JEFFRY DAVID MADURA

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Education

1986-1990	Post-Doctoral Fellow, University of Houston Sponsor: J. Andrew McCammon
1985	PhD in Physical Chemistry, Purdue University Advisor: Prof. William L. Jorgensen
1980	BA in Chemistry, *cum laude*, Thiel College

Honors and Awards

2007	Duquesne University President's Award for Excellence in Scholarship.
2008	Duquesne University Office of Research Hall of Fame, 2008 Inductee.
2007	Bayer School of Natural & Environmental Sciences Award for Excellence in Scholarship.
2002	Bayer School of Natural & Environmental Sciences Award for Excellence in Service.
1998	Computational Chemistry Gordon Research Conference Chair, 1998.
1997	Henry Dreyfus Teacher-Scholar, 1997.
1996	Computational Chemistry Gordon Research Conference vice-chair, 1996.

Appointments held

7/13-present	Lambert F. Minucci Endowed Chair in Engineering and Computational Sciences, Duquesne University
7/04 - present	Professor, Duquesne University
7/00 - 6/10	Chair, Duquesne University
1/98- 6/04	Associate Professor, Duquesne University
3/06 - present	Visiting Adjunct Professor, Department of Computational & Systems Biology, University of Pittsburgh
2002 - present	Research Associate, Department of Chemistry, University of Pittsburgh
9/00 - 3/06	Associate Faculty, Center for Computational Biology & Bioinformatics, University of Pittsburgh
1/91-8/97	Assistant Professor, University of South Alabama
9/97-12/97	Associate Professor, University of South Alabama
9/88-12/90	Director of Chem. Computing/Visiting Assistant Professor, University of Houston
2/87-12/90	Chief Scientist, Institute for Molecular Design, University of Houston
11/85-1/87	Research Associate in Chemistry, University of Houston
7/82-11/85	Research Assistant, Purdue University
9/80-6/82	Teaching Assistant, Purdue University

Professional Activities

8/11	Elected as an ACS Fellow
7/09- present	Journal of Molecular Graphics and Modeling, Co-Editor
1/12- 12/12	ACS Computers in Chemistry Division Chair
8/10-12/11	ACS Computers in Chemistry Division Chair-Elect
1/07-8/10	ACS Computers in Chemistry Program Chair
3//05 - 12/06	ACS Computers in Chemistry Assistant Program Chair

University, School or Department Service

2011-present	Teacher Education Council (Duquesne University).
7/00-6/10	Department Chair.
1/99-7/00; 7/10-present	Bayer School of Natural & Environmental Sciences Tenure and Promotion Committee.
9/99-12/01	Bayer School of Natural & Environmental Sciences and University Education Technology Committee.
1/00-5/06	Duquesne University Core Committee.
7/01-7/03	Department Seminar Coordinator.
1/98-7/00	Department Undergraduate Curriculum Committee.
5/98-12/00	Department Summer Undergraduate Research Representative.
5/02-present	Development of "Topics in Mathematics" course (along with Mathematics Department) for BSNES core.

External Activities

2013	Supercomputer Allocations Board, NRC Anton Supercomputer Allocation Committee, DOE INCITE Allocations Panel, NIH post doctoral fellowship panel, NSF ad hoc.
2012	Supercomputer Allocations Board, NIH K01, NIH New Innovator Awards - Phase I, NIH Biomedical Technology Center Panel, NIH SBIR/STTR Drug Discovery.
2011	NIH Small Business: Drug Discovery Study Section.
2010	NIH Small Business: Drug Discovery Study Section.
2010	Molecular Science Computing: Greenbook .
2010	Co-leader and co-author to the chapter on Biological Science Drivers.
2009	NIH study section panels.
2009	NSF CRCNS review panel.
2009-present	INCITE Allocations Panel.
2008	NIH Pre- and Post-doctoral Fellowship Panel.
2007	NIH MBRS Study Section member.
2004-2007	NIH BMQC (Biomolecular Structure & Function B) NIH Study Section member.
2003	NIH BBCA ad hoc Member.
2002-2005	NSF Bioinformatics Fellowship panel.
2002-present	Member of the NSF Supercomputer Allocation Board.
2002	NSF ITR Small Grant panel.
2002-present	Alliance Allocation Board and National Resource Allocation Committee for NSF Supercomputer Resources.
2001-2002	NIH Post-doctoral Fellowship Study Section.
2000	NIH Special Program Study Section.
1999	NIH Special Program Study Section.
9/99	Co-organizer of a Centre Européen de Calcul Atomique et Moléculaire (CECAM) Workshop titled "Molecular Modeling of Proteins at Interfaces".
8/98	Organizer for an American Chemical Society National Meeting Symposium titled "Computational Chemistry and the Classroom" (Comp. Division)..
1998	NSF Special Panel Member (Biophysics).

1998	NIH BBCA Study Section ad hoc Member.
1997	NSF Postdoctoral Panel Member.
1996	NIH Special Program Study Section.
1993-1997	American Chemical Society Student Affiliate Advisor (Univ. Of S. Alabama chapter.).
1992-1996	Co-chairman of the Chemistry Olympiad for the Mobile Section of the American Chemical Society.
1992-1995	Member of the Steering Committee for Molecular Simulations, Inc. User's Group.
1991-present	Reviewer for the following journals: J. Phys. Chem., J. Amer. Chem. Soc., J. Comput. Chem., J. Org. Chem., Biophys. J., and Biopolymers.
1991-present	External reviewer for NSF and PRF.

Scholarly Activities

Grants

(Currently active grants listed, total funding: >$10 M)

$0.62 M 2012-2017	**NSF S-STEM** Scholarships for Academically Talented and Financially Disadvantaged Undergraduate and Graduate Students
$0.36 M 2013-2016	**NSF REU** REU Site: Integrated Computational and Experimental RE/DoD Site
$1.25 M 2009-2014	**NIH RO1** Computational and Experimental Study of Monoamine Transporters
$0.45 M 2011-2016	**NIH R25** Summer Research Program for Undergraduates
$0.25 M 2010-2012	**NSF MRI** Purchase of SGI Supercomputer

Teaching

- Created and currently run a Pennsylvania Junior Academy of Sciences Workshop in the Fall 2000, 2001, 2003, 2004 and 2005, 2006, 2007, 2008, 2009, 2010 and 2012 for one-half day.
- Developed and taught six-hours of lecture and nine-hours of lab for the NSF/NIH Bioengineering and Bioinformatics Summer Institute. SU03, SU04, SU05, SU06, SU07, SU08, SU09
- Developed and taught six-hours of lecture for the NSF sponsored TECBio program at the University of Pittsburgh. SU10, SU11

Academic Advisement or Supervision

High School Students: 20
Undergraduate Students: 80
Total Graduate Students Advised at Duquesne: 25
Dissertation Committee: 35

Dissertations/Theses

1. Manepalli, Sankar, Ph.D. Degree (**2012**) Structure Based Ligand Design for Monoamine Transporters and Mitogen Activated Kinase 5.
2. Ziegler, Michael, Ph.D. Degree (**2011**) Understanding the Effect of Cation and Solvation on the Structure and Reactivity of Nitrile Anions.

