

## **Joseph J. Urban, Ph. D.**

Professor and Chair  
Chemistry Department  
U.S. Naval Academy

### **EDUCATION AND PROFESSIONAL EXPERIENCE**

Professor: U. S. Naval Academy, Aug 2010 – present  
Associate Professor: U.S. Naval Academy, Aug 1999 – Aug 2010  
Assistant Professor: U.S. Naval Academy, Aug 1994 – Aug 1999  
Postdoctoral Fellowship: Nat'l Research Council Postdoctoral Fellow, U.S. Army ERDC, 1991-1994  
Graduate Education: University of Delaware, Ph.D. in Organic Chemistry, 1991  
Undergraduate Education: Villanova University, B.S. in Chemistry, 1985

### **SELECTED USNA ADMINISTRATIVE ACTIVITIES**

#### **Yard-Wide:**

- USNA Promotion and Tenure Committee, Co-Chair, 2013 – 2015
- USNA Faculty Senate, 2013 - 2015
- USNA Premedical/Predental Advising Committee, 2004 - 2016
- Faculty Senate Academic Affairs Committee, 2008 - 2012
- Faculty Teaching Award Selection Committee, 2008 - 2012
- USNA Middle States Self Study Committee, 2003 - 2005

#### **Department:**

- Chemistry Department Chair, July 2016 - present
- Faculty Development Committee, Chair, 2010 - 2016
- Midshipmen Research Liaison , 2010 - 2013
- Chemistry Department Assessment Committee, 2000-2009, Chair 2002-2004
- Premedical Advisor/Medical Internship Coordinator, 2004 - present
- Course Coordinator for Plebe Chemistry, 1999 - 2001

### **HONORS AND AWARDS**

USNA Benac Teaching Excellence Award Recipient, 2015  
Navy Meritorious Civilian Service Award, 2015  
Kinnear Research Fellow, 2002, 2005  
USNA Apgar Teaching Award Recipient, 1998

### **RESEARCH INTERESTS**

The research focuses on the application of molecular modeling techniques to problems in Physical Organic and Bioorganic Chemistry such as conformational analysis, solvation, reactivity, and binding affinity. The systems currently under study are analogs to proteins generated by the incorporation of non-natural amino acids or replacements for the peptide bond. Of particular interest is the impact of these substitutions in terms of self-assembly and molecular recognition. The work has applications in the development of novel sensors, catalysts, and biologically-inspired nanomaterials. The methods employed include high-level computational chemistry techniques conducted at DoD High Performance Computing centers. A heavy emphasis is placed on the involvement of undergraduates in the research.

**COURSES TAUGHT AT U.S.N.A.**

SC111-112 : Fundamentals of Chemistry I and II      SC263-264: Integrated Lab I and II  
SC225-226 Organic Chemistry I and II              SC325: Advanced Organic Chemistry  
SC486C: Special Topics in Organic Chemistry      SC495-496: Undergraduate Research

**COURSES COORDINATED AT U. S. N. A.**

SC111-112: Fundamentals of Chemistry I and II, AY 00, 01  
SC225-226; Organic Chemistry, AY 03, 97  
SC263-264: Integrated Lab I and II, AY 02, 09, 10, 11

**MIDSHIPMEN RESEARCH STUDENTS**

Mac Hastings '14 *Chemistry Department Research Award Honorable Mention*  
Alec Emerling '13  
Eric Emerling '13 *Chemistry Department Research Award Honorable Mention*  
Robert Crutcher '13  
Gary Beier '12  
Nathan Erxleben '12  
Rex Atwood '11 *Chemistry Department Research Award Winner*  
Genevieve Harmon '11  
William Eucker '08 *Trident, Bowman Scholar*  
Brian McKinney '08 *Chemistry Department Research Award Honorable Mention*  
Jami Gann '05  
Brendon Tillman '05 *Chemistry Department Research Award Winner*  
William Andrew Cronin '04  
Sean Driscoll '04  
Curtis Cronin '98

