11/9/15

Ilya Vakser, Ph.D.

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785-766-7152 (cell), Fax: 785-864-5558
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Home: 1625 N First St, Baldwin City, KS 66006; Phone: 785-594-3043
Citizenship: United States
Personal: Married, 2 children

EXPERIENCE

2005 – pres. Director and Professor, Computational Biology Program and Center for Computational Biology (Bioinformatics, until 2014), University of Kansas
Professor, Department of Mol. Biosciences, University of Kansas, Lawrence, KS

2001 – 2004 Associate Professor (tenured), Bioinformatics Laboratory, Department of Applied Mathematics and Statistics, SUNY at Stony Brook, Stony Brook, NY
Adjunct Associate Professor, Department of Biochemistry and Cell Biology, SUNY at Stony Brook, Stony Brook, NY
Investigator, Brookhaven National Laboratory, Upton, NY

1997 – 2001 Associate Professor (2000-2001), Assistant Professor (1997-2000), Department of Cell and Molecular Pharmacology, Medical University of South Carolina, Charleston, SC

1995 - 1997 Research Associate, The Rockefeller University, New York, NY

1993 - 1995 Postdoctoral Assoc., Center for Mol. Design, Washington University, St. Louis, MO

1990 - 1993 Research Fellow, Dept. of Biophysics, Weizmann Inst. of Science, Rehovot, Israel

1982 - 1989 Research Assistant/Junior Scientist, Genetics Research Institute, Minsk, Belarus

EDUCATION

Post PhD: Washington University, St. Louis, MO; Rockefeller University, New York, NY
PhD, biophysics: Moscow State University, Russia, 1989
MS, physics: Belarus State University, Belarus, 1982

MEMBERSHIP IN PROFESSIONAL SOCIETIES

Current
American Association for the Advancement of Science
American Chemical Society
Biophysical Society
The Protein Society

Past
The New York Academy of Sciences
Sigma Xi

SELECT HONORS AND AWARDS

Fellow of American Association for the Advancement of Science (AAAS)
Leading Light award, University of Kansas, 2012, 2013
Chancellor's service recognition award, University of Kansas, 2010
Feinberg Fellow, Weizmann Institute of Science, 1991-1992

FUNDING

Current

NIH R01 GM074255, Vakser (PI), $1,142,506 (2013-2017 budget period), 03/01/05-08/31/17
Integrated resource for protein recognition studies

NSF DBI 1262621, Vakser (PI), $757,958, 09/01/13-08/31/16
Target-template structural and functional relationships in modeling of protein-protein interactions

NSF CNS 1337899, Huan (PI), Vakser (Co-PI), $700,000, 08/01/13-07/31/16
MRI Acquisition of computing equipment to support data-intensive bioinformatics research at the University of Kansas

NIH T32GM008359, Siahaan (PI), $2,096,732 (current budget period), 7/1/07-6/30/19
Pharmaceutical aspects of biotechnology training

Pending

NSF DBI 1565107, Vakser (PI), $ 873,278, 09/01/16-08/31/19
Bilateral BBSRC-NSF/BIO: Modeling protein interactions to interpret genetic variation

Past

NSF MCB 1158469, Rivera (PI), $615,503, 6/1/12-5/31/15
Protein interactions in the utilization of iron by pathogenic bacteria

NIH R01GM074255-05S1, Vakser (PI), $148,828, 09/01/09-08/31/11
Integrated resource for protein recognition studies

NIH R01 GM61889, Vakser (PI), $819,300, 08/01/00-08/31/05
Docking in large databases of modeled proteins

NSF DBI 9808093, Vakser (PI), $309,152, 09/15/98-08/31/02
Development of GRAMM method and software for protein-protein docking

South Carolina Commission on Higher Education, Vakser (PI), $73,609, 01/01/00-07/31/01
Predicting protein interactions in structural bioinformatics

NSF DBI 0097883, Vakser (PI), $25,000, 05/31/01-12/31/03
Conference: Modeling of Protein Interactions in Genomes

DOE, Vakser (PI), $10,000, 09/15/00-09/14/01
Conference: Modeling of Protein Interactions in Genomes

NIH P20RR017708, Hanzlik (PI), $30,000, 04/01/10-03/31/12
Dynamics and interprotein interactions in the release of iron stored in bacterioferritin

NIH R13 Vajda (PI), $5,000, 09/01/07-08/31/08
Conference on Modeling of Protein Interactions

NIH R13 GM 075726, Vajda (PI), $5,000, 05/01/05-04/30/06
Conference on Modeling of Protein Interactions in Genomes

NIH R01 CA78887, Rosenzweig (PI), $1,281,195, 04/01/00-03/31/05
Inhibition of IGF mediated tumorigenesis

NIH R01 EY08239, Knapp (PI), $1,015,854, 12/01/99-11/30/03
Structural studies of visual transduction proteins

NIH R13 GM063722, Vajda (PI), $5,000, 05/01/01-04/30/02
Conference: Modeling of Protein Interactions in Genomes

Belarusian Foundation for Fundamental Research, Tuzikov (PI), 04/01/08-03/31/12
Protein structure alignment and prediction of protein interactions

NSF/EPSCoR, $1,392,346, 7/1/96-7/31/00
Interdisciplinary Program in Signal Transduction

NSF DBI 9732152, $50,000, 06/15/98-05/31/01
REU Site in Cellular Signal Transduction

Ministry of Science and Technology, Israel, Vakser (PI), $120,000, 1991-93
Design of k-opiate receptor agonists as a basis for novel analgesic drugs

Ministry of Integration Fellowship, Israel; 1992-93

Feinberg Fellowship, Israel; 1991-92

COMMITTEES

International

Advisory Board for Drug Design & Med. Chem. Conf., Berlin, Germany, Member, 2015 – 2016
Conference on Modeling of Protein Interactions, Organizer, 2000 – present
Critical Assessment of Predicted Interactions (CAPRI) Initiative Group, Chairman, 2001
Crit. Assessment of Predict. Inter. (CAPRI) Management Committee, Member, 2002 – present
Organizing Committee of CAPRI Meeting, Utrecht, the Netherlands, Member, 2012 – 2013
Program Committee of CAPRI Evaluation Meeting, Toronto, Canada, Member, 2006 – 2007
American Chemical Society, Protein Interactions Symposium, Organizer, 2010 – 2011
Health Informatics &Technology Conference, Organizing Committee Member, 2014 (declined)
Program Cmte Intelligent Syst. Mol. Biol. & European Conf. Comp. Biol., Member, 2007 – present
Biomedical Engineering Society Annual Symposium Program Committee, Member, 2015
GTC Drug Design & Med. Chem. (Europe) Conf., Advisory Board Member, 2013 (declined)
Journal of Advances Applic. Bioinformatics Chem., Editorial Board Member, 2008 – present
Journal of Open Access Bioinformatics, Editorial Board Member, 2009 – present
Agency for Science, Research & Technology, Singapore, 2014
National Science Center, Poland, Reviewer, 2012 – present
Science Foundation of Ireland, Reviewer, 2012
PLoS Computational Biology, guest Associate Editor, 2008
Intl. Program Committee for Conf. on Advanced Inform. Tech. for Health, Belarus, Member, 2008
Institute of Physics, Chinese Academy of Science, Evaluator, 2007
United States-Israel Bi-national Science Foundation, Board of Reviewers, Reviewer, 2002 – pres.
Israel Science Foundation, Board of Reviewers, Reviewer, 2002 – present
Indo-US Science & Technology Forum, Reviewer, 2010 – 2011
Wellcome Trust, Reviewer, 2004 – 2005
Protein Information Resource (PIR) - Expert Scientific Council, Consultant, 2000 – 2005
International Business Communications USA Conf., Advisory Board, Member, 1995– 1996

