gniewek & A. Kolinski, "Note. A simple picture of sub-diffusive polymer motion from stochastic simulations", *J. Chem. Phys.* **134**:056101 (2011)
203. P. Gniewek, S. U. Leelananda, A. Kolinski, R. L. Jernigan & A. Kloczkowski, "Multibody Coarse-Grained Potentials for Native Structure Recognition and Quality Assessment of Protein Models", *Proteins* **79**:1923-1929 (2011)
204. I. Horwacik, M. Kurcinski, M. Bzowska, A. Kowalczyk, D. Czaplicki, A. Kolinski & H. Rokita, "Analysis and optimization of interactions between peptides mimicking GD2 ganglioside and monoclonal antibody 14G2a", *Int. J. Mol. Medicine* **28**:47-57 (2011)
205. K. Steczkiewicz, M. Kurcinski, M. T. Zimmermann, B. Lewis, D. Dobbs, A. Kloczkowski, R. L. Jernigan, A. Kolinski, & K. Ginalski, "Human Telomerase Model Shows the Role of the TEN Domain in Advancing Double Helix for the Next Polymerization Step", *Proc. Natl. Acad. Sci. USA* **108**:9443-9448 (2011)
206. K. Kamel & A. Kolinski, "Computational study of binding of epothilone A to  $\beta$ -tubulin", *Acta Biochimica Polonica* **58**:255-260 (2011)
207. S. Kmiecik & A. Kolinski, "Simulation of chaperonin effect on protein folding: a shift from nucleation-condensation to framework mechanism", *J. American Chem. Soc.* **133**:10283-10289 (2011)
208. M. Blaszczyk, M. Jamroz, D. Gront, A. Kolinski, "Protein Structure Prediction Using CABS – a Consensus Approach", in: *From Computational Biophysics to Systems Biology (CBSB11) Proceedings, NIC Series* **8**:29-32, 2012
209. D. Gront, M. Blaszczyk, J. Wabik, A. Kolinski, "Modeling Protein Structures and their Complexes with Sparse Experimental Data", in: *From Computational Biophysics to Systems Biology (CBSB11) Proceedings, NIC Series* **8**:49-52, 2012

210. S. Kmiecik, M. Blaszczyk, A. Kolinski, "Prediction of experimental phi values in protein folding by simulation with knowledge-based potentials: B domain of protein A.", in: *From Computational Biophysics to Systems Biology (CBSB11) Proceedings, NIC Series* **8**:79-82, 2012
211. A. Kolinski, M. Blaszczyk, S. Kmiecik, "Coarse-grained Protein Modeling: Dynamics, Folding Pathways and Mechanical Unfolding.", in: *From Computational Biophysics to Systems Biology (CBSB11) Proceedings, NIC Series* **8**:83-90, 2012
212. J. Wabik, D. Gront, S. Kmiecik, A. Kolinski, "Multiscale approach to thermodynamics and dynamics of a  $\beta$ -hairpin folding." in: *From Computational Biophysics to Systems Biology (CBSB11) Proceedings, NIC Series* **8**:213-216, 2012
213. P. Gniewek & A. Kolinski, "Coarse-grained modeling of mucus barrier properties", *Biophys. J.* **102**:195-200 (2012)
214. P. Gniewek, A. Kolinski, A. Kloczkowski & R. L. Jernigan, "How noise in force fields can affect the structural refinement of protein models", *Proteins* **80**:335-341 (2012)
215. M. Jamroz, A. Kolinski & D. Kihara, "Structural features that predict real-value fluctuation of globular proteins", *Proteins* **80**:1425-1435 (2012)
216. D. Gront, S. Kmiecik, M. Blaszczyk, D. Ekonomiuk & A. Kolinski, "Optimization of protein models", *WIREs Computational Molecular Sciences* **2**:479-493 (2012)
217. P. Gniewek, A. Kolinski, R. L. Jernigan & A. Kloczkowski, "Elastic network modes provide a basis for protein structure refinement", *J. Chem. Phys.* **136**:195101 (2012)
218. S. Saraswathi, J. L. Fernandez-Martinez, A. Kolinski, R. L. Jernigan & A. Kloczkowski, "Fast learning optimized prediction methodology (FLOPRED) for protein secondary structure prediction", *J. Mol. Modeling* **18**:4275-4289 (2012)
