

MARCEY L. WATERS

Department of Chemistry, CB 3290
The University of North Carolina at Chapel Hill
Chapel Hill, NC 27599

Office: (919) 843-6522
FAX: (919) 962-2388
mlwaters@unc.edu

EDUCATION AND PROFESSIONAL POSITIONS

- 2009-present Professor of Chemistry, UNC Chapel Hill
- 2008-present Vice Chair of Undergraduate Studies
- 2005-2009 Associate Professor of Chemistry, UNC Chapel Hill
- 1999-2005 Assistant Professor of Chemistry, UNC Chapel Hill
- 1997-1999 NIH Postdoctoral Fellow, Columbia University, Advisor: Professor Ronald Breslow
- 1997 Ph.D., The University of Chicago, Advisor: Professor William D. Wulff
- 1992 B. A., Chemistry, The University of California at San Diego, Advisor: Professor Charles L. Perrin
- 1991 NSF Undergraduate Research Fellow, Columbia University, Advisor: Professor Gerard Parkin

AWARDS AND MEMBERSHIPS

- Alfred P. Sloan Fellowship, 2004-2006
- NSF Career Award, 2001-2006
- NIH Postdoctoral Fellowship, 1997-1999
- ACS Organic Division Research Fellow, sponsored by John Wiley & Sons, 1995-1996
- GAANN Fellow, 1992-1993
- Phi Beta Kappa
- Howard Hughes Honors Research Fellow, UCSD, 1991
- NSF REU Fellow, Columbia University, 1991
- Member, American Chemical Society
- Member, American Peptide Society
- Section Editor, "Supramolecular Chemistry: From Molecules to Nanomaterials", to be published by John Wiley and Sons.
- Guest Editor, *Current Opinion in Chemical Biology*, December 2009 issue.
- Advisory Board Member, International Symposia on Macrocyclic and Supramolecular Chemistry, 2008 – present
- Mentor, TANDEMplusIDEA, international mentoring program for female scientists, 2007 - 2009
- Board of Directors, Mesilla Chemistry Workshop, July 2006 – present

PEER REVIEWED PUBLICATIONS AT UNC (* indicates corresponding author)

1. A. J. Riemen, **M. L. Waters***, "Dueling Post-Translational Modifications Control Folding and Unfolding of a beta-Hairpin Peptide", *J. Am. Chem. Soc.* **2010**, *132*, 9007-9013.
2. Chung, M.-K.; Severin, K.; Lee, S. J.; **Waters, M. L.**; Gagné, M. R.*, "Constitutional, Diastereo- and Enantioselective Amplification of 84-Membered Macrocyclic Hosts for (-)-Cytidine", *J. J. Am. Chem. Soc.*, *submitted 5-21-10*.
3. S. Ghosh, L. A. Ingerman, A. G. Frye, S. J. Lee, M. R. Gagné,* **M. L. Waters***, "Dynamic Cyclic Thiopeptide Libraries From Thiol-Thioester Exchange", *Org Lett*, **2010**, *12*, 1860-1863.