**MEMBERSHIP**

American Chemical Society  
    Division of Chemical Education  
    Division of Organic Chemistry  
    Division of Computers in Chemistry  
American Association for the Advancement of Science

**EXTERNAL REVIEWING**

Ad hoc reviewer for :  
    *Journal of Organic Chemistry*                      *Journal of Physical Organic Chemistry*  
    *Journal of Physical Chemistry*                  *Computational and Theoretical Chemistry*  
    National Science Foundation

**FUNDING**

DoD High Performance Computing Modernization Office, DTRA

**PUBLICATIONS** (bold=midshipman coauthor)

1. **Erxleben, Nathan, D.**; Kedziora, Gary. S; Urban, Joseph J. “Anomeric Effects in Fluoro and Trifluoromethyl Piperidines: A Computational Study of Conformational Preferences and Hydration”, *Theoretical Chemistry Accounts*, 133(7), 1-13, (2014).
2. **Atwood, R. E.**; Urban, J. J. “Conformations of the Model Peptide Ac-Gly-Gly-NHMe: A Computational Study Including Aqueous Solvation Effects” *Journal of Physical Chemistry A*, 116, 1396-1408, (2012).
3. Reichert, W. M.; Henderson, W. A.; Trulove, P. C.; Urban, J. J.; De Long, H. C. “Effects of Crystal Packing on the Thermal Behavior of N,N'-alkylpiperidinium and N,N'-alkylmorpholinium Iodide Salts”, *Electrochemical Society Transactions*, 33(7), 667, (2010).
4. Piotrowski, P. I.; Cannara, R. J.; Gao, G; Urban, J. J.; Carpick, R. W.; Harrison, J. A. “Atomistic Factors Governing Adhesion between Diamond, Amorphous Carbon, and Model Diamond Nanocomposite Surfaces”, *Journal of Adhesion Science and Technology*, 24, 2471-2498, (2010).
5. **McKinney, B. E.**; Urban, J. J. “Fluoroolefins as Peptide Mimetics 2. A Computational Study of the Conformational Ramifications of Peptide Bond Replacement”, *Journal of Physical Chemistry A.*, 114, 1123-1133, (2010).
6. Reichert, M.; **Eucker IV, W.**; Trulove, P. C.; Urban, J. J.; De Long, H. C. “The Mechanism of Absorption of CO<sub>2</sub> in Ionic Liquids: a Computational and Raman Spectroscopy Study” *Electrochemical Society Transactions*, 16(49), 151, (2009).
7. Urban, J. J.; **Tillman, B. G.**; **Cronin, W. A.** “Fluoroolefins as Peptide Mimetics: A Computational Study of Structure, Charge Distribution, Hydration, and Hydrogen Bonding” *Journal of Physical Chemistry A* 110, 11120-11129, (2006).
8. Urban, J. J. “Computational Study of Stereoelectronic Effects in Fluorinated Alkylamines”, *Journal of Physical Organic Chemistry*, 18, 1061-1071 (2005).
9. Urban, J. J., von Tersch, R. L. “A Computational Study of Charge Delocalization and Ring Fluoro Substituent Effects in 4-Fluoromethylphenoxides”, *Journal of Organic Chemistry*, 64, 3409-3416, (1999).
10. Urban, J. J.; von Tersch, R. L. “Conformational Analysis of the Isomers of Lewisite”, *Journal of Physical Organic Chemistry*, 12, 95-102, (1999).

