

JEFFRY DAVID MADURA

Professor

Department of Chemistry & Biochemistry

Duquesne University

600 Forbes Avenue

Pittsburgh, PA 15282-1530

Phone: (412) 396-4129

Email: Madura@duq.edu

URL: <http://www.scienceresearch.duq.edu/chem/chemfac/jmadura/>

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;	Bayer School of Natural & Environmental Sciences Tenure and Promotion Committee.
7/10-present	
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 BSNE 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 Bio-engineering 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.

- Dick, Thomas J., Ph.D. Degree (**2007**) Chemical and physical influences of salts on CO₂ solubility and water phase changes.
- Foukes, Richard, Ph.D. Degree (**2006**) Approximating interfacial adhesion energies of thermal barrier coatings.
- Esposito, Emilio Xavier, Ph.D. Degree (**2003**) Computational study of human melatonin receptors, MT-1 and MT-2.
- Zhou, Zhigang, Ph.D. Degree (**2003**) Computational Studies of HIV-1 RT and Quinone Oxidoreductase -Interaction, Activity, and Mechanism.

Publications & talks

BOOKS

- Petrucci, Harwood, Herring, and Madura *General Chemistry*, 9th edition, **2006** (co-author)
- Petrucci, Bissonette, Herring, and Madura *General Chemistry*, 10th edition, **2010** (co-author)
- Bissonette, Herring, and Madura *General Chemistry*, 11th edition, **2013** (co-author)
- Metiu *Physical Chemistry* volumes 1-4, **2006** (author of the Mathcad documents on accompanying CD-ROM)
- Waldeck and Madura *Solutions Manual for Physical Chemistry*, **2009**.

BOOK CHAPTERS

- 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
- 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.
- 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**).
- 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.
- 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.
- Esposito EX, Tobi D, Madura JD. *Comparative Protein Modeling. Reviews in Computational Chemistry (2005)*, 22, 57-167.
- Dick, Thomas J.; Madura, Jeffrey D. *A Review of TIP4P: TIP4P-Ew, TIP5P and TIP5P-E Water Models Annual Reports in Computational Chemistry (2005)*, 1, 59-74.
- Esposito, Emilio X; Hopfinger, Anton J; Madura, Jeffrey D. *Methods for Applying the Quantitative Structure-Activity Relationship Paradigm. Methods in Molecular Biology (2004)*, 275 (Cheminformatics), 131-213.

9. Madura, Jeffrey 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, Jeffrey D. *3D- and nD-QSAR Methods*, in *Cheminformatics-From Data to Knowledge, Volume II: Advanced Topics*; Johann Gasteiger and Thomal Engel, Eds.: Wiley-VCH: Germany, (2003) 4, 1576-1603.
11. Madura, Jeffrey D.; Wierzbicki, Andrzej. *Modeling of antifreeze proteins. Theoretical and Computational Chemistry* (1999), 8(Computational Molecular Biology), 537-568.
12. Young, Sidney, H.; Madura, Jeffrey 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, Jeffrey 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, Jeffrey 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, Jeffrey 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, Jeffrey 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](https://doi.org/10.1021/cn500133b)
2. Thomas, James R. ; Gedeon, Patrick C.; Madura, Jeffrey 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](https://doi.org/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](https://doi.org/10.1021/tx400350b)
5. Ascitutto, 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 Multi-scale Hybrid Methodology: Application to Adenylate Kinase. *Biophys. J.* (2013) 105 (7) 1643-1652. DOI: [10.1016/j.bpj.2013.07.058](https://doi.org/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. Ascitutto, E. K.; Young, M. J.; Madura, J.; Pochapsky, S. S.; Pochapsky, T. C. Solution Structural Ensembles of Substrate-Free Cytochrome P450_{cam}. *Biochemistry* (2012) 51, 3383-3393.
14. Jain, Prashi; Flaherty, Patrick T.; Yi, Shuyan; Chopra, Ishveen; Bleasdel, Gwentyth; Lipay, Josh; Ferandin, Yoan; Meijer, Laurent; Madura, Jeffrey 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, Jeffrey 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. Ascitutto, Eliana K.; Dang, Marina; Pochapsky, Susan Sondej; Madura, Jeffrey 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, Jeffrey 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, Jeffrey 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, Jeffrey 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. Ascitutto, Eliana K. General, Ignacio J. Xiong, Kan; Asher, Sanford; Madura, Jeffrey. 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. Ascitutto, Jeffrey D. Madura and Sanford A Asher. Salt Dependence of α -helical Peptide Folding Energy Landscapes. *Biochemistry* (2009), 48, 10818-10826.
25. Ascitutto, Eliana K.; Madura, Jeffrey 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. Ascitutto, Eliana K.; Mikhonin, Aleksandr V.; Asher, Sanford A.; Madura, Jeffrey, 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, Jeffrey, 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, Jeffrey, 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, Jeffrey, 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, Jeffrey, 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.; Ascitutto, Eliana K.; Madura, Jeffrey, 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, Jeffrey 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, Jeffrey, 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 antiviral 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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1063/1.2138704)
39. Esposito, Emilio Xavier; Tobi, Dror; Madura, Jeffrey 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](https://doi.org/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/jao53973d>
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](https://doi.org/10.1529/biophysj.104.058503)
43. Berberich, Jason, A.; Yang, Lee, W.; Madura, Jeffrey 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. *Acta Biomaterialia* (2005), 1, 173-181. doi:[10.1016/j.actbio.2004.11.006](https://doi.org/10.1016/j.actbio.2004.11.006)
44. Zhou, Zhigang; Madura, Jeffrey 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](https://doi.org/10.1002/prot.20223).
45. Esposito, Emilio Xavier; Hopfinger, Anton J.; Madura, Jeffrey 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, Jeffrey 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](https://doi.org/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](https://doi.org/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, Jeffrey 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](https://doi.org/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/jpo305988](https://doi.org/10.1021/jpo305988)
51. Zhou, Zhigang; Fisher, Derek; Spidel, Jared; Greenfield, Jodi; Patson, Brian; Fazal, Aleem; Wigal, Carl; Moe, Owen A.; Madura, Jeffrey 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/bio26518s>
52. Madura, Jeffrey D.; Salter, Edward A.; Wierzbicki, Andrzej; Dalal, Pranav; Harrington, John P. Homology Models for the Tetrameric and Dodecameric Complexes of *Lumbricus terrestris* Hemoglobin. *Theochem.* (2002), 592, 173-181. doi:[10.1016/S0166-1280\(02\)00238-5](https://doi.org/10.1016/S0166-1280(02)00238-5)
53. Walsh, Mary Beth; Moss, Connie M.; Johnson, Benny G.; Holder, Dale A.; Madura, Jeffrey 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](https://doi.org/10.1333/s00897020620a)
54. Zhou, Zhigang; Madrid, Marcela; Madura, Jeffrey 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](https://doi.org/10.1002/prot.10233)
55. Carlier, Paul R.; Madura, Jeffrey 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/j00255633>
56. Dick, Thomas J.; Acevedo, Orlando; Dalal, Pranav; Madura, Jeffrey 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.
57. Lakshminarasimhulu, Pasupulati; Madura, Jeffrey D. A Cell Multipole Based Domain Decomposition Algorithm For Molecular Dynamics Simulation of Systems of Arbitrary Shape. *Computer Physics Communications* (2002), 144(2), 141-153. DOI: [10.1016/S0010-4655\(02\)00157-1](https://doi.org/10.1016/S0010-4655(02)00157-1)
58. Esposito, Emilio Xavier; Baran, Kelli; Kelly, Ken; Madura, Jeffrey D. Docking Substrates To Metalloenzymes. *Molecular Simulation* (2001), 24(4-6), 293-306.
59. Madrid, Marcela; Lukin, Jonathan A.; Madura, Jeffrey D.; Ding, Jianping; Arnold, Edward. Molecular Dynamics of HIV-1 Reverse Transcriptase Indicates Increased Flexibility Upon DNA Binding. *Proteins: Structure, Function, and Genetics* (2001), 45(3), 176-182. DOI: [10.1002/prot.1137](https://doi.org/10.1002/prot.1137)
60. Dalal, Pranav; Knickelbein, Jared; Haymet, A.D.J.; Sonnichsen, Frank D.; Madura, Jeffrey D. Hydrogen Bond Analysis of Type 1 Antifreeze Protein in Water and the Ice/Water Interface. *PhyChem Comm (online computer file)* (2001, Paper No. 7. DOI: [10.1039/b101331i](https://doi.org/10.1039/b101331i)
61. Harris, Michael N.; Madura, Jeffrey D.; Ming, Li-June; Harwood, Valerie J. Kinetic and Mechanistic Studies of Prolyl Oligopeptidase from the Hyperthermophile *Pyrococcus Furius*. *Journal of Biological Chemistry* (2001), 276(22), 19310-19317. DOI: [10.1074/jbc.M010489200](https://doi.org/10.1074/jbc.M010489200)
62. Ravichandran, S.; Madura, Jeffrey D.; Talbot, J. A Brownian Dynamics Study of the Initial Stages of Hen Egg-White Lysozyme Adsorption at a Solid Interface. *Journal of Physical Chemistry B* (2001), 105(17), 3610-3613. <http://pubs.acs.org/doi/pdf/10.1021/jpo10223r>

