**MARY JO ONDRECHEN**

**Present Position; Permanent address**:

Professor of Chemistry & Chemical Biology

Department of Chemistry & Chemical Biology

Northeastern University (NU)

Boston, Massachusetts 02115

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**Education**:

Ph.D. (Chemistry) 1978 Northwestern University, Evanston, Illinois

B.A. (Chemistry, ACS certified) 1974 Reed College, Portland, Oregon

**Previous Appointments**:

Assistant Professor (1980-86), Associate Professor (1986-90), NU, Boston

NATO Postdoctoral Fellow (1980), Tel Aviv University, Tel Aviv, ISRAEL

Postdoctoral Research Associate (1978-1979), The University of Chicago

**Honors and Awards**:

Alfred P. Sloan Foundation Fellowship (1987-1991)

NATO Postdoctoral Fellowship (1980)

Excellence in Teaching Award, Northeastern (1989)

Phi Beta Delta International Honor Society Medal (1999)

Outstanding Contributions Award, Interstate Technology & Regulatory Council – ITRC (2014)

Outstanding Service Award, ITRC (2005)

Outstanding Native American Student Mentor Award, SACNAS (2018)

Eminent Scientist Lecturer, American Chemica Society National Meeting (2018)

**Board Memberships, Editorial Appointments:**

Regional Editor, **Current Bioinformatics** (2007-2017); Editorial Board:(2005-2017)

Editorial Board, **Journal of Enzymology & Proteomics Research** (2017-)

Committee of Visitors, National Science Foundation Chemistry Division (2007)

Committee of Visitors, National Science Foundation MCB Division (2011 & 2014)

Board of Directors, **Telluride Research Center**, Telluride, CO 2005-2007

Board of Directors, **North American Indian Center of Boston (NAICOB)**, Boston, MA 1999-2016

Board of Advisors, **Interstate Technology & Regulatory Council**, Washington, DC (2008-2013)

Board of Directors, **American Indian Science & Engineering Society (AISES)**, Albuquerque, NM(2007-2010), Chair 2011-2013

**Professional Societies**: American Chemical Society; American Physical Society;

International Society for Computational Biology (ISCB); American Indian Science and Engineering Society (AISES); Society for the Advancement of Chicanos & Native Americans in Science (SACNAS); The Biophysical Society; The Protein Society

**Research Interests**: Theoretical and computational chemistry; ­Functional genomics; Applications of statistics and physicochemical methods to genomics; Bioinformatics; understanding enzyme function; structure-based drug discovery; enzyme design

**Special Skills & Experience:**

Theoretical Chemistry

Computational Chemistry and Chemical Biology

Applications of Statistics to Genomics

Applications of Physicochemical methods to Genomics

Molecular Modeling

Molecular Dynamics

Biological Modeling

Functional genomics

Protein structure analysis & function prediction

Advocacy for environmental remediation

Advocacy for Native American rights

Advocacy for Tribal and stakeholder involvement in environmental

remediation decisions

Analysis of toxic and radioactive waste treatment systems

Cultural perspectives on technical issues

Environmental justice

Communication of technical concepts to a non-technical audience

Advocacy for the Urban Indian Community

Service on non-profit Boards of Directors

**Other Professional service:**

Presidential Task Force on Diversity, **American Chemical Society,** 2009-2010

Committee on Minority Affairs, **American Chemical Society**, 2011-

Advisory Board, Open Chemistry Collaborative in Diversity Equity (OXIDE), 2012-

COACh Board of Advisors 2016-

**Community involvement and leadership:**

Enrolled member, Mohawk tribe of Iroquois Nation

Board of Directors, **North American Indian Center of Boston**

**(NAICOB)**, Boston, MA 1999-2016

## **Hopkinton Conservation Commission** (1998-2001; dealt

## primarily with wetlands protection law)

**Community Leaders Network**, U.S. Department of Energy, Office

of Science and Technology, Washington, D.C. 1997

High-Level Waste Tank Remediation Subgroup of the Community

Leaders Network, 1997

Sequoyah Fellow, American Indian Science and Engineering

Society (AISES), 1997-

**Interstate Technology and Regulatory Council (ITRC)** of the

Western Governor's Association, Denver, CO, 1997-1999

Interstate Technology and Regulatory Council (ITRC) of the

Environmental Council of the States (ECOS),

Washington, D.C., 1999-

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**Current and Recent Research and Education Grants**

“Distal Residues in Enzyme Catalysis and Protein Design”

National Science Foundation – MCB-1517290

PI: Mary Jo Ondrechen; co-PI: Penny Beuning

$818,211

07/01/2015 – 06/30/2019

"Chemical Signatures for the Discovery of Protein Function"

National Science Foundation – CHE-1305655

PI: Mary Jo Ondrechen; co-PI: Penny Beuning

$318,000.