11. Urban, J. J.; Cronin, C. W.; Roberts, R. R.; Famini, G. R. "Conformational Preferences of 2-Phenethylamines. A Computational Study of Substituent and Solvent Effects on the Intramolecular Amine-Aryl Interactions in Charged and Neutral 2-Phenethylamines" *Journal of the American Chemical Society*, 119, 12292-12299, (1997).
12. Urban, J.J.; Famini, G. R.; Eds. *Theochem* Special Issue: Conformational Analysis, 370 (2,3), Elsevier, NY(1996).
13. Lowrey, A. H.; Cramer, C. J.; Urban, J. J.; Famini, G. R. "Quantum Chemical Descriptors for Linear Solvation Energy Relationships", *Computers in Chemistry*, 19 (1995), 209-15, (1994).
14. Urban, J. J.; von Tersch, R. L.; Famini, G. R. "Effect of Fluorine Substitution on Phenol Acidities in the Gas Phase and in Aqueous Solution. A Computational Study Using Continuum Solvation Models." *Journal of Organic Chemistry* **59**: 5239-5245 (1994).
15. Urban, J. J. and Famini, G. R. "The Conformational Dependence of Electrostatic Potential Derived Charges of Dopamine. Ramifications in Molecular Mechanics Force Field Calculations in the Gas Phase and in Aqueous Solution." *Journal of Computational Chemistry* **14**(3): 353-362, (1992).
16. Urban, J. J.; Cramer, C. J.; Famini, G. R. "A Computational Study of Solvent Effects on the Conformation of Dopamine." *Journal of the American Chemical Society* **114**: 8226, (1992).
17. Urban, J. J. "Computational Investigations of Molecular Recognition", Ph. D. dissertation, University of Delaware, (1991).
18. Urban, J., J. and Damewood, J. R., Jr. "Accurate Free Energy Perturbation Calculation of the Hydration Free Energies of  $\text{Fe}^{3+}$  and  $\text{Fe}^{2+}$ ." *Journal of the Chemical Society, Chemical Communications*, 1636-1638, (1990).
19. Damewood, J. R., Jr.; Kumpf, R. A.; Urban, J. J.; Mühlbauer, W. C. F.; Eksterowicz, J. E. "Parameterization of Molecular Modeling Calculations for the Accurate Description of Hydrogen Bonding." *Journal of Physical Chemistry* **94**, 6619-6626, (1990).
20. Damewood, J. R., Jr.; Anderson, W. P.; Urban, J. J. "A Molecular Mechanics Study of Neutral Molecule Complexation with Crown Ethers." *Journal of Computational Chemistry* **9**, 111-124, (1988).
21. Damewood, J. R., Jr.; Urban, J. J.; Williamson, T. C.; Rheingold, A. R. "Isomer-Dependent Complexation of Malononitrile by Dicyclohexano-18-Crown-6." *Journal of Organic Chemistry* **53**: 167, (1988).

**PRESENTATIONS** (bold=midshipman coauthor)

1. Urban, Joseph J.; Kedziora, Gary S.; Hastings, McMillan; Erxleben, Nathan; Crutcher, Robert; Atwood, Rex “Computational Studies of Fluorinated Biomimetic Molecules”, 249<sup>th</sup> ACS National Meeting, 22-26 March, 2015, Denver, CO.
2. Urban, Joseph J. “Computational Investigations of Biomimetic Molecules”, Invited Lecture, Oliver G. Ludwig Symposium, Villanova University, Villanova, PA, 14 March 2014.
3. **Hastings, McMillan J.**, Urban, Joseph J. “Modulation of Hydrogen Bonding by the Anomeric Effect: Computational Studies of Hydrated Complexes of 2-Fluoropiperidine and 2-Trifluoromethylpiperidine.”, 247<sup>th</sup> ACS National Meeting, 16-20 March, 2014, Dallas, TX.
4. **Crutcher, Robert M., Atwood, Rex E.**, Urban, Joseph J. “Computational Investigations of Fluoroalkene Tripeptide Analog Mimics: A Computational Study of Beta Turn Formation.”, 245<sup>th</sup> ACS National Meeting, 7-11 April, 2013, New Orleans, LA.
5. **Emerling, Alec, D.**, Kedziora, Gary. S., Urban, Joseph J. “Conformational Influence of Fluorine Substitution on Peptides Derived From Beta Amino Acids”, 245<sup>th</sup> ACS National Meeting, 7-11 April, 2013, New Orleans, LA.
6. **Emerling, Eric, W.**, Kedziora, Gary. S., Urban, Joseph J. “Conformational Preferences for C-F Bonds Adjacent to Carbonyls”, 245<sup>th</sup> ACS National Meeting, 7-11 April, 2013, New Orleans, LA.
7. **Erxleben, Nathan, E.**; Kedziora, Gary. S; Urban, Joseph J. “Anomeric Effects in Fluoro and Trifluoromethylpiperidines”, Eastern Collegiate Science Conference, Wayne, NJ, April, 2012.
8. **Crutcher, Robert M.**; Urban, Joseph J. “Computational Investigations of Fluoroalkene Peptide Mimics of the Alanine Tripeptide Analog”, 3<sup>rd</sup> Interacademy Chemistry Symposium, Annapolis, MD, March, 2012.
9. **Erxleben, Nathan, E.**; Kedziora, Gary. S; Urban, Joseph J. “Anomeric Effects in Fluoro and Trifluoromethylpiperidines”, 243<sup>rd</sup> ACS National Meeting, San Diego, CA, March, 2012.