219. S. Kmiecik, D. Gront, M. Kouza & A. Kolinski, "From Coarse-Grained to Atomic-Level Characterization of Protein Dynamics: Transition State for the Folding of B Domain of Protein A", *J. Phys. Chem. B* **116**:7026-7032 (2012)
220. D. Gront, P. Wojciechowski, M. Blaszczyk & A. Kolinski, "BioShell Threader: protein homology detection based on sequence profiles and secondary structure profiles", *Nucleic Acids Research* **40**(W1):W257-W262 (2012)
221. P. Gniewek, A. Kolinski & D. Gront, "Optimization of profile-to-profile alignment parameters for one-dimensional threading", *J. Computational Biology* **19**(7):879-886 (2012)
222. K. Kamel & A. Kolinski, "Assessment of free binding energy of 1,25-dihydroxyvitamin D<sub>3</sub> and analogs with human VDR receptor", *Acta Biochimica Polonica* **59**:653-660 (2012)
223. A. Dawid, M. Koliński, A. Koliński & S. Kmiecik, "Modelowanie Molekularne Białek Błonowych" ("Molecular Modeling of Membrane Proteins"), *Na pograniczu chemii i biologii (At the Treshold of Chemistry and Biology)*, H. Koroniak, J. Barciszewski, (red.). Wydawnictwo Naukowe UAM, Poznań, pp. 223-238, 2013
224. M. Jamroz, M. Orozco, A. Kolinski & S. Kmiecik, "A Consistent View of Protein Fluctuations from All-atom Molecular Dynamics and Coarse-Grained Dynamics with Knowledge-based Force-field", *J. Chem. Theo. Comp.* **9**:119-125 (2013)
225. M. Jamroz & A. Kolinski, "CluSco: Clustering and Scoring of Protein Models" *BMC Bioinformatics* **14**:62 (2013)
226. J. Wabik, S. Kmiecik, D. Gront, M. Kouza & A. Kolinski, "Combining coarse-grained protein models with replica-exchange all-atom molecular dynamics", *International Journal of Molecular Science*, **14**:9893-9905 (2013)
227. M. Blaszczyk, M. Jamroz, S. Kmiecik & A. Kolinski, "CABS-fold: server for de novo and consensus-based prediction of protein structure" *Nucleic Acids Research* **41**(W1):W406-W411 (2013)
228. M. Jamroz, A. Kolinski & S. Kmiecik, "CABS-flex: server for fast simulation of protein structure fluctuations" *Nucleic Acids Research* **41**(W1):W427-W431 (2013)
229. S. Saraswathi, J. L. Fernandez-Martinez, A. Kolinski, R. L. Jernigan & A. Kloczkowski, "Distributions of amino acids suggest that certain residue types more effectively determine protein secondary structure" *J. Mol. Mod.* **19**(10):4337-4348 (2013)
230. M. Kouza, Chin-Kun Hu, Mai Suan Li & A. Kolinski, "A structure-based model fails to probe the mechanical unfolding pathway of titin I27 domain", *J. Chem. Phys.* **139**:065103 (2013)
231. M. Blaszczyk, D. Gront, S. Kmiecik, K. Ziolkowska, M. Panek & A. Kolinski, "Coarse grained protein models in structure prediction" in: *Computational Methods to Study the Structure and Dynamics of Biomolecules and Biomolecular Processes - From Bioinformatics to Molecular Quantum Mechanics*, A. Liwo, Ed. Springer Series in Bio-Neuroinformatics, pp:25-53, 2014

232. S. Kmiecik, J. Wabik, M. Kolinski, M. Kouza & A. Kolinski, "Coarse grained models of protein dynamics" in: *Computational Methods to Study the Structure and Dynamics of Biomolecules and Biomolecular Processes - From Bioinformatics to Molecular Quantum Mechanics*, A. Liwo, Ed. Springer Series in Bio-Neuroinformatics, pp:55-79, 2014
233. M. Jamroz, A. Kolinski & S. Kmiecik, "Protocols for efficient simulations of long time protein dynamics using coarse-grained CABS models" in: *Protein Structure Prediction – Methods in Molecular Biology*, Vol. 1137, D. Kihara, Ed. Springer, pp:235-250, 2014
