October 1, 2006

Curriculum Vitae

1. NAME AND PERSONAL DATA

Jaroslaw (Jarek) Meller
10842 Lake Thames Drive, Cincinnati, OH 45242
Personal web sites: http://folding.chmcc.org

2. EDUCATION

2A. Pre-doctoral training

1985-1991	M.Sc. in Physics (major in computer physics, joint undergraduate/graduate program), Nicholas Copernicus University, Torun, Poland
1988-1993	M.Sc. in Mathematics (major in computer science, joint undergraduate/graduate program), Nicholas Copernicus University, Torun, Poland
1994-1995	Graduate training in computational chemistry, mentor: Prof. Jean-Paul Malrieu, Paul Sabatier University, Toulouse, France
1991-1996	Ph.D. in Computational Chemistry (computational methods for electronic structure of molecules, thesis advisor: Prof. Wlodzislaw Duch), Nicholas Copernicus University, Torun, Poland

2B. Post-doctoral training

1996-1997	Postdoctoral fellow, **Hebrew University**, Jerusalem, Israel (mentor: Prof. Ron Elber, research subjects: *computational biology*, computer simulations of proteins, Molecular Dynamics, protein folding)
1999-1998	Japan Society for the Promotion of Science fellow, **Kyoto University**, Japan (mentor: Prof. Hiroshi Nakatsuji, research subjects: *computational chemistry*, ab initio studies on electronic structure of biomolecules, modeling of the hydrophobic effect and dispersion interactions in chromatography)
1999-2001	Research fellow, **Cornell University**, Ithaca, USA (mentor: Prof. Ron Elber, research subjects: *bioinformatics*, computational biology, structural genomics, protein structure and function recognition)
2004	**Doctorate** (Habilitation) in Biocybernetics and Biomedical Engineering, Institute of Biocybernetics and Biomedical Engineering, Polish Academy of Sciences, Warsaw, Poland

3. **ACADEMIC APPOINTMENTS**

1995-1998	Teaching Assistant, Department of Informatics, Nicholas Copernicus University, Torun, Poland
1998-present	Assistant Professor, Department of Informatics, Nicholas Copernicus University, Torun, Poland
2001-2005	Assistant Professor, Division of Biomedical Informatics, Children's Hospital Research Foundation, Cincinnati, Ohio, USA
2004-2006	Assistant Professor (secondary appointment), Department of Biomedical Engineering, University of Cincinnati, Ohio, USA
2005-2006	Associate Professor, Division of Biomedical Informatics, Children's Hospital Research Foundation, Cincinnati, Ohio, USA
2006-present	Associate Professor, Department of Environmental Health, University of Cincinnati Medical College, Cincinnati, Ohio, USA
2006-present	Associate Professor (secondary appointment), Department of Biomedical Engineering, University of Cincinnati, Ohio, USA
2006-present	Associate Professor (tertiary appointment), Division of Biomedical Informatics, Children's Hospital Research Foundation, Cincinnati, Ohio, USA

4. **AWARDS AND HONORS**

1993	European Union TEMPUS Program fellowship
1994	European Union TEMPUS Program fellowship
1995	Polish-French Scientific Collaboration Program fellowship
1997	Polish-French Scientific Collaboration Program fellowship
1998	Japan Society for the Promotion of Science fellowship
1999	Center for Advanced Studies of the Hebrew University fellowship
2000	Selected to represent Cornell University during the press release and inaugural meeting of the Tri-institutional Initiative (Cornell University, Rockefeller University and Sloan-Kettering Cancer Institute) in bioinformatics

5. **PROFESSIONAL ACTIVITIES:**

1997	Visiting scientist, IRSAMC, Paul Sabatier University, Toulouse, France
1999	Visiting scientist, Center for Advanced Studies, Hebrew University, Jerusalem, Israel
2001	Co-organizer of a mini-symposium, Tenth SIAM Conference on Parallel Processing for Scientific Computing, Portsmouth, VA
2001-present	Member, American Association for the Advancement of Science
2003	Co-organizer of a bioinformatics workshop, *Genes, Proteins, Interactions and Expressions*, BioInformatics Research Center, Nanyang Technological University, Singapore

2003 Co-organizer of a bioinformatics workshop, *BIT 2003*, Nicholas Copernicus University, Torun, Poland

2004-present Member, International Society for Computational Biology

2004 Co-organizer and leader of a bioinformatics session, Life Sciences Without Boundaries, OVALS 2004, University of Louisville, KY

2004 Co-organizer of a bioinformatics workshop, *BIT 2004*, Nicholas Copernicus University, Torun, Poland

2005 Organizer of a computational biology mini-symposium, Joint Annual Meeting of the Interface and the Classification Society of North America, *Interfaces 2005*, Washington University, Saint Lois

2005 Organizer of a bioinformatics workshop, *Computational Studies of Protein-Protein Interactions*, University of Cincinnati

2005 Co-organizer of a satellite *Workshop on Applications of Statistical and Machine Learning in Bioinformatics*, ICANN 2005, Warsaw, Poland

6. **SERVICE**

6A. **Manuscripts review**

Biophysical Journal, Proteins: Structure, Function and Bioinformatics, BMC Bioinformatics, Bioinformatics, Multiscale Modeling and Simulation, various conference papers

6B. **Committee Involvement**

Core Curriculum Review Committee, College of Medicine, UC, member (Dr. R. Brackenbury, chair), 2004; Computational Medicine Center Scientific Committee, CHRF & UC, member (Dr. B. Aronow, chair), 2004-05; Bioinformatics Curriculum Committee, Dept. of Biomedical Engineering, UC, member (Dr. M. Wagner, chair), 2003-05, multiple faculty search committees.