National

NIH ZRG1 BCMB-U (40) P01 Program Project Review, Member, 2015
NIH Macromolecular Struct. & Function MSFD Study Section, Member (ad hoc), 2007 – 2014
NIH NIAID Modeling Immunity for Biodefense ZAI1 QV-I (J3) 1 Study Section, Member, 2014
NIH NIGMS Complex Phenotypes ZGM1 GDB-7 (CP) Study Section, Member, 2012
NIH Small Business: Biol. Chem. Biophysics and Drug Discovery Study Section, Member, 2012
NIH NIAID Struct. Genom. Centers for Infectious Diseases Study Section, Member, 2011– 2012
NIH NIGMS PSI Centers for High-Throughput Struct Determination Study Section, Member, 2010
NIH NCI Centers of Cancer Nanotechnology Study Section, Member, 2010
NIH NCI Intramural Review and site visit, Member, 2006, 2010
NIH Special Topic in Bioengineering ZRG1 BST-J (03) M Study Section, Member, 2009
NIH RCMI COBRE Study Section, Member, 2008 – 2009
NIH Challenge grants ZRG1 BCMB-P (58) Study Section, Member, 2009
NIH Challenge grants ZRG1 BST-M (58) Study Section, Member, 2009
NIH Computational Biophysics BCMB Study Section, Member, 2006 – 2007
NIH Protein Structure Initiative CBB-3 Study Section, Member, 2005 – 2006
NIH Biochemistry and Biophysics Fellowship F04B Study Section, Member, 2005 – 2007
NIH Minority Biomedical Research Support MBRS Study Section, Member, 2003 – 2004
NIH NCRR P41 Review and site visit, Member, 2006
NIH/NSF Mathematical Biology Study Section, Member, 2004 – 2005
NSF, Advances in Biological Informatics Review Panel, Member, 2014
NSF, Board of Reviewers, Reviewer, 2000 – present
NSF, Computational Biology Activities Review Panel, Member, 1999
DOE, Genomes to Life Advisory Group, Member, 2002
DOE, Structural Biology Review Panel, Member, 2000
Department of Veteran Affairs, Board of Reviewers, Reviewer, 2000

Regional/Institutional

Kansas City Area Life Sci. Institute Bioinformatics Steering Committee, Member, 2013 – present
NIH COBRE Center for Translational Bioinformatics Steering Committee, Member, 2013
State of Kansas Bioscience and Innovation Roadmap, Team Member, 2005 – 2009
Kansas City Proteomics Consortium, Member, 2005 – 2008
Nebraska Research Initiative, Reviewer, 2008
University of Wyoming, External Advisory Committee for INBRE Program (declined)
Louisiana Board of Regents, Research Grants Review Committee (declined)

University

Medical University of SC
Bioinformatics Program Committee, Chairman, 1999 – 2001
Pharmacology Graduate Training Committee, Member, 1999 – 2001
Bioinformatics Seminar Series, Organizer, 1998 – 2001
Structural Biology Track Committee, Member, 1998 – 2001
Informatics Curriculum Committee, Member, 1998 – 2001
Information Technology Committee, Member, 1998 – 2001
Biomolecular Computing Resource Advisory Committee, Member, 1999 – 2001
Institutional Research Funds, Member, 2000 – 2001
University Research Council, Board of Reviewers, Reviewer, 2000
Computational Biology and Bioinformatics Faculty Search Committee, Member, 2000 – 2001
Thesis Advisory Committee for PhD students, Member, 2000 – 2002

SUNY Stony Brook
Bioinformatics Graduate Program Committee, Chairman, 2001 – 2002

Biomathematics Hiring Committee, Member, 2001 – 2005
Postdoc Hiring Committee, Member, 2001 – 2005
Bioinformatics and Computational Biology Seminar Series, Organizer, 2002 – 2005
Biocomputing Program Initiative, Member, 2001 – 2003

University of Kansas
Bioinformatics Faculty Search Committee, Chairman, 2004 – 2014
Bioinformatics Sabbatical Leave Committee, Member, 2012
Bioinformatics Coordinating Committee, Member, 2004 – 2006
Bioinformatics Graduate Program Development Committee, Chairman, 2005 – 2009
Comp. Biol. (Bioinformatics) Graduate Program Admission Committee, Member, 2009 – present
Comp. Biol. (Bioinformatics) Graduate Program Executive Committee, Member, 2009 – present
Thesis Advisory Committees for PhD students, Member, 2005 – present
Advisory Committee to Molecular Biosciences Graduate Admission, Member, 2006 – present
Molecular Biosciences Industry Consortium Committee, Member, 2012 – present
Molecular Biosciences Promotion & Tenure Cmte for Full Professors, Member, 2014 – present
Molecular Biosciences Awards Committee, Member, 2014 – 2015
Mallinckrodt Foundation Internal Review Committee, Member, 2015
NSF MRI Internal Review Committee, Member, 2014
Pew Review Committee, Member, 2012
Genomics development at KU group, Member, 2013 – present

PROGRAMS AND CENTERS

Medical University of SC
Hollings Cancer Center, Member, 2000 – 2001
Graduate College, Member, 1997 – 2001

SUNY Stony Brook
Biomedical Engineering Graduate Program, Member, 2002 – 2004
Biochemistry and Structural Biology Graduate Program, Member, 2003 – 2004
Center for Molecular Toxicology, Member, 2001 – 2004

University of Kansas
Computational Biology (Bioinformatics) Program, Director, 2005 – present
Bioengineering Graduate Program, Member, 2006 – present
Biotechnology Graduate Training Program, Member, 2007 – present

TEACHING

Medical University of SC
Course Director: Protein Modeling and Structural Bioinformatics, PCOL-745
Lecturer: Drug-Receptor Interaction, PCOL-734
Lecturer: Molecular Genetics
Lecturer: Special Topics in Computational Biology

SUNY Stony Brook
Course Director: Structural Bioinformatics, AMS-691
Course Director: Linear Algebra, AMS-210
Lecturer: Introduction to Computational Biology, CSE-549
Lecturer: Biochemistry, MCB-520

University of Kansas
Lecturer: Bioinformatics Core, BINF-701
Lecturer: Bioinformatics Core, BINF-702
Lecturer: Introduction to Biomedical Engineering, CPE 656/756

PEOPLE IN THE LAB

Total number of postdocs sponsored: 17
Total number of graduate students advised: 13

REFEREEING JOURNALS / BOOKS

ACS Chemical Biology, Annals of Biomedical Engineering, Annual Review & Research in Biology, Biochemistry, Bioinformatics, Biomacromolecules, Biomedical Engineering and Computational Biology, Biophysical Journal, Biopolymers, BMC Bioinformatics, BMC Biophysics, BMC Genomics, BMC Structural Biology, BMC Systems Biology, Briefings in Bioinformatics, Cellular & Molecular Biology Letters, Chemical Physics Letters, Chemical Reviews, Computational Biology and Chemistry: Advances and Applications, Computational Methods for Protein Structure Prediction and Modeling Springer-Verlag, Computational Molecular Biology Series MIT Press, Critical Reviews in Biochemistry and Molecular Biology, Current Medicinal Chemistry, Current Opinion in Structural Biology, Current Pharmaceutical Biotechnology, Current Pharmaceutical Design, eLife, Experimental and Computational Cell Biology Series Kluwer Academic Publishers, FEBS Journal, FEBS Letters, Genome Research, IEEE Decision and Control Proceedings, IEEE/ACM Transactions on Computational Biology and Bioinformatics, In Silico Biology, International Journal of Molecular Sciences, International Journal of Robotics Research, ISMB Proceedings, Journal of Bioinformatics and Computational Biology, Journal of Biomolecular Structure & Dynamics, Journal of Biosciences, Journal of Chemical Information and Modeling, Journal of Chemical Physics, Journal of Chemical Theory and Computation, Journal of Computational Chemistry, Journal of Computer-Aided Molecular Design, Journal of Molecular Biology, Journal of Molecular Graphics and Modelling, Journal of Molecular Modeling, Journal of Nutrition, Journal of Proteome Research, Journal of the Taiwan Institute of Chemical Engineers, Journal of Theoretical Biology, Medicinal Chemistry, Molecules, Nature Scientific Reports, Nature Protocols, Nucleic Acids Research, Peptides, PLoS Computational Biology, PLoS One, Proceedings of the National Academy of Science USA, Pacific Symposium on Biocomputing, Protein Engineering, Design and Selection, Protein Science, Proteins: Structure, Function and Bioinformatics, Structure