3. Dick, Thomas J., Ph.D. Degree (**2007**) Chemical and physical influences of salts on CO_2 solubility and water phase changes.

4. Foukes, Richard, Ph,D. Degree (**2006**) Approximating interfacial adhesion energies of thermal barrier coatings.

5. Esposito, Emilio Xavier, Ph.D. Degree (**2003**) Computational study of human melatonin receptors, MT-1 and MT-2.

6. Zhou, Zhigang, Ph.D. Degree (**2003**) Computational Studies of HIV-1 RT and Quinone Oxidoreductase -Interaction, Activity, and Mechanism.

Publications & talks

Books

1. Petrucci, Harwood, Herring, and Madura *General Chemistry*, 9th edition, **2006** (co-author)

2. Petrucci, Bissonette, Herring, and Madura *General Chemistry*, 10th edition, **2010** (co-author)

3. Bissonette, Herring, and Madura *General Chemistry*, 11th edition, **2013** (co-author)

4. Metiu *Physical Chemistry* volumes 1-4, **2006** (author of the Mathcad documents on accompanying CD-ROM)

5. Waldeck and Madura *Solutions Manual for Physical Chemistry*, **2009**.

Book Chapters

1. Gedeon, P. C.; Thomas, J. R.; and Madura, J. D. *Accelerated Molecular Dynamics and Protein Conformational Change: A Theoretical and Practical Guide Using a Membrane Embedded Model Neurotransmitter Transporter Molecular Modeling of Proteins, Methods in Molecular Biology*, vol. 1215, DOI 10.1007/978-1-4939-1465-4_12

2. Merchant, B. A; Madura, J. D. *A Review of Coarse-Grained Molecular Dynamics Techniques to Access Extended Spatial and Temporal Scales in Biomolecular Simulations Annual Reports in Computational Chemistry* (**2011**), 7, 68-84.

3. Madura, J. D.; Wierzbicki, A.; Cui, J. and Battle, K. *Antifreeze Proteins: A computational perspective from the past 10 years., Biochemistry and Function of Antifreeze Proteins*, Stefan P. Gaether, editor (**2010**).

4. Dick, T. J., Wierzbicki, A., Madura, J. D. *CO2(aq) Parameterization through FEP/MC Simulations for use in CO2 Sequestration* (**2009**) in Practical Aspects of Computational Chemistry, Chapter 17.

5. Dick, T. J., Wierzbicki, A., Madura, J. D. *CO2(aq) Calculation of Salt Influences on Aqueous Freezing Point Depression* (**2009**) in Practical Aspects of Computational Chemistry, Chapter 18.

6. Esposito EX, Tobi D, Madura JD. *Comparative Protein Modeling. Reviews in Computational Chemistry* (**2005**), 22, 57-167.

7. Dick, Thomas J.; Madura, Jeffry D. *A Review of TIP4P: TIP4P-Ew, TIP5P and TIP5P-E Water Models Annual Reports in Computational Chemistry* (**2005**), 1, 59-74.

8. Esposito, Emilio X; Hopfinger, Anton J; Madura, Jeffry D. *Methods for Applying the Quantitative Structure-Activity Relationship Paradigm. Methods in Molecular Biology* (**2004**), 275 (Cheminformatics), 131-213.

9. Madura, Jeffry D; Wierzbicki, Andrzej. *Molecular Modeling of Adsorption at Crystal Surfaces and Interfaces, in From Fluid-Solid Interfaces to Nanostructural Engineering*; Eds.: DeYoreo, Jim; Liu, Xiang Yang, (**2004**), 2, 1-53.

10. Esposito, Emilio X.; Hopfinger, Anton J.; Madura, Jeffry D. *3D- and nD-QSAR Methods, in Chemoinformatics- From Data to Knowledge, Volume II: Advanced Topics*; Johann Gasteiger and Thomal Engel, Eds.: Wiley-VCH: Germany, (**2003**) 4, 1576-1603.

11. Madura, Jeffry D.; Wierzbicki, Andrzej. *Modeling of antifreeze proteins. Theoretical and Computational Chemistry* (**1999**), 8(Computational Molecular Biology), 537-568.

12. Young, Sidney, H.; Madura, Jeffry D.; Rioux, Frank. Department of Chemistry, University of South Alabama, Mobile, AL, USA. *Software for Teaching and Using Numerical Methods In Physical Chemistry.* Editor(s): Zielinski, Theresa Julia; Swift, Mary L. Using Computers in Chemistry and Chemical Education (**1997**), 163-185. Publisher: American Chemical Society, Washington, D.C.

13. Madura, Jeffry D.; Davis, Malcolm E.; Gilson, Michael K.; Wade, Rebecca C.; Luty, Brock A.; McCammon, J. Andrew. Department of Chemistry, University of South Alabama, Mobile, AL, USA. *Biological Applications of Electrostatic Calculations and Brownian Dynamics Simulations. Rev. Comput. Chem.* (**1994**), 5 229-67.

14. DeKock, Roger L.; Madura, Jeffry D.; Rioux, Frank; Cassanova, Joseph. Dept. Chem., Calvin College, Grand Rapids, MI, USA. *Computational Chemistry in the Undergraduate Curriculum. Rev. Comput. Chem.* (**1993**), 4 149-228.

15. Davis, Malcolm E.; Madura, Jeffry D.; Sines, Jacqueline; Luty, Brock A.; Allison, Stuart A.; McCammon, J. Andrew. *Diffusion-controlled enzyme reactions. Methods Enzymol.* (**1991**) 202(Mol. Des. Model.: Concepts Appl., Pt A), 473-97.

16. Jorgensen, William L.; Blake, James F.; Madura, Jeffry D.; Wierschke, Scott D. *Computer simulations of organic reactions in solution. ACS Symp. Ser.* (**1987**) 353(Supercomput. Res. Chem. Chem. Eng.), 200-17.

Articles (Refereed)

1. Nolan, T. L., Geffert, L. M.; Kolber, B. J.; Madura, J. D.; Surratt, C. K. Discovery of novel-scaffold monoamine transporter ligands via in silico screening with the S1 pocket of the serotonin transporter. *ACS Chemical Neuroscience* (**2014**) 5, 784-792, DOI: 10.1021/cn500133b

2. Thomas, James R. ; Gedeon, Patrick C.; Madura, Jeffry D. Structural dynamics of the monoamine transporter homolog LeuT from accelerated conformational sampling and channel analysis. *Proteins* (**2014**) 82, 2289-2302, DOI: 10.1002/prot.24588

3. Pope, D.; Madura, J. D.; Cascio, M. B-amyloid and neprilysin computational studies identify critical residues implicated in binding specificity. *J. Chem. Inform. Modeling* (**2014**) 54, 1157-1165.