63. Spreitzer, Glen; Whitling, Jacqueline M.; Madura, Jeffrey D.; Wright, David W. Peptide-encapsulated CdS Nanoclusters from a Combinatorial Ligand Library. *Chemical Communications (Cambridge)* (2000), (3), 209-210. DOI: [10.1039/a907178d](https://doi.org/10.1039/a907178d)
64. Esposito, E.X.; Baran, K.; Kelly, K.; Madura, J.D. Docking of Sulfonamides To Carbonic Anhydrase II and IV. *Journal of Molecular Graphics & Modeling* (2000), 18(3), 283-289. DOI: [10.1016/S1093-3263\(00\)00040-1](https://doi.org/10.1016/S1093-3263(00)00040-1)
65. Madura, Jeffrey D.; Baran, Kelli; Wierzbicki, Andrzej. Molecular Recognition and Binding of Thermal Hysteresis Proteins to Ice. *Journal of Molecular Recognition* (2000), 13(2), 101-113. DOI: [10.1002/\(SICI\)1099-1352\(200003/04\)13:2<101::AID-JMR493>3.0.CO;2-9](https://doi.org/10.1002/(SICI)1099-1352(200003/04)13:2<101::AID-JMR493>3.0.CO;2-9).
66. Madura, J. D.; Lombardini, J.B.; Briggs, J.M.; Minor, D.L.; Wierzbicki, A. Physical and Structural Properties of Taurine and Taurine Analogues. *Amino Acids* (1997), 13(2), 131-139. DOI: [10.1007/BF01373211](https://doi.org/10.1007/BF01373211) DOI: [10.1007/BF01373211](https://doi.org/10.1007/BF01373211)
67. Aronson, Nathan N.; Blanchard, Christopher, J.; Madura, Jeffrey D. Homology Modeling of Glycosyl Hydrolase Family 18 Enzymes and Proteins. *Journal of Chemical Information and Computer Sciences* (1997), 37(6), 999-1005. <http://pubs.acs.org/doi/pdf/10.1021/ci970236v>
68. Wierzbicki A.; Madura, Jeffrey D.; Salmon, C.; Sonnichsen, F. Modeling Studies of Binding of Sea Raven Type II Antifreeze Protein to Ice. *Journal of Chemical Information and Computer Sciences* (1997), 37(6), 1006-10. <http://pubs.acs.org/doi/pdf/10.1021/ci9702353>
69. Wierzbicki, A.; Taylor, M.S.; Knight, C.A.; Madura, J.D.; Harrington, J.P.; Sikes, C.S. Analysis of Shorthorn Sculpin Antifreeze Protein Stereospecific Binding To (2-1 0) Faces of Ice. *Biophysics Journal* (1996), 71(1), 8-18. doi: [10.1016/S0006-3495\(96\)79204-4](https://doi.org/10.1016/S0006-3495(96)79204-4)
70. Wierzbicki, Andrzej; Salter, Edward A.; Hoffman, Norris W.; Stevens, Edwin D.; Van Do, Liem; VanLoock, Margaret S.; Madura, Jeffrey D. Structural Investigations of trans-Rh(PY₃)₂(CO)X (X=F, Cl, NCO; Y=H, Me, Ph) Using Density Functional Theory and X-ray Analysis. *Journal of Physical Chemistry* (1996), 100(27), 11250-11254. DOI: [10.1021/jp952918w](https://doi.org/10.1021/jp952918w)
71. Huang, Ching-Li; Harrison, B. Keith; Madura, Jeffrey; Dolfing, Jan. Gibbs Free Energies of Formation of PCDDs: Evaluation of Estimation Methods and Application For Predicting Dehalogenation Pathways. *Environ. Toxicol. and Chem.* (1996), 15(6), 824-836. DOI: [10.1897/1551-5028\(1996\)015<0824:GFEOF0>2.3.CO;2](https://doi.org/10.1897/1551-5028(1996)015<0824:GFEOF0>2.3.CO;2)
72. Madura, Jeffrey D.; Nakajima, Yasushi; Hamilton, Rodney M.; Wierzbicki, Andrzej; Warshel, Arieh. Calculations of the Electrostatic Free Energy Contributions to the Binding Free Energy of Sulfonamides to Carbonic Anhydrase. *Struct. Chem.* (1996), 7(2), 131-138. DOI: [10.1007/BF02278738](https://doi.org/10.1007/BF02278738)
73. Davis, James H., Jr.; Madura, Jeffrey D. Synthesis and Computational Evaluation of a Boronium Ion Analogue of the Tropane Ring System. *Tetrahedron Lett.* (1996), 37(16), 2729-30. DOI: [10.1016/0040-4039\(96\)00372-3](https://doi.org/10.1016/0040-4039(96)00372-3)
74. Madura, Jeffrey D.; Taylor, Mark S.; Wierzbicki, Andrzej; Harrington, John P.; Sikes, C.S.; Soennichsen, Frank. The Dynamics and Binding Of A Type III Antifreeze Protein In Water And On Ice. *THEOCHEM* (1996), 388 65-77. doi: [10.1016/S0166-1280\(96\)80020-0](https://doi.org/10.1016/S0166-1280(96)80020-0)
75. Madura, Jeffrey D.; Briggs, James M.; Wade, Rebecca C.; Davis, Malcolm E.; Luty, Brock A.; Llin, Andrew; Antosiewicz, Jan; Gilson, Michael K.; Bagherri, Babak; et al. Electrostatics and Diffusion of Molecules in Solution: Simulations with the University of Houston Brownian Dynamics Program. *Comput. Phys. Commun.* (1995), 91-(1-3), 57-95. doi: [10.1016/S0166-1280\(96\)80020-0](https://doi.org/10.1016/S0166-1280(96)80020-0)