REFEREEING OTHER

External Tenure and Promotion/Appointment Referee for faculty in 18 institutions
External Referee for Romnes Faculty Fellowship Award, University of Wisconsin - Madison
Foreign Thesis Examiner, West Bengal University of Technology, India
Foreign Thesis Examiner, Anna University, Chennai, India

INVITED LECTURES (accepted)

9th Conf. of Young Scientists on Biologically Active Compounds; Riga, Latvia, April 1987
Weizmann Institute of Science; Rehovot, Israel, December 1990
13th Annual Conf. of the Molecular Graphics Society; Chicago, IL, July 1994
10th Int. Conf. on Methods in Protein Structure Analysis; Snowbird, Utah, September 1994
Hebrew University, School of Pharmacy, Jerusalem, Israel, December 1994
Weizmann Institute of Science; Rehovot, Israel, December 1994
Tel Aviv University, Dept of Biotechnology and Dept of Immunology; Israel, December 1994
TRIPOS Users Group Meeting; St. Louis, MO, May 1995
Terrapin Technologies; San Francisco, CA, December 1995
IBC's Conf. on Comput. Approaches to Protein-Ligand Interaction; Coronado, CA, Dec.1995
Scripps Research Institute, Dept of Molecular Biology; La Jolla, CA, December 1995
University of Arizona, Dept of Chemistry; Tucson, AZ, December 1995
Center for Studies in Physics and Biology, Rockefeller University; New York, NY, January 1996

DuPont Merck Pharmaceutical Company; Wilmington, DE, February 1996
Mount Sinai School of Medicine, Dept of Physiology & Biophysics, New York, NY, February 1996
Molecular Research Institute, Palo Alto, CA, December 1996
Second Meeting on the Protein Structure Prediction, Asilomar, CA, December 1996
A&PC Pharmaceuticals, Minneapolis, MN, February 1997
Oak Ridge National Laboratory, Oak Ridge, TN, March 1997
Saint Louis University, Department of Biochemistry, Saint Louis, MO, March 1997
University of Florida, Department of Chemistry, Gainesville, FL, May 1997
College of Charleston, Dept. of Chemistry and Biochemistry, Charleston, SC, October 1997
Australian Molecular Modelling Workshop (plenary lecture), Melbourne, Australia, October 1997
National Cancer Institute, Laboratory of Exper.& Comput. Biology, Frederick, MD, March 1998
Structural Bioinformatics, Inc., San Diego, CA, July 1998
Boston University, Department of Biomedical Engineering, Boston, MA, July 1999
American Chemical Society National Meeting, New Orleans, LA, August 1999
College of Charleston, Department of Physics, Charleston, SC, October 1999
Tel Aviv University, Dept of Biochemistry, Israel, November 1999
Hebrew University, School of Pharmacy, Jerusalem, Israel, November 1999
Conference on Molecular Approaches to Biological Problems, Isle of Palms, SC, January 2000
Georgia Institute of Technology, School of Biology, Atlanta, GA, March 2000
Washington University, Department of Biochemistry, St. Louis, MO, May 2000
Texas A&M University, Department of Biochemistry, College Station, TX, December 2000
Brookhaven National Laboratory, Upton, NY, December 2000
Indiana University, Department of Physics, Bloomington, IN, January 2001
University of North Carolina at Chapel Hill, Dept Pharmacology, Chapel Hill, NC, February 2001
University of California Irvine, Department of Biochemistry, Irvine, CA, February 2001
University of Michigan at Ann Arbor, Department of Pharmacology, Ann Arbor, MI, March 2001
American Chemical Society National Meeting, Chicago, IL, August 2001
Applied Biomathematics, Setauket, NY, November 2001
Critical Assessment of Predicted Interactions, La Londe-des-Maures, France, September 2002
Frontiers in Bioinformatics Symposium, Buffalo, NY, June 2003
American Chemical Society National Meeting, New York, NY, September 2003
University of Kansas, Bioinformatics Program, Lawrence, KS, February 2004
University of California Davis, Genome Center, Davis, CA, February 2004
Brown University, Center for Computational Biology, Providence, RI, March 2004
Critical Assessment of Predicted Interactions, Gaeta, Italy, December 2004
Iowa State University, Baker Center for Bioinformatics, Ames, IA, November 2005
Nebraska Research Expo, Lincoln, NE, March 2006
Conf. on Exploring Mechanisms & Landscapes of Cellular Network, Telluride, CO, August 2006
Biomedical Engineering Society National Meeting, Chicago, IL, October 2006
Critical Assessment of Predicted Interactions, Toronto, Canada, April 2007
Stochastic Adaptive Seminar, University of Kansas, Math Department, Lawrence, KS, April 2007
Moscow Conference on Computational Molecular Biology, Moscow, Russia, July 2007
United Institute of Informatics Problems, National Academy of Sci., Minsk, Belarus, May 2008
Grand Challenges in Computational Biology, Barcelona, Spain, June 2008
Intl. Conf. Advanced Information & Telemedicine Technologies for Health, Belarus, October 2008
Critical Assessment of Predicted Interactions, Barcelona, Spain, December 2009
University of Texas, Institute for Comput. Engineering & Sciences, Austin, TX, March 2010
Conf. Coarse-Grained Modeling Struct. & Dynamics Biomacromolecules, Telluride, CO, July 2010
Informatics Institute, University of Missouri, Columbia, MO, November 2010
Hebrew University, School of Pharmacy, Jerusalem, Israel, March 2011
University of California San Diego, School of Pharmacy, La Jolla, CA, April 2011
Conference on Protein-Protein Interactions as Drug Targets, San Diego, CA, April 2011
Schrodinger Drug Design Software Users Meeting, La Jolla, CA, April 2011
University of California San Francisco, San Francisco, CA, April 2011
Conf. Modeling Biomolecular Structures, Interactions, and Functions, Telluride, CO, June 2011
University of Wyoming Summer Undergraduate Research Program, Laramie, WY, June 2011

Pittsburg State University, Department of Chemistry, Pittsburg, KS, September 2011
Protein and RNA Structure Prediction Conference, Cancun, Mexico, December 2011
Conference on Protein-Protein Interactions as Drug Targets, San Diego, CA, April 2012
Conf. Coarse-Grained Modeling Struct. & Dynamics Biomacromolecules, Telluride, CO, July 2012
Comput. Theor. Biology Symposium, Rice University, Houston, TX, November-December 2012
Discovery Chemistry Congress, Munich, Germany, March 2013
Critical Assessment of Predicted Interactions, Utrecht, Netherlands, April 2013
Conf. Modeling Biomolecular Structures, Interactions, and Functions, Telluride, CO, July 2013
Huazhong University of Science and Technology, Wuhan, China, October 2013
Protein and RNA Structure Prediction Conference, Cancun, Mexico, December 2013
Protein Folding Conference, Punta Cana, Dominican Republic, July 2014
Conf. Coarse-Grained Modeling of Biomacromolecules, Telluride, CO, July 2014
Hebrew University, School of Medicine, Jerusalem, Israel, February 2015
University of California Riverside, Riverside, CA, March 2015
Kansas City Area Life Sciences Regional Translational Medicine, Lawrence, KS, April 2015
American Chemical Society National Meeting, Boston, MA, August 2015
Intl. Conf. Protein RNA Structure Prediction, Punta Cana, Dominican Republic, December 2015
American Chemical Society National Meeting, San Diego, CA, March 2016
Biochemistry Seminar, University of Kansas Medical Center, Kansas City, KS, April 2016
Critical Assessment of Predicted Interactions, Israel, April 2016