4. Esposito, E. X.; Stouch, T. R.; Wymore, T. Madura, J. D. Exploring the Physicochemical Properties of Oxime-Reactivation Therapeutics for Cyclosarin, Sarin, Tabun, and VX Inactivated Acetylcholinesterase. *Chem. Res. Toxicol.* (**2014**) 27, 99-110. DOI:10.1021/tx400350b

5. Asciutto, E. K.; Gaborek, T.; Madura, J. D. Sodium versus potassium effects on the glutamic acid side-chains interaction on a heptapeptide. *ASAP* (**2014**).

6. Gur, M.; Madura, J.D.; Bahar, I. Global Transitions of Proteins Explored by a Multiscale Hybrid Methodology: Application to Adenylate Kinase. *Biophys. J.* (**2013**) 105 (7) 1643-1652. DOI: 10.1016/j.bpj.2013.07.058; PMID:24094405

7. Immadisetty, K.; Geffert, L.M.; Surratt, C.K.; Madura, J.D. New design strategies for antidepressant drugs. *Expert Opinion on Drug Discovery* (**2013**), 8, 1399-1414. DOI:10.1517/17460441.2013.830102

8. Immadisetty, K; Madura, J. D. A Review of Monoamine Transporter-Ligand Interactions. *Current Computer-aided Drug Design* (**2013**), 9, 556-568. PMID:24138394

9. Gaborek, T. J.; Chipot, C.; Madura, J. D. Using multiple collective variables to examine salt effects on peptide conformational stability. *Biophys. J.* (**2012**), 103, 2513-2520.

10. Manepalli, Sankar; Surratt, C. K.; Madura, J. D.; Nolan, T. L. Monoamine Transporter Structure, Function, Dynamics, and Drug Discovery:A Computational Perspective. *The AAPS Journal* (**2012**), 14, p 820-831. DOI: 10.1208/s12248-012-9391-0

11. Merchant, Bonnie A.; Madura, J. D. Insights from molecular dynamics: The binding site of cocaine in the dopamine transporter and permeation pathways of substrates in the leucine and dopamine transporters. *J. Mol. Graphics and Modeling* (**2012**), 338, 1-12. DOI:10.1016/j.jmgm.2012.05.007

12. Thomas, James; Gedeon, P.; Grant, B.; Madura, J. D. LeuT Conformational Sampling Utilizing Accelerated Molecular Dynamics and Principal Component Analysis. *Biophys. J.* (**2012**), 103, p 1-3.

13. Asciutto, E. K.; Young, M. J.; Madura, J; Pochapsky, S. S.; Pochapsky, T. C. Solution Structural Ensembles of Substrate-Free Cytochrome P450cam. *Biochemistry* (**2012**) 51, 3383-3393.

14. Jain, Prashi; Flaherty, Patrick T.; Yi, Shuyan; Chopra, Ishveen; Bleasdell, Gwenyth; Lipay, Josh; Ferandin, Yoan; Meijer, Laurent; Madura, Jeffry D. Design, synthesis, and testing of an 6-O-linked series of benzimidazole based inhibitors of CDK5/p25. *Bioorganic & Medicinal Chemistry* (**2011**), 19(1), 359-373. DOI:10.1016/j.bmc.2010.11.022

15. Manepalli, Sankar; Geffert, Laura M.; Surratt, Christopher K.; Madura, Jeffry D. Discovery of Novel Selective Serotonin Reuptake Inhibitors through Development of a Protein-Based Pharmacophore. *Journal of Chemical Information and Modeling* (**2011**), 51(9), 2417-2426. DOI:10.1021/ci200280m

16. Asciutto, Eliana K.; Dang, Marina; Pochapsky, Susan Sondej; Madura, Jeffry D.; Pochapsky, Thomas C. Experimentally Restrained Molecular Dynamics Simulations for Characterizing the Open States of Cytochrome $P450_{cam}$. *Biochemistry* (**2011**), 50(10), 1664-1671. DOI:10.1021/bi101820d

17. Nolan, Tammy L.; Lapinsky, David J.; Talbot, Jeffery N.; Indarte, Martin; Liu, Yi; Manepalli, Sankar; Geffert, Laura M.; Amos, Mary Ellen; Taylor, Phillip N.; Madura, Jeffry D.; Surratt, Christopher, K. Identification of a Novel Selective Serotonin Reuptake Inhibitor by Coupling Monoamine Transporter-Based Virtual Screening and Rational Molecular Hybridization. *Chemical Neuroscience* (**2011**), 2(9), 544-552. DOI:10.1021/cn200044x

18. Ziegler, Michael J.; Madura, Jeffry D. Solvation of Metal Cations in Non-aqueous Liquids. *Journal of Solution Chemistry* (**2011**), 40(8), 1383-1398. DOI:10.1007/s10953-011-9732-0

19. Kuhel J. J., Wheeler M. C., Miele P. E., Holder D. A., Johnson B., Paterno Parsi A. A., Madura J. D. Quantitative Impact of an Artificial Intelligence Tutoring System on Student Performance in Assigning Oxidation Numbers in Chemical Formulas. *Chem. Educator* (**2010**), 15, 455-460.

20. Zaheer-ul-Haq; Halim, Sobia Ahsan; Uddin, Reaz; Madura, Jeffry D. Benchmarking docking and scoring protocol for the identification of potential acetylcholinesterase inhibitors. *Journal of Molecular Graphics & Modeling* (**2010**), 28(8), 870-882.

21. Indarte, M., Liu, Y., Madura, J.D., Surratt. C.K., Receptor-Based Discovery of a Plasmalemmal Monoamine Transporter Inhibitor via High-Throughput Docking and Pharmacophore. *Modeling Chemical Neuroscience* (**2010**), 1(3), 223-233.

22. Asciutto, Eliana K. General, Ignacio J. Xiong, Kan; Asher, Sanford; Madura, Jeffry. D. Sodium perchlorate effects on the helical stability of a mainly alanine peptide. *Bipohys. J.* (**2010**), 98(2), 186-196.

23. Gedeon, P. G.; Indarte, M; Surratt, C. K.; Madura, J. D. Molecular Dynamics of Leucine and Dopamine Transporter Proteins in a Model Cell Membrane Lipid Bilayer. *Proteins: Structure, Function and Bioinformatics* (**2010**), 78(4), 797-811.

24. Kan Xiong, Eliana K. Asciutto, Jeffry D. Madura and Sanford A Asher. Salt Dependence of ?-helical Peptide Folding Energy Landscapes. *Biochemistry* (**2009**), 48, 10818-10826.

25. Asciutto, Eliana K.; Madura, Jeffry D.; Pochapsky, Susan Sondej; OuYang, Bo; Pochapsky, Thomas C. Structural and Dynamic Implications of an Effector-induced Backbone Amide cis-trans Isomerization in Cytochrome $P450_{cam}$. *J. Mol. Biol.* (**2009**) 388, 801-814.