6C. **Other services**

Established and organized the Bioinformatics Journal Club (BJC); Invited speakers and organized several monthly research seminars for the Div. of Biomedical Informatics (2002-2005).

Participated in a number of faculty searches, faculty candidate interviews, candidates for the BME graduate program interviews; served as a member on several Ph.D. Qualifying Exam Committees.

Served as an ad hoc reviewer for the NIH Virology Study Section panel on bio-defense and emerging infectious diseases (Dr. J. D. Mosca, coordinator).

Co-organized (with Dr. R. Brackenbury) several bioinformatics workshops (2003, 2004, 2005) within the framework of the Summer Undergraduate Research Program of the College of Medicine, UC; Co-organized and taught several workshops and training sessions in bioinformatics for CHRF and UC researchers.

Developed Protein Modeling Laboratory, with multiple simulation, data mining and bioinformatics software packages (obtained in part thanks to the funding from the Ohio Board of Regents) to be used for research and to enhance teaching at UC & CHRF.

7. **SELECTED TALKS**

1st Annual Ohio Collaborative Conference on Bioinformatics, OCCB 2006, Ohio University (June 2006), invited speaker: *Prediction of Solvent Accessibility in Soluble and Membrane Proteins*

Workshop on Applications of Statistical and Machine Learning in Bioinformatics, ICANN 2005, Poland (September 2005), co-organizer, speaker: *Recognition of Protein-Protein Interaction Sites and Membrane Domains with Prediction-based Structural Profiles*

Bioinformatics Workshop: Computational Studies of Protein-Protein Interactions, University of Cincinnati (September 2005), organizer, speaker: *Identification of Protein-Protein Interaction Sites Using Solvent Accessibility Prediction*

Joint Annual Meeting of the Interface and the Classification Society of North America, Interfaces 2005, Washington University, Saint Lois (June 2005), mini-symposium organizer, speaker: *Classification and Regression-based Approaches to Protein Structure Prediction*

Midwest Computational Structural Biology Workshop, Michigan State University (May 2005), invited speaker: *Protocols for Functional Annotations of Proteins*

Cornell University, Ithaca (July 2004), speaker: *Prediction of Secondary Structures and Solvent Accessibility of Amino Acid Residues in Proteins: Can We Do Better?* (invited by Prof. R. Elber)

Institute of Biocybernetics and Biomedical Engineering, Polish Academy of Sciences, Warsaw (June 2004), invited speaker (habilitation proceedings): *Gene Finding in Eukaryotic Genomes*

Bioinformatics Workshop, BIT 2004, Nicholas Copernicus University, Torun (June 2004), invited speaker: *Sequence-independent filters for protein folding simulations*

Physics Seminar Series, University of Cincinnati (June 2004), invited speaker: *Knowledge-based protocols for protein structure prediction: from protein threading to solvent accessibility prediction and back to protein structure prediction by threading*

Life Sciences without Boundaries, OVALS 2004, University of Louisville (March 2004), invited speaker: *Bioinformatics at the University of Cincinnati and Children's Hospital Research Foundation*

The Second International Conference on Computational Intelligence, Robotics and Autonomous Systems, CIRAS 2003, Singapore (December 2003), invited speaker: *Maximum Feasibility Approach for Consensus Classifiers*

Genes, Proteins, Interactions and Expressions Workshop, BioInformatics Research Center, Nanyang Technological University, Singapore (December 2003), invited speaker: *A Novel Method for Predicting Relative Solvent Accessibility Using Neural Networks Based Regression*

The 15th Congress of the International Society for Human and Animal Mycology, ISHAM 2003, San Antonio (May 2003) invited speaker: *Gone Fishing – Computational Strategies for Gene Finding in the Pneumocystis and Other Fungal Genomes*

Biomedical Engineering Seminar Series, University of Cincinnati (April 2003), invited speaker: *Predicting Protein Structure and Protein-Protein Interactions Using Sequence-to-Structure Matching*

Bioinformatics Workshop, BIT 2002, Nicholas Copernicus University, Torun (June 2002), invited speaker, lecturer: *Introduction to Bioinformatics*, *Sequence Alignment Methods*, *Hidden Markov Models in Bioinformatics*

Computational Challenges in the Post-genomic Era, SUN and Duke University (March 2002), invited speaker: *Novel Threading Algorithm for Recognition of Remote Homologs: from Design of Scoring Functions to Biological Discovery*

MCS Divisional Seminars & Colloquia, Argonne National Lab (July 2001), invited speaker: *Protein Recognition by Sequence-to-Structure Fitness: from Design of Energy Functions to Annotations of Genomic Sequences*