PARTICIPATION IN SCIENTIFIC MEETINGS

1985a: Math. Methods for Studying Polymers and Biopolymers, Pushchino, Russia. Abstract: Leonova, V.I., Tseytin, V.M., Vakser, I.A., *et al.*, *Human protein data bank and modeling of protein degradation process*

1985b: Phys.-Chem. Properties of Biopolymers in Solution: COMECON Intl Symp., Pushchino, Russia. Abstract: Tseytin, V.M., Galaktionov, S.G., Vakser, I.A., *et al.*, *Amphiphilic properties and biological activity of peptides*

1986a: 7th Symp. Intermolecular Interactions, Pushchino, Russia. Abstract: Galaktionov, S.G., Tseytin, V.M., Vakser, I.A. *Computation of peptide molecules conformations at the water - lipophilic phase boundary*

1986b: Complex Methods of Environmental Control: COMECON International Symp., Moscow. Abstract: Galaktionov, S.G., Yurin, V.M., Vakser, I.A., *Interpreting the water quality bioassay results in terms of concentrations standards*

1987a: Synthesis and Investigation of Biologically Active Compounds: 9th Conf. of Young Scientists, Riga, Latvia. Lecture and Abstract: Vakser, I.A., Prokhorchik, E.V. *Amphiphilicity and membranotropic properties of biologically active peptides*

1987b: 5th Conf. on Organic Crystallochemistry, Chernogolovka, Russia. Abstract: Vakser, I.A., *et al.*, *Stable conformations of biologically active peptides in heterogeneous environment*

1987c: Cell Biology: 5th Universities Conf., Tbilisi, Georgia. Abstracts: Vakser, I.A., *A theoretical study of steric factors in receptor binding sites*; Vakser, I.A., Tseytin, V.M., *Amphiphilicity and biologically active conformations of angiotensin*

1987d: Hydration of Biopolymers: COMECON International Symposium, Pushchino, Russia.

1988a: Theoretical Research and Databanks on Mol. Biology and Genetics, Novosibirsk, Russia. Abstract: Vakser, I.A., *et al.*, *Calculation of spatial structure of peptide molecules in heterogeneous environment*

1988b: Biological Membranes: Norm and Pathology: 6th Universities Conf., Kutaisi, Georgia. Abstracts: Vakser, I.A., Tseytin, V.M., Shenderovich, M.D., *Hydrophobic forces in peptide-receptor interactions*; Markovski, G.A., Vakser, I.A., Galaktionov, S.G., Oniani, D.A., *Bioassay methods for environmental control*; Tseytin, V.M., Vakser, I.A., Birger, P.S. *et al.*, *Peptides as protectors from membranotropic effects of "middle molecules"*

1988c: Structure of Immunoregulatory Peptides, Moscow. Abstract: Galaktionov, S.G., Birger, P.S., Prokhorchik, E.V., Vakser, I.A., Mikhneva, L.M., *Mechanisms of effect of "middle molecule" peptides on cellular immunity*

1988d: 2nd Intl Symp. Molecular Aspects of Chemotherapy, Gdansk, Poland. Abstracts: Nikolaichik, V.V., Tseytin, V.M., Vakser, I.A., *et al.*, *Specific oligopeptide bioregulators - fragments of fibrin: A study of "conformation-activity" relationships*; Oniani, D.A., Okropiridze, I.A., Vakser, I.A., *et al.*, *Calculation of stable conformations of peptides in heterogeneous environment.*

1989a: 9th International Symp. Chemistry of Natural Products, Riga, Latvia. Abstract: Galaktionov, S.G., Vakser, I.A., Tseytin, V.M., *Structure-function relationships and computer-aided design of peptide bioregulators*

1989b: Intl Conf. Transport in Biol. Membranes, Tbilisi, Georgia. Abstract: Oniani, D.A., Galaktionov, S.G., Vakser, I.A., *et al.*, *The modulation of ion transport across erythrocyte membrane by peptides of "middle molecules" group*

1989c: FECS 5th International Conf. on Chemistry and Biotechnology of Biologically Active Natural Products, Varna, Bulgaria. Abstract: Galaktionov, S.G., Tseytin, V.M., Vakser, I.A., *Calculation of stable conformations of peptide molecules in a heterogeneous environment*

1990a: International Conf. on Modeling and Computer Methods in Molecular Biology and Genetics, Novosibirsk, Russia. Abstract: Tseytin, V.M., Vakser, I.A., Galaktionov, S.G., *Interaction of peptide and protein molecules with lipophilic environment*

1990b: 2nd World Congress of Theoretical Organic Chemists, Toronto, Canada. Abstract: Galaktionov, S.G., Tseytin, V.M., Vakser, I.A. *Molecular mechanics in heterogeneous environment*

1991: Advances in Biomolecular Simulations: Int. Meeting, Obernai, France. Abstract: Tseytin, V.M., Vakser, I.A., Galaktionov, S.G., Okropiridze, I.A., Oniani, J.A. *Calculation of peptide molecule conformations in heteropolar environment*

1992: Weizmann-Strasbourg Sympos., Strasbourg, France. Abstract: Katchalski-Katzir, E., Shariv, I., Eisenstein, M., Aflalo, C., Vakser, I.A. *et al.*, *The role of geometric fit between proteins and their ligands in determining biological specificity*

1993: Int. Workshop on Protein Dynamics and Thermodynamics, Jerusalem, Israel. Poster: Vakser, I.A., Aflalo, C. *Solvation effects in intermolecular structure prediction*

1994a: TRIPOS Users Group Meeting, St. Louis, MO. Poster: Vakser, I.A., Aflalo, C. *Hydrophobic properties in protein docking*

1994b: Protein Engineering and Design: The Pfizer-Beckman Institute Sympos., Urbana, IL. Abstract: Vakser, I.A. *Molecular recognition beyond local interactions*

1994c: 13th Annual Conf. of the Molecular Graphics Society, Chicago, IL. Abstract: Vakser, I.A., Aflalo, C. *Hydrophobic properties in molecular surface recognition*

1994d: Gordon Research Conference on Biomolecular Recognition, Wolfeboro, NH

1994e: 6th Biothermokinetics Meeting, Shroken, Austria. Poster: Aflalo, C., Vakser, I.A. *Hydrophobic docking*

1994f: 10th International Conference on Methods in Protein Structure Analysis, Snowbird, Utah. Abstract: Vakser, I.A., *Protein docking in the absence of detailed molecular structures*, J. Prot. Chem., 1994, 13:541.

1995a: Gordon Research Conference on Enzyme Organization, Oxnard, CA

1995b: TRIPOS Users Group Meeting, St. Louis, MO. Lecture and Abstract: Vakser, I.A. *Ligand-receptor interactions for underdetermined structures*

1995c: Protein Interactions: The Pfizer-Beckman Institute Sympos., Urbana, IL. Abstract: Vakser, I.A. *Long-distance potentials: an approach to the multiple-minima problem in protein interactions*

1995d: 14th Amer. Peptide Sympos., Columbus, OH. Abstract: Galaktionov, S.G., Tseytin, V.M., Vakser, I.A., Marshall, G.R. *Calculation of peptide orientation at lipophilic surface: an useful tool for "conformation - function" analysis*

1995e: 9th Sympos. of The Protein Society, Boston, MA. Abstract: Vakser, I.A., *Protein recognition at low resolution*, Protein Sci., 1995, 4(suppl. 2): 86

1995f: The Year of Louis Pasteur Int. Symp. on Stereospecificity and Molecular Recognition, New York, NY

1995g: IBC's Fourth Rational Drug Design Conf. on Computational Approaches to Analyze Protein-Ligand Interaction, Coronado, CA. Lecture: *Protein-ligand docking for underdetermined structures*