234. J. Wabik, M. Kurcinski & A. Kolinski, "Flexible docking of the fragment of the troponin I to the troponin C", Proceedings IWBBIO 2014: International Work-Conference on Bioinformatics and Biomedical Engineering, Granada 7-9 April, 2014, pp:1064-1073, 2014
235. P. Gniewek, A. Kolinski, A. Kloczkowski & D. Gront, "BioShell-Threading: versatile Monte Carlo package for protein threading" *BMC Bioinformatics* **15**:22 (2014)
236. M. Jamroz, A. Kolinski & S. Kmiecik, "CABS-flex predictions of protein flexibility compared with NMR ensembles", *Bioinformatics* **30(15)**:2150-2154 (2014)
237. M. Kurcinski, A. Kolinski & S. Kmiecik, "Mechanism of folding and binding of an intrinsically disordered protein as revealed by ab initio simulations", *J. Chem. Theo. Comp.* **10(6)**:2224-2231 (2014)
238. A. Kolinski, S. Kmiecik, M. Jamroz, M. Blaszczyk, M. Kouza & M. Kurcinski, "Coarse-grained modeling of protein structure, dynamics and protein-protein interactions", From Computational Biophysics to Systems Biology (CBSB14) Proceedings, *TASK Quarterly* **18(3)**:219-229 (2014)
239. M. Kouza, M. Jamroz, D. Gront, S. Kmiecik, & A. Kolinski, "Mechanical unfolding of DDFLN4 studied by the coarse-grained knowledge-based CABS model", From Computational Biophysics to Systems Biology (CBSB14) Proceedings, *TASK Quarterly* **18(4)**:373-378 (2014)
240. L. Wieteska, M. Ionov, J. Szymraj, A. Kolinski, C. Feller & D. Gront, "Improving thermal stability of thermophilic L-threonine aldolase from *Thermatoga maritima*", *J. Biotechnology* **199**:69-76 (2015)
241. M. Kouza, Nguyen Trong Co, Phuong H. Nguyen, A. Kolinski & Mai Suan Li, "Preformed template fluctuations promote fibril formation: Insights from lattice and all-atom models", *J. Chem. Phys.* **142**:145104 (2015)
242. J. Wabik, M. Kurcinski & A. Kolinski, "Multiscale modeling of peptide docking associated with large conformation transitions of the binding protein", *Molecules* **20**:10763-10780 (2015)
243. M. Kurcinski, M. Jamroz, M. Blaszczyk, A. Kolinski & S. Kmiecik, "CABS-dock: web server for flexible docking of peptides to proteins without prior knowledge of the binding site", *Nucleic Acids Research* **43(W1)**: W419-W424 (2015)
244. M. Kurcinski, M. Jamroz, M. Blaszczyk, A. Kolinski & S. Kmiecik, "CABS-dock web server for protein-peptide docking with significant conformational changes and without prior knowledge of the binding site", *Protein Sci.* **24(S1)**:247-247 (2015)
245. M. Blaszczyk, M. Jamroz, M. Kurcinski, A. Szczasiuk, A. Kolinski & S. Kmiecik, "Web server tools for modeling of protein structure, flexibility, aggregation and protein-peptide interactions", *Protein Sci.* **24(S1)**:247-248 (2015)
246. M. Blaszczyk, M. Kurcinski, M. Kouza, L. Wieteska, A. Debinski, A. Kolinski & S. Kmiecik "Modeling of protein-peptide interactions using the CABS-dock web server for binding site search and flexible docking", *Methods* **93**:72-83 (2016)
247. A. Bielenica, E Kedzierska, M. Kolinski, S. Kmiecik, A. Kolinski, F. Fiorino, B. Saverino, E. Magli, I. Rossi, P. Masserelli, A. Koziol & M. Struga, „5-HT<sub>2</sub> receptor affinity, docking studies and pharmacological evaluation of a series of 1,3-disubstitued thiourea derivatives", *Euro. J. Medicinal. Chem.* **116**:173-1086 (2016)
248. M. Jamroz, A. Kolinski & D. Kihara, "Ensemble-Based Evaluation of Protein Structure Models", *Bioinformatics* **32(12)**:314-321 (2016)
249. M. Kurcinski, M. Ciemny, M. Blaszczyk, A. Kolinski & S. Kmiecik, "Flexible protein-peptide docking using CABS-dock with knowledge about the binding site", Proceedings IWBBIO 2016, International Work-Conference on Bioinformatics and Biomedical Engineering, Granada, pp: 195-201, 2016