4. L. A. Ingerman, M. E. Cuellar, **M. L. Waters***, "A Small Molecule Receptor that Selectively Recognizes Trimethyl Lysine in a Histone Peptide with Native Protein-like Affinity", *Chem. Commun.*, **2010**, 46, 1839-41 (*selected as a "hot article"*).
5. A. J. Riemen, **M. L. Waters***, "Controlling Peptide Folding with Repulsive Interactions between Phosphorylated Amino Acids and Tryptophan", *J. Am. Chem. Soc.*, **2009**, 39, 14081–14087.
6. L. L. Cline, **M. L. Waters***, "Design of a β -Hairpin Peptide-Intercalator Conjugate for Simultaneous Recognition of Single Stranded and Double Stranded Regions of RNA", *Org. Biomol. Chem.*, **2009**, 7, 4622-30 (*selected for a feature in Highlights in Chemical Biology*).
7. L. L. Cline, **M. L. Waters***, "The Structure of Well-folded β -Hairpin Peptides Promotes Resistance to Peptidase Degradation", *Peptide Science*, **2009**, 92, 502-507.
8. A. R. Riemen, **M. L. Waters***, "Design of Highly Stabilized β -Hairpin Peptides through Cation- π Interactions of Lysine and N-Methyllysine with an Aromatic Pocket", *Biochemistry* **2009**, 48, 1525-31.
9. A. L. Stewart, M. L. **Waters***, "Structural Effects on DNA Recognition by a Designed beta-Hairpin", *ChemBiochem*, **2009**, 10, 539-544.
10. L. A. Ingerman, **M. L. Waters***, "Photoswitchable Dynamic Combinatorial Libraries: Coupling Azobenzene Photoisomerization with Hydrazone Exchange", *J. Org. Chem.* **2009**, 74, 111-117.
11. Z. R. Laughrey, S. E. Kiehna, A. J. Riemen, **M. L. Waters***, "Carbohydrate- π Interactions: What Are They Worth?", *J. Am. Chem. Soc.* **2008**, 130, 14625–14633.
12. A. J. Riemen, **M. L. Waters***, "Stabilization of the N-Terminal β -Hairpin of Ubiquitin by a Terminal Hydrophobic Cluster", *Peptide Science*, **2008**, 90, 394-398 (*for the Merrifield Memorial Issue*).
13. S. E. Kiehna, Z. R. Laughrey, **M. L. Waters***, "Evaluation of a Carbohydrate- π Interaction in a Peptide Model System", *Chem. Commun.*, **2007**, 4026-4028 (*selected as a "hot article"*).
14. S. E. Kiehna, Z. R. Laughrey, **M. L. Waters***, "Folding Induced CO₂-Soluble Peptides", *Chem. Commun.*, **2007**, 4297-4298.
15. R. M. Hughes, K. R. Wiggins, S. Khorasanizadeh, **M. L. Waters***, "Molecular Recognition of Trimethyllysine by Chromodomain Is Not Just the Hydrophobic Effect", *Proc. Natl. Acad. Sci., USA*, **2007**, 104, 11184-11188.
16. R. M. Hughes, M. L. Benshoff, **M. L. Waters***, "Effects of Chainlength and N-Methylation on a Cation- π Interaction in a β -Hairpin Peptide", *Chem. Eur. J.*, **2007**, 5753-5764.
17. R. M. Hughes, **M. L. Waters***, "Effects of Lysine Acylation in a β -Hairpin Peptide: Comparison of an Amide- π and a Cation- π Interaction", *J. Am. Chem. Soc.*, **2006**, 128, 13586-13591.
18. R. M. Hughes, **M. L. Waters***, "Arginine Methylation in a β -Hairpin Peptide: Implications for Arg- π Interactions, ΔC_p° , and the Cold Denatured State", *J. Am. Chem. Soc.*, **2006**, 128, 12735-12742.
19. D. G. Barrett, C. M. Minder, M. U. Mian, S. J. Whittington, W. J. Cooper, K. M. Fuchs, A. Tripathy, **M. L. Waters**, T. P. Creamer, G. J. Pielak, "Pressure Perturbation Calorimetry of Helical Peptides", *Proteins-Structure Function and Bioinformatics* **2006**, 63, 322-326.
20. W. J. Cooper, **M. L. Waters***, "Turn Residues in β -Hairpin Peptides as Points for Covalent Modification", *Org. Lett.*, **2005**, 7, 3825-3828.
21. R. M. Hughes, **M. L. Waters***, "Influence of N-Methylation on a Cation- π Interaction Produces a Remarkably Stable β -Hairpin Peptide", *J. Am. Chem. Soc.*, **2005**, 127, 6518-9.
22. S. M. Butterfield, W. J. Cooper, **M. L. Waters***, "Minimalist Protein Design: a β -Hairpin Peptide that Binds ssDNA", *J. Am. Chem. Soc.*, **2005**, 127, 24-25.