76. Gilson, Michael, K.; McCammon, J. Andrew; Madura, Jeffrey D. Molecular Dynamics Simulation With A Continuum Electrostatic Model of the Solvent. *Journal of Computational Chemistry* (1995), 16(9), 1081-95. DOI: [10.1002/jcc.540160904](https://doi.org/10.1002/jcc.540160904)
77. Young, Sidney, H.; Madura, Jeffrey D.; Wierzbicki, Andrzej. Integration of Numerical Methods Into The Undergraduate Physical Chemistry Curriculum Using MATHCAD. *J. Chem. Educ.* (1995), 72(7), 609-10.
78. Schaffer, S. W.; Azuma, J.; Madura, J.D. Mechanisms Underlying Taurine-Mediated Alterations In Membrane Function. *Amino Acids* (1995), 8(3), 231-46. DOI: [10.1007/BF00806821](https://doi.org/10.1007/BF00806821)
79. Wierzbicki, A.; Sikes, C.S.; Sallis, J.D.; Madura, J.D.; Stevens, E.D.; Martin, K.L. Scanning Electron Microscopy and Molecular Modeling of Inhibition of Calcium Oxalate Monohydrate Crystal Growth by Citrate and Phosphocitrate. *Calcified Tissue International* (1995), 56(4), 297-304. DOI: [10.1007/BF00318050](https://doi.org/10.1007/BF00318050)
80. Wierzbicki, A.; Sikes, C. S.; Madura, J. D.; Drake, B. Atomic Force Microscopy and Molecular Modeling of Protein and Peptide Binding to Calcite. *Calcified Tissue International* (1994), 54, 133-141. DOI: [10.1007/BF00296064](https://doi.org/10.1007/BF00296064)
81. Madura, J. D.; Wierzbicki, A.; Harrington, J. P.; Maughon, R. H.; Raymond, J. A.; Sikes, C. S. Interactions of the D and L Forms of Winter Flounder Antifreeze Peptide with the 201 Planes of Ice. *J. Amer. Chem. Soc.* (1994), 116, 417-418. <http://pubs.acs.org/doi/pdf/10.1021/ja00080a066>
82. Salter, E. A.; Wierzbicki, A.; Seminario, J. M.; Hoffman, N. W.; Easterling, M. L.; Madura, J. D. The Structure of trans-Rh(PH₃)₂(CO)X (X=F, Cl) Using Hartree-Fock/MBPT(2) Theory and Density Functional Theory. *J. Phys. Chem.* (1994), 98, 12945-12948. DOI: [10.1021/j100100a022](https://doi.org/10.1021/j100100a022)
83. Wade, Rebecca C.; Luty, Brock A.; Demchuk, Eugene; Madura, Jeffrey D.; Davis, Malcolm, E.; Briggs, James M.; McCammon, J. Andrew. Simulation of Enzyme-Substrate Encounter With Gated Active Sites. *Struct. Biol.* (1994), 1(1), 65-9. doi: [10.1038/nsbo194-65](https://doi.org/10.1038/nsbo194-65)
84. Wade, Rebecca C.; Davis, Malcolm E.; Luty, Brock A.; Madura, Jeffrey D.; McCammon, J. Andrew. Department Gating of the active site of triose phosphate isomerase: Brownian dynamics simulations of flexible peptide loops in the enzyme. *Biophys. J.* (1993), 64(1), 9-15. doi: [10.1016/S0006-3495\(93\)81335-3](https://doi.org/10.1016/S0006-3495(93)81335-3)
85. Cannon, William R.; Madura, Jeffrey D.; Thummel, Randolph P.; McCammon, J. Andrew. Molecular Recognition: Effect of Rotational Isomers on Host-Guest Binding. *J. Am. Chem. Soc.* (1993), 115(3), 879-84. DOI: [10.1021/ja00056a009](https://doi.org/10.1021/ja00056a009)
86. Luty, Brock A.; Wade, Rebecca C.; Madura, Jeffrey D.; Davis, Malcolm E.; Briggs, James M.; McCammon, J. Andrew. Brownian Dynamics Simulations of Diffusional Encounters Between Triose Phosphate Isomerase and Glyceraldehyde Phosphate: Electrostatic Steering of Glyceraldehyde Phosphate. *J. Phys. Chem.* (1993), 97(1), 233-7. DOI: [10.1021/j100103a040](https://doi.org/10.1021/j100103a040)
87. Sikes, C. S.; Mueller, E.; Madura, J. D.; Drake, B. Polyamino acids as Antiscalants, Corrosion Inhibitors, and Dispersants: Atomic Force Microscopy and Mechanisms of Action. *Proceedings for the National Association of Corrosion Engineers* (1993).
88. Davis, M. E.; Madura, J. D.; Luty, B. A.; McCammon, J. A. Electrostatics and Diffusion of Molecules in Solution: Simulations with the University of Houston Brownian Dynamics Program. *Computer Phys. Comm.*(1991), 62, 187-197. doi: [10.1016/0010-4655\(91\)90094-2](https://doi.org/10.1016/0010-4655(91)90094-2)
89. Davis, M. E.; Madura, J. D.; Sines, J.; Luty, B.A.; Allison, S.A.; McCammon, J.A. Diffusion-Controlled Enzymatic Reactions. *Methods in Enzymology* (1991), 202, 473-79. doi: [10.1016/0076-6879\(91\)02024-4](https://doi.org/10.1016/0076-6879(91)02024-4)