07/01/2013 - 06/30/2018

“Tethering SOD1 Cysteine Pairs with Cyclic Disulfides: a New Method for Protein Stabilization”

ALS Association – 18-IIA-420

PI: Jeffrey Agar; Co-PIs: Mary Jo Ondrechen & Roman Manetsch

$300,000

10/01/2017 – 09/30/2020

“Northeastern University Skills and Capacity for Inclusion (NU-SCI): Inclusive Excellence Catalyzed by Experiential Education”

Howard Hughes Medical Institute

PD: Mary Jo Ondrechen; co-PD: Wendy A. Smith

$1,010,000.

09/01/2017 – 08/31/2022

“Lighting the Pathway to Faculty Careers for Natives in STEM”

NSF-DBI-1444853

PI: Sarah Echohawk; co-PIs: Mary Jo Ondrechen, Chris J. Cornelius, Melinda McClanahan, Robert E. Megginson

$1,438,505

08/15/2014 – 07/31/2019

**ACADEMIC RESEARCH PUBLICATIONS -- MARY JO ONDRECHEN**

1. "A Treatment of Vibrational Relaxation Without the Rotating Wave Approximation," M.J. Ondrechen, A. Nitzan, and M.A. Ratner, Chem. Phys. 16, pp. 49-59 (1976).
2. "Intramolecular Electron Transfer: Simple Theory of Purely Electronic Effects,: M.A. Ratner and M.J. Ondrechen, Mol. Phys. 32, pp. 1233-1245 (1976).
3. "Intramolecular Electron Transfer in Simple Model Systems. A Propagator Study," M.J. Ondrechen and M.A. Ratner, J. Chem. Phys. 66, pp. 938-946 (1977).
4. "Effect of Basis Function Overlap on Intramolecular Electron Transfer Amplitudes: Some Results for a Two-Site Hubbard Model," M.J. Ondrechen and M.A. Ratner, Chem. Phys. Lett. 51, pp. 573-577 (1977).
5. "Intramolecular Electron Transfer Theory: A Study of Purely Electronic Effects," M.J. Ondrechen, Ph.D. Thesis, chapters I-VIII, Northwestern University, Evanston, Illinois, 1978.
6. "The Role of Anharmonicity in the Breakdown of the Grüneisen Scaling Law in Molecular Crystals," M.J. Ondrechen, Ph.D. Thesis, chapter IX, Northwestern University, Evanston, Illinois, 1978.
7. "Electron Transfer in Fixed-Nuclei Systems: A Comparison of Propagator Descriptions," M.J. Ondrechen, M.A. Ratner, and J.R. Sabin, J. Chem. Phys. 71, pp. 2244-2249 (1979).
8. "Thermodynamics in Finite Time: A Chemically-Driven Engine," M.J. Ondrechen, R.S. Berry, and B. Andresen, J. Chem. Phys. 72, pp. 5118-5124 (1980).
9. "Thermodynamics in Finite Time: Processes with Temperature-Dependent Chemical Reactions," M.J. Ondrechen , B. Andresen, and R.S. Berry, J. Chem. Phys. 73, pp. 5838-5843 (1980).
10. "Hexammineruthenium (II,III) and Pentamminedinitrogenruthenium (II). A Hartree-Fock-Slater Study," M.J. Ondrechen, M.A. Ratner, and D.E. Ellis, J. Am. Chem. Soc. 103, pp. 1656-1659 (1981).
11. "Maximum Work from a Finite Reservoir by Sequential Carnot Cycles," M.J. Ondrechen, B. Andresen, M. Mozurkewich, and R.S. Berry, Am. J. Phys. 49, pp. 681-685 (1981).
12. "Model Calculations of Potential Surfaces of van der Waals Complexes Containing Large Aromatic Molecules," M.J. Ondrechen, Z. Berkovitch-Yellin, and J. Jortner, J. Am. Chem. Soc. 103, pp. 6586-6592 (1981).
13. "Through-Bridge Electron Transfer: A Propagator Study of a Simple Three-Site Model," L.J. Root and M.J. Ondrechen, Chem. Phys. Lett. 88, pp. 538-542 (1982).
14. "Adiabatic Potentials for a Bridged Three-Site Electron-Transfer System," L.J. Root and M.J. Ondrechen, Chem. Phys. Lett. 93, p. 421-424 (1982).