23. S. M. Butterfield, M. M. Sweeney, **M. L. Waters***, “Recognition of Nucleotides with Model β -Hairpin Receptors: Investigation of Critical Contacts and Recognition Selectivity”, *J. Org. Chem.*, **2005**, *70*, 1105 - 1114 (*highlighted on the cover of issue 4*).
24. C. D. Tatko, **M. L. Waters***, “Effect of Halogenation on Edge-Face Aromatic Interactions in a β -Hairpin Peptide: Enhanced Affinity with Iodo-Substituents”, *Org. Lett.*, **2004**, *6*, 3969-3972.
25. M. J. Rashkin, R. M. Hughes N. T. Calloway, **M. L. Waters***, “Orientation and Alkylation Effects on Cation- π Interactions”, *J. Am. Chem. Soc.* **2004**, *126*, 13320-13325.
26. C. D. Tatko, **M. L. Waters***, “Investigation of the Nature of the Methionine- π Interaction in a β -Hairpin peptide Model System”, *Protein Science*, **2004**, *13*, 2515-2522.
27. C. D. Tatko, **M. L. Waters***, “Comparison of C-H $\cdots\pi$ and Hydrophobic Interactions in a β -Hairpin Peptide: Impact on Stability and Specificity”, *J. Am. Chem. Soc.*, **2004**, *126*, 2028-2034.
28. S. M. Butterfield, C. M. Goodman, V. M. Rotello, **M. L. Waters***, A Peptide Flavoprotein Mimic: Flavin Recognition and Redox Potential Modulation in Water Using a Designed β -Hairpin” *Angew. Chem. Int. Ed.*, **2004**, *43*, 724-727.
29. C. D. Tatko, **M. L. Waters***, “The Geometry and Efficacy of Cation- π Interactions in Diagonal Positions of a Designed β -Hairpin”, *Protein Science*, **2003**, *12*, 2443-2452.
30. S. E. Kiehna, **M. L. Waters***, “Sequence Dependence of β -Hairpin Structure: Comparison of a Salt Bridge and an Aromatic Interaction”, *Protein Science*, **2003**, *12*, 2657-2667.
31. S. M. Butterfield, **M. L. Waters***, “A Rationally Designed β -Hairpin Peptide for Molecular Recognition of ATP in Water”, *J. Am. Chem. Soc.*, **2003**, *125*, 9580-9581.
32. L. K. Tsou, C. D. Tatko, **M. L. Waters***, “A Simple Cation- π Interaction Between a Phenyl Ring and a Protonated Amine Stabilizes an α -Helix in Water”, *J. Am. Chem. Soc.*, **2002**, *124*, 14917-14921.
33. S. M. Butterfield, P. R. Patel, **M. L. Waters***, “Contribution of Aromatic Interactions to α -Helix Stability”, *J. Am. Chem. Soc.*, **2002**, *124*, 9751-9755.
34. C. D. Tatko, **M. L. Waters***, “Selective Aromatic Interactions in β -Hairpin Peptides”, *J. Am. Chem. Soc.*, **2002**, *124*, 9372-9373.
35. M. J. Rashkin, **M. L. Waters***, “Unexpected Substituent Effects in Offset π - π Stacked Interactions in Water”, *J. Am. Chem. Soc.*, **2002**, *124*, 1860-1861.

REVIEW ARTICLES AT UNC

36. **M. L. Waters**, “Studying Biologically Relevant Noncovalent Interactions using beta-Hairpin Peptides”, *Accounts of Chemical Research*, manuscript in preparation.
37. **M. L. Waters**, Daniel H. Appella, “Mimicking Nature: from Fundamentals to Applications”, *Curr. Opin. Chem. Biol.* **2009**, available online at www.sciencedirect.com.
38. E. T. Kool, **M. L. Waters**, “The Model Student: What model systems can teach us about Biology”, *Nat. Chem. Biol.*, **2007**, *3*, 70-73.
39. R. M. Hughes, **M. L. Waters***, “Model Systems for β -Hairpins and β -Sheets”, *Curr. Opin. Struct. Biol.*, **2006**, *514-524*.
40. W. J. Cooper, **M. L. Waters***, “Molecular Recognition with Designed Peptides and Proteins”, *Curr. Opin. Chem. Biol.*, **2005**, *9*, 627-631.
41. **M. L. Waters***, “Aromatic Interactions in Peptides”, *Biopolymers, Peptide Science*, **2004**, *76*, 435-445.
42. **M. L. Waters***, “Aromatic Interactions in Model Systems”, *Curr. Opin. Chem. Biol.*, **2002**, *6*, 736-741.