26. Asciutto, Eliana K.; Mikhonin, Aleksandr V.; Asher, Sanford A.; Madura, Jeffry, D. Computational and Experimental Determination of the α-Helix Unfolding Reaction Coordinate. *Biochemistry* (**2008**), 47(7), 2046-2050.
http://pubs.acs.org/doi/pdf/10.1021/bi702112v

27. Snyder, James A.; Madura, Jeffry, D. Interaction of the phospholipid head group with representative quartz and aluminosilicate structures: an ab initio study. *Journal of Physical Chemistry B* (**2008**), 112(23), 7095-7103.
http://pubs.acs.org/doi/pdf/10.1021/jp7103769

28. Cui, Jun; Battle, Keith; Wierzbicki, Andrzej; Madura, Jeffry, D. Investigations of structure and dynamics of water solvation of the type I antifreeze protein. *International Journal of Quantum Chemistry* (**2008**), 109(1), 73-80. DOI: 10.1002/qua.21857

29. Zaheer-ul-Haq; Uddin, Reaz; Yuan, Hongbin; Petukhov, Pavel A.; Choudhary, M. Iqbal; Madura, Jeffry, D. Receptor-Based Modeling and 3D-QSAR for a Quantitative Production of the Butyrylcholinesterase Inhibitors Based on Genetic Algorithm. *Journal of Chemical Information and Modeling* (**2008**), 48(5), 1092-1103.
http://pubs.acs.org/doi/pdf/10.1021/ci8000056

30. Wierzbicki, Andrzej; Knight, Charles A.; Salter, E. Alan; Henderson, Camden N.; Madura, Jeffry, D. Role of Nonpolar Amino Acid Functional Groups in the Surface Orientation-Dependent Adsorption of Natural and Synthetic Antifreeze Peptides on Ice. *Crystal Growth & Design* (**2008**), 8(9), 3420-3429. DOI: 10.1021/cg8003855

31. General, Ignacio J.; Asciutto, Eliana K.; Madura, Jeffry, D. Structure of Aqueous Sodium Perchlorate Solutions. *Journal of Physical Chemistry B* (**2008**), 112(48), 15417-15425.
http://pubs.acs.org/doi/pdf/10.1021/jp806269w

32. Indarte, Martin; Madura, Jeffry D.; Surratt, Christopher K. Dopamine transporter comparative molecular modeling and binding site prediction using the LeuTAa leucine transporter as a template. *Proteins: Structure, Function, and Bioinformatics* (**2008**) 70(3), 1033-1046.
DOI: 10.1002/prot.21598

33. Wierzbicki, Andrzej; Dalal, Pranav; Cheatham, Thomas E., III; Knickelbein, Jared E.; Haymet, A. D. J.; Madura, Jeffry, D. Antifreeze proteins at the ice/water interface: Three calculated discriminating properties for orientation of type I proteins. *Biophysical Journal* (**2007**), 93(5), 1442-1451. doi:10.1529/biophysj.107.105189

34. ul-Haq, Z.; Dalal, P.; Aronson, Jr., N. N.; Madura, J. D. Family 18 chitolectins: Comparison of MGP40 and HUMGP39. *Biochem. Biophys. Res. Commun.* (**2007**), 359(2), 221-226.
doi:10.1016/j.bbrc.2007.05.074

35. Zhou, Z., Lin, X., Madura, J. D. HIV-1 RT nonnucleoside inhibitors and their interaction with RT for antivirtal drug development. *Infectious Disorders: Drug Targets* (**2006**) 6(4), 391-413.

36. Zhou, Z.; Bates, M.; Madura, J. D. Structure modeling, ligand binding, and binding affinity calculation (LR-MM-PBSA) of human heparanase for inhibition and drug design. *Proteins* (**2006**) 65(3), 580-592. DOI: 10.1002/prot.21065

37. Krouskop, P. E.; Garrison, P. C.; Gedeon, P. C.; Madura, J. D. A novel hybrid simulation for study of multiscale phenomena. *Mol. Sim.* (**2006**) 32(10-11), 825-830. DOI: 10.1080/08927020600779368

38. Krouskop, P; Madura, JD; Paschek, D; Krukau, A. Solubility of simple, nonpolar compounds in TIP4P-Ew. *Journal of Chemical Physics* (**2006**) 124(1), 016102/1-06102/2. DOI: 10.1063/1.2138704

39. Esposito, Emilio Xavier; Tobi, Dror; Madura, Jeffry D. Comparative protein modeling. *Reviews in Computational Chemistry* (**2006**), 22, 57-167.

40. Munshi, R; Coalson, RD; Ermentrout, GB; Madura, JD; Meirovitch, H; Stiles, JR; Bahar, I. An Introduction to Simulation and Visualization of Biological Systems at Multiple Scales: A Summer Training Program for Interdisciplinary Research. *Biotechnology Progress* (**2006**) 22(1), 179-185. DOI: 10.1021/bp0501773

41. Zhou Z; Madrid M; Evanseck JD; Madura JD. Effect of a bound non-nucleoside RT inhibitor on the dynamics of wild-type and mutant HIV-1 Reverse Transcriptase. *J. Amer. Chem. Soc.* (**2005**) 127:17253-17260. http://pubs.acs.org/doi/pdf/10.1021/ja053973d

42. Dalal, P; Zanotti, K; Wierzbicki, A; Madura, JD; Cheung, HS. Molecular dynamics simulation studies of the effect of phosphocitrate on crystal-induced membranolysis. *Biophysical J.* (**2005**) 89(4) 2251-2257. DOI: 10.1529/biophysj.104.058503

43. Berberich, Jason, A.; Yang, Lee, W.; Madura, Jeffry D.; Bahar, I. and Russell, Alan, J. A stable three-enzyme creatinine biosensor. 1. Impact of structure, function and environment on PEGylated and immobilized sarcosine oxidase. *ActaBiomaterialia* (**2005**), 1, 173-181. doi:10.1016/j.actbio.2004.11.006

44. Zhou, Zhigang; Madura, Jeffry D Relative free energy of binding and binding mode calculations of HIV-1 RT inhibitors based on dock-MM-PB/GS. *Proteins: Structure, Function, and Bioinformatics* (**2004**), 57(3), 493-503. DOI: 10.1002/prot.20223..

45. Esposito, Emilio Xavier; Hopfinger, Anton J.; Madura, Jeffry D Methods for applying the quantitative structure-activity relationship paradigm. *Methods in Molecular Biology* (**2004**), 275(Chemoinformatics), 131-213.

46. Horn, Hans W.; Swope, William C.; Pitera, Jed W.; Madura, Jeffry D.; Dick, Thomas J.; Hura, Greg L.; Head-Gordon, Teresa. Development of an improved four-site water model for biomolecular simulations: TIP4P-Ew. *Journal of Chemical Physics* (**2004**), 120(20), 9665-9678. DOI: 10.1063/1.1683075

47. Zhou, Z.; Madura, J. D. CoMFA 3D-QSAR Analysis of HIV-1 RT Nonnucleoside Inhibitors, TIBO Derivatives Based on Docking Conformation and Alignment. *J. Chem. Infor. Comput. Sci.* (**2004**), 44, 2167-2178. DOI: 10.1021/ci049893v.