250. M. Ciemny, M. Kurcinski, A. Kolinski & S. Kmiecik, "Towards protein-protein docking with significant structural changes using CABS-dock", Proceedings IWBBIO 2016, International Work-Conference on Bioinformatics and Biomedical Engineering, Granada, pp: 207-213, 2016
251. S. Kmiecik, D. Gront, M. Kolinski, L. Wieteska, A. Dawid & A. Kolinski, "Coarse-grained protein models and their applications", *Chemical Reviews* **116(14)** 7898–7936 (2016)
252. S. Rashid, S. Saraswathi, A. Kloczkowski, S. Sundaram & A. Kolinski, "Protein secondary structure prediction using a small training set (Compact Model) combined with a Complex-valued neural network approach" *BMC Bioinformatics* **17**:362 (2016)

253. W. Pulawski, M. Jamroz, M. Kolinski, A. Kolinski & S. Kmieciak, "Coarse-grained simulations of membrane insertion and folding of small helical protein using CABS model", *J. Chem. Info. Mod.* (2016) DOI: 10.1021/acs.jcim.6b00350
254. M. P. Ciemny, A. Debinski, M. Paczkowska, A. Kolinski, M. Kurcinski & S. Kmieciak, "Protein-peptide molecular docking with large-scale conformational changes: the p53-MDM2 interaction", *Scientific Reports - Nature*, in press
255. M. Kurcinski, M. Blaszczyk, M. P. Ciemny, A. Kolinski & S. Kmieciak, "A protocol for CABS-dock protein-peptide docking driven by side-chain contact information", *Biomedical Engineering Online (BMC)*, in press
256. M.P. Ciemny, M. Kurcinski, M. Blaszczyk, A. Kolinski & S. Kmieciak, "Modeling EphB4-EphrinB2 protein-protein interaction using flexible docking of a short linear motif", *Biomedical Engineering Online (BMC)*, in press
257. S. Kmieciak & A. Kolinski, "One dimensional structural properties of proteins in coarse-grained CABS model" in: *Prediction of Protein Secondary Structure and Other One-dimensional Structural Properties-Methods in Molecular Biology*, Yaoqi Zhou, Eshel Faraggi, Yuedong Yang and Andrzej Kloczkowski, Editors, Springer, *Methods Mol. Biol.* **1484**:83-114 (2017)
258. L. Peterson, M. Jamroz, A. Kolinski & D. Kihara, "Predicting real-valued protein residue fluctuation using FlexPred" in: *Prediction of Protein Secondary Structure and Other One-dimensional Structural Properties-Methods in Molecular Biology*, Yaoqi Zhou, Eshel Faraggi, Yuedong Yang and Andrzej Kloczkowski, Editors, Springer, *Methods Mol. Biol.* **1484**:175-186 (2017)
259. M. Kouza, A. Faraggi, A. Kolinski & A. Kloczkowski, "GOR Method of Protein Secondary Structure Prediction, and its Application as Protein Aggregation Prediction Tool" in: *Prediction of Protein Secondary Structure and Other One-dimensional Structural Properties-Methods in Molecular Biology*, Yaoqi Zhou, Eshel Faraggi, Yuedong Yang and Andrzej Kloczkowski, Editors, Springer, *Methods Mol. Biol.* **1484**:7-24 (2017)
260. M. P. Ciemny, M. Kurcinski, K. Kozak, A. Kolinski & S. Kmieciak, "Highly flexible protein-peptide docking using CABS-dock" in: *Modeling of Peptide-Protein Interactions-Methods in Molecular Biology*, Ora Schueler-Furman and Nir London, Editors, Springer, *Methods Mol. Biol.* **1561**:xxx-xxx, in press

## STATISTICS:

1. About 100 invited lectures at international conferences.
2. About 50 invited lectures (or series of lectures) at foreign Universities, Research Institutes and Pharmaceutical/Biotech Companies.
3. 7712 citations (6268 excluding self-citations) according to ISI Web of Knowledge, Hirsch Index H=50.
4. 10009 (2713 since 2013) citations according to Google Scholar, Hirsch Index H=54.