From Genes to Proteins and to Biological Function: Computational Approaches, Cornell University (October 2000), invited speaker: *Designing an efficient and accurate threading algorithm: from optimization of energy functions to relating a new class of plant regulatory genes to a human Ras protein.*

Press release and inauguration meeting of the Tri-institutional (Cornell University, Rockefeller University and Sloan-Kettering Cancer Institute) initiative in bioinformatics, New York City (June, 2000), invited speaker: *Computational Short Cuts from Genes to Drugs.*

Workshop on Computational Biology Tools, Ithaca (November, 1999), invited speaker, lecturer:
1) *Protein structure prediction by means of threading and sequence alignments*
2) *Locally Enhanced Sampling for molecular dynamics and energy minimization*

International Conference on Optimization in Computational Chemistry and Molecular Biology, Princeton (May, 1999), speaker: *Novel folding potentials for efficient threading based on optimization with linear constraints*

Nagoya University (October, 1998), speaker: *Novel algorithms for electronic structure of molecules* (invited by Prof. S. Yamamoto)

Kyoto University (January, 1998), speaker: *Novel computational algorithms based on the CI method* (invited by Prof. H. Nakatsuji)

Paul Sabatier University, Toulouse (October, 1997), speaker: *Computer Simulations of Carbon Monoxide Photodissociation in Myoglobin* & *Size-consistent multireference CI method through the dressing of the norm of determinants* (invited by Prof. J-P. Malrieu)

Fritz Haber Center, Jerusalem (July, 1997), speaker: *Computer Simulations of Carbon Monoxide Photodissociation in Myoglobin: Structural Interpretation of the B state* (invited by Prof. B. Gerber)

8. **TEACHING**

Co-authored (with Dr. M. Wagner) a revised curriculum for the Dept. of Biomedical Engineering (BME) graduate program in bioinformatics, which is being implemented now.

In collaboration with Drs. M. Cushion and R. Brackenbury developed a revamped and extended (to include bioinformatics, computational biology and computer hands-on labs with the use of Protein Modeling Lab and other computer resources) Introduction to Functional Genomics course, UC, College of Medicine (JM, co-director); taught a block of four lectures (and computer labs) in 2002/2003, 2003/2004 as well as in 2004/2005 courses.

Proposed, developed and taught an Introduction to Bioinformatics and Advance Computational Biology courses (BME); developed web resources, course materials and electronic exams and quizzes enabling instant evaluation for the course (http://folding.chmcc.org/intro2bioinfo/intro2bioinfo.html).

In addition to lectures and other materials developed specifically for the courses described above, additional educational materials, lectures and web resources developed by JM are available at http://folding.chmcc.org/online/online.html and other Web pages developed and maintained by JM (see http://folding.chmcc.org).

At present, actively mentoring and supervising: one junior faculty, one postdoc, three Ph.D. students as advisor (BME program in bioinformatics) and two Ph.D. students as co-advisor.

9. **GRANTS AND CONTRACTS**

"Protein Modeling Laboratory"
Funded by the Ohio Board of Regents to Dr. R. Brackenbury (UC) and subcontracted to CCHMC with Jarek Meller coordinating and supervising the development of the Lab and its subsequent use for training, graduate education and research applications; approximately $90,000 for hardware, software and personnel support; Period: 2003-2005

"Annotation of Divergent Genomic Sequences"
Principal Investigator: Jarek Meller
Agency: Trustee Grant, Cincinnati Children's Hospital Research Foundation; Period: 2002-2004.

"Large-scale Integrated Analysis of Genomics Landscapes in JRA"
Principal Investigator: Sue Thompson, Co-PI: Jarek Meller (30% time effort)
Agency: National Institutes of Health (NIAMS, R01 AR050688); $426,228; Period: 2003-2007.

The major goals of this project are the development of new pattern recognition and data mining techniques applicable to large scale classification problem, in particular those arising in the context of Juvenile Rheumatoid Arthritis integrated studies with gene expression, polymorphisms and clinical data.

"Optimization of Folding and Threading Potentials"

Principal Investigator: Ron Elber, PI of the CCHMC subcontract: Jarek Meller (15% effort)
Agency: National Institutes of Health (NIHGM, 1 R01 GM67823-01A1); $150,929; Period: 2004-2008.

The major goals of this project are the development of large-scale optimization techniques and novel algorithms for protein structure prediction and for classification of genomic data. These algorithms are of interest also in the context of other projects, with the focus on analysis of multidimensional expression and clinical data pertaining to specific diseases.

Development of Genomics Research Center
Principal Investigator: John Pestian, co-I: Jarek Meller (5%); Period: 2002-2005
Ohio Board of Regents (BRTT)

"Gene Identification and Functional Annotations for the Pneumocystis Genome"
Principal Investigator: Jarek Meller (30% time effort)
Agency: National Institutes of Health (NIAID, 5 R21 AI055338-02); $300,000; Period: 2003-2006.

This project aims at unraveling the genome of a fungal pathogen Pneumocystis carinii by providing new algorithms and computational tools for gene identification and functional annotations, specifically tailored to the Pneumocystis genome. The clinical relevance lies in the potential to discover new drug targets and therapies that might improve the treatment of Pneumocystis pneumonia, especially in AIDS patients.