15. "Energetics and Dynamics of Large van der Waals Molecules," U. Even, A. Amirav, S. Leutwyler, M.J. Ondrechen, Z. Berkovitch-Yellin, and J. Jortner, Faraday Discuss. Chem. Soc. 73, pp. 153-172 (1982).
16. "The Generalized Carnot Cycle: A Working Fluid Operating in Finite time Between Finite Heat Sources and Sinks," M.J. Ondrechen, M.H. Rubin, and Y.B. Band, J. Chem. Phys. 78, pp. 4721-4727 (1983).
17. "Thermodynamics for Processes in Finite Time," B. Andresen, R.S. Berry, M.J. Ondrechen, and P. Salamon, Accts. Chem. Res. 17, pp. 266-271 (1984).
18. "The Electronic Structure of the Creutz-Taube Ion: A Hartree-Fock-Slater Study," M.J. Ondrechen, D.E. Ellis, and M.A. Ratner, Chem. Phys. Lett. 109, pp. 50-55 (1984).
19. "Two-Dimensional Potential Surfaces for Bridged Mixed-Valence Dimers," M.J. Ondrechen, J. Ko, and L.J. Root, J. Phys. Chem. 88, pp. 5919-5923 (1984).
20. "A Model for the Intervalence Transfer Band Profile of Bridged Mixed-Valence Dimers," J. Ko and M.J. Ondrechen, Chem. Phys. Lett. 112, pp. 507-512 (1984).
21. "Lineshape of the Intervalence Transfer Band in Bridged Mixed-Valence Dimers: The Delocalized Case," J. Ko and M.J. Ondrechen, J. Am. Chem. Soc. 107, pp. 6161-6167 (1985).
22. "Models for the Spectra of Bridged Mixed-Valence Dimers," M.J. Ondrechen, J. Ko, and L.-T. Zhang, Int. J. Quantum Chem.: Quantum Chem. Symposium 19, pp. 393-401 (1986).
23. "The Creutz-Taube Ion: A Model for the EPR g Tensor which Includes the Bridging Ligand," J. Ko, L.-T. Zhang and M.J. Ondrechen, J. Am. Chem. Soc. 108, pp. 1712-1713 (1986).
24. "An Analysis of the Absorption and Fluorescence Spectra of Trimethylamine: Determination of the A~-X~ Origin and the Ground State Inversion Barrier," A.M. Halpern, M.J. Ondrechen and L.D. Ziegler, J. Am. Chem. Soc. 108, pp. 3907-3912 (1986).
25. "Electronic Structure of the Creutz-Taube Ion," L.-T. Zhang, J. Ko, and M.J. Ondrechen, J. Am. Chem. Soc. 109, 1666-1671 (1987).
26. "A Model for the Optical Absorption Spectrum of (μ-Pyrazine) Decaamminediruthenium (5+): What Hath Creutz and Taube Wrought?" M.J. Ondrechen, J. Ko and L.-T. Zhang, J. Am. Chem. Soc. 109, pp. 1672-1676 (1987).
27. "A Non-Adiabatic Quantum Mechanical Treatment of the Absorption Lineshape of Bridged Mixed-Valence Dimers," L.-T. Zhang, J. Ko and M.J. Ondrechen, J. Phys. Chem. 93, pp. 3030-3034 (1989).
28. "Bridged Mixed-Valence Systems: How Polarizable Bridging Ligands Can Lead to Interesting Spectroscopic and Conductive Properties," M.J. Ondrechen, S. Gozashti, L.-T. Zhang and F. Zhou, ACS Symposium Series No. 226, Electron Transfer in Biology and the Solid State: Inorganic Compounds with Unusual Properties, 225-235 (1990).
29. "A Hybrid Hubbard Model for Discrete and Periodic Backbonded Complexes," S. Gozashti, L.-T. Zhang, M.X. Wu, F. Zhou and M.J. Ondrechen, Chem. Phys. Lett. 165, 208-212 (1990).
30. "Non-Lorentz Cycles in Nonequilibrium Thermodynamics," M.J. Ondrechen, Advances in Thermodynamics 4, 139-152 (1990).
31. "Mixed-Valency Oligomers: Model Pathways for the Control of Their Properties," M.J. Ondrechen and X.M. Wu, Mixed Valency Systems: Applications in Chemistry, Physics and Biology, K. Prassides, Ed. (Kluwer, Dordrecht) 335-340 (1991).