48. Nunes, S.; Zhou, Z.; Evanseck, J. D.; Madura, J. D. Computational analysis of Cadmium Sulfide (CdS) Nanocrystals. *Encyclopedia of Nanoscience and Nanotechnology* (2004), MarcelDekker Inc.

49. Aronson, Nathan N., Jr.; Halloran, Brian A.; Alexyev, Mikhail F.; Amable, Lauren; Madura, Jeffry D.; Pasupulati, Lakshminarasimhulu; Worth, Catherine; Van Roey, Patrick. Family

18 chitinase-oligosaccharide substrate interaction: subsite preference and anomer selectivity of Serratia marcescens chitinase A. *Biochemical Journal* (**2003**), 376(1), 87-95. DOI: 10.1042/BJ20030273

50. Wierzbicki, A.; Dalal, P.; Madura, J.D. Molecular Dynamics Simulations of Crystal Induced Membranolysis. *J. Phys. Chem. B* (**2003**), 107, 12345-12351. DOI: 10.1021/jp0305988

51. Zhou, Zhigang; Fisher, Derek; Spidel, Jared; Greenfield, Jodi; Patson, Brian; Fazal, Aleem; Wigal, Carl; Moe, Owen A.;Madura, Jeffry D. Kinetic and Docking Studies of the Interaction of Quinones with the Quinone Reductase Active Site. *Biochemistry* (**2003**), 42, 1985-1994. http://pubs.acs.org/doi/pdf/10.1021/bi026518s

52. Madura, Jeffry D.; Salter, Edward A.; Wierzbicki, Andrzej; Dalal, Pranav; Harrington, John P. Homology Models for the Tetrameric and Dodecameric Complexes of *Lumbricus terresitris* Hemoglobin. *Theochem.* (**2002**), 592, 173-181. doi:10.1016/S0166-1280(02)00238-5

53. Walsh, Mary Beth; Moss, Connie M.; Johnson, Benny G.; Holder, Dale A.; Madura, Jeffry D.. Quantitative of a cognitive modeling intelligent tutoring system on student performance in balancing chemical equations. *Chemical Educator* (**2002**), 7(6), 379-383. DOI: 10.1333/s00897020620a

54. Zhou, Zhigang; Madrid, Marcela; Madura, Jeffry D. Docking of Non-nucleoside Inhibitors: Neotripterifordin and its Derivatives to HIV-1 Reverse Transcriptase. *Proteins: Structure, Function, and Genetics* (**2002**), 49, 529-541. DOI: 10.1002/prot.10233

55. Carlier, Paul R.; Madura, Jeffry D., Effective Computational Modeling of Constitutional Isomerism and Aggregation States of Explicit Solvates of Lithiated Phenylacetonitrile. *Journal of Organic Chemistry* (**2002**), 67 (11), 3832-3840. http://pubs.acs.org/doi/pdf/10.1021/jo0255633

56. Dick, Thomas J.; Acevedo, Orlando; Dalal, Pranav; Madura, Jeffry D.; Evanseck, Jeffrey D.; Mathews, Jonathan P. Molecular Basis For Carbon Dioxide Sequestration In Coal. *Reprints of Symposia-American Chemical Society, Division of Fuel Chemistry* (**2002**), 47(1), 14-16.

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Articles (Non-Refereed)

103. Madura, Jeffry D. Chemistry entry for Scribner Dictionary of American History. (**2003**).

104. Stouch, Terry R.; Brooks, Bernard R.; Swope, William C.; Madura, Jeffry D.; Halgren, Thomas A.; Houk, Kendall N.; McKelvey, John; Jorgensen, William L.; Lipkowitz, Kenny B.; Boyd, Donald B. A Letter to the Community of Computational Chemists- The Gordon Research Conferences on Computational Chemistry. *J. Mol. Graphics Modelling* (**2001**), 19(6), 617.

105. Madura, Jeffry D. Using MOE to Visualize Molecular Orbitals. *Journal of Molecular Graphics and Modeling* (**1999**), 17(2), 150-1.

106. Madura, Jeffry D. Computational Chemistry on a Shoestring: Software from QCPE. *Council on Undergraduate Research Quarterly.* (**1995**), 155-157.

107. Madura, Jeffry D. MOBY 1.5. *J. Chem. Inf. Comput. Sci.* (**1993**).

108. Madura, Jeffry D. Brownian Dynamics Simulations. *Annu. Tech. Conf.- Soc. Plast. Eng.* (**1992**), 50th(2), 2274-6.

109. Madura, Jeffry D. Software Review of Dimensional Reasoner. *Computers Chem.* (**1992**), 16(4), 347.

Talks

1. Biomolecular Simulations of Neurotransmitter Transporters Carnegie Mellon University School of Chemical Engineering, Nov. 11, 2014. (Invited)

2. Conformational analysis of peptides in salt solutions 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, Sept. 8-12, (2013), PHYS-294.

3. Evaluation of electrostatic binding free energies in protein-substrate complexes 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, Sept. 8-12, (2013), COMP-95.

4. Computational neuroscience advances in drug abuse and addition 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, (2013), SOCED-1.

5. Peptides in Salt Solution University of Texas Medical Branch Galveston, November 2012 . (Invited)

6. Monoamine Transporters: Structure, Function and Dynamics University of Texas Medical Branch Galveston, July 2012 . (Invited)

7. Monoamine Transporters: Structure, Function and Dynamics McGill University, June 2012 (Invited).

8. Structure-based virtual screening for monoamine transporter inhibitors 243rd ACS National Meeting & Exposition, San Diego, CA, United States, March 25-29, (2012), COMP-627. (Invited)

9. Monoamine transporter dynamics 243rd ACS National Meeting & Exposition, San Diego, CA, United States, March 25-29, (2012), COMP-139. (Invited)

10. Biomolecular Simulations: Proteins and Transporters University of Pittsburgh -Johnstown, October 2011. (Invited)

11. Biomolecular Simulations, Chemical Computing Group User Group Meeting, Montreal, CANADA June 2011 (Invited)

12. Structure, Function and Dynamics of Monoamine Transporters St. Francis University, October 2010. (Invited)

13. Electrostatic Free Energy Calculations, Chemical Computing Group User Group Meeting, Montreal, CANADA June 2010 (Invited)

14. Biomolecular Simulations: Proteins and Transporters Thiel College, Greenville, PA, October 2009 (Invited).

15. Monoamine Transporter Modeling, Chemical Computing Group User Group Meeting, Montreal, CANADA June 2009 (Invited)

16. Biomolecular Simulations: Proteins and Transporters University of Pittsburgh, Pittsburgh, PA, November 2008 (Invited).

17. Biomolecular Simulations: Proteins and Transporters. IUPUI, Indianapolis, IN, November 2007 (Invited).

18. Biomolecular Simulations: Interplay between mathematics, physics, chemistry, biology, and computer science, SUNY-New Paltz, New Paltz, NY, October 2007 (Invited).

19. Biomolecular Simulations: Interplay between mathematics, physics, chemistry, biology, and computer science, St. Francis University, Lorreto, PA, September 2007 (Invited).