"Computational Medicine Center"
Consortium with UC, Principal Investigator: Thomas F. Boat; co-I: Jarek Meller (20% effort)
Ohio BRTT Partnership Award; $1,086,909; Period: 2004-2007

One of the central premises of the CMC grant is to facilitate (and subsequently capitalize on, also in the commercial sense) personalized therapeutic interventions based on predictive fingerprints of diseases states to be identified using advanced machine learning, pattern recognition and data mining approaches.

"Norwalk-like Viruses and Their Receptors"
Principal Investigator: Xi Jiang, co-PI: Jarek Meller (15% time effort)
Agency: National Institutes of Health (NIAID); $800,000; Period: 2005-2009

The major goals of this project are elucidating the interaction between Norwalk-like viruses (NLVs) with histo-blood group antigens and unraveling the structural determinants of strain-specific patterns of NLV binding to their antigen receptors.

10. **PEER-REVIEWED PUBLICATIONS**

10A. **Papers:**

1) B. G. Wybourne and **J. Meller**; *Enumeration of the order 14 invariants formed from the Riemann tensor*, **Journal of Physics, A: Mathematics and General**, 25 (1992)
2) W. Duch and **J. Meller**; *On multireference superdirect configuration interaction in third order*, **International Journal of Quantum Chemistry**, 50 (1994)

3) **J. Meller**, J. L. Heully and J. P. Malrieu; *Size-consistent self consistent combination of selected CI and perturbation theory*, **Chemical Physics Letters**, 218 (1994)
4) R. S. Ingarden and **J. Meller**; *Temperature in Linguistics as a Model of Thermodynamics*, **Open Systems and Informational Dynamics**, Vol. 2, No 2 (1994)
5) **J. Meller**, J. P. Malrieu and J. L. Heully; *Multireference size-consistent self-consistent CI method: a few applications to ground and excited states*, **Chemical Physics Letters**, 244, 440 (1995)
6) **J. Meller**, J.P. Malrieu and R. Caballol; *State-specific Coupled Cluster type dressing of Multireference Singles and Doubles Configuration Interaction matrix*, **Journal of Chemical Physics**, 104, 4068 (1996)
7) L. Adamowicz, R. Caballol, J.P. Malrieu and **J. Meller**; *A general bridge between CI and CC methods: a multistate solution*, **Chemical Physics Letters**, 259, 619 (1996)
8) **J. Meller** and R. Elber; *Computer Simulations of Carbon Monoxide Photodissociation in Myoglobin: Structural Interpretation of the B states*, **Biophysical Journa**l, 74, 789-802 (1998)
9) M. Turowski, N. Yamakawa, **J. Meller**, K. Kimata, T. Ikegami, K. Hosoya and N. Tanaka; *Deuterium isotope effect in chromatography as examined by various HPLC systems. Comments on the retention and H/D differentiation mechanism*, **Chromatography**, 19 (1998)
10) R. Elber, **J. Meller** and R. Olender; *Stochastic Path Approach to Compute Atomically Detailed Trajectories: Application to the Folding of C Peptide*, **Journal of Physical Chemistry B**, 103, 899-911 (1999)
11) **J. Meller** and W. Duch; *SGA derivation of matrix elements between spin-adapted perturbative wavefunctions*, **International Journal of Quantum Chemistry**, 74, 123-133 (1999)
12) A. Frary, T. C. Nesbitt, A. Frary, S. Grandillo, E. van der Knaap, B. Cong, J. Liu, **J. Meller**, R. Elber, K. B. Alpert, S. D. Tanksley; *fw2.2: A Quantitative Trait Locus Key to the Evolution of Tomato Fruit Size*, **Science**, 289: 85-88 (2000)
13) Wan J, **Meller J**, Hada M, Ehara M, Nakatsuji H; *Electronic excitation spectra of furan and pyrrole: Revisited by the symmetry adapted cluster-configuration interaction method*, **Journal of Chemical Physics**, 113: 7853-7866 (2000)
14) **J. Meller**, R. Elber; *Linear Optimization and a Double Statistical Filter for Protein Threading Protocols*, **Proteins: Structure, Function and Genetics**, 45: 241-261 (2001)
15) **J. Meller**, M. Wagner, R. Elber; *Maximum Feasibility Guideline to the Design and Analysis of Protein Folding Potentials*, **Journal of Computational Chemistry**, 23: 111-118 (2002)
16) A. V. Kuznetsova, **J. Meller**, P. O. Schnell, J. A. Nash, Y. Sanchez, J. W. Conaway, R. C. Conaway and M. F. Czyzyk-Krzeska; *VHL binds hyperphosphorylated large subunit of RNA Polymerase II through a proline hydroxylation motif and targets it for ubiquitination*, **PNAS** vol. 100 (5), 2706-2711 (2003)
17) **J. Meller**, J. P. Malrieu and J. L. Heully; *Size-consistent multireference CI through the dressing of the norm of determinants*, **Molecular Physics**, vol. 101 (13), 2029-2041 (2003)
18) M. Turowski, N. Yamakawa, **J. Meller**, K. Kimata, T. Ikegami, K. Hosoya, N. Tanaka and E.R. Thornton; *Deuterium Isotope Effects on Hydrophobic Interactions. The Importance of Dispersion Interactions in the Hydrophobic Phase*, **Journal of American Chemical Society**, 125: 13836-13849 (2003)
19) M. Tan, P. Huang, **J. Meller**, W. Zhong, T. Farkas and X. Jiang; *Mutations within P2 Domain of Norovirus Capsid Affect Binding to Human Histo-Blood Group Antigens: Evidence for a Binding Pocket*, **Journal of Virology**, 77 (23): 12562-71 (2003)