1996a: New York Structural Biology Discussion Group Meeting, New York, NY

1996b: Gordon Research Conference on Chemistry and Biology of Peptides, Ventura, CA

1996c: 10th Sympos. of The Protein Society, San Jose, CA. Abstract: Vakser, I.A., Sali, A., *Large-scale structural complementarity in protein complexes*, Protein Sci. 1996, 5 (suppl. 1): 98

1996d: 2nd Meeting on the Critical Assessment of Techniques for Protein Structure Prediction, Asilomar, CA. Lecture and Abstract: Vakser, I.A. *GRAMM: a systematic approach to protein docking*

1997a: New York Structural Biology Discussion Group Meeting, New York, NY

1997b: Australian Molecular Modelling Workshop, Melbourne, Australia. Plenary lecture: *Protein docking by GRAMM methodology*

1998a: Innovative Techniques for New Lead Discovery and Development, Isle of Palms, SC

1998b: Gordon Research Conference on Biopolymers, Newport, RI

1998c: 12th Sympos. of The Protein Society, San Diego, CA. Abstract: Vakser, I.A. *Protein docking by GRAMM methodology,* Protein Sci., 1998,.7 (suppl.1):155

1998d: 3rd Meeting on the Critical Assessment of Techniques for Protein Structure Prediction, Asilomar, CA

1999a: Innovative Techniques for New Lead Discovery and Development, Isle of Palms, SC. Lecture and Abstract: Vakser, I.A., Matar, O.G., Lam, C.F. *Protein docking for structural genomics*

1999b: 16th Enzyme Mechanisms Conference, Napa, CA. Abstract: Bridges, A., Gruenke, L., Chang, Y.-T., Loew, G., Vakser, I.A., Waskell, L. *Identification of the binding sites on Cytochrome P450 2B4 for Cytochrome b5 and Cytochrome P450 Reductase and identification of the binding site on Cytochrome b5 for Cytochrome P450 2B4*

1999c: 13th Sympos. of The Protein Society, Boston, MA. Abstract: Vakser, I.A., Matar, O.G., Lam, C.F. *A systematic study of low-resolution recognition in protein-protein complexes,* Protein Sci., 1999, 8 (suppl.1):111

1999d: American Chemical Society National Meeting, New Orleans, LA. Lecture and Abstract: Vakser, I.A., Matar, O.G., Lam, C.F. *Low-resolution recognition in protein-protein complexes*

2000a: Molecular Approaches to Biological Problems, Isle of Palms, SC. Lecture: *Protein modeling in structural genomics*

2000b: Quantitative Challenges in the Post-Genomic Sequence Era, San Diego, CA. Abstract: Vakser, I.A., Tovchigrechko, A., Matar, O.G., Lam, C.F. *Protein docking in structural genomics*

2000c: 14th Sympos. of The Protein Society, San Diego, CA. Abstracts: Vakser, I.A., Tovchigrechko, A. *Estimating the quality of protein-protein docking,* Protein Sci. , 2000, 9 (suppl.1):.81; Tovchigrechko, A., Vakser, I.A. *Docking protein models*, p.80*;* Jiang, S., Vakser, I.A*. Side chains in transmembrane helices are shorter at helix-helix interfaces*, p.148

2001a: RECOMB - 5th International Conference on Computational Molecular Biology, Montreal, Canada. Abstract: White, C.N., Vakser, I.A., Hazard, E.S., Zhang, Z. *Using physicochemical properties in alignment of multiple protein sequences*

2001b: Conference on Modeling of Protein Interactions in Genomes, Charleston, SC. Session Chair; Lecture: *Docking of protein models*

2001c: American Chemical Society National Meeting, Chicago, IL. Lecture and Abstract: Vakser, I.A., Tovchigrechko, A. *Docking of protein models*

2001d: 8th Nemethy Memorial Symposium, New York, NY.

2002a: Workshop Mathematics for Genomes-to-Life Program, Washington, DC.

2002b: Conf. Critical Assess. Predicted Interaction (CAPRI), La Londe-des-Maures, France. Session Chair; Lecture: *Docking of shapes: flexibility needed*

2003a: Frontiers in Bioinformatics Symposium, Buffalo, NY. Lecture: *Modeling of protein-protein complexes in structural genomics*

2003b: Conference on Modeling of Protein Interactions in Genomes, Stony Brook, NY. Session Chair; Lecture: *High-throughput protein-protein docking for entire genomes*

2003c: American Chemical Society National Meeting, New York, NY. Lecture and Abstract: Vakser, I.A., Tovchigrechko, A., *Modeling of protein-protein complexes in structural genomics*

2003d: Biomedical Engineering Symposium, Nashville, TN. Lecture: *High-throughput protein-protein docking for entire genomes*

2004a: Pacific Symposium on Biocomputing, Big Island, HI.

2004b: Conf. Critical Assess. Predicted Interaction (CAPRI), Gaeta, Italy. Session Chair; Lecture: *Development and testing of an automated approach to protein docking*

2005: Conference on Modeling of Protein Interactions in Genomes, Lawrence, KS. Session Chair.

2006a: Nebraska Research Expo, Lincoln, NE. Session Chair; Lecture: Modeling of protein interactions in genomes

2006b: 20th Symposium of The Protein Society, San Diego, CA.

2006c: Conf. on Exploring Mechanisms & Landscapes of Cellular Network, Telluride, CO. Lecture: *Modeling of protein interactions in genomes*

2006d: Biomedical Engineering Society National Meeting, Chicago, IL. Lecture: Modeling of protein interactions in genomes

2007a: Pacific Symposium on Biocomputing, Maui, HI.

2007b: Conf. Critical Assess. Predicted Interaction (CAPRI), Toronto, Canada. Session Chair; Lecture: *Dockground integrated system of databases for protein docking, 2nd release*

2007c: Moscow Conference on Computational Molecular Biology, Moscow, Russia. Session Chair; Plenary Lecture: *Modeling of protein-protein interactions in structural genomics.*

2007d: Conference on Modeling of Protein Interactions, Lawrence, KS. Session Chair; Lecture: *Multiscale modeling of protein interactions*

2008a: Biophysical Soc. 52nd Annual Meeting/16th Int. Biophys. Congress (IUPAB), Long Beach, CA. Abstract: Ruvinsky, A.M, Vakser, I.A. *Revealing physical basis for ruggedness of protein-protein energy landscapes: Interaction cutoff effect*

2008b: Grand Challenges in Computational Biology, Barcelona, Spain. Session Chair; Lecture: *Modeling of protein-protein interactions in structural genomics*

2008c: International Conference on Advanced Information and Telemedicine Technologies for Health, Minsk, Belarus. Session Chair; Plenary Lecture: *Modeling of protein-protein interactions in structural genomics*

2008d: Critical Assessment of Structure Prediction (CASP) meeting, Sardinia, Italy

2009a: Pacific Symposium on Biocomputing, Big Island, HI

2009b: Biophysical Soc. 53nd Annual Meeting, Boston, MA. Abstract: Kundrotas, P.J., Vakser, I.A. *Template-based modeling of protein-protein interfaces*

2009c: International Conference on Intelligent Systems for Molecular Biology, Stockholm, Sweden. Abstract: Kundrotas, P.J., Zhu, Z., Vakser, I.A. *Genome-wide structural modeling of protein-protein interactions*

2009d: Moscow Conference on Computational Molecular Biology, Moscow, Russia. Abstract: Kirys, T., et al. *Conformational preferences of the side chains in protein-protein complexes*

2009e: Conference on Critical Assessment of Predicted Interaction (CAPRI), Barcelona, Spain. Session Chair; Lecture: *Docking by structural similarity at the interface*; Abstracts: Kirys, T., Ruvinsky, A.M., Tuzikov, A.V., Vakser, I.A. *A systematic study of the side-chain conformational changes upon protein-protein binding*; Kundrotas, P., Zhu, Z., Vakser, I.A., *Genome-wide structural modeling of protein-protein interactions*; Liu, S., Vakser, I.A. *Protein-protein scoring by statistical potentials and machine learning techniques*