32. "An Electronic Mechanism for Electron Pairing in Antiferromagnetic Bridged Mixed-Valence Systems," M.J. Ondrechen, S. Gozashti and X.M. Wu, J. Chem. Phys. 96, 3255-3261 (1992).
33. “Third-Order Nonlinear Optical Properties of Finite Bridged Polymers," X.M. Wu and M.J. Ondrechen, Chem. Phys. Lett. 205, 85 (1993).
34. "The Electronic Structure of Pentaammine (Pyrazine) Ruthenium (II) and (III): The Metal-Ligand Pi Conjugation and Its Implications in Electron Transfer," L.-T. Zhang and M.J. Ondrechen, Inorg. Chim. Acta 226, 43-51 (1994).
35. “Comment on the Calculation of Absorption Lineshapes for Mixed-Valence Dimers," M.J. Ondrechen, A. Ferretti, A. Lami, and G. Villani, J. Phys. Chem. 98, 11230-11232 (1994).
36. "Potential Energy Surfaces for a Mixed-Valence Dimer in an Applied Electric Field," L.F. Murga and M.J. Ondrechen, Theor. Chim. Acta 90,331-339 (1995).
37. "Electron Donor-Acceptor Couples," M.J. Ondrechen, Int. Revs. Phys. Chem. 14, 1-14 (1995).
38. "The Role of Vibronic Coupling and Correlation Effects on the Optical Properties of Mixed-Valent and Monovalent Dimer Compounds: The Creutz-Taube Ion and Its Monovalent Analogues," A. Ferretti, A. Lami, M.J. Ondrechen and G. Villani, J. Phys. Chem. 99, 10484-10491 (1995).
39. “The Intrinsic Anodic Stability of Several Anions Comprising Solvent-Free Ionic Liquids," V.R. Koch, L.A. Dominey, C. Nanjundiah, and M.J. Ondrechen, J. Electrochem. Soc.. 143, 798-803 (1996).
40. “Theory of the Stark Effect Spectral Lineshape for a Delocalized Mixed-Valence Complex,” L.F. Murga, A. Ferretti, A. Lami, M.J. Ondrechen and G. Villani, Inorganic Chemistry Communications 1, 137-140 (1998).
41. "Theory of the Stark Effect in Protein Systems Containing an Electron Donor- Acceptor Couple," L.F. Murga and M.J. Ondrechen, J. Inorg. Biochem.70 245-252 (1998).
42. **“**A Hubbard Model for the Second Hyperpolarizability in Alternating Polymers,” I.A. Shehadi, L.F. Murga, M.J. Ondrechen and J. Linderberg,Chem. Phys. Lett. 291 325-332 (1998).
43. **“**Theory of Electroabsorption Spectroscopy in Pyrazine Bridged Ru Dimers**,”** A. Ferretti, A. Lami, L.F. Murga, I.A. Shehadi, M.J. Ondrechen and G. Villani, J.Am. Chem. Soc. 121, 2594-2596 (1999).
44. "Introducing a Practice-Oriented Approach in the Physical Chemistry Instructional Laboratory," D.E. Budil, L.R. Khundkar, I.A. Shehadi and M.J. Ondrechen, J. Chem. Ed. 76, 601-602 (1999).
45. "Models for Chemical Control of Third-Order Nonlinear Optical Properties in Finite Polymers," L.F. Murga, I.A. Shehadi, M.J. Ondrechen, Trends in Chemical Physics 7, 233-245 (1999).
46. "Numerical Aspects of the Calculation of Second Hyperpolarizabilities Using the Finite Field Method Coupled with a Simple Lanczos Algorithm," L.F. Murga and M.J. Ondrechen, **Journal of Computational Chemistry** **22**, 468-474 (2001).
47. "A Model for Enzyme-Substrate Interaction in Alanine Racemase," M.J. Ondrechen, J.M. Briggs and J.A. McCammon, **Journal of the American Chemical Society** **123**, 2830-2834 (2001). PMID: 11456969