10. **Erxleben, Nathan, E.**; Urban, Joseph J. “Fluorinated Alkylamine Groups as Peptide Bond Mimics: A Computational Investigation of Hydrogen Bonding”, 243<sup>rd</sup> ACS National Meeting, San Diego, CA, March, 2012.
11. **Beier, Gary, J.**; Urban, Joseph J. “Molecular Modeling Studies of Trifluoroethylamine Peptide Mimics”, 243<sup>rd</sup> ACS National Meeting, San Diego, CA, March , 2012.
12. **Crutcher, Robert M.**; Urban, Joseph J. “Computational Investigations of Fluoroalkene Peptide Mimics of the Alanine Tripeptide Analog”, 243<sup>rd</sup> ACS National Meeting, San Diego, CA, March , 2012.
13. Reichert, W. M.; Tumulak, E. G.; Foley, M. P.; Urban, J. J.; Trulove, P. C.; De Long, H. C. “Exploring Thermal Conformation Transitions of N,N'-Alkylpyrrolidinium and N,N'-alkylpiperidinium Iodide Salts”, 243<sup>rd</sup> ACS National Meeting, San Diego, CA, March , 2012.
14. **Erxleben, Nathan, E.**; Urban, Joseph J. Hydrogen Bonding in Fluoroethylamine Peptide Mimics: A Computational Study, Eastern Collegiate Science Conference, Fairfield, CT, 30 March, 2011.
15. **Atwood, Rex E.**; Urban, Joseph J. “Glycine Tripeptide Analog and its Fluoroalkene Mimics: A Computational Study of the Impact of Peptide Bond Replacement on Conformational Preferences” 241st ACS National Meeting & Exposition, Anaheim, CA, United States, March 27-31, 2011.
16. **Harmon, Genevieve A.**; Urban, Joseph J., “Conformational Preferences of Model Peptides and Fluorinated Peptidomimetics: A Computational Study”, 241st ACS National Meeting & Exposition, Anaheim, CA, United States, March 27-31, 2011.
17. Reichert, W. M.; Haverhals, Luke; Henderson, Wesley A.; Trulove, Paul C.; Urban, Joseph. J.; De Long, Hugh C. “Exploring the Effects of Structure Conformation on the Thermal Properties of Ionic Liquids: Dialkylpyrrolidinium and Dialkylpiperidinium Iodide Salts” , 241st ACS National Meeting & Exposition, Anaheim, CA, United States, March 27-31, 2011.
18. Urban, Joseph J.; Reichert, W. M.; Henderson, Wesley A.; Haverhals, Luke; Trulove, Paul C.; De Long, Hugh C. Dialkylpyrrolidinium and dialkylpiperidinium ions: A Computational Investigation of the Conformational Profiles of Ionic Liquid Cations” 241st ACS National Meeting & Exposition, Anaheim, CA, United States, March 27-31, 2011.
19. Keating, P. I.; Cannara, R. J.; Gao, G; Urban, J. J.; Carpick, R. W.; Harrison, J. A. “Atomistic Factors Governing Adhesion between Diamond, Amorphous Carbon, and

Model Diamond Nanocomposite Surfaces”, Gordon Research Conference on Tribology, Waterville, ME, 27 Jun – 2 July, 2010.