PUBLICATIONS prior to UNC

43. **M. L. Waters**, M. E. Bos, W. D. Wulff, "Mechanistic Studies on the Reaction of Fischer Carbene Complexes with Alkynes. Does the Alkyne Insertion Intermediate form Irreversibly?" *J. Am. Chem. Soc.*, **1999**, *121*, 6403-6413.
44. **M. L. Waters**, T. A. Brandvold, L. Isaacs, W. D. Wulff, A. L. Rheingold "Stereochemical Effects on Product Formation from the E- and Z-Isomers of η^1, η^3 -Vinyl Carbene Complexed Intermediates in the Reactions of Fischer Carbene Complexes with Alkynes." *Organometallics*, **1998**, *17*, 4298-4308.
45. W. A. Howard, T. M. Trnka, **M. Waters**, G. Parkin, "Terminal Chalcogenido Complexes of Zirconium: Synthesis and Reactivity of Cp*Zr(E)(NC₅H₅) (E = O, S, Se, Te)." *J. Organomet. Chem.* **1997**, *528*, 95-121.
46. S. Chamberlin, **M. L. Waters**, W. D. Wulff, "Contrasteric Regiochemical Incorporation of Stannylacetylenes in the Benzannulation Reaction." *J. Am. Chem. Soc.* **1994**, *116*, 3113-3114.
47. W. A. Howard, **M. Waters**, G. Parkin, "Terminal Zirconium Oxo Complexes: Synthesis, Structure, and Reactivity of (η^5 -C₅Me₄R)₂Zr(O)(NC₅H₄R')." *J. Am. Chem. Soc.* **1993**, *115*, 4917-4918.

BOOK CHAPTERS

- M. L. Waters**, W. D. Wulff, "The Synthesis of Phenols and Quinones via Fischer Carbene Complexes", in *Organic Reactions*, Denmark, S. E., Ed.; John Wiley and Sons, Vol. 70, 2008.
- M. L. Waters**, "The Role of Aromatic Interactions in Biomolecular Recognition: Contributions to Affinity and Specificity", *Beilstein Workshop Proceedings*, 2008.

INVITED ACADEMIC AND INDUSTRIAL LECTURES

2010

- *Keynote Speaker*, Vaughan Symposium, University of Michigan, *August 18, 2010*
- Hope College, Department of Chemistry, *February 26, 2010*
- Calvin College, Department of Chemistry, *February 25, 2010*
- Arizona State University, Department of Chemistry, *January 29, 2010*
- Albert Einstein School of Medicine, Dept of Biochemistry and Biophysics, *January 19, 2009*

2009

- Glaxo SmithKline, *October 7, 2009*
- Boston College, *September 15, 2009*
- Mt. Holyoke College, South Hadley, MS, *February 18, 2009*

2008

- University of New Orleans, Department of Chemistry, *September 23, 2008*
- Tulane University, Department of Chemistry, *September 22, 2008*
- 3^{ème} Cycle Lectureship, University of Basel, Basel Switzerland, *April 24,25, 2008*
- 3^{ème} Cycle Lectureship, University of Neuchatel, Neuchatel, Switzerland, *April 23, 2008*
- 3^{ème} Cycle Lectureship, University of Lausanne, Lausanne, Switzerland, *April 22, 2008*
- 3^{ème} Cycle Lectureship, University of Geneva, Geneva, Switzerland, *April 21, 2008*
- Rice University, Department of Chemistry, *March 12, 2008*
- Trinity University, Department of Chemistry, *March 13, 2008*
- University of Virginia, Department of Chemistry, *February 22, 2008*

2007

- Virginia Tech, Department of Chemistry, *October 19, 2007*
- UNC School of Pharmacy, Department of Medicinal Chemistry, *February 14, 2007*

2006

- National Institutes of Health, NIDDK, Laboratory of Bioorganic Chemistry, *December 15, 2006*
- University of Tokyo, *November 8, 2006*
- NYU, Department of Chemistry, *September 15, 2006*

- University of Rochester, Department of Biochemistry and Biophysics, *May 10, 2006*
- University of Texas at Austin, Dept of Chemistry, *May 5, 2006*
- Stanford University, Department of Chemistry, *May 3, 2006*
- Wesleyan University, Dept of Chemistry, *April 14, 2006*
- Yale University, Dept of Chemistry, *February 1, 2006*

2005

- *Eli Lilly Seminar*, Northwestern University, Dept of Chemistry, *December 5, 2005*
- Eastern Carolina University, Dept of Chemistry, *November 18, 2005*
- Bowdoin College, Dept of Chemistry, *November 4, 2005*
- Duke University, Dept of Chemistry, *November 1, 2005*
- University of Florida, Dept of Chemistry, *October 6, 2005*
- University of Pennsylvania, Dept of Chemistry, *May 16, 2005*
- Cornell University, Dept of Chemistry, *March 30, 2005*