48. “THEMATICS: A Simple Computational Predictor of Enzyme Function from Structure,” M.J. Ondrechen, J.G. Clifton & D. Ringe, **Proc. Nat. Acad. Sci. USA 98,** 12473-12478 (2001). PMID: 11606719
49. “Future Directions in Protein Function Prediction,” I.A. Shehadi, H. Yang and M.J. Ondrechen, **Molecular Biology Reports 29**, 329-335 (2002).
50. “THEMATICS as a Tool for Functional Genomics,” M.J. Ondrechen, **Genome Informatics 13**, 563-564 (2002).
51. “Prediction of Protein Function with THEMATICS,” M.J. Ondrechen, L.F. Murga, J.G. Clifton and D. Ringe, **Currents in Computational Molecular Biology**, 21-22, 2003.
52. “THEMATICS is Effective for Active Site Prediction in Comparative Model Structures,” I.A. Shehadi, A. Uzun, L.F. Murga, V. Ilyin and M.J. Ondrechen, **Conferences in Research and Practice in Information Technology, Vol. 29**, Yi-Ping Phoebe Chen, Editor, 209-215 (2004).
53. “Protein Structure to Function: Insights from Computation,” D. Ringe, Y. Wei, K.R. Boino and M.J. Ondrechen, **Cellular and Molecular Life Sciences** **61**, 387-392 (2004).
54. “Identifying Functional Sites Based on Prediction of Charge Group Behavior,” M.J. Ondrechen, **Protocols in Bioinformatics**, A.D. Baxevanis, et al., Editors, John Wiley & Sons: Hoboken, N.J. p. 8.6.1 - 8.6.10 (2004).
55. “Statistical Metrics for Protein Active Site Prediction with THEMATICS,” J. Ko, P. Andre, L.F. Murga and M.J. Ondrechen, Proceedings of the Fourth International Conference on Bioinformatics of Genome Regulation and Structure BGRS 2004, 1, 282-285, Novosibirsk, Russia (2004).
56. “Physicochemical Methods for Prediction of Functional Information for Proteins, L.F. Murga, Y. Wei, P. Andre, J.G. Clifton, D. Ringe and M.J. Ondrechen, **Israel Journal of Chemistry** **44**, 299-308 (2004).
57. “Active Site Prediction for Comparative Model Structures with THEMATICS,” I.A. Shehadi, A. Abyzov, A. Uzun, Y. Wei, L.F. Murga, V. Ilyin, and M.J. Ondrechen, **Journal of Bioinformatics and Computational Biology 3**, 127-143 (2005).
58. “Statistical Criteria for Protein Active Site Prediction with THEMATICS,” J. Ko, L.F. Murga, P. Andre, H. Yang, M.J. Ondrechen, R.J. Williams, A. Agunwamba, and D.E. Budil, **Proteins: Structure Function Bioinformatics 59**, 183-195 (2005).
59. “Prediction of Active Sites for Protein Structures from Computed Chemical Properties,” J. Ko, L.F. Murga, Y.Wei, and M.J. Ondrechen, **Bioinformatics** **21**, i258-i265 (2005).
60. “Central Moments Based Statistical Analysis for the Determination of Functional Sites in Proteins with THEMATICS,” L.F. Murga, J. Ko, Y. Wei, and M.J. Ondrechen, in Bioinformatics of Genome Regulation and Structure II, N. Kolchanov and R. Hofestaedt, Eds., Springer Science & Business Media, Inc, pp 215-224 (2005).
61. “Identification of Functional Subclasses in the DJ-1 Superfamily Proteins,” Y. Wei, D. Ringe, M.A. Wilson, and M.J. Ondrechen, **PloS Computational Biology 3**, e10, 120-126 (2007). PMID: 17257049
62. “Selective Prediction of Interaction Sites in Protein Structures with THEMATICS,” Y. Wei, J. Ko, L.F. Murga, and M.J. Ondrechen, **BMC Bioinformatics 8:**119**,** (2007).PMID: 17419878
