Curriculum Vita

Joseph J. Urban, Ph. D.
Chemistry Department
U.S. Naval Academy

EDUCATION AND PROFESSIONAL EXPERIENCE

Undergraduate Education:	Villanova University, B.S. in Chemistry, 1985
Predoctoral Internship:	Du Pont Biomedical Products, Summer 1985
Graduate Education:	University of Delaware, Ph.D. in Organic Chemistry, 1991
Postdoctoral Fellowship:	Nat'l Research Council Postdoctoral Fellow, U.S. Army Edgewood Research, Develop., and Engineering Ctr, 1991-1994
Assistant Professor:	Villanova University, Aug 1990-May 1991 (one-year appointment)
	U.S. Naval Academy, Aug 1994 – Aug 1999
Associate Professor:	U.S. Naval Academy, Aug 1999 – Aug 2010
Professor:	U. S. Naval Academy, effective Aug 2010

SELECTED USNA ADMINISTRATIVE ACTIVITIES

Yard-Wide:

- USNA Premedical/Predental Advising Committee
- Faculty Senate Academic Affairs Committee
- Faculty Teaching Award Selection Committee
- USNA Middle States Self Study Committee, Academic Years 03/04, 04/05
- USNA Technical Core Improvement Group (Co-Chair), Academic Years 99/00, 00/01

Department:

- Chemistry Department Assessment Committee
- Chemistry Majors Curriculum Committee
- Medical Internship Coordinator
- PreMed/PreDental Advisor
- Course Coordinator for Plebe Chemistry, Academic Years 1999/2000, 2000/2001

HONORS AND AWARDS

Kinnear Research Fellow, 2002, 2005
Apgar Teaching Award Recipient, 1998
Merck Index Award, 1985

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. Currently, the properties of fluorinated organics that mimic biologically relevant compounds are being investigated.

COURSES TAUGHT AT U.S.N.A.

SC111-112 : Fundamentals of Chemistry I and II
SC225-226 Organic Chemistry I and II
SC486C: Special Topics in Organic Chemistry
SC263-264: Integrated Lab I and II
SCSC485C: Advanced 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

MIDSHIPMEN RESEARCHERS
Nathan Erxleben '12
Rex Atwood '11
Genevieve Harmon '11
William Eucker '08 Trident Scholar
Brian McKinney '08 Chem. Dept. Research Award Honorable Mention
Jami Gann '05
Brendon Tillman '05 Chem. Dept. 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
Journal of Molecular Structure (Theochem)

Member, Unclassified Bulletin Review Panel, Chemical Security Analysis Center, U. S. Dept. of Homeland Security

PUBLICATIONS (bold=midshipman coauthor)

1. **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).

2. 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", (2010), *Journal of Adhesion Science and Techonlogy*., accepted.

3. Reichert, M.; **Eucker IV, W**.; Trulove, P. C.; Urban, J. J.; De Long, H. C. "The Mechanism of Absorption of CO_2 in Ionic Liquids: a Computational and Raman Spectroscopy Study" *Electrochemical Society Transactions.*, 16(49), 151, (2009).

4. 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).

5. Urban, J. J. "Computational Study of Stereoelectronic Effects in Fluorinated Alkylamines", *Journal of Physical Organic Chemistry*, 18, 1061-1071 (2005).

6. 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)

7. Urban, J. J.; von Tersch, R. L. "Conformational Analysis of the Isomers of Lewisite", *Journal of Physical Organic Chemistry*, 12, 95-102, (1999).

8. 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*, (1997), 119, 12292-12299.

9. Urban, J.J.; Famini, G. R.; Eds. *Theochem* Special Issue: Conformational Analysis, (1996), 370 (2,3) Elsevier, NY.

10. Lowrey, A. H.; Cramer, C. J.; Urban, J. J.; Famini, G. R. (1994), "Quantum Chemical Descriptors for Linear Solvation Energy Relationships", *Computers in Chemistry*, 19 (1995), 209-15.

11. Urban, J. J.; von Tersch, R. L.; Famini, G. R. (1994). "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.

12. Urban, J. J. and Famini, G. R. (1992). "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.

13. Urban, J. J.; Cramer, C. J.; Famini, G. R. (1992). "A Computational Study of Solvent Effects on the Conformation of Dopamine." *Journal of the American Chemical Society* **114**: 8226.

14. Urban, J. J (1991) "Computational Investigations of Molecular Recognition", Ph. D. dissertation, University of Delaware.

15. Urban, J., J. and Damewood, J. R., Jr. (1990). "Accurate Free Energy Perturbation Calculation of the Hydration Free Energies of Fe^{3+} and Fe^{2+}." *Journal of the Chemical Society, Chemical Communications,* 1636-1638.