20) M. Wagner, **J. Meller** and R. Elber; *Large-Scale Linear Programming Techniques for the Design of Protein Folding Potentials*, **Mathematical Programming**, vol. 101 (2): 301-318 (2004)
21) M. F. Czyzyk-Krzeska and **J. Meller**; *Von Hippel-Lindau Tumor Suppressor: Not Only HIF's Executioner*, **Trends in Molecular Medicine**, vol. 10 (4), 146-149 (2004)
22) R. Adamczak, A. Porollo and **J. Meller**; *Accurate Prediction of Solvent Accessibility Using Neural Networks Based Regression*, **Proteins: Structure, Function and Bioinformatics**, 56(4):753-67 (2004)
23) R. Adamczak and **J. Meller**; *On the Transferability of Folding and Threading Potentials and Sequence-Independent Filters for Protein Folding Simulations*, **Molecular Physics**, vol. 102 (11-12): 1291-1305 (2004)
24) M.-D. Filippi, C. E. Harris, **J. Meller,** Y. Zheng and D. A. Williams; *Localization of Rac2 Specifies Superoxide Generation, Actin Polarity and Chemotaxis in Neutrophils*, **Nature Immunology** 5, 744 - 751 (2004)
25) A. Porollo, R. Adamczak and **J. Meller**; *Polyview: A Flexible Visualization Tool for Structural and Functional Annotations of Proteins*, **Bioinformatics**, vol. 20 (15): 2460-62 (2004)
26) R. Adamczak, A. Porollo and **J. Meller**; *Combining Prediction of Secondary Structures and Solvent Accessibility in Proteins*, **Proteins: Structure, Function and Bioinformatics**, 59(3): 467-75 (2005)
27) M. Wagner, R. Adamczak, A. Porollo and **J. Meller**; *Linear Regression Models for Solvent Accessibility Prediction in Proteins*, **Journal of Computational Biology**, Vol. 12 (3): 355-369 (2005)
28) C. E. Petre-Draviam, E. B.Williams, C. J. Burd, A. Gladden, H. Moghadam, **J. Meller**, J. A. Diehl, and K. E. Knudsen; *A Central Domain of Cyclin D1 Mediates Nuclear Receptor Co-repressor Activity*, **Oncogene**, 24(3): 431-44 (2005)
29) V. V. Ivanenko, **J. Meller**, and T. L. Kirley; *Characterization of disulfide bonds in human nucleoside triphosphate diphosphohydrolase 3 (NTPDase3): implications for NTPDase structural modeling*, **Biochemistry**, 44(25):8998-9012 (2005)
30) B. Cao, A. Porollo, R. Adamczak, M. Jarrell and **J. Meller**; *Enhanced Recognition of Protein Transmembrane Domains*, **Bioinformatics**, 22 (3): 303-309 (2006)
31) W. Duch, K. Swaminathan and **J. Meller**; *Artificial Intelligence Approaches for Rational Dug Design and Discovery*, **Pharmaceutical Design**, to appear (2006)
32) M. Tan, **J. Meller** and X. Jiang; *The C-Terminal Arginine Cluster Is Essential for Receptor-Binding of Norovirus*, **Journal of Virology**, to appear (2006)
33) A. Porollo and **J. Meller**; *Prediction-based Fingerprints of Protein-protein Interactions*, **Proteins: Structure, Function and Bioinformatics**, to appear (2006)

10B. **Books, chapters and encyclopedia articles:**

1) **J. Meller**, *Molecular Dynamics*, in **Encyclopedia of Life Sciences**, http://www.els.net (on-line), ISBN 0-333-72621-9 (print), Nature Publishing Group, 2001 Macmillan Publishers Ltd
2) With updates and modifications published also as: **J. Meller**, *Molecular Dynamics*, in **Encyclopedia of the Human Genome**, Nature Publishing Group 2003
3) **J. Meller**, R. Elber; *Protein Recognition by Sequence-to-Structure Fitness: Bridging Efficiency and Capacity of Threading Models*, in **Computational Methods for Protein Folding**: A Special Volume of Advances in Chemical Physics, ed. R. A. Friesner, John Wiley & Sons 2002

4) **J. Meller**, *Advances in Protein Structure Predictions: Algorithms and Applications*, IBIB, Polish Academy of Sciences, ISSN 0239-7455, Warsaw 2004