63. “Computed Protonation Properties: Unique Capabilities for Protein Functional Site Prediction,” L.F. Murga, Y. Wei, and M.J. Ondrechen, **Genome Informatics** **19**, 107-118 (2007).
64. “Enhanced Sensitivity in Prediction of Protein Active Sites with THEMATICS and Support Vector Machines,” W. Tong, Y. Wei, L.F. Murga, J. Ko, M.J. Ondrechen, and R. J. Williams, **Protein Science 17**, 333-341 (2008).
65. “Prediction of Interaction Sites from Apo 3D Structures When the Holo Conformation is Different,” L.F. Murga, M.J. Ondrechen, and D. Ringe, **Proteins: Structure Function Bioinformatics** **72:**3, 980-992 (2008).
66. “Identification of a twin-arginine leader peptide binding site in DmsD; Defined through random and bioinformatics-directed mutagenesis,” C.S. Chan, T.M.L. Winstone, L. Chang, H. Li, C. Stevens, M.L. Workentine, Y. Wei, M.J. Ondrechen, M. Paetzel, and R.J. Turner, **Biochemistry** **47**, 2749-2759 (2008). PMID: 18247574
67. “pH-dependent Interdomain Tethers of CD1b Regulate Its Antigen Capture**,”** M. Relloso, T.-Y. Cheng, J.S. Im, E. Parisini, C. Roura-Mir, C. DeBono, D. M. Zajonc, L. F. Murga, M.J. Ondrechen, I.A. Wilson, S.A. Porcelli, and D.B. Moody, **Immunity 28**, 774-786 (2008). PMID: 18538591
68. “Partial Order Optimum Likelihood (POOL): Maximum Likelihood Prediction of Active Site Residues Using 3D Structure and Sequence Properties,” W. Tong, Y. Wei, L.F. Murga, M.J. Ondrechen, and R.J. Williams, **PLoS Computational Biology**, **5**(1): e1000266 (2009). PMID: 9148270
69. "High Conservation of Amino Acids with Anomalous Protonation Behavior," D.G.C. Hildebrand, H. Yang, M.J. Ondrechen, and R.J. Williams, **Current Bioinformatics**, **5**(2), 134-140 (2010).
70. "Functional Classification of Protein 3D Structures from Predicted Local Interaction Sites," R. Parasuram, J.S. Lee, P. Yin, S. Somarowthu, M.J. Ondrechen, **Journal of Bioinformatics and Computational Biology**, **8**, 1-15 (2010).
71. "High Performance Prediction of Functional Residues in Proteins with Machine Learning and Computed Input Features," S. Somarowthu, H. Yang, D.G.C. Hildebrand, and M.J. Ondrechen, **Biopolymers** **95**(6), 390-400 (2011). PMID: 21254002
72. "Electrostatic Properties for Protein Functional Site Prediction," J.S. Lee and M.J.Ondrechen, in Protein Function Prediction for Omics Era, D. Kihara, Ed., Springer, Dordrecht, pp. 183-196 (2011).
73. "Crystal structure of a metal-dependent phosphoesterase (YP\_910028.1) from Bifidobacterium adolescentis: Computational prediction and experimental validation of phosphoesterase activity," G.W. Han, J. Ko, C.L. Farr, M.C. Deller, Q. Xu, H.-J. Chiu, M.D. Miller, J. Sefcikova, S. Somarowthu, P.J. Beuning, M.-A.´ Elsliger, A.M. Deacon, A. Godzik, S.A. Lesley, I.A. Wilson,\* and M.J. Ondrechen\*, **Proteins 79**(7), 2146-2160 (2011). PMID: 21538547
74. "Evidence of the Participation of Remote Residues in the Catalytic Activity of Co-Type Nitrile Hydratase from Pseudomonas putida," Heather R. Brodkin, Walter R. P. Novak, Amy C. Milne, J. Alejandro D’Aquino, N. M. Karabacak, Ilana G. Goldberg, Jeffrey N. Agar, Mark S. Payne, Gregory A. Petsko, Mary Jo Ondrechen, Dagmar Ringe, **Biochemistry 50**(22), 4923-4935 (2011). PMID: 21473592