90. Hegde, Vidyadhar; Madhukar, Puttannachetty; Madura, Jeffrey D.; Thummel, Randolph P. Fischer Route to pyrido[3,2-g]indoles. A Novel Receptor for Urea Derivatives. *J. Am. Chem. Soc.*(**1990**), 112(11), 4549-50. DOI: [10.1021/ja00167a066](https://doi.org/10.1021/ja00167a066)
91. Madura, Jeffrey D.; McCammon, J. Andrew. Department of Chemistry, Brownian Dynamics Simulation of Diffusional Encounters Between Triose Phosphate Isomerase and D-glyceraldehyde Phosphate. *J. Phys. Chem.* (**1989**), 93(21), 7285-7. DOI: [10.1021/j100358a002](https://doi.org/10.1021/j100358a002)
92. Madura, J. D.; Pettitt, B. M.; Calef, D. Water under High Pressure. *Mol. Phys.* (**1988**), 64(2), 325-336. DOI: [10.1080/00268978800100253](https://doi.org/10.1080/00268978800100253)
93. Madura, Jeffrey D.; Pettitt, B. Montgomery. Effects of Truncating Long-Range Interactions in Aqueous Ionic Solution Simulations. *Chem. Phys. Lett.* (**1988**), 150(1-2), 105-8. doi:[10.1016/0009-2614\(88\)80404-4](https://doi.org/10.1016/0009-2614(88)80404-4)
94. Madura, Jeffrey D.; Pettitt, B. Montgomery; McCammon, J. Andrew. Geometric Considerations in the Calculation of Relative Free Energies of Activation. *Chem. Phys. Lett.* (**1987**), 141(1-2), 83-7. doi:[10.1016/0009-2614\(87\)80096-9](https://doi.org/10.1016/0009-2614(87)80096-9)
95. Speedy, Robin J.; Madura, Jeffrey D.; Jorgensen, William L. Network Topology in Simulated Water. *J. Phys. Chem.* (**1987**), 91(4), 909-13. DOI: [10.1021/j100288a029](https://doi.org/10.1021/j100288a029)
96. Madura, Jeffrey D.; Jorgensen, William L. Ab initio and Monte Carlo Calculations for a Nucleophilic Addition Reaction in the Gas Phase and in Aqueous Solution. *J. Am. Chem. Soc.* (**1986**), 108(10), 2517-27. DOI: [10.1021/ja00270a005](https://doi.org/10.1021/ja00270a005)
97. Jorgensen, W. L.; Chandrasekhar, J.; Buckner, J. K.; Madura, J. D. Computer Simulations of Organic Reactions in Solution. *Ann. N. Y. Acad. Sci.* (**1986**), 482, 198-209. DOI: [10.1111/j.1749-6632.1986.tb20951.x](https://doi.org/10.1111/j.1749-6632.1986.tb20951.x)
98. Jorgensen, William L.; Madura, Jeffrey D. Temperature and size dependence for Monte Carlo Simulations of TIP4P Water. *Mol. Phys.* (**1985**), 56(6), 1381-92. DOI: [10.1080/00268978500103111](https://doi.org/10.1080/00268978500103111)
99. Jorgensen, W. L.; Madura, J. D.; Swenson, C. J. Optimized Intermolecular Potential Functions for liquid Hydrocarbons. *J. Amer. Chem. Soc.* (**1984**), 106, 6638-6646. <http://pubs.acs.org/doi/pdf/10.1021/ja00270a005>
100. Houk, K.N.; Rondan, Nelson G.R.; Brown, Frank K.; Jorgensen, William L.; Madura, Jeffrey D.; Spellmeyer, David C. Electronic Origins and Consequences of Pyramidalization of Asymmetric Alkenes in Ground and Triplet Excited States. *J. Am. Chem. Soc.* (**1983**), 105(19), 5980-8. DOI: [10.1021/ja00357a004](https://doi.org/10.1021/ja00357a004)
101. Jorgensen, William L.; Chandrasekhar, Jayaraman; Madura, Jeffrey D. Impey, Roger W.; Klein, Michael L. Comparison of Simple Potential Functions for Simulating Liquid Water. *J. Chem. Phys.* (**1983**), 79(2), 926-35. DOI:[10.1063/1.445869](https://doi.org/10.1063/1.445869)
102. Jorgensen, William L.; Madura, Jeffrey D. Solvation and Conformation of Methanol in Water. *J. Am. Chem. Soc.* (**1983**), 105(6), 1407-13. DOI: [10.1021/ja00344a001](https://doi.org/10.1021/ja00344a001)

ARTICLES (NON-REFEREED)

103. Madura, Jeffrey D. Chemistry entry for Scribner Dictionary of American History. (**2003**).
104. Stouch, Terry R.; Brooks, Bernard R.; Swope, William C.; Madura, Jeffrey 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, Jeffrey D. Using MOE to Visualize Molecular Orbitals. *Journal of Molecular Graphics and Modeling* (**1999**), 17(2), 150-1.