10C. **Selected Conference papers:**

5) **J. Meller**, *Protein Recognition by Sequence-to-Structure Fitness: from Design of Scoring Functions to Biological Discovery*, in Lecture Notes of the ICB Seminars: Statistics and Clinical Practice, ed. L. Bobrowski, Warsaw 2002
6) A. Porollo, R. Adamczak, M. Wagner and **J. Meller**; *Maximum Feasibility Approach for Consensus Classifiers: Applications to Protein Structure Prediction*, Proceedings of The Second International Conference on Computational Intelligence, Robotics and Autonomous Systems, CIRAS 2003
7) B. E. Slaven, A. Porollo, T. Sesterhenn, A. G. Smulian, M. T. Cushion and **J. Meller**; *Large-Scale Characterization of Introns in the Pneumocystis carinii Genome*, Journal of Eukaryotic Microbiology, to appear (2006)
8) B. E. Slaven, **J. Meller**, A. Porollo, T. Sesterhenn, A. G. Smulian, and M. T. Cushion; *Draft Assembly and Annotation of the Pneumocystis carinii Genome*, Journal of Eukaryotic Microbiology, to appear (2006)
9) **J. Meller**, R. Adamczak, M. P. Scola, M. Barnes, S. D. Thompson, M. H. Passo, H. I. Brunner, D. N. Glass, and A. A. Grom; *Machine Learning Analysis of Expression Profiles of Synovial Tissue Cytokines Helps Identify Patients with Systemic Onset Juvenile Rheumatoid Arthritis*, in **Applications of Statistical and Machine Learning in Bioinformatics**: a volume in the series Advances in Computational and Systems Biology, eds. J. Meller and W. Nowak, Peter Lang, to appear (2006)
10) B. Cao, M. Medvedovic, and **J. Meller**; *Prediction of Transmembrane Domains and Pore-facing Residues in Beta-barrel Membrane Proteins*, in **Applications of Statistical and Machine Learning in Bioinformatics**: a volume in the series Advances in Computational and Systems Biology, eds. J. Meller and W. Nowak, Peter Lang, to appear (2006)

10D. **Assessment of the impact of selected publications**

The following table includes selected publications that had been cited at least twice as many times as the impact factor of the journal they were published in (in other words these are publications with an impact that appears to be higher than an average impact of papers published in a given journal). Acronyms used in the table: IF – *impact factor* of a journal (according to http://www.bioreference.net/impact/if2002c.htm), NoC – the number of citations as of October 2006 according to the Science Citation Index (excluding self-citations by JM but not necessarily by all other co-authors).

No.	Authors, title, journal, issue, year	IF	NoC
1	W. Duch and **J. Meller**; *On multireference superdirect configuration interaction in third order*, **International Journal of Quantum Chemistry**, 50 (1994)	1.5	5
2	**J. Meller**, J. P. Malrieu and J. L. Heully; *Multireference size-consistent self-consistent CI method: a few applications to ground and excited states*, **Chemical Physics Letters**, 244, 440 (1995)	2.5	21
3	**J. Meller**, J.P. Malrieu and R. Caballol; *State-specific Coupled Cluster type dressing of Multireference Singles and Doubles Configuration Interaction matrix*, **Journal of Chemical Physics**, 104, 4068 (1996)	3.0	41
4	L. Adamowicz, R. Caballol, J.P. Malrieu and **J. Meller**; *A general bridge between CI and CC methods: a multistate solution*, **Chemical Physics Letters**, 259, 619 (1996)	2.5	7
5	**J. Meller** and R. Elber; *Computer Simulations of Carbon Monoxide Photodissociation in Myoglobin: Structural Interpretation of the B states*, **Biophysical Journal**, 74, 789-802 (1998)	4.6	28
6	R. Elber, **J. Meller** and R. Olender; *Stochastic Path Approach to Compute Atomically Detailed Trajectories: Application to the Folding of C Peptide*, **Journal of Physical Chemistry B**, 103, 899-911 (1999)	3.6	52
7	A. Frary, T. C. Nesbitt, A. Frary, S. Grandillo, E. van der Knaap, B. Cong, J. Liu, **J. Meller**, R. Elber, K. B. Alpert, S. D. Tanksley; *fw2.2: A Quantitative Trait Locus Key to the Evolution of Tomato Fruit Size*, **Science**, 289: 85-88 (2000)	29.0	251
8	Wan J, **Meller J**, Hada M, Ehara M, Nakatsuji H; *Electronic excitation spectra of furan and pyrrole: Revisited by the symmetry adapted cluster-configuration interaction method*, **Journal of Chemical Physics**, 113: 7853-7866 (2000)	3.0	31
9	**J. Meller**, R. Elber; *Linear Optimization and a Double Statistical Filter for Protein Threading Protocols*, **Proteins: Structure, Function and Genetics**, 45: 241-261 (2001)	4.1	51
10	**J. Meller**, M. Wagner, R. Elber; *Maximum Feasibility Guideline to the Design and Analysis of Protein Folding Potentials*, **Journal of Computational Chemistry**, 23: 111-118 (2002)	2.9	12
11	A. V. Kuznetsova, **J. Meller**, P. O. Schnell, J. A. Nash, Y. Sanchez, J. W. Conaway, R. C. Conaway and M. F. Czyzyk-Krzeska; *VHL binds hyperphosphorylated large subunit of RNA Polymerase II through a proline hydroxylation motif and targets it for ubiquitination*, **PNAS** vol. 100 (5), 2706-2711 (2003)	10.1	57
12	M. Turowski, N. Yamakawa, **J. Meller**, K. Kimata, T. Ikegami, K. Hosoya, N. Tanaka and E.R. Thornton; *Deuterium Isotope Effects on*	6.2	22