# "A Tale of Two Isomerases: Compact versus Extended Active Sites in Ketosteroid Isomerase and Phosphoglucose Isomerase," Srinivas Somarowthu, Heather R. Brodkin, J. Alejandro D'Aquino, Dagmar Ringe, Mary Jo Ondrechen, and Penny J. Beuning, **Biochemistry 50**(43) 9283-9295 (2011).

1. "Pharmacological Validation of Trypanosoma brucei Phosphodiesterases B1 and B2 as Druggable Targets for African Sleeping Sickness," Nicholas D. Bland, Cuihua Wang, Craig Tallman, Alden E. Gustafson, Zhouxi Wang, Trent D. Ashton, Stefan Ochiana, Gregory McAllister, Kristina Cotter, Anna P. Fang, Lara Gechijian, Norman Garceau, Rajiv Gangurde, Ron Ortenberg, Mary Jo Ondrechen, Robert K. Campbell, and Michael P. Pollastri, **J. Medicinal Chemistry 54**(23), 8188-8194 (2011). PMID: 22023548
2. “POOL server: Machine learning application for functional site prediction in proteins,” Srinivas Somarowthu and Mary Jo Ondrechen, **Bioinformatics 28**(15), 2078-2079 (2012). PMID: 22661648
3. “Effects of non-catalytic, distal amino acid residues on activity of *E. coli* DinB (DNA Polymerase IV),” Jason M. Walsh, Ramya Parasuram, Pradyumna R. Rajput, Eriks Rozners, Mary Jo Ondrechen, and Penny J. Beuning, **Environmental and Molecular Mutagenesis 53**(9), 766-776 (2012). PMID: 23034734
4. “The human Aurora kinase inhibitor danusertib is a lead compound for anti-trypanosomal drug discovery via target repurposing,” Stefan O. Ochiana, Vidya Pandarinath, Zhouxi Wang, Rishika Kapoor, Mary Jo Ondrechen, Larry Ruben, and Michael P. Pollastri, **European Journal Medicinal Chemistry**, **62**, 777-784 (2013). PMID: 22889561
5. “Protein Function Annotation with Structurally Aligned Local Sites of Activity (SALSAs), Zhouxi Wang, Pengcheng Yin, Joslynn S. Lee, Ramya Parasuram, Srinivas Somarowthu,” and Mary Jo Ondrechen, **BMC Bioinformatics**, **14**(Suppl 3):S13 (2013). PMID: 23514271
6. “Design and evaluation of xanthine based adenosine receptor antagonists: Potential hypoxia targeted immunotherapies,” R. Thomas, J. Lee, V. Chevalier, S. Sadler, K. Selesniemi, S. Hatfield, M. Sitkovsky, M.J. Ondrechen, and G.B. Jones, **Bioorganic and Medicinal Chemistry 21**, 7453-7464 (2013). PMID: 24126093
7. “American Indian Science and Engineering Society (AISES): Building a Successful Model for Diversity and Inclusion,” Mary Jo Ondrechen, in **Career Challenges and Opportunities in the Global Chemistry Enterprise**, **ACS Symposium Series 1169,** edited by H. N. Cheng, Sadiq Shah, and Marinda Li Wu, Oxford University Press (2014).
8. “Synthesis and evaluation of 2-halogenated-1,1-bis(4-hydroxyphenyl)-2-(3-hydroxyphenyl)-ethylenes as potential estrogen receptor-targeted radiodiagnostic and radiotherapeutic agents,” Robert N. Hanson, Pakamas Tongcharoensirikul, Kelton Barnsley, Mary Jo Ondrechen, Alun Hughes, Eugene R. DeSombre, **Steroids 96**, 50-62 (2015). PMID: 25637676
9. “Biochemical Functional Predictions for Protein Structures of Unknown or Uncertain Function,” Caitlyn L. Mills, Penny J. Beuning, Mary Jo Ondrechen, **Computational and Structural Biotechnology Journal** **13**, 182-191 (2015). PMID: 25848497
10. “Prediction of distal residue participation in enzyme catalysis,” Heather R. Brodkin, Nicholas A. DeLateur, Srinivas Somarowthu, Caitlyn L. Mills, Walter R. Novak, Penny J. Beuning, Dagmar Ringe, Mary Jo Ondrechen, **Protein Science 24 (5)**, 762-778 (2015). PMID: 25627867
11. “Local structure based method for prediction of the biochemical function of proteins: Applications to glycoside hydrolases,” Ramya Parasuram, Caitlyn L. Mills, Zhouxi Wang, Saroja Somasundaram, Penny J. Beuning, Mary Jo Ondrechen, **Methods 93**, 51-63 (2016). PMID: 28462720
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