

MARY JO ONDRECHEN

Present Position; Permanent address:

Professor of Chemistry & Chemical Biology
Department of Chemistry & Chemical Biology
Northeastern University (NU)
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Affiliated Faculty Member: Department of Bioengineering, Northeastern University

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 Chemical Society National Meeting (2018)
Fulbright Faculty Research Scholar (2021)
Technical Excellence Award, American Indian Science and Engineering Society (2024)

Board Memberships, Editorial Appointments:

Regional Editor, **Current Bioinformatics** (2007-2017); Editorial Board: (2005-2017)
Editorial Board, **Journal of Enzymology & Proteomics Research** (2017- 2020)
Associate Editor – Theoretical & Computational Chemistry, **Frontiers in Chemistry**, 2023-
Committee of Visitors, National Science Foundation Chemistry Division (2007 & 2020)
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 (2007-2013), Chair of the Board 2011-2013

Research Interests: Theoretical and computational chemistry; Functional genomics; Understanding enzyme function; Bioinformatics; Structure-based drug discovery; Applications of statistics and physicochemical methods to genomics; enzyme design; protein engineering; mutation effects on enzymes

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

Special Skills & Experience:

Theoretical Chemistry; Computational Chemistry and Chemical Biology;
Applications of Artificial Intelligence (AI) to Protein Chemistry and Genomics;
Applications of Physicochemical methods to Protein Chemistry and Genomics;
Molecular Modeling; Molecular Dynamics; Functional genomics
Protein structure analysis & function prediction

Advocacy for environmental remediation; Advocacy for Native American rights;
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

Other Professional service:

Presidential Task Force on Diversity, **American Chemical Society**, 2009-2010
Committee on Minority Affairs, **American Chemical Society**, 2011-2020
Committee on Chemistry and Public Affairs, **American Chemical Society**, 2021-
Advisory Board, Open Chemistry Collaborative in Diversity Equity (OXIDE), 2012-
COACH (originally Committee on the Advancement of Women Chemists), Board of
Advisors 2016-

SELECTED RESEARCH PUBLICATIONS

1. "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
2. "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
3. "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).
4. "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
5. "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
6. "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
7. "Evidence of the Participation of Remote Residues in the Catalytic Activity of Co-Type Nitrile Hydratase from *Pseudomonas putida*," Heather R. Brodtkin, 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
 8. "A Tale of Two Isomerases: Compact versus Extended Active Sites in Ketosteroid Isomerase and Phosphoglucose Isomerase," Srinivas Somarowthu, Heather R. Brodtkin, J. Alejandro D'Aquino, Dagmar Ringe, Mary Jo Ondrechen, and Penny J. Beuning, **Biochemistry** 50(43) 9283-9295 (2011).
 9. "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
 10. "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
 11. "Functional classification of protein structures by local structure matching in graph representation," Caitlyn L. Mills, Rohan Garg, Joslynn S. Lee, Liang Tian, Alexandru Suciuc, Gene Cooperman, Penny J. Beuning, Mary Jo Ondrechen, **Protein Science** 27, 1125-1135 (2018). PMID: 29604149
 12. "Analysis of electrostatic coupling throughout the laboratory evolution of a designed retroaldolase," Timothy A. Coulther, Moritz Pott, Cathleen Zeymer, Donald Hilvert, Mary Jo Ondrechen, **Protein Science**, 30(8), 1617-1627 (2021).
 13. "Amino acid interactions that facilitate enzyme catalysis," Timothy A. Coulther, Jaeju Ko, and Mary Jo Ondrechen, **J. Chem. Phys.** 154, 195101; <https://doi.org/10.1063/5.0041156> (2021).
 14. "Functional Characterization of Structural Genomics Proteins in the Crotonase Superfamily," Caitlyn L. Mills, Pengcheng Yin, Becky Leifer, Lori Ferrins, George A. O'Doherty, Penny J. Beuning*, Mary Jo Ondrechen*, (ACS) **Chemical Biology** 17, 395-403 (2022).
 15. "Electrostatic fingerprints of catalytically active amino acids in enzymes," Suhasini M. Iyengar, Kelly K. Barnsley, Rholee Xu, Aleksandr Prystupa, Mary Jo Ondrechen. **Protein Science** 31(5), e4291 (2022).
 16. "Identification and characterization of alternative sites and molecular probes for SARS-CoV-2 target proteins," Suhasini M. Iyengar, Kelly K. Barnsley, Hoang Yen Vu, Ian Jef A. Bongalonta, Alyssa S. Herrod, Jasmine A. Scott, Mary Jo Ondrechen, **Frontiers in Chemistry** 10, <https://doi.org/10.3389/fchem.2022.1017394> (2022).
 17. "Hydration sphere structure of architectural molecules: poly-ethylene glycol and poly-oxymethylene oligomers," Ahmed M. Rozza, Danny E. P. Vanpoucke, Eva-Maria Krammer, Julie Bouckaert, Ralf Blossey, Mark F. Lensink, Mary Jo Ondrechen, Imre Bakó, Julianna Oláh, Goedele Roos, **Journal of Molecular Liquids** 384, 122172 <https://doi.org/10.1016/j.molliq.2023.122172> (2023).