	Hydrophobic Interactions. The Importance of Dispersion Interactions in the Hydrophobic Phase, **Journal of American Chemical Society**, 125: 13836-13849 (2003)		
13	M. Tan, P. Huang, **J. Meller**, W. Zhong, T. Farkas and X. Jiang; *Mutations within P2 Domain of Norovirus Capsid Affect Binding to Human Histo-Blood Group Antigens: Evidence for a Binding Pocket*, **Journal of Virology**, 77 (23): 12562-71 (2003)	5.2	15
	Most recent publications (last two years) with a limited data regarding the number of citations:		
15	M. F. Czyzyk-Krzeska and **J. Meller**; *Von Hippel-Lindau Tumor Suppressor: Not Only HIF's Executioner*, **Trends in Molecular Medicine**, vol. 10 (4), 146-149 (2004)	7.2	8
16	M. Wagner, **J. Meller** and R. Elber; *Large-Scale Linear Programming Techniques for the Design of Protein Folding Potentials*, **Mathematical Programming**, vol. 101 (2): 301-318 (2004)	1.2	5
17	R. Adamczak, A. Porollo and **J. Meller**; *Accurate Prediction of Solvent Accessibility Using Neural Networks Based Regression*, **Proteins: Structure, Function and Bioinformatics**, 56(4):753-67 (2004)	4.1	25
18	A. Porollo, R. Adamczak and **J. Meller**; *Polyview: A Flexible Visualization Tool for Structural and Functional Annotations of Proteins*, **Bioinformatics**, vol. 20 (15): 2460-62 (2004)	4.6	3
19	M.-D. Filippi, C. E. Harris, **J. Meller,** Y. Zheng and D. A. Williams; *Localization of Rac2 Specifies Superoxide Generation, Actin Polarity and Chemotaxis in Neutrophils*, **Nature Immunology**, 5, 744 - 751 (2004)	27.9	26
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21	C. E. Petre-Draviam, E. B.Williams, C. J. Burd, A. Gladden, H. Moghadam, **J. Meller**, J. A. Diehl, and K. E. Knudsen; *A Central Domain of Cyclin D1 Mediates Nuclear Receptor Co-repressor Activity*, **Oncogene**, 24(3): 431-44 (2005)	6.0	5
22	R. Adamczak, A. Porollo and **J. Meller**; *Combining Prediction of Secondary Structures and Solvent Accessibility in Proteins*, **Proteins: Structure, Function and Bioinformatics**, 59(3): 467-75 (2005)	4.1	5
23	M. Wagner, R. Adamczak, A. Porollo and **J. Meller**; *Linear Regression Models for Solvent Accessibility Prediction in Proteins*, **Journal of Computational Biology**, Vol. 12 (3): 355-369 (2005)	3.5	2
24	V. V. Ivanenko, **J. Meller**, and T. L. Kirley; *Characterization of disulfide bonds in human nucleoside triphosphate diphosphohydrolase 3 (NTPDase3): implications for NTPDase structural modeling*, **Biochemistry**, 44(25):8998-9012 (2005)	3.9	2
25	B. Cao, A. Porollo, R. Adamczak, M. Jarrell and **J. Meller**; *Enhanced Recognition of Protein Transmembrane Domains*, **Bioinformatics**, 22 (3): 303-309 (2006)	4.6	-

A total of 631 citations as of September 2006 (without excluding self-citations, annual breakdown included below).

Publication Year	Record Count	% of 631	
2005	147	23.2964 %	23.2964%
2004	117	18.5420 %	18.5420%
2006	103	16.3233 %	16.3233%
2003	81	12.8368 %	12.8368%
2002	79	12.5198 %	12.5198%
2001	49	7.7655 %	7.7655%
2000	16	2.5357 %	2.5357%
1999	14	2.2187 %	2.2187%
1998	10	1.5848 %	1.5848%
1996	7	1.1094 %	1.1094%
1997	4	0.6339 %	0.6339%
1994	3	0.4754 %	0.4754%

10E. **Quality review of selected works:**

1) A. Frary, T. C. Nesbitt, A. Frary, S. Grandillo, E. van der Knaap, B. Cong, J. Liu, **J. Meller**, R. Elber, K. B. Alpert, S. D. Tanksley; *fw2.2: A Quantitative Trait Locus Key to the Evolution of Tomato Fruit Size*, **Science**, 289: 85-88 (2000).

   A plant gene, which regulates the tomato fruit size, was predicted by JM in collaboration with R. Elber (using the LOOPP protocol) to share a 3D structure with human Ras (oncogene) proteins, suggesting an evolutionary link between genesis of tumors and control of cell division in humans and development and growth of a plant fruit. This paper was included in highlights in Science, was also discussed in many popular publications (e.g. Associated Press interviewed JM on that occasion). The article was cited more than 200 times as of Sep. 2005. The discovery and the role of the LOOPP protocol was also described in the textbook in genomics: "*A Primer of Genome Science*" by G. Gibson and S. V. Muse, Sinauer Associates, Inc. Publishers, 2002.