106. Madura, Jeffrey D. Computational Chemistry on a Shoestring: Software from QCPE. *Council on Undergraduate Research Quarterly*. (1995), 155-157.
107. Madura, Jeffrey D. MOBY 1.5. *J. Chem. Inf. Comput. Sci.* (1993).
108. Madura, Jeffrey D. Brownian Dynamics Simulations. *Annu. Tech. Conf.- Soc. Plast. Eng.* (1992), 50th(2), 2274-6.
109. Madura, Jeffrey 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 addiction 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 Moléculaire (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 Moléculaire (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-Dienatonickel (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, Jeffrey 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, Jeffrey 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, Jeffrey 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, Jeffrey 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, Jeffrey 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, Jeffrey 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, Jeffrey 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, Jeffrey 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, Jeffrey 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; Karuppanan, Balamurugan; Madura, Jeffrey D.; Aitken, Jennifer A. Abstracts of Papers, 243rd ACS National Meeting & Exposition, San Diego, CA, United States, March 25-29, 2012 (2012), INOR-97
13. Salt effects on the conformational stability of small peptides Gaborek, Timothy J.; Madura, Jeffrey D. Abstracts of Papers, 243rd ACS National Meeting & Exposition, San Diego, CA, United States, March 25-29, 2012 (2012), COMP-358.
14. Free energy calculations on monoamine transporters Immadisetty, Kalyan; Madura, Jeffrey D. Abstracts of Papers, 243rd ACS National Meeting & Exposition, San Diego, CA, United States, March 25-29, 2012 (2012), COMP-338.
15. Analysis of structural dynamics from a conformational sampling of the bacterial monoamine transporter homologue LeuT Thomas, James R.; Gedeon, Patrick C.; Madura, Jeffrey D. Abstracts of Papers, 243rd ACS National Meeting & Exposition, San Diego, CA, United States, March 25-29, 2012 (2012), COMP-334.
16. Pathways and dynamics of the dopamine transporter in the presence of an explicit sodium gradient Merchant, Bonnie A.; Madura, Jeffrey D. Abstracts of Papers, 243rd ACS National Meeting & Exposition, San Diego, CA, United States, March 25-29, 2012 (2012), COMP-64.
17. Free energy perturbation of AEA and AKA to AAA in salt solutions Litzenberger, Emily A.; Gaborek, Timothy J.; Madura, Jeffrey D. Abstracts of Papers, 243rd ACS National Meeting & Exposition, San Diego, CA, United States, March 25-29, 2012 (2012), CHED-1349.
18. Design and synthesis of aminothiazole meriolin hybrid compounds as CDK5 inhibitors Shah, Dhruv; Jain, Prashi; Flaherty, Patrick T.; Manepalli, Sankar G.; Madura, Jeffrey D. Abstracts of Papers, 242nd ACS National Meeting & Exposition, Denver, CO, August 28-September 1, 2011 (2011), MEDI-282.
19. Effects of serotonin transporter mutations E493A and E494T on the free energy of binding of psychoactive molecules Brancho, James J.; Manepalli, Sankar; Immadisetty, Kalyan C.; Madura, Jeffrey D. Abstracts of Papers, 241st ACS National Meeting & Exposition, Anaheim, CA, March 27-31, 2011 (2011), COMP-161.
20. Homology modeling and membrane insertion of the human reduced folate carrier Link, Katie; Madura, Jeffrey D. Abstracts of Papers, 241st ACS National Meeting & Exposition, Anaheim, CA, March 27-31, 2011 (2011), COMP-138.
21. Investigation of the dopamine active transporter: A study in the motion and communication stochastics of transporter proteins in the neurotransmitter sodium symporter family Gibbons, Jonathon D.; Chennubhotla, Chakra; Madura, Jeffrey D.; Bahar, Ivet Abstracts of Papers, 241st ACS National Meeting & Exposition, Anaheim, CA, March 27-31, 2011 (2011), COMP-214.
22. MAT homologue LeuT transport mechanism and conformational sampling using Principal Component Analysis Thomas, James R.; Gedeon, Patrick C.; Madura, Jeffrey D. Abstracts of Papers, 241st ACS National Meeting & Exposition, Anaheim, CA, March 27-31, 2011 (2011), COMP-151.

23. Ortho-amido diphenylamines as MEK5 inhibitors Chakrabarty, Suravi; Flaherty, Patrick T.; Monlish, Darlene; Cavanaugh, Jane; Manepalli, Sankar G.; Madura, Jeffrey D. Abstracts of Papers, 242nd ACS National Meeting & Exposition, Denver, CO, August 28-September 1, 2011 (2011), MEDI-248.
24. Exploration of novel benzimidazole core as selective CDK5/p25 inhibitors Jain, Prashi; Yi, Shuyan; Flaherty, Patrick T.; Madura, Jeffrey D.; Meijer, Laurent Abstracts of Papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010 (2010)
25. Aminothiazole analogs as CDK5 inhibitors Jain, Prashi; Shah, Dhruv; Flaherty, Patrick; Madura, Jeffrey D.; Meijer, Laurent Abstracts of Papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010 (2010)
26. Parameterization of small drug-Like ligands using CHARMM General Force Field Immadisetty, Kalyan C.; Gibbons, Jonathan; Brancho, James; Madura, Jeffrey D. Abstracts of Papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010 (2010)
27. Comparison of the performance of different scoring functions in docking of antidepressants to serotonin transporter Manepalli, Sankar G. ; Madura, Jeffrey D.; Surratt, Chris Abstracts of Papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010 (2010)
28. Computational investigation of the transport mechanism for monoamine transporters Merchant, Bonnie A. ; Madura, Jeffrey D. From Abstracts of Papers, 240th ACS National Meeting, Boston, MA, United States, August 22-26, 2010 (2010)
29. Computational investigation of the transport mechanism for monoamine transporters Merchant, Bonnie A. ; Madura, Jeffrey D. Abstracts of Papers, 239th ACS National Meeting, San Francisco, CA, United States, March 21-25, 2010 (2010)
30. Simulation of monoamine transporter protein ligands' crystal structures using CHARMM Brancho, James; Madura, Jeffrey D. Abstracts of Papers, 239th ACS National Meeting, San Francisco, CA, United States, March 21-25, 2010 (2010)
31. Sodium phosphate effects on the helical stability of a mainly alanine peptide Batey, Nichole L.; Ascitto, Eliana K. ; Madura, Jeffrey D. Abstracts of Papers, 239th ACS National Meeting, San Francisco, CA, United States, March 21-25, 2010 (2010)
32. Design, synthesis, and testing of 4-substituted benzimidazole analogs as CDK5/p25 inhibitors Jain, Prashi; Chopra, Ishveen; Yi, Shuyan; Flaherty, Patrick T. ; Madura, Jeffrey D. Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009 (2009)
33. Development of novel photoaffinity ligands for the dopamine transporter based on pyrovalerone Aggarwal, Shaili; Lapinsky, David J.; Huang, Yurong; Surratt, Christopher K.; Lever, John R.; Foster, James D.; Vaughan, Roxanne A.; Manepalli, Sankar; Madura, Jeffrey D. Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009 (2009)
34. Potential of mean force calculations of the free energy of binding of Type I antifreeze proteins at water/ice interface Wierzbicki, A.; Battle, Keith; Madura, Jeffrey D. Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009 (2009)
35. Parameterization of desipramine, imipramine, and clomipramine Gibbons, Jonathon D. ; Madura, Jeffrey D. Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009 (2009)