20. Using NSF supercomputer resources to study biomolecular structure and function, 234th National ACS Meeting, Boston, MA. Aug. 20-24, 2007 (Invited).

21. Simulations of Type I AFPs at the ice/water interface. 234th National ACS Meeting, Boston, MA. Aug. 20-24, 2007 (Invited).

22. Protein-Carbohydrate Interactions, Chemical Computing Group User Group Meeting, Montreal, CANADA June 2007 (Invited)

23. Homology Modeling, Docking and Binding Free Energy, St.Vincent College, Latrobe, PA, November, 2006 (Invited).

24. Homology Modeling, Docking and Binding Free Energy, Southwest Regional ACS meeting, Houtson, TX, October 2006, Invited.

25. Homology Modeling, Docking, Electrostatics and MOE, Chemical Computing Group User Group Meeting, Montreal, CANADA June 2006 (Invited)

26. Interfacial Simulations, North Dakota State University, April 27, 2006 (Invited)

27. Protein-Carbohydrate Interactions, University of Houston, Houston, TX, March, 10, 2006. (Invited)

28. Proteins at Ice/Water Interfaces, University of Houston, Houston, TX, September, 8, 2005. (Invited)

29. The merging of physical chemistry and computer algebra systems, 230th ACS National Meeting, Washington, DC, Aug. 28-Sept 1, 2005, (Invited)

30. The role of hydrogen bonding at interfaces, 229th ACS National Meeting, San Diego, CA, March 13-17, 2005 (Invited)

31. Proteins at Ice/Water Interface, University of Western Michigan, Nov. 2004 (Invited)

32. NNRTI's, University of Pittsburgh Medical School, April 2004 (Invited)

33. Influence of HIV-RT inhibitors on RT dynamics: Molecular arthritis, 227th ACS National Meeting, Anaheim, CA, March 28-April 1, 2004 (Invited)

34. Influence of inorganic crystals and peptides on the structure and dynamics of lipid bilayers, 227th ACS National Meeting, Anaheim, CA, March 28-April 1, 2004 (Invited)

35. Ice/water and lipid/water Interfacial Simulations, Bowling Green University, Bowling Green, KY, October 8, 2003 (Invited)

36. Ice/water and lipid/water Interfacial Simulations, University of Pittsburgh, Pittsburgh, PA, September 25, 2003 (Invited)

37. Development of a QM/MM model for peptide-encapsulated CdS nanocrystals, 225th ACS National Meeting, New Orleans, LA, March 23-27, 2003 (Invited)

38. Ab initio and DFT modeling of CdS nanoclusters, 225th ACS National Meeting, New Orleans, LA, March 23-27, 2003. (Invited)

39. Interfacial Simulations, 90th Birthday Celebration for Dr. Robert Feeney, Bodega Bay, CA March 7-9, 2003. (Invited)

40. Antifreeze Proteins, Wright State University, Dayton, OH October 2002. (Invited)

41. Computational studies of explicit solvates of lithiated phenylacetonitrile, 224th ACS National Meeting, Boston, MA, Aug 18-22, 2002 (Invited)

42. Docking Study of Non-nucleoside inhibitors of HIV-1 Reverse Transcriptase, 223rd ACS National Meeting, Orlando, FL, April 7-11, 2002, (Invited).

43. Protein-interface simulations, 223rd ACS National Meeting, Orlando, FL, April 7-11, 2002, (Invited)

44. Computational Biochemistry, SSP Retired Chemists Club. Pittsburgh, PA, April 2002.

45. Antifreeze Proteins, Computational Chemistry GRID Conference, October 2001, (Invited).

46. Antifreeze Proteins, School Seminar, New Palz, NY, September 2001, (Invited).

47. Computational methods throughout the curriculum at Duquesne University, 222nd ACS National Meeting, Chicago, IL, August 26-30, 2001.

48. Proteins at Interfaces, 222nd ACS National Meeting, Chicago, IL, August 26-30, 2001, (Invited).

49. Antifreeze Proteins, University of Pittsburgh's Condensed Matter Lunchtime Seminar, University of Pittsburgh, March 2001, (Invited Talk).

50. Computational chemistry skills course, 221st ACS National Meeting, CHED-1045. 2001, (Invited Talk).

51. Computational methods throughout the curriculum at Duquesne University, 222nd ACS National Meeting, PHYS-010. 2001, (Invited Talk).

52. Making a Better Ice Cream, SSP Retired Chemists Club, Pittsburgh, PA February 2000.

53. Designing Melatonin Receptor Ligands for MT1 and MT2 Receptors, National ACS Meeting, San Francisco, CA, March 2000.

54. Designing Melatonin Receptor Ligands for MT1 and MT2 Receptors, Discovery 2000, San Diego, CA, April 2000, (Invited Talk).

55. Drug-Surface Interaction, International Biophysics 2000, Nice, France, June 2000, (Invited Talk).

56. Computer, the Internet, and Chemistry, University of Miami (FL), January 1999, (Invited Talk).

57. Chemistry and the Internet: Today, Tomorrow, and the Future, Penn-Ohio ACS, Kent, OH, March 1999, (Invited Talk).

58. Simulations of Antifreeze Proteins at the Ice/Water Interface, CECAM Conference, Lyon, France. September 1999, (co-organizer).

59. Computational Modeling of Glycosyl Hydrolases, Duquesne University, March 1998.

60. Computer Modeling of Antifreeze Proteins, 219th National ACS Meeting, Boston, MA, August 1998, (Invited Talk).

61. Building an Understanding of Proteins and Enzymes using the Tools of Computational Chemistry, Duquesne University, July 1997.

62. Coupled Poisson-Boltzmann Electrostatics with Molecular Dynamics Simulations, 218th National ACS Meeting, Las Vegas, NV, August 1997.

63. Molecular Dynamics Simulations in an Implicit Solvent Continuum, 6th Current Trends in Computational Chemistry, Jackson, MS, November 1997.

64. Molecular Modeling of Structure-Function relationship in the Antifreeze Activity of Engineered Antifreeze Polypeptides, 6th Current Trends in Computational Chemistry, Jackson, MS, November 1997.

65. Computational Modeling of Antifreeze Proteins at the Ice/Water Interface. Chemical Engineering, Department at Tulane, New Orleans, LA, December 1995.

66. Antifreeze Proteins: A Computational Perspective, National Institute of Chemistry, Ljubljana, Slovenia, August 1995, (Invited).

67. Molecular Modeling of Taurine-Phospholipid Interactions, 4th International Congress on Amino Acids, Vienna, Austria, August 1995, (Invited).