2004

- Michigan State University, Dept of Chemistry, *November 17, 2004*
- *Invited Speaker, Symposium on Nanotechnology for the Life Sciences*, Univ. of Maryland, *Nov. 4, 2004*
- Memorial Sloan-Kettering Cancer Center, Molecular Pharmacology and Chemistry Dept, *Oct. 26, 2004*
- Purdue University, Dept of Chemistry and Biochemistry, *August 31, 2004*
- University of California at San Diego, Dept of Chemistry, *April 26, 2004*
- University of Michigan, Dept of Chemistry, *April 20, 2004*
- Penn State University, Dept of Chemistry, *April 6, 2004*
- Florida State University, Dept of Chemistry, *March 25, 2004*
- University of California at Irvine, Dept of Chemistry, *March 17, 2004*
- Colorado State University, Dept of Chemistry, *March 1, 2004*
- University of Pennsylvania, Dept of Biochemistry and Biophysics, *February 25, 2004*
- *Cherry Emerson Lecture*, Georgia Institute of Technology, Dept of Chemistry, *February 10, 2004*
- University of Illinois, Dept of Chemistry, *February 4, 2004*
- University of Wisconsin, Dept of Chemistry, *February 3, 2004*

2003

- Boston College, Dept of Chemistry, *November 12, 2003*
- University of Chicago, Dept of Chemistry, *October 24, 2003*
- *Keynote Speaker*, Society of Fellows Symposium, Scripps Research Institute, *October 17, 2003*
- Indiana University, Dept of Chemistry, *October 13, 2003*
- Emory University, Dept of Chemistry, *March 3, 2003*

2002

- University of Georgia, Dept of Chemistry, *November 7, 2002*
- Louisiana State University, Dept of Chemistry, *September 27, 2002*
- UNC Charlotte, Dept of Chemistry, *April 1, 2002*
- Wake Forest University, *February 20, 2002*

2001

- North Carolina State University, Dept of Chemistry, *December 4, 2001*
- UNC Greensboro, Dept of Chemistry, *October 12, 2001*

INVITED CONFERENCE LECTURES

- *Keynote Speaker*, International Symposium on Macrocyclic and Supramolecular Chemistry, Brighton, UK, *July 2011*
- *Breslow Symposium*, 241st National ACS Meeting, Anaheim, CA, *March 2011*
- *Supramolecular Symposium*, Joint SE/SW Regional ACS Meeting, New Orleans, LA, *December 2010*
- *Advances in Physical Organic Chemistry*, 93rd Canadian Chemistry Conference, Toronto, Canada, *May 2010*
- 5th Peptide Engineering Meeting (PEM5), Barcelona, Spain, *Oct 2009*
- International Symposium on Macrocyclic and Supramolecular Chemistry, Las Vegas, NV, *July 2008*
- Reaction Mechanisms Conference, Chapel Hill, NC, *June 2008*

- *James Flack Norris Award Symposium*, 235th National ACS Meeting, New Orleans, LA, *March 2008*
- *International Symposium on Dynamic Combinatorial Chemistry*, Boston, MA, *November 2007*
- *Ralph Hirschmann Award Symposium*, 233rd National ACS Meeting, Chicago, IL, *March 2007*
- *Japanese Peptide Symposium*, Yokohama, Japan, *November, 2006*
- *International Symposium on Macrocyclic and Supramolecular Chemistry*, Victoria, BC, *June, 2006*
- *Beilstein-Bozen Workshop, "Molecular Interactions-Bringing Chemistry to Life"*, Bozen, Italy, *May, 2006*
- *Peptides Gordon Conference*, Ventura, CA *February, 2006*
- *Organic Structures and Properties Gordon Conference*, Santa Barbara, CA *January, 2006*
- *NSF Workshop on Synthetic Organic Chemistry*, Lake Arrowhead, CA, *June 2005*
- *Symposium on Biomimetic Polymers*, National ACS Meeting, San Diego, CA, *March, 2005*
- *NSF Workshop in Supramolecular Chemistry*, Sanibel Island, FL *January, 2004*
- *Plenary Speaker*, American Peptide Symposium, Boston, MA *July, 2003*
- *Bioorganic Gordon Conference*, Andover, NH *June, 2003*
- *NSF Workshop in Physical Organic Chemistry*, Hilton Head, SC *June, 2002*
- *SERMACS*, Savannah, GA, *September, 2001*
- *Bioorganic Gordon Conference*, Andover, NH *June, 2001*