36. Elucidation of binding profile similarities across structurally diverse ligands using a 3D dopamine transporter model Manepalli, Sankar; Madura, Jeffrey D.; Lapinsky, David J.; Surratt, Christopher K. Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009 (2009)
37. Continuum electrostatic and free energy perturbation calculations on leucine transporter complexed with tricyclic antidepressants Immadisetty, Kalyan; Gibbons, Jonathon D. ; Madura, Jeffrey D. Abstracts of Papers, 238th ACS National Meeting, Washington, DC, United States, August 16-20, 2009 (2009)
38. Comparison of popular force fields for use by pharmaceutical industry by computation of hydration free energies of drug-like molecules William C. Swope; Julia E. Rice; Jed W. Pitera; Hans W. Horn; Goundla Srinivas; Dan Price; Martha S. Head; Jeffrey D. Madura. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 237th ACS National Meeting, Salt Lake City, UT, USA, March 22-26, (2009)
39. Computational investigation of the leucine transport mechanism in LeuTAA Bonnie A. Merchant; Thomas J. Dick; Jeffrey D. Madura. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 237th ACS National Meeting, Salt Lake City, UT, USA, March 22-26, (2009)
40. Parameterization of small molecules that interact with the dopamine active transporter Jonathon D. Gibbons and Jeffrey D. Madura. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 237th ACS National Meeting, Salt Lake City, UT, USA, March 22-26, (2009)
41. Destabilization effects of sulfate on a polyalanine peptide Kathryn K. Myer; Jeffrey D. Madura; Eliana K. Ascitto. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 237th ACS National Meeting, Salt Lake City, UT, USA, March 22-26, (2009)
42. Non-tenure track faculty at Duquesne University Jeffrey 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)
43. Design, synthesis and testing of benzimidazole based inhibitors of CDK5 Prashi Jain; Shuyan Yi; Ishveen Chopra; Gwenyth Bleasdel; Patrick T. Flaherty; Jeffrey 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)
44. Drug discovery workbooks for high school and undergraduate students Jeffrey 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)
45. Structure based design of benzimidazole inhibitors of CDK5 Patrick T. Flaherty; Jeffrey D. Madura; Gwenyth Bleasdel; Prashi Jain; Shuyan Yi; Ishveen Chopra; 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)
46. Comprehensive comparison and assessment of force fields for pharmaceutical applications by computation of hydration free energy William C. Swope; Jed W. Pitera; Julia

- Rice; Hans W. Horn; Goundla Srinivas; Dan Price; Martha S. Head; Jeffrey 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)
47. Using a computational serotonin transporter model to identify likely binding pocket residues Sankar Manepalli; Jeffrey D. Madura; Martin Indarte; Chris Surratt. 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)
 48. Salt effects on the conformational preferences of alanine peptides Eliana K. Ascitutto and Jeffrey 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)
 49. COARSE: Enhanced sugar and lectin interaction scoring and energy function Emilio Xavier Esposito; Sankar Manepalli; Jeffrey 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)
 50. Molecular modeling at Duquesne University Jeffrey D. Madura and Eliana K. Ascitutto. 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 Jeffrey 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 Jeffrey 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; Jeffrey 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 Jeffrey 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)
 55. Unfolding of AAAAA(AAARA)₃A: A molecular dynamics study Eliana Ascitutto; Jeffrey D. Madura; Sandy Asher. 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)
 56. Comparative modeling and ligand binding of the dopamine transporter Jeffrey D. Madura; Martin Indarte; Christopher Surratt. 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)
57. Comparative modeling of plasma membrane permease Git1p from *Saccharomyces cerevisiae* Sophie Okolo; Jeffry D. Madura; Jana L. Patton-Vogt. 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)
 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)
 59. Comparative modeling and ligand binding Jeffry D. Madura. Department of Chemistry & Biochemistry, Center for Computational Sciences, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts, 62nd Southwest Regional Meeting of the American Chemical Society, Houston, TX, USA, October 19-22, (2006)
 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)
 63. A novel MD/BD model for the simulation of multi-scale 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, 230th ACS National Meeting, Washington, DC, USA, August 28-September 1, (2005)
 64. Structure and reactivity of nitrile anions Justine N. Geidosch; Jeffry D. Madura, Fraser F. Fleming. Department of Chemistry and Biochemistry, Duquesne University, 600 Forbes Avenue, 308 Mellon Hall, Pittsburgh, PA 15282. Abstracts of Papers, 229th ACS National Meeting, San Diego, CA, USA, March 13-17, (2005)
 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)

68. Analysis of protein-oligosaccharide docking interactions using principal component analysis Jennifer Leiss; Pranav Dalal; 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)
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 pK_as 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, NY, USA, September 7-11, (2003)
81. MD simulation of resistant 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)
83. Determining pK_a values for metallochaperones Jeffry D. Madura; Rasha Abd El-Rahman; Zhigang Zhou; Charles T. Dameron, 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)
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 chitinase 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)
86. Theoretical applications of chemical and physical CO₂ sequestration. Dick, Thomas J.; Dalal, Pranav; Madura, Jeffry D. Abstracts of Papers, 224th ACS National Meeting, Boston, MA, USA, August 18-22, 2002 (2002)
87. Computational studies of explicit solvates of lithiated phenylacetonitrile. Carlier, Paul R.; Madura, Jeffry D. Abstracts of Papers, 224th ACS National Meeting, Boston, MA, USA, August 18-22, 2002 (2002)
88. Unusual binding of oligosaccharides in the active-site cleft of family 18 chitinases. Dalal, Pranav; Aronson, Nathan N., Jr.; Alexyev, Mikhail F.; Amable, Lauren; Halloran, Brian A.; VanRoey, Patrick; Madura, Jeffry D.. Abstracts of Papers, 224th ACS National Meeting, Boston, MA, USA, August 18-22, 2002 (2002)