2010a: Pacific Symposium on Biocomputing, Big Island, HI

2010b: American Chemical Society 239th National Meeting, San Francisco, CA. Lecture: Ruvinsky, A.M., Vakser, I.A. *Advances in coarse-grained statistical mechanics of protein vibrations: Theory and calculation*

2010c: Biophysical Soc. 54th Annual Meeting, San Francisco, CA. Abstracts: Kundrotas, P.J., Sinha, R., Vakser, I.A. *Docking by structural similarity at protein-protein interfaces*; Ruvinsky, A.M., Vakser, I.A. *Structure fluctuations in proteins and their relationship to amino acid propensities*

2010d: Conf. Coarse-Grained Modeling of Struct.& Dynamics Biomacromolecules, Telluride, CO. Session Chair; Lecture: *Modeling of protein interactions in genomes*

2010e: 24th Symposium of The Protein Society, San Diego, CA. Abstracts: Kundrotas, P.J., Zhu, Z., Vakser, I.A. *Genome-wide structural modeling of protein-protein interactions*; Kundrotas, P.J., Sinha, R., Vakser, I.A. *Modeling of protein-protein interactions by structural similarity at the interfaces*

2010f: Conference on Modeling of Protein Interactions, Lawrence, KS. Session Chair; Lecture: *Protein docking methodology for structural genomics;* Abstracts: Kirys, T., Ruvinsky, A.M., Tuzikov, A.V., Vakser, I.A. *Direction of the side-chain conformational transitions upon protein-protein binding;* Ruvinsky, A.M., Kirys, T., Tuzikov, A.V., Vakser, I.A. *Side-chain conformational changes in protein-protein* association; Ruvinsky, A.M., Vakser, I.A. *Structure fluctuations in proteins and their relationship to amino acid propensities;* Kundrotas, P.J., Sinha, R., Vakser, I.A. *Docking by structural similarity at protein-protein interfaces;* Kundrotas, P.J., Zhu, Z., Vakser, I.A. *Genome-wide structural modeling of protein-protein interactions*

2010g: Critical Assessment of Structure Prediction (CASP) meeting, Asilomar, CA

2011a: Biophysical Soc. Annual Meeting, Baltimore, MD. Lecture and Abstract: Ruvinsky, A.M., Kirys, T., Tuzikov, A.V., Vakser, I.A. *Structural fluctuations and conformational changes in proteins and protein complexes*; Abstract: Kundrotas, P.J., Anishchenko, I., Tuzikov, A.V., Vakser, I.A. *Docking benchmark set of protein models*

2011b: Conference on Protein-Protein Interactions as Drug Targets, San Diego, CA. Lecture: *Multiscale modeling of protein-protein interactions*

2011c: Schrodinger Drug Design Software Users Meeting, La Jolla, CA. Lecture: *Computational proteomics*

2011d: Conference on Modeling Biomolecular Structures, Interactions, and Functions, Telluride, CO. Lecture: *Modeling of protein-protein interactions in structural genomics*

2011e: 9th European Symposium of The Protein Society, Stockholm, Sweden. Abstract: Kundrotas, P.J., Anishchenko, I., Tuzikov, A.V., Vakser, I.A. *Docking benchmark set of protein models*

2011f: 4th Symposium on Methods and Applications of Computational Chemistry, Lviv, Ukraine. Lecture: Ruvinsky, A.M., Vakser, I.A. *Thermodynamic and evolutionary aspects of structure fluctuations in proteins*

2011g: Moscow Conference on Computational Molecular Biology, Moscow, Russia. Lecture Ruvinsky, A.M., Vakser, I.A. *Structure fluctuations and configuration instabilities in proteins*

2011h: American Chemical Society National Meeting, Denver, CO. Lecture: *Multiscale modeling of protein-protein interactions*

2011i: Protein and RNA Structure Prediction Conference, Cancun, Mexico. Lecture: *Learning from Nature: Data-driven docking*

2012a: Conference on Protein-Protein Interactions as Drug Targets, San Diego, CA. Discussion Leader; Lecture: *Protein docking and conformational properties of the interfaces*

2012b: Conf. Coarse-Grained Modeling of Struct.& Dynamics Biomacromolecules, Telluride, CO. Session Chair; Lecture: *Comparative docking*

2012c: Conference on Modeling of Protein Interactions, Lawrence, KS. Discussion leader; Session chair; Lecture: Vakser, I.A. *Comparative docking*; Abstracts: Anishchenko, I., Kundrotas, P.J., Tuzikov, A.V., Vakser, I.A. *Docking benchmark set of protein models*; Badal, V.D., Zhu, Z., Kundrotas, P.J., Vakser, I.A. *Genome-Wide Docking Database*.

2012d: Computational and Theoretical Biology Symposium, Rice University, Houston, TX. Lecture: *Modeling of protein interactions in structural genomics*

2013a: Discovery Chemistry Congress, Munich, Germany. Lecture: *Protein docking and conformational properties of the interfaces*

2013b: Conference on Critical Assessment of Predicted Interaction (CAPRI), Utrecht, Netherlands. Lecture: *Target-template structural relationships in modeling of protein-protein complexes*; Abstract: Kundrotas, P.J., Sinha, R., Vakser, I.A. *The diversity of similarity: Target-template structural relationships in modeling of protein-protein complexes, Proc. of CAPRI Evaluation Meeting, University of Utrecht, Netherlands, 2013, p. 20.*

2013c: Symposium on Integrating Technology into Translational Research, Kansas City, MO.

2013d: Workshop on Materials by Advanced Technologies, Lawrence, KS. Lecture: *Molecular docking methodologies*

2013e: Conference on Modeling Biomolecular Structures, Interactions, and Functions, Telluride, CO. Lecture: *Knowledge-based modeling of PPI*

2013f: Protein and RNA Structure Prediction Conference, Cancun, Mexico. Discussion Leader; Lecture: *Comparative protein-protein docking*

2014a: Biophysical Soc. Annual Meeting, San Francisco, CA. Abstracts: Kundrotas, P.J., Vakser, I.A., Janin, J. *Structural similarity in modeling of homodimers;* Anishchenko, I., Kundrotas, P.J., Tuzikov, A.V., Vakser, I.A. *Docking benchmark set of protein models*

2014b: Protein Folding Conference, Punta Cana, Dominican Republic. Lecture: *The binding of the poorly folded: A systematic modeling study*

2014c: 28th Symposium of The Protein Society, San Diego, CA.

2014d: American Chemical Society 248th National Meeting, San Francisco, CA. Abstract: Ruvinsky, A.M., Vakser, I.A., Rivera, M. *Allosteric networks in ferritin-like molecules*

2014e: Conference on Modeling of Protein Interactions, Lawrence, KS. Discussion leader; Session chair; Lecture: Vakser, I.A. *Comparative docking*; Abstracts: Anishchenko, I., Kundrotas, P.J., Tuzikov, A.V., Vakser, I.A. *2nd docking benchmark set of protein models*; Das, M., Kundrotas, P.J., Vakser, I.A. *Genome-Wide Docking Database*; Singla, D., Kundrotas, P.J., Vakser, I.A. DOCKGROUND: *A platform for protein-protein interactions*; Badal, V.D., Kundrotas, P.J., Vakser, I.A. *Generating constraints for protein docking by text-mining*; Dauzhenka, T.A., Kundrotas, P.J., Vakser, I.A. *Exhaustive search in the rotameric space of side-chain conformations: An implementation on GPU*; Belkin, S., Kundrotas, P.J., Vakser, I.A. *A systematic study of potential modulators of protein-protein interactions*.

2014f: Critical Assessment of Structure Prediction (CASP) meeting, Cancun, Mexico. Discussion Leader; Abstract: Anishchenko, I., Kundrotas, P.J., Vakser, I.A. *Modeling CAPRI Targets 68 – 94 by Template-Based and Free Docking*.