112. "Functional annotation of haloacid dehalogenase superfamily structural genomics proteins," Lakindu S. Pathira Kankanamge, Lydia A. Ruffner, Mong Mary Touch, Manuel Pina, Penny J. Beuning and Mary Jo Ondrechen, **Biochemical Journal** **480**, 1553-1569 (2023).

113. "Biochemical activity of seventeen cancer associated variants of DNA polymerase kappa predicted by electrostatic properties," Lakindu S. Pathira Kankanamge, Alexandra Mora, Mary Jo Ondrechen, Penny J. Beuning, **Chemical Research in Toxicology**, **36**, 1789-1803 (2023).

114. "A community effort in SARS-CoV-2 drug discovery," Schimunek, J., Seidl, P., Elez, K., Hempel, T., Le, T., Noé, F., Olsson, S., Raich, L., Winter, R., Gokcan, H., Gusev, F., Gutkin, E.M., Isayev, O., Kurnikova, M.G., Narangoda, C.H., Zubatyuk, R., Bosko, I.P., Furs, K.V., Karpenko, A.D., Kornoushenko, Y.V., Shulda, M., Yushkevich, A., Benabderrahmane, M., Bousquet-Melou, P., Bureau, R., Charton, B., Cirou, B., Gil, G., Allen, W.J., Sirimulla, S., Watowich, S., Antonopoulos, N., Epitropakis, N., Krasoulis, A., Pitsikalis, V., Theodorakis, S., Kozlovskii, I., Maliutin, A., Medvedev, A., Popov, P., Zaretckii, M., Eghbal-zadeh, H., Halmich, C., Hochreiter, S., Mayr, A., Ruch, P., Widrich, M., Berenger, F., Kumar, A., Yamanishi, Y., Zhang, K., Bengio, E., Bengio, Y., Jain, M., Korablyov, M., Liu, C., Gilles, M., Glaab, E., Barnsley, K., Iyengar, S.M., **Ondrechen, M.J.**, Haupt, V.J., Kaiser, F., Schroeder, M., Pugliese, L., Albani, S., Athanasiou, C., Beccari, A., Carloni, P., D'Arrigo, G., Gianquinto, E., Goßen, J., Hanke, A., Joseph, B.P., Kokh, D.B., Kovachka, S., Manelfi, C., Mukherjee, G., Muñoz-Chicharro, A., Musiani, F., Nunes-Alves, A., Paiardi, G., Rossetti, G., Sadiq, S.K., Spyraakis, F., Talarico, C., Tsengenes, A., Wade, R., Copeland, C., Gaiser, J., Olson, D.R., Roy, A., Venkatraman, V., Wheeler, T.J., Arthanari, H., Blaschitz, K., Cespugli, M., Durmaz, V., Fackeldey, K., Fischer, P.D., Gorgulla, C., Gruber, C., Gruber, K., Hetmann, M., Kinney, J.E., Das, K.M.P., Pandita, S., Singh, A., Steinkellner, G., Tesseyre, G., Wagner, G., Wang, Z., Yust, R.J., Druzhilovskiy, D.S., Filimonov, D., Pogodin, P.V., Poroikov, V., Rudik, A.V., Stolbov, L.A., Veselovsky, A.V., De Rosa, M., Simone, G.D., Gulotta, M.R., Lombino, J., Mekni, N., Perricone, U., Casini, A., Embree, A., Gordon, D.B., Lei, D., Pratt, K., Voigt, C.A., Chen, K., Jacob, Y., Krischuns, T., Lafaye, P., Zettor, A., Rodríguez, M.L., White, K.M., Fearon, D., von Delft, F., Walsh, M.A., Horvath, D., Brooks, C.L., Falsafi, B., Ford, B., García-Sastre, A., Lee, S.Y., Naffakh, N., Varnek, A., Klambauer, G. and Hermans, T.M., **Molecular Informatics** **43(1)**, e202300262 (2024).

115. "Evaluating protein cross-linking as a therapeutic strategy to stabilize SOD1 variants in a mouse model of familial ALS," Md Amin Hossain, Richa Sarin, Daniel P. Donnelly, Brandon C. Miller, Alexandra Weiss, Luke McAlary, Svetlana V. Antonyuk, Joseph P. Salisbury, Jakal Amin, Jeremy B. Conway, Samantha S. Watson, Jenifer N. Winters, Yu Xu, Novera Alam, Rutali R. Brahme, Haneyeh Shahbazian, Durgalakshmi Sivasankar, Swathi Padmakumar, Aziza Sattarova, Aparna C. Ponmudiyan, Tanvi Gawde, David E. Verrill, Wensheng Yang, Sunanda Kannapadi, Leigh D. Plant, Jared R. Auclair, Lee Makowski, Gregory A. Petsko, Dagmar Ringe, Nathalie Y. R. Agar, David J. Greenblatt, **Mary Jo Ondrechen**, Yunqiu Chen, Justin J. Yerbury, Roman Manetsch, S. Samar Hasnain, Robert H. Brown Jr., Jeffrey N. Agar, **PLoS Biology**, <https://doi.org/10.1371/journal.pbio.3002462> (2024).

116. "Revisiting the roles of catalytic residues in human ornithine transcarbamylase," Samantha S. Watson, Emily Micheloni, Lisa Ngu, Kelly K. Barnsley, Lee Makowski, Penny J. Beuning, **Mary Jo Ondrechen**, **Biochemistry** **63**, 1858-1875 (2024).