20. Reichert, W. M.; Henderson, W. A.; Trulove, P. C.; Urban, J. J.; De Long, H. C, “Effects of Crystal Packing on the Thermal Behavior of N,N’-alkylpiperidinium and N,N’-alkylmorpholinium Iodide Salts”, 218<sup>th</sup> Electrochemical Society Meeting, Las Vegas, NV, 10 – 15 Oct 2010.
21. **W. Eucker**, W. Reichert, P. Trulove, J. Urban and H. De Long, "The Mechanism of Absorption of CO<sub>2</sub> in Ionic Liquids: A Computational and Raman Spectroscopy Study" 214<sup>th</sup> Electrochemical Society Meeting, Honolulu HI, 14 Oct 2008.
22. **Eucker, William**, Trulove, Paul C., Urban, Joseph J., Reichert, Matthew, “Probing the Interaction of Room Temperature Ionic Liquids with CO<sub>2</sub>: A Raman Spectroscopy and Ab Initio Study”, Seventh Annual Conference on Carbon Capture and Sequestration, 5 - 8 May 2008, Pittsburgh, PA.
23. **McKinney, Brian E.**; Urban, Joseph J., “Fluoroalkenes as Peptide Bond Replacements: A Computational Study of the Conformational Ramifications”. Poster, 235<sup>th</sup> National ACS Meeting, New Orleans, LA, 6 – 10 April 2008.
24. **Tillman, Brendon G.**; **Cronin, William A.**; Urban, Joseph J. “Hydrogen Bonding in Fluorinated Peptide Mimetics: A Computational Investigation”, Oral, 231<sup>st</sup> National ACS Meeting, Atlanta, GA, 26 – 30 March 2006.
25. **Gann, J. L.**, Urban, J. J. “Computational Studies of the Conformational Preferences of Fluorinated Amino Acids”, Poster, 229<sup>th</sup> National ACS Meeting, San Diego, CA, 14 March, 2005.
26. **Tillman, B. G.**; Urban, J. J. “Computational Studies of Fluoroolefins as Peptide Mimetics” Poster, 229<sup>th</sup> National ACS Meeting, San Diego, CA, 14 March, 2005.
27. Urban, J. J. “Computational Evaluation of Stereoelectronic Effects in Fluorinated Amines”, Poster, 228<sup>th</sup> National ACS Meeting, Philadelphia, PA, 24 August 2004.
28. Urban, J. J.; **Cronin, W. A.** “Fluorinated Peptide Mimetics: A Computational Investigation”, Poster, 227<sup>th</sup> National ACS Meeting, Anaheim, CA, 29 March 2004.
29. Urban, J. J.; **Cronin, C. W.** “Conformational Analysis of the Neurotransmitter Acetylcholine” 215<sup>th</sup> National Meeting of the American Chemical Society, Dallas, TX, March, 1998.
30. Urban, Joseph J., Assistant Professor, and Von Tersch, Robert, L., CAPT, USA "A

Computational Study of the Fluoro Substituent Effects on Fluoromethylphenoxides"  
213<sup>th</sup> National Meeting of the American Chemical Society, San Francisco, CA, 15 April,  
1997.