2015a: American Chemical Society 249th National Meeting, Denver, CO. Abstracts: Kundrotas, P.J., Anishchenko, I., Vakser, I.A. *Docking of protein models;* Anishchenko, I., Kundrotas, P.J., Vakser, I.A. *Benchmark set of models for protein docking*

2015b: Kansas City Area Life Sciences Institute Regional Translational Medicine Meeting, Lawrence, KS. Invited lecture: Vakser, I.A. *Structural modeling of interactome*

2015c: Moscow Conference on Computational Molecular Biology, Moscow, Russia. Abstract: Hadarovich, A., Anishchenko, I., Kundrotas, P.J., Tuzikov, A.V., Vakser, I.A. *Quantitative comparison of functional properties in protein-protein complexes*

2015d: 23rd Annual International Conference on Intelligent Systems for Molecular Biology and 14th European Conference on Computational Biology, Dublin, Ireland. Abstracts: Kundrotas, P.J., Anishchenko, I., Vakser, I.A. *Docking of protein models*; Badal, V.D., Kundrotas, P.J., Vakser, I.A. *Text mining for protein docking*

2015e: 29th Symposium of The Protein Society, Barcelona, Spain. Abstracts: Anishchenko, I., Kundrotas, P.J., Vakser, I.A. *Docking of protein models*; Das, M., Kundrotas, P.J., Vakser, I.A. *GWIDD Genome-Wide Docking Database*

2015f: American Chemical Society 250th National Meeting, Boston, MA. Invited lecture; Abstracts: Anishchenko, I., Kundrotas, P.J., Vakser, I.A. *Structural modeling of interactome*; Belkin, S., Kundrotas, P.J., Vakser, I.A. *Docking of PPI inhibitors to the protein-bound structures*; Singla, D., Kundrotas, P.J., Vakser, I.A. *DOCKGROUND resource for protein recognition studies*

2015g: Biomedical Engineering Society Annual National Meeting, Tampa, FL. Chair of Session 'Molecules and Molecular Systems'

2015h: 3rd International Conference on Protein and RNA Structure Prediction, Punta Cana, Dominican Republic. Invited lecture: Vakser, I.A. *Structural modeling of interactome*

2016a: American Association for the Advancement of Science Annual Meeting, Washington, DC.

2016b: American Chemical Society 251st National Meeting, San Diego, CA. Invited lecture: Vakser, I.A. *Structural modeling of interactome*

2016c: Conference on Critical Assessment of Predicted Interaction (CAPRI), Israel.

PUBLICATIONS

Articles in Refereed Journals

1. **Vakser, I.A.**, Oniani, D.A., 1987, Amphiphilic properties and membranotropic action of peptides, *Bull. Acad. Sci. Georgia,* 126:397-400.
2. Galaktionov, S.G., Tseytin, V.M., **Vakser, I.A.**, Prokhorchik, E.V., 1988, Amphiphilic properties of angiotensin and its fragments, *Biophysics,* 33:595-598.
3. Galaktionov, S.G., Tseytin, V.M., **Vakser, I.A.**, 1990, Computer-aided design of biologically active peptides: Some new possibilities, *Biopolymers & Cell,* 6:48-52.
4. Katchalski-Katzir, E., Shariv, I., Eisenstein, M., Friesem, A.A., Aflalo, C., **Vakser, I.A.**, 1992, Molecular surface recognition: Determination of geometric fit between proteins and their ligands by correlation techniques, *Proc. Natl. Acad. Sci. USA,* 89:2195-2199.
5. **Vakser, I.A.**, Aflalo, C., 1994, Hydrophobic docking: A proposed enhancement to molecular recognition techniques, *Proteins,* 20:320-329.
6. **Vakser, I.A.**, 1995, Protein docking for low-resolution structures, *Protein Eng.*, 8:371-377.
7. **Vakser, I.A.**, 1996, Long-distance potentials: An approach to the multiple-minima problem in ligand-receptor interaction, *Protein Eng.*, 9:37-41.
8. **Vakser, I.A.**, 1996, Low-resolution docking: Prediction of complexes for underdetermined structures, *Biopolymers*, 39:455-464.
9. **Vakser, I.A.**, 1996, Main-chain complementarity in protein-protein recognition, *Protein Eng.*, 9:741-744.
10. Chang, Y.-T., Stiffelman, O.B., **Vakser, I.A.**, Loew, G.H., Bridges, A., Waskell, L., 1997, Construction of a 3D model of cytochrome P450 2B4, *Protein Eng.*, 10:119-129.
11. **Vakser, I.A.**, 1997, Evaluation of GRAMM low-resolution docking methodology on the hemagglutinin-antibody complex, *Proteins*, Suppl.1:226-230.
12. Bridges, A., Gruenke, L., Chang, Y.-T., **Vakser, I.A.**, Loew, G. H., Waskell, L., 1998, Identification of the binding site on cytochrome P450 2B4 for cytochrome b5 and cytochrome P450 reductase, *J. Biol. Chem.*, 273:17036-17049.
13. **Vakser, I.A.**, Matar, O.G., Lam, C.F., 1999, A systematic study of low-resolution recognition in protein-protein complexes, *Proc. Natl. Acad. Sci. USA*, 96:8477-8482.
14. Jiang, S., **Vakser, I.A.**, 2000, Side chains in transmembrane helices are shorter at helix-helix interfaces, *Proteins*, 40:429-435.
15. Glaser, F., Steinberg, D., **Vakser, I.A.**, Ben-Tal, N., 2001, Residue frequencies and pairing preferences at protein-protein interfaces, *Proteins*, 43:89-102.
16. Tovchigrechko, A., **Vakser, I.A.**, 2001, How common is the funnel-like energy landscape in protein-protein interactions? *Protein Sci.*, 10:1572-1583.

17. Tovchigrechko, A., Wells, C.A., **Vakser, I.A.**, 2002, Docking of protein models, *Protein Sci.*, 11:1888-1896.

18. Vajda, S., **Vakser, I.A.**, Sternberg, M.J.E., Janin, J., 2002, Modeling of protein interactions in genomes, *Proteins*, 47: 444-446.

19. Jiang, S., Tovchigrechko, A., **Vakser, I.A.**, 2003, The role of geometric complementarity in secondary structure packing: A systematic docking study, *Protein Sci.*, 12:1646-1651.

20. Janin, J., Henrick, K., Moult, J., Ten Eyck, L.F., Sternberg, M.J.E., Vajda, S., **Vakser, I.A.**, Wodak, S.J. 2003, CAPRI: A Critical Assessment of PRedicted Interactions, *Proteins*, 52:2-9.

21. Jiang, S., **Vakser, I.A.**, 2004, Shorter side chains optimize helix-helix packing, *Protein Sci.*, 13:1426-1429.

22. **Vakser, I.A.**, 2004, Protein-protein interfaces are special, *Structure*, 12:910-912.

23. Tovchigrechko, A., **Vakser, I.A.**, 2005, Development and testing of an automated approach to protein docking, *Proteins*, 60:296-301.

24. Tovchigrechko, A., **Vakser, I.A.**, 2006, GRAMM-X public web server for protein-protein docking, *Nucl. Acids Res.*, 34:W310-W314.

25. Douguet, D., Chen, H.C., Tovchigrechko, A., **Vakser, I.A.** 2006, DOCKGROUND resource for studying protein-protein interfaces, *Bioinformatics*, 22:2612-2618.

26. Nicola, G., **Vakser, I.A.**, 2007, A simple shape characteristic of protein-protein recognition, *Bioinformatics*, 23:789-792.

27. Gao, Y., Douguet, D., Tovchigrechko, A., **Vakser, I.A.**, 2007, DOCKGROUND system of databases for protein recognition studies: Unbound structures for docking, *Proteins*, 69:845-851.