2) **J. Meller**, R. Elber; *Linear Optimization and a Double Statistical Filter for Protein Threading Protocols*, **Proteins: Structure, Function and Genetics**, 45: 241-261 (2001) & **J. Meller** and R. Elber, *LOOPP – Learning, Observing and Outputting Protein Patterns* (2000), http://cbsu.cornell.edu/software/loopp, a public domain package for protein recognition and design of folding potentials, available as part of NIH resources at the Cornell Theory Center.

   The LOOPP protein recognition protocol had been described in an invited book chapter published in the prestigious series of the Advances of Chemical Physics. However, as it is most of the time cited as an electronic link rather than a citation to a paper (which has been cited 33 times so far), the overall impact of the server is presented here. During the second edition of the Critical Assessment of Fully Automated protein Structure Prediction (CAFASP2) LOOPP was ranked as the third best server in the category of targets with distant homology to known proteins. LOOPP was also included among the eight servers described in the paper summarizing CAFASP2 competition. There were more than 20,000 submissions to the server from more than 5,000 different researchers (data collected by the Cornell Theory Center).

3) R. Elber, **J. Meller** and R. Olender; *Stochastic Path Approach to Compute Atomically Detailed Trajectories: Application to the Folding of C Peptide*, **Journal of Physical Chemistry B**, 103, 899-911 (1999)

   Explicit simulations of protein folding, while clearly a desired milestone in structural genomics because of the importance of structural and kinetic aspects of protein folding, remain a challenging problem. The basic difficulty with attacking this problem is that of time scales. Using the novel path integral based simulation technique for long time dynamics introduced by R. Elber and extended in this paper to systems in solution with separation of subsystems with different intrinsic time scales, it became possible to study folding of the smallest α-helical peptide. In extensive parallel simulations early nucleation events in the folding and the formation of the helical structure in the C peptide were observed for the first time. The article was cited 32 times as of Sep. 2004.

4) **J. Meller**, J.P. Malrieu and R. Caballol; *State-specific Coupled Cluster type dressing of Multireference Singles and Doubles Configuration Interaction matrix*, **Journal of Chemical Physics**, 104, 4068 (1996)

   In collaboration with J. P. Malrieu and R. Caballol, JM proposed a novel state-specific multi-reference coupled cluster-type method for ground and excited electronic states of molecules that opened new directions in the search for efficient and correctly scaling with size algorithms for excited states of large molecular systems. This paper represents JM's contributions to the field of quantum chemistry and was cited 33 times as of Dec. 2004, which is a relatively high number for methodological developments in this field.

5) R. Adamczak, A. Porollo and **J. Meller**; *Accurate Prediction of Solvent Accessibility Using Neural Networks Based Regression*, **Proteins: Structure, Function and Bioinformatics**, 56(4):753-67 (2004)

   Even though this paper was published in 2004, the related protein structure prediction server SABLE has become relatively widely used since its inception in 2003, allowing one to assess the impact of this work. In particular, the SABLE server uses a novel regression-based (rather than classification-based) approach to relative solvent accessibility prediction (RSA) that was introduced in this paper. RSA is one of important intermediate attributes of amino acid residues in proteins, that if known can be used to enhance folding simulations and protein structure prediction. According to our rigorous tests, SABLE is currently the most accurate RSA prediction method. Several groups used SABLE in the recent CASP6 competition. The improved secondary structure prediction in SABLE was also shown in independent evaluation by the EVA meta-server (http://cubic.bioc.columbia.edu/eva/sec/res_sec.html) to achieve the state-of-the-art accuracy. So far, there have been more than 70,000 submissions to the SABLE server from over 1,200 users and more than 20,000 submissions from over 1,700 users to the related POLYVIEW server.

6) A. V. Kuznetsova, **J. Meller**, P. O. Schnell, J. A. Nash, Y. Sanchez, J. W. Conaway, R. C. Conaway and M. F. Czyzyk-Krzeska; *VHL binds hyperphosphorylated large subunit of RNA Polymerase II through a proline hydroxylation motif and targets it for ubiquitination*, **PNAS** vol. 100 (5), 2706-2711 (2003)

   RNA Polymerase II is the major transcription complex in eukaryotes, which interacts with many co-factors in larger transcription initiation and transcription elongations complexes (with transformation between the two stages being dependent among other things on post-translation modifications). In this paper (JM one of the two first authors), in collaboration with the group of Dr. Czyzyk-Krzeska, we show that the tumor suppressor pVHL binds the largest subunit of RNA Pol II and targets it for ubiquitination. The interaction between pVHL and the largest subunit of RNA Pol II was first predicted computationally, using sequence-to-structure matching and other modeling approaches, and then confirmed experimentally in Dr. Czyzyk-Krzeska's Lab. These new findings shed light onto the potential VHL-dependent role of hypoxia in the regulation of transcription, opening an exciting new avenue in the studies on hypoxia and cancer. Despite the fact that this paper was published recently, it has already been cited more than 50 times.

References: available upon request