31. Urban, J. J.; von Tersch, R. L., "A Computational Study of the Fluoro Substituent Effects on Fluoromethylphenoxides" 213<sup>th</sup> National Meeting of the American Chemical Society, San Francisco, CA, 15 April, 1997.
32. Urban, J. J. "Electrostatic Potentials as Teaching Tools in Undergraduate Organic Chemistry" 213<sup>th</sup> National Meeting of the American Chemical Society, San Francisco, CA, 13 April, 1997.
33. Urban, J. J. "NavApps: An Auxiliary Text for the Plebe Chemistry Course", Curriculum Development Presentation at USNA, Oct. 2001.
34. Urban, J. J. "SNAC: An Auxiliary Text for the Plebe Chemistry Course", Curriculum Development Presentation at USNA, Oct. 2000.
35. Urban, J. J. "Use of 3-D Molecular Models in Instructional Chemistry Web Pages" Curriculum Development Presentation at USNA, Oct. 1999.
36. Urban, J. J. "Use of 3-D Molecular Models in Instructional Chemistry Web Pages" Curriculum Development Presentation at USNA, 22 Sept. 1998.
37. Balková, A.; Urban, J. J., "Computational Investigations of Conformational Effects Involving Aromatic Rings. I. The Gas-Phase Study, Sanibel Symposium, St. Augustine, FL, March, 1996.
38. Urban, J. J. "Conformational Analysis of Bioactive Compounds," USNA Chemistry Department Seminar, 29 Nov. 1995.
39. von Tersch, R. L.; Urban, J. J., "Ab Initio Analysis of the Conformations of Lewisite Using Effective Core Potentials," 208<sup>th</sup> National Meeting of the American Chemical Society, Anaheim, CA, 3 April, 1995.
40. Urban, J. J.; Famini G. R. co-chairs "Conformational Analysis: Methods and Applications" symposium held at the American Chemical Society National Meeting, Anaheim, CA, April, 1995.
41. Urban, J. J.; Houk, K. N. co-chairs "Computational Organic Chemistry" symposium held at the American Chemical Society National Meeting, San Diego, CA, March, 1994

42. Urban, J. J.; Famini, G. R. "Modeling Substituent Effects in the Gas Phase and in Aqueous Solution" U. S. Army Conference on Chemical Defense, Aberdeen Proving Ground, MD November, 1993.
43. Urban, J. J. "Molecular Modeling in Aqueous Solution" 1993 Summit for Scientific Computing and Automation, Washington, DC, October 1993.
44. Smith, J. R.; Logan, T. P.; von Tersch, R. L.; Jakubowski, E. M.; Dolzine, T. W.; Szafraniec, L L.; Urban, J. J. "Identification of the Isomeric Forms of Lewisite Using Mass Spectrometry, Nuclear Magnetic Resonance, Infrared Spectroscopy, and Molecular Modeling" poster presented at the U. S. Army Medical Research and Development Command 1993 Medical Defense Bioscience Review, May 1993.
45. Urban, J. J.; von Tersch; R. L.; Famini, G. R. "Computational Studies of the Aqueous Phase Conformation of Fluorotyrosines" poster presented at the American Chemical Society National Meeting in Denver, April, 1993.
46. Urban, J. J.; Famini, G. R. "Theoretical Studies of the Conformation of Dopamine and Structural Analogues" poster presented at the U. S. Army Conference on Chemical Defense, Aberdeen Proving Ground, MD November, 1992.
47. Urban, J. J.; Famini, G. R. "Atomic Charges in Molecular Mechanics Force Fields: The Dependence of Electrostatic Potential-Derived Charges for Dopamine on Conformation" poster presented at the American Chemical Society National Meeting in Washington, DC, August, 1992.
48. Urban, J. J.; Famini, G. R. "The Conformational Dependence of the Electrostatic Potential-Derived Charges of Dopamine. Ramifications in Molecular Mechanics Force Field Calculations in the Gas Phase and in Aqueous Solution" Presented at the Second Solute-Solvent Interactions Meeting, U. S. Army ERDEC, Aberdeen Proving Ground, MD, May, 1992.
49. Urban, J. J. "Molecular Modeling in Aqueous Solution: Free Energy Calculations" invited seminar at Villanova University, April, 1992.
50. Urban, J. J.; Famini, G. R. "Examination of the Degree of Convergence in Amino Acid Interconversions with the Molecular Dynamics/Free Energy Perturbation Technique" poster presented at the American Chemical Society National Meeting, April, 1992.
51. Urban, J. J.; Famini, G. R. "Studies of the Application of the Molecular Dynamics/Free Energy Perturbation Technique to Models for Acetylcholine-Acetylcholine Receptor" poster presented at the U. S. Army Conference on Chemical Defense Research, Nov, 1992.