89. Use of dock and PB in reproducing the binding mode and predicting the binding-free energies of non-nucleoside inhibitors to HIV-1 reverse transcriptase. Zhou, Zhigang; Madura, Jeffrey. Abstracts of Papers, 224th ACS National Meeting, Boston, MA, United States, August 18-22, 2002 (2002)
90. Docking and binding affinity calculations of TIMBO analog inhibitors in HIV-1 RT. Zhou, Zhigang; Madura, Jeffrey D.. Abstracts of Papers, 224th ACS National Meeting, Boston, MA, USA, August 18-22, 2002 (2002)
91. Docking of novel Melatonin ligands to homology models of MT1 and MT2. Esposito, Emilio Xavier; Wymore, Troy; Li, Pui-Kai; Madura, Jeffrey D.. Abstracts of Papers, 224th ACS National Meeting, Boston, MA, USA, August 18-22, 2002 (2002)
92. Determination of pKa's in Proteins. AbdEl-Rahman, Rasha R.; Madura, Jeffrey D.; Dameron, Charles T. Abstracts of Papers, 224th ACS National Meeting, Boston, MA, USA, August 18-22, 2002 (2002)
93. Theoretic model and experimental verification of temperature dependence of MAE recovery from solid materials. Zhou, Zhigang; Shah, Sejal; Kingston, H. M.; Madura, Jeffrey. Abstracts of Papers, 224th ACS National Meeting, Boston, MA, USA, August 18-22, (2002)
94. Molecular basis for carbon dioxide sequestration in coal. Dick, Thomas J.; Acevedo, Orlando; Dalal, Pranav; Madura, Jeffrey D.; Evanseck, Jeffrey D.; Mathews, Jonathan P. Center of Computational Sciences, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, USA, April 7-11, (2002)
95. Computational modeling of Brine/CO₂ sequestration. Dick, Thomas J.; Dalal, Pranav; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, USA, April 7-11, (2002)
96. Molecular dynamics studies of interaction between crystals of calcium pyrophosphate dihydrate and phospholipid membranes. Dalal, Pranav; Wierzbicki, Andrzej; Madura, Jeffrey D.; Cheung, H.S. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, USA, April 7-11, (2002)
97. Protein folding using an on/off lattice simulation protocol. Rumon, Meredith P.; Brooks, Charles L., III; Feig, Michael; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, USA, April 7-11, (2002)
98. Effects of different force fields on antifreeze protein helical stability. Knickelbein, Jared E.; Dalal, Pranav; Haymet, A.D.J.; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, USA, April 7-11, (2002)
99. Computational gas phase calculations on hen egg white lysozyme. Forward, Paul A.; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, USA, April 7-11, (2002)
100. Binding thermodynamics of substrate-receptor interactions using isothermal titration calorimetry. Dean, Aaron; Enz, Kristy; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 223rd ACS National Meeting, Orlando, FL, USA, April 7-11, (2002)
101. Solvent effects on acetonitrile anion: Ab-initio modeling. Kulkarni, Vinod V.; Fleming, Fraser F.; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, USA, August 26-30, (2001)

102. 4D-QSAR study of melatonin receptor ligands for MT₁ and MT₂ receptors. Esposito, Emilio X.; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, USA, August 26-30, (2001)
103. Quinone inhibitors docking structures in its Oxidoreductase and binding free energy calculations. Zhou, Zhigang; Moe, Owen A.; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, USA, August 26-30, (2001)
104. Hydrogen bond analysis of the type 1 antifreeze protein in the water and the ice/water interfacial region. Dalal, Pranav; Knickelbein, Jared E.; Haymet, A.D.J.; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, USA, August 26-30, (2001)
105. Non-nucleoside inhibitors of HIV-1 reverse transcriptase binding calculations. Zhou, Zhigang; Madrid, Marcela; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 222nd ACS National Meeting, Chicago, IL, USA, August 26-30, (2001)
106. Protein folding using an on/off lattice simulation protocol. Rumon, Meredith P.; Evanseck, Jeffrey D.; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 221st ACS National Meeting, (2001)
107. Crambin energy landscape using CHARMM and MOPAC2000. Forward, Paul A.; Gomez, Michael E.; Evanseck, Jeffrey D.; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 221st ACS National Meeting (2001)
108. Antifreeze proteins at the ice/water interface. Dalal, Pranav; Knickelbein, Jared E.; Sonnichsen, Frank; Haymet, A.D.J.; Madura, Jeffrey D. Physiology and Biophysics, Case Western Reserve University, Cleveland, OH, USA. Abstracts of Papers, 221st ACS National Meeting (2001)
109. Nitrile anions: Ab initio modeling. Kulkarni, Vinod V.; Fleming, Fraser F.; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 220th ACS National Meeting, (2000)
110. Computational modeling of antifreeze protein: Ice interactions. Dalal, Pranav; Madura, Jeffrey D.; Sonnichsen, Frank. Physiology and Biophysics, Case Western Reserve University, Cleveland, OH, USA. Abstracts of Papers, 220th ACS National Meeting, (2000)
111. QSAR Study and design of melatonin receptor ligands for MT₁ and MT₂ receptors. Esposito, Emilio X.; Madura, Jeffrey D.; Li, Pui-Kai. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 220th ACS National Meeting, (2000)
112. Simulation of a Type II thermal hysteresis protein at the ice/water interface. Knickelbein, Jared E.; Madura, Jeffrey D. Duquesne University, Pittsburgh, PA, USA. Abstracts of Papers, 220th ACS National Meeting, (2000)
113. Comparison of CoMFA and QSAR in the study of melatonin receptor ligands for MT₁ and MT₂ receptors. Madura, Jeffrey D.; Esposito, Emilio; Li, Pui-Kai. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Book of Abstracts, 219th ACS National Meeting, San Francisco, CA, March 26-30, (2000)
114. Simulations of ice/protein/water interfaces. Knickelbein, Jared E.; Madura, Jeffrey D. Duquesne University, Pittsburgh, PA, USA. Book of Abstracts, 219th ACS National Meeting, San Francisco, CA, March 26-30, (2000)

115. Simulations of *Tenebrio molitor* in water. Baran, Kelli L.; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Book of Abstracts, 219th ACS National Meeting, San Francisco, CA, March 26-30, (2000)
116. Semiempirical calculation of hen egg-white lysozyme using Mopac2000. Forward, Paul A.; Madura, Jeffrey D. Duquesne University, Pittsburgh, PA, USA. Book of Abstracts, 219th ACS National Meeting, San Francisco, CA, March 26-30, (2000)
117. Using MOE/SVL to solve the PB equation and study protein electrostatics. Hampton, Edward S.; LaBute, Paul; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Book of Abstracts, 218th ACS National Meeting, New Orleans, August 22-26, (1999)
118. Predicted 3-D structure for thermal hysteresis protein of *Dendroidis candius*. Baran, Kelli L.; Moreland, Robert B.; Kelly, Ken; Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Book of Abstracts, 218th ACS National Meeting, New Orleans, August 22-26, (1999)
119. Molecular modeling lectures over the Internet. Madura, Jeffrey D.; Laaksonen, Leif; Ayling, June. SCS, Finland. Book of Abstracts, 216th ACS National Meeting, Boston, August 23-27 (1998)
120. Modeling antifreeze proteins at the ice/water interface. Madura, Jeffrey D. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Book of Abstracts, 216th ACS National Meeting, Boston, MA, August 23-27, (1998)
121. Investigation of the binding pocket of chitinase A. Hampton, Edward S.; Madura, Jeffrey D.; Pasupulati Lakshminarasimhulu; Aronson, Nathan N. Department of Chemistry and Biochemistry, Duquesne University, Pittsburgh, PA, USA. Book of Abstracts, 216th ACS National Meeting, Boston, MA, August 23-27, (1998)
122. Molecular dynamics simulation with Poisson-Boltzmann electrostatics. Madura, Jeffrey D.; Gilson, Michael; Wierzbicki, Andrzej. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 214th ACS National Meeting, Las Vegas, NV, September 7-11, (1997)
123. New data analysis methods for the Physical Chemistry laboratory using the Mathcad software. Young, S.H.; Madura, J.D.; Wierzbicki, A. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 214th ACS National Meeting, Las Vegas, NV, September 7-11, (1997)
124. Homology modeling of GP39. Blanchard, Chris J.; Madura, Jeffrey D.; Aronson, Nathan N. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 214th ACS National Meeting, Las Vegas, NV, September 7-11, (1997)
125. Molecular dynamics, circular dichroism and ice crystal growth studies of synthetic antifreeze compounds. Wierzbicki, A.; Knight, C.A.; Muccio, D.D.; Madura, J.D.; Harrington, J.P. University of South Alabama, Mobile, AL, USA. Book of Abstracts, 213th ACS National Meeting, San Francisco, April 13-17, (1997)
126. Binding of a type II AFP to ice. Salmon, Chris; Madura, Jeffrey D.; Sonnichsen, Frank; Wierzbicki, Andrzej. University of South Alabama, Mobile, AL, USA. Book of Abstracts, 213th ACS National Meeting, San Francisco, April 13-17, (1997)
127. Simulation of winter flounder antifreeze protein at the ice/water interface. Madura, Jeffrey D.; Ward, W.A.; Murrill, S.; Wierzbicki, A. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 212th ACS National Meeting, Orlando, FL, August 25-29, (1996)