68. Antifreeze Proteins: A Computational Perspective, ETH, Zurich, Switzerland, August 1995.

69. Molecular Dynamics for Undergraduates, 216th National ACS Meeting, Chicago, IL, August 1995.

70. Antifreeze Proteins: A Computational Perspective, EMBL, Heidelberg, Germany, July 1995.

71. Molecule-Surface Interactions: A Computational Perspective, ACT 95, Charlottesville, VA, March 1995.

72. Antifreeze Proteins: A Computational Perspective, Miami University, Miami, FL, October 1994.

73. Theory of Enzyme-Drug Interactions, Southern Mississippi University, Hattiesburg, MS, October 1994.

74. Antifreeze Proteins: A Computational Perspective, Cornell University, Ithaca, NY, September 1994.

75. Brownian Dynamics Simulation of Polymers, 215th National ACS Meeting, Washington, DC, August 1994.

76. Modeling Molecule-Surface Interactions, 215th National ACS Meeting, San Diego, CA, April 1994.

77. Theory of Enzyme-Drug Interactions, Auburn University, Auburn, AL, November 1993.

78. Applications of Electrostatics Calculations using UHBD, Molecular Simulations Users Group Meeting, Denver, CO, April 1993.

79. Modeling Molecule-Surface Interactions, Colorado School of Mines, Golden, CO, April 1993.

80. Application of Electrostatics and Brownian Dynamics Simulations using UHBD, Polygen Users Group Meeting, San Francisco, CA, April 1992.

81. Molecular Modeling: Methods and Applications, National Institute of Health, Bethesda, MD, May 1990.

82. Development of Potential Functions for Sulfonamides, Centre European de Calcul Atomique et Moleculaire (CECAM) Free Energy of Biopolymers Workshop, Orsay, France, February 1990.

83. Molecular Modeling: Methods and Applications, Supercomputing in the Agricultural and Life Sciences Symposium Texas A&M, College Station, TX, February 1990.

84. Molecular Modeling: A New Tool in Chemical Education, 198th ACS National Meeting, Miami, FL, September 1989.

85. Modeling and Simulation of Enzymes, Institute for Molecular Design, Houston, TX, March 1989.

86. Effects of Truncating Long-Range Interactions in Free Energy Simulations, Centre European de Calcul Atomique et Moleculaire (CECAM) Free Energy of Biopolymers Workshop, Orsay, France, June 1988.

87. Molecular Modeling: Methods and Computation, Tripos Associates, St. Louis, MO, January 1988.

88. Molecular Modeling: Methods and Computation, IBM, Palo Alto, CA, April 1987.

89. Thermal Analysis of 5,7,7,12,14,14-Hexamethyl-1, 4,8,11-Tetraazacyclo-tetradeca-4, 11-Dieenatonickel (II) Iodine, 211th ACS National Meeting, Houston, TX, April 1980.

Poster Presentations

1. Impact of inhibitors on the tertiary structure of acetylcholinesterase Esposito, Emilio X.; Stouch, Terry R.; Wymore, Troy; Madura, Jeffry D. Abstracts of Papers, 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013 (2013), COMP-104.

2. Assessing the role of potassium in resetting the conformation of dopamine transporter Benner, Emily M.; Madura, Jeffry D. Abstracts of Papers, 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013 (2013), COMP-254.

3. Lead optimization of a selective serotonin reuptake inhibitor Jean, Bernandie; Madura, Jeffry D. Abstracts of Papers, 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013 (2013), COMP-257.

4. Conformational energy landscape of aqueous polyglutamine peptides from metadynamics calculations Workman, Riley J.; Madura, Jeffry D. Abstracts of Papers, 246th ACS National Meeting & Exposition, Indianapolis, IN, United States, September 8-12, 2013 (2013), COMP-258.

5. Predictive models for the better understanding of oxime-reactivation for organophosphate inactivated Acetylcholinesterase Esposito, Emilio X.; Stouch, Terry R.; Wymore, Troy; Madura, Jeffry D. Abstracts, 44th Central Regional Meeting of the American Chemical Society, Mount Pleasant, MI, United States, May 15-17 (2013), CERM-67.

6. Application of the free energy perturbation method to monoamine transporters Immadisetty, Kalyan; Madura, Jeffry D. Abstracts of Papers, 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, 2013 (2013), COMP-356.

7. Predictive models to better understand the nuances for the oxime-reactivation of cyclosarin, sarin, tabun, and VX inactivated acetylcholinesterase Esposito, Emilio X.; Stouch, Terry R.; Wymore, Troy; Madura, Jeffry D. Abstracts of Papers, 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, 2013 (2013), COMP-48.

8. Correlation between band gap and electronegativity of substituted atoms in the TiO2 crystalline structure Glaid, Andrew J.; Srnec, Matthew N.; Aitken, Jennifer A.; Madura, Jeffry D. Abstracts of Papers, 245th ACS National Meeting & Exposition, New Orleans, LA, United States, April 7-11, 2013 (2013), CHED-538.

9. Global Transitions or Proteins Explored by a Multiscale Hybrid Methodology: Application to Dopamine Transporter Gur, Mert; Madura, J.; Bahar, I. Biophys. J. 104, 226a-227a.

10. The Conformational Energy Landscape of Aqueous Polyglutamine Peptides from Metadynamics Calculations Workman, R.; Madura, J. Biophys. J. 104. 107a.

11. Synthesis and biological evaluation of selective MEK-5 inhibitors Chakrabarty, Suravi; Qin, Si; Flaherty, Patrick T.; Monlish, Darlene; Cavanaugh, Jane; Manepalli, Sankar; Madura, Jeffry D. Abstracts of Papers, 244th ACS National Meeting & Exposition, Philadelphia, PA, United States, August 19-23, 2012 (2012), MEDI-319.

12. Electronic structure calculations for quaternary diamond-like semiconductors using density functional theory Daley, Kimberly R.; Brunetta, Carl D.; Srnec, Matthew; Karuppannan, Balamurugan; Madura, Jeffry D.; Aitken, Jennifer A. Abstracts of Papers, 243rd ACS National Meeting & Exposition, San Diego, CA, United States, March 25-29, 2012 (2012), INOR-97

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44. Drug discovery workbooks for high school and undergraduate students Jeffry D. Madura. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 236th ACS National Meeting, Philadelphia, PA, USA, August 17-21, (2008)

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Rice; Hans W. Horn; Goundla Srinivas; Dan Price; Martha S. Head; Jeffry D. Madura; Alexander D. MacKerell, Jr.; Kenno Vanommeslaeghe. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 236th ACS National Meeting, Philadelphia, PA, USA, August 17-21, (2008)

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50. Molecular modeling at Duquesne University Jeffry D. Madura and Eliana K. Asciutto. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 236th ACS National Meeting, Philadelphia, PA, USA, August 17-21, (2008)

51. Computational study of the counterion and solvent effect on stereoselectivity in SN2 reactions of cyclic nitrile anions Lisa N. Morkowchuk and Jeffry D. Madura. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 235th ACS National Meeting, New Orleans, LA, USA, April 6-10, (2008)

52. Simulations of Type I AFPs at the ice/water interface Jeffry D. Madura. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 234th ACS National Meeting, Boston, MA, USA, August 19-23, (2007)

53. Molecular dynamics simulations of antifreeze proteins at a lipid/water interface E. J. Smith; Pranav Dalal; Jeffry D. Madura; A. D. J. Haymet. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 234th ACS National Meeting, Boston, MA, USA, August 19-23, (2007)