28. O'Toole, N., **Vakser, I.A.**, 2008, Large-scale characteristics of the energy landscape in protein-protein interactions, *Proteins*, 71:144-152.

29. Ruvinsky, A.M., **Vakser, I.A.**, 2008, Interaction cutoff effect on ruggedness of protein-protein energy landscape, *Proteins*, 70:1498-1505.

30. Hunjan, J., Tovchigrechko, A., Gao, Y., **Vakser, I.A.**, 2008, The size of the intermolecular energy funnel in protein-protein interactions, *Proteins*, 72:344–352.

31. Zhu, Z., Tovchigrechko, A., Baronova, T., Gao, Y., Douguet, D., O'Toole, N., **Vakser, I.A.**, 2008, Large-scale structural modeling of protein complexes at low resolution, *J. Bioinformatics Comp. Biol.*, 6:789–810.

32. Ruvinsky, A.M., **Vakser, I.A.**, 2008, Chasing funnels on protein-protein energy landscapes at different resolutions, *Biophys. J.*, 95:2150–2159.

33. Liu, S., Gao, Y., **Vakser, I.A.**, 2008, DOCKGROUND protein-protein docking decoy set, *Bioinformatics*, 24:2634-2635.

34. **Vakser, I.A.**, Kundrotas, P., 2008, Predicting 3D structures of protein-protein complexes, *Curr. Pharm. Biotech.*, 9:57-66.

35. **Vakser, I.A.**, 2008, PSI has to live and become PCI - Protein Complex Initiative, *Structure*, 16:1-3.

36. Ruvinsky, A.M., **Vakser, I.A.**, 2009, The ruggedness of protein-protein energy landscape and the cutoff for $1/r^n$ potentials, *Bioinformatics*, 25:1132-1136.

37. Kundrotas, P.J., Zhu, Z., **Vakser, I.A.**, 2010, GWIDD: Genome-Wide Protein Docking Database, *Nucl. Acids Res.,* 38:D513-517.

38. Kundrotas, P.J., **Vakser, I.A.**, 2010, Accuracy of protein-protein binding sites in high-throughput template-based modeling, *PLoS Comp. Biol.*, 6: e1000727.

39. Sinha, R., Kundrotas, P.J., **Vakser, I.A.**, 2010, Docking by structural similarity at protein-protein interfaces, *Proteins*, 78:3235-3241.
40. Ruvinsky, A.M., **Vakser, I.A.**, 2010, Sequence composition and environment effects on residue fluctuations in protein structures, *J. Chem. Phys.*, 133:155101 *(Cover story; JCP Top 6 Most Downloaded Articles in October 2010).*
41. Ruvinsky, A.M., Kirys, T., Tuzikov, A.V., **Vakser, I.A.**, 2011, Side-chain conformational changes upon protein-protein association, *J. Mol. Biol.*, 408: 356–365.
42. Liu, S., **Vakser, I.A.**, 2011, DECK: Distance and environment-dependent, coarse-grained, knowledge-based potentials for protein-protein docking, *BMC Bioinformatics*, 12: 280.
43. Sinha, R., Kundrotas, P.J., **Vakser, I.A.**, 2012, Protein docking by the interface structure similarity: How much structure is needed?, *PLoS ONE*, 7: e31349.
44. Kundrotas, P.J., Zhu, Z., **Vakser, I.A.**, 2012, GWIDD: A comprehensive resource for genome-wide structural modeling of protein-protein interactions, *Human Genomics*, 6: 7.
45. Ruvinsky, A.M., Kirys, T., Tuzikov, A.V., **Vakser, I.A.**, 2012, Structure fluctuations and conformational changes in protein binding, *J. Bioinformatics Comput. Biol.*, 10: 1241002.
46. Kundrotas, P.J., Zhu, Z., Janin, J., **Vakser, I.A.**, 2012, Templates are available to model nearly all complexes of structurally characterized proteins, *Proc. Natl. Acad. Sci. USA*, 109: 9438–9441.
47. Kirys, T., Ruvinsky, A.M., Tuzikov, A.V., **Vakser, I.A.**, 2012, Rotamer libraries and probabilities of transition between rotamers for the side chains in protein-protein binding, *Proteins*, 80: 2089–2098.
48. Yao, H., Wang, Y., Lovell, S., Kumar, R., Ruvinsky, A.M., Battaile, K.P., **Vakser, I.A.**, Rivera, M., 2012, The structure of the BfrB-Bfd complex reveals protein-protein interactions enabling iron release from bacterioferritin, *J. Amer. Chem. Soc.*, 134: 13470-13481 (*Highlighted in Nature Chemical Biology, October, 2012*).
49. Kirys, T., Ruvinsky, A.M., Tuzikov, A.V., **Vakser, I.A.**, 2012, Correlation analysis of the side-chains conformation distributions in bound and unbound proteins, *BMC Bioinformatics*, 13: 236.
50. Ruvinsky, A.M., Kirys, T., Tuzikov, A.V., **Vakser, I.A.**, 2013, Ensemble-based characterization of unbound and bound states on protein energy landscape, *Protein Sci.*, 22: 734-744.
51. Kundrotas, P.J., **Vakser, I.A.**, 2013, Protein-protein alternative binding modes do not overlap, *Protein Sci.*, 22: 1141-1145 (*Highlighted in "In This Issue" section*).
52. Kundrotas, P.J., **Vakser, I.A.**, Janin, J., 2013, Structural templates for modeling homodimers, *Protein Sci.* 22: 1655—1663 (*Vakser and Janin corresponding authors*).
53. Kundrotas, P.J., **Vakser, I.A.**, 2013, Global and local structural similarity in protein-protein complexes: Implications for template-based docking, *Proteins*, 81: 2137–2142.
54. **Vakser, I.A.**, 2013, Low-resolution structural modeling of protein interactome, *Curr. Opin. Struc. Biol.*, 23: 198–205.
55. Anishchenko, I., Kundrotas, P.J., Tuzikov, A.V., **Vakser, I.A.**, 2014 Protein models: The Grand Challenge of protein docking, *Proteins*, 82: 278–287.
56. Lensink, M.F., Moal, I.H., Bates, P.A., Kastritis, P.L., Melquiond, A.S. J., Karaca, E., Schmitz, C., van Dijk, M., Bonvin, A.M.J.J., Eisenstein, M., Jimenez-Garcia, B., Grosdidier, S., Solernou, A., Prez-Cano, L., Pallara, C., Fernandez-Recio, J., Xu, J., Muthu, P., Kilambi, K.P., Gray, J.J., Grudinin, S., Derevyanko, G., Mitchell, J.C., Wieting, J., Kanamori, E., Tsuchiya, Y., Murakami, Y., Sarmiento, J., Standley, D.M., Shirota, M., Kinoshita, K., Nakamura, H., Chavent, M., Ritchie, D.W., Park, H., Ko, J., Lee, H., Seok, C., Shen, Y.,

Vajda, S., Kundrotas, P.J., **Vakser, I.A.**, Pierce, B.G., Hwang, H., Vreven, T., Weng, Z., Buch, I., Farkash, E., Wolfson, H. J., Zacharias, M., Zhou, H.X., Huang, S.Y., Zou, X., Wojdyla, J., Kleanthous, C. & Wodak, S.J., 2014, Blind prediction of interfacial water positions in CAPRI. *Proteins*, 82: 620-632.

57. Ruvinsky, A.M., **Vakser, I.A.**, Rivera, M., 2014, Local packing modulates diversity of iron pathways and cooperative behavior in eukaryotic and prokaryotic ferritins, *J. Chem. Phys.*, 140: 115104.
58. **Vakser, I.A.**, 2014, Protein-protein docking: From interaction to interactome, *Biophys. J.*, 107: 1785-1793.
59. Anishchenko, I., Kundrotas, P.J., Tuzikov, A.V., **Vakser, I.A.**, 2015, Structural templates for comparative protein docking, *Proteins*, 83: 1563–1570.
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