128. Analysis of shorthorn sculpin antifreeze protein stereospecific binding to ice. Wierzbicki, A.; Taylor, M.S.; Knight, C.A.; Madura, J.D.; Harrington, J.P.; Sikes, C.S. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 212th ACS National Meeting, Orlando, FL, August 25-29, (1996)
129. Evaluation of estimation methods and application for predicting dehalogenation pathways. Madura, Jeffrey D.; Harrison, B. Keith; Huang, C.L.; Dolfing, J. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 212th ACS National Meeting, Orlando, FL, August 25-29, (1996)
130. Determining the 3-D structure of an antifreeze protein from amino acid primary sequence. Madura, Jeffrey D.; Moreland, Robert B.; Piche, Joseph; Duman, John G. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 212th ACS National Meeting, Orlando, FL, August 25-29, (1996)
131. Structural studies of trans-Rh(PY₃)₂(CO)X (X=F, Cl, NCO; Y=H, Me, Ph) using density functional theory. Wierzbicki, A.; Salter, E.A.; Hoffman, N.W.; Stevens, E.D.; Van Do, L.; Vanloock, M.S.; Madura, J.D. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 211th ACS National Meeting, New Orleans, LA, March 24-28, (1996)
132. Computational investigation of the bonding in Cp*Ru(C₆H₅X)₂(X=H, OH, OCH₃). Madura, Jeffrey D.; Nolan, Steve; Wierzbicki, Andrzej. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 211th ACS National Meeting, New Orleans, LA, March 24-28, (1996)
133. Computer Simulation of a Type I Antifreeze Protein at the Ice/Water Interface. Biophysical Society Meeting, Baltimore, MD, February (1996)
134. Modeling studies of the heme-containing chains of the multimeric lumbricus terrestris hemoglobin. Garber, R.; Madura, J.D.; Harrington, J.P.; Hirsch, R.E. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 211th ACS National Meeting, New Orleans, LA, March 24-28, (1996)
135. A modeling study of the noncovalent complexes of mechanism-based inhibitors with porcine pancreatic elastase. Henderson, Leigh Ann; Kerrigan, John E.; Madura, Jeffrey D. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 211th ACS National Meeting, New Orleans, LA, March 24-28, (1996)
136. Investigation of peptide secondary structure by FT-IR and molecular modeling. Davis, Tammy K.; Madura, Jeffrey D.; Harrington, John P. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 211th ACS National Meeting, New Orleans, LA, March 24-28, (1996)
137. Electrostatic free energy of binding between carbonic anhydrase and sulfonamides. Nakajima, Y.; Wierzbicki, A.; Madura, J.D. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 210th ACS National Meeting, Chicago, IL, August 20-24, (1995)
138. Molecular dynamics for undergraduates. Madura, Jeffrey D. Department of Chemistry, University of South Alabama, Mobile, AL, USA. Book of Abstracts, 210th ACS National Meeting, Chicago, IL, August 20-24, (1995).
139. Using UHBD to Study Biomolecular Interactions. 4th Conference on Current Trends in Computational Chemistry, Vicksburg, MS, November (1995).
140. Enzyme Inhibitor Interactions: Determining Free Energies of Binding for Sulfonamides Binding to Carbonic Anhydrase Using FDPB and PDL. ACS National Meeting, San Diego, CA, April (1994).

141. Enzyme Inhibitor Interactions: Determining Free Energies of Binding for Sulfonamides Binding to Carbonic Anhydrase Using FDPB and PDL. Gordon Research Conference (Computational), New Hampton, NH, June (1994).
142. Enzyme Inhibitor Interactions. Current Trends in Computational Chemistry Workshop, Vicksburg, MS, November (1994).
143. Coupling Poisson-Boltzmann finite-Difference Methods with Molecular Mechanics and Molecular Dynamics. Biophysical Society, Washington, DC, February (1993).
144. Coupling Poisson-Boltzmann Finite-Difference Methods with Molecular Mechanics and Molecular Dynamics. Gordon Research Conference (Proteins), New Hampton, NH, June (1993).
145. Modeling Molecule-Surface Interactions. Current Trends in Computational Chemistry Workshop, Vicksburg, MS, November (1993).
146. Molecular Dynamics Simulation of Alanine Dipeptide in Chloroform. ASBMB/ -Biophysical Society, Houston, TX, February (1992).
147. Brownian Dynamics Simulations. 69th Annual Meeting of the Alabama Academy of Science, Tuscaloosa, AL, April (1992).
148. Brownian Dynamics Simulations. Society of Plastic Engineers, Detroit, MI, May (1992).
149. Coupling Poisson-Boltzmann Finite-Difference Methods with Molecular Mechanics and Molecular Dynamics. Current Trends in Computational Chemistry Workshop, Jackson, MS, November (1992).
150. Rotation and Inversion Barriers of Sulfonamides. 197th ACS National Meeting, Dallas, TX, April (1989)
151. Computer Collection and Analysis of Data from Spectrophotometer. 30th Annual Pennsylvania Association of College Chemistry Teachers, Duquesne University, Pittsburgh, PA, April (1981)