54. Using NSF supercomputer resources to study biomolecular structure and function Jeffry D. Madura. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 234th ACS National Meeting, Boston, MA, USA, August 19-23, (2007)

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58. Academic success through LSAMP and PUI participation Jeffrey D. Evanseck; Ellen S. Gawalt; Jeffry D. Madura. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 233rd ACS National Meeting, Chicago, IL, USA, March 25-29, (2007)

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60. Quantum mechanical analysis of cadmium sulfide/selenium quantum dots Jacqueline M. Bair and Jeffry D. Madura. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 231st ACS National Meeting, Atlanta, GA, USA, March 26-30, (2006)

61. Carbon dioxide sequestration: MM CO2/ brine simulations Thomas J. Dick and Jeffry D. Madura. Department of Chemistry & Biochemistry, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 230th ACS National Meeting, Washington, DC, USA, August 28-September 1, (2005)

62. Ionic activities in brine solution from computer simulation Peter E. Krouskop; Jeffry D. Madura; Thomas J. Dick. Department of Chemistry and Biochemistry, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 230th ACS National Meeting, Washington, DC, USA, August 28-September 1, (2005)

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65. A Computational Study of Cadmium Sulfide Quantum Dots Jacqueline M. Stoll; Athena R. Spencer; Stacie S. Nunes; Jeffry D. Madura. Department of Chemistry, State University of New York at New Paltz, NY. Abstracts, 32nd Northeast Regional Meeting of the American Chemical Society, Rochester, NY, USA, October 31-November 3, (2004)

66. Studies of brine using TIP4P-Ew and DYNAMO Peter E. Krouskop and Jeffry D. Madura. Department of Chemistry and Biochemistry, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 228th ACS National Meeting, Philadelphia, PA, USA, August 22-26, (2004)

67. Development of an improved four-site water model for bio-molecular simulations: TIP4P-Ew Hans W. Horn; William Swope; Jed Pitera; Jeffry D. Madura; Thomas J. Dick; Greg L. B. Hura; Teresa Head-Gordon. IBM Almaden Research Center, San Jose, CA. Abstracts of Papers, 228th ACS National Meeting, Philadelphia, PA, USA, August 22-26, (2004)

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69. Determining pK a values for metallochaperones Jeffry D. Madura, Rasha Abd El-Rahman, Zhigang Zhou, and Charles T. Dameron. Department of Chemistry & Biochemistry, Center for Computational Sciences and Duquesne University, 308 Mellon Hall, 600 Forbes Ave., Pittsburgh, PA 15282. Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, USA, March 23-27, (2003)

70. Determination of cysteine pKas in a copper chaperone Rasha R. Abd ElRahman; Jeffry D. Madura; Charles T. Dameron. Department of Chemistry and Biochemistry/Computational Chemistry, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 228th ACS National Meeting, Philadelphia, PA, USA, August 22-26, (2004)

71. Characterization of the ice/water interface with TIP4P-Ew water Thomas J. Dick; Jeffry D. Madura; Pranav Dalal, Department of Chemistry and Biochemistry, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 228th ACS National Meeting, Philadelphia, PA, USA, August 22-26, (2004)

72. Family 18 chitolectins: Comparison of MGP40 and GP39 Pranav Dalal; Jeffry D. Madura; Nathan N. Aronson, Department of Chemistry and Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 228th ACS National Meeting, Philadelphia, PA, USA, August 22-26, (2004)

73. Investigation of natural gas clathrate hydrate formation and stability through Monte Carlo simulations Laura L. Thomas; Thomas J. Dick; Jeffry D. Madura, Department of Chemistry and Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 227th ACS National Meeting, Anaheim, CA, USA, March 28-April 1, (2004)

74. Investigation of HIV-RT inhibitors on RT dynamics: Molecular arthritis Jeffry D. Madura, Department of Chemistry and Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 227th ACS National Meeting, Anaheim, CA, USA, March 28-April 1, (2004)

75. Analysis of protein-sugar interactions Pranav Dalal; Laura L. Thomas; Nathan N. Aronson; Jeffry D. Madura, Department of Chemistry and Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 226th ACS National Meeting, New York, NY, USA, September 7-11, (2003)

76. Antifreeze" proteins at the ice/water interface Pranav Dalal; Jared E. Knickelbein; A. D. Haymet; Jeffry D. Madura, Department of Chemistry and Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 226th ACS National Meeting, New York, NY, USA, September 7-11, (2003)

77. Testing simple models of protein folding with computer simulation Laura L. Thomas; Jed Pitera; Julie Rice; Jeffry D. Madura; William Swope, Department of Chemistry and Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 226th ACS National Meeting, New York, NY, USA, September 7-11, (2003)

78. Development of a QM/MM model for peptide-encapsulated CdS nanocrystals James Worthington and Jeffry D. Madura, Center of Computational Sciences, Duquesne University, Department of Chemistry and Biochemistry, 600 Forbes Avenue, Pittsburgh, PA 15282. Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, USA, March 23-27, (2003)

79. Combination of receptor-based and ligand-based drug design: Application in 3D-QSAR of HIV-1 RT non-nucleoside inhibitors Zhigang Zhou and Jeffry D. Madura, Department of Chemistry & Biochemistry, Center for Computational Sciences and Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 226th ACS National Meeting, New York, NY, USA, September 7-11, (2003)

80. Solubility of CO2 in brines through FEP/MC simulations Thomas J. Dick and Jeffry D. Madura, Department of Chemistry and Biochemistry, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 226th ACS National Meeting, New York, NU, USA, September 7-11, (2003)

81. MD simulation of resistent effect of HIV-1 RT mutation to NNRTI Zhigang Zhou1, Jeffry D. Madura1, and Marcela Madrid2. (1) Department of Chemistry & Biochemistry, Center for Computational Sciences and Duquesne University, 600 Forbes Avenue, Mellon Hall 320, Pittsburgh, PA 15282, (2) Pittsburgh Supercomputer Center, Pittsburgh, PA. Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, USA, March 23-27, (2003)

82. Ab initio and DFT modeling of CdS nanoclusters James C. Worthington and Jeffry D. Madura, Department of Chemistry & Biochemistry, Center for Computational Sciences and Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, USA, March 23-27, (2003)

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84. Ab initio and DFT survey of solvated acetonitrile anion lithium complexes Andrea Goncher, Jeffry D. Madura, and Fraser F. Fleming. Department of Chemistry and Biochemistry, Center for Computational Sciences, Duquesne University, 308 Mellon Hall, 600 Forbes Avenue, Pittsburgh, PA 15282 Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, USA, March 23-27, (2003)

85. Investigation of interactions between chitnase and oligosaccharides Laura L. Thomas1, Pranav Dalal1, Nathan N. Aronson Jr.2, and Jeffry D. Madura1. (1) Department of Chemistry and Biochemistry, Center for Computational Sciences, Duquesne University, 308 Mellon Hall, 600 Forbes Avenue, Pittsburgh. Abstracts of Papers, 225th ACS National Meeting, New Orleans, LA, USA, March 23-27, (2003)

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