16. Damewood, J. R., Jr.; Kumpf, R. A.; Urban, J. J.; Mühlbauer, W. C. F.; Eksterowicz, J. E. (1990). "Parameterization of Molecular Modeling Calculations for the Accurate Description of Hydrogen Bonding." *Journal of Physical Chemistry* **94**, 6619-6626.

17. Damewood, J. R., Jr.; Anderson, W. P.; Urban, J. J. (1988). "A Molecular Mechanics Study of Neutral Molecule Complexation with Crown Ethers." *Journal of Computational Chemistry* **9**, 111-124

18. Damewood, J. R., Jr.; Urban, J. J.; Williamson, T. C.; Rheingold, A. R. (1988). "Isomer-Dependent Complexation of Malononitrile by Dicyclohexano-18-Crown-6." *Journal of Organic Chemistry* **53**: 167.

PRESENTATIONS (bold=midshipman coauthor)

1. **W. Eucker**, W. Reichert, P. Trulove, J. Urban and H. De Long ,"The Mechanism of Absorption of CO_2 in Ionic Liquids: A Computational and Raman Spectroscopy Study" 214th Electrochemical Society Meeting, Honolulu HI, 14 Oct 2008.

2. **Eucker, William**, Trulove, Paul C., Urban, Joseph J., Reichert, Matthew, "Probing the Interaction of Room Temperature Ionic Liquids with CO_2: A Raman Spectroscopy and Ab Initio Study", Seventh Annual Conference on Carbon Capture and Sequestration, 5 - 8 May 2008, Pittsburgh, PA.

3. **McKinney, Brian E**.; Urban, Joseph J., "Fluoroalkenes as Peptide Bond Replacements: A Computational Study of the Conformational Ramifications". Poster, 235th National ACS Meeting, New Orleans, LA, 6 – 10 April 2008

4. **Tillman, Brendon G.**; **Cronin, William A.**; Urban, Joseph J. "Hydrogen Bonding in Fluorinated Peptide Mimetics: A Computational Investigation", Oral, 231st National ACS Meeting, Atlanta, GA, 26 – 30 March 2006

5. **Gann, J. L.**, Urban, J. J. "Computational Studies of the Conformational Preferences of Fluorinated Amino Acids", Poster, 229th National ACS Meeting, San Diego, CA, 14 March, 2005

6. **Tillman, B. G**.;Urban, J. J. "Computational Studies of Flouroolefins as Peptide Mimetics" Poster, 229th National ACS Meeting, San Diego, CA, 14 March, 2005

7. Urban, J. J. "Computational Evaluation of Stereoelectronic Effects in Fluorinated Amines", Poster, 228th National ACS Meeting, Philadelphia, PA, 24 August 2004

8. Urban, J. J.; **Cronin, W. A.** "Fluorinated Peptide Mimetics: A Computational Investigation", Poster, 227th National ACS Meeting, Anaheim, CA, 29 March 2004

9. Urban, J. J.; **Cronin, C. W.** "Conformational Analysis of the Neurotransmitter Acetylcholine" 215th National Meeting of the American Chemical Society, Dallas, TX, March, 1998

10. Urban, Joseph J., Assistant Professor, and Von Tersch, Robert, L., CAPT, USA "A Computational Study of the Fluoro Substituent Effects on Fluoromethylphenoxides" 213th National Meeting of the American Chemical Society, San Francisco, CA, 15 April, 1997.

11. Urban, J. J.; von Tersch, R. L., "A Computational Study of the Fluoro Substituent Effects on Fluoromethylphenoxides" 213th National Meeting of the American Chemical Society, San Francisco, CA, 15 April, 1997.

12. Urban, J. J. "Electrostatic Potentials as Teaching Tools in Undergraduate Organic Chemistry" 213th National Meeting of the American Chemical Society, San Francisco, CA, 13 April, 1997.

13. Urban, J. J. "NavApps: An Auxiliary Text for the Plebe Chemistry Course", Curriculum Development Presenation at USNA, Oct. 2001

14. Urban, J. J. "SNAC: An Auxiliary Text for the Plebe Chemistry Course", Curriculum Development Presenation at USNA, Oct. 2000.

15. Urban, J. J. "Use of 3-D Molecular Models in Instructional Chemistry Web Pages" Curriculum Development Presentation at USNA, Oct. 1999

16. Urban, J. J. "Use of 3-D Molecular Models in Instructional Chemistry Web Pages" Curriculum Development Presentation at USNA, 22 Sept. 1998

17. 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
18. Urban, J. J. "Conformational Analysis of Bioactive Compounds," USNA Chemistry Department Seminar, 29 Nov. 1995

19. von Tersch, R. L.; Urban, J. J., "Ab Initio Analysis of the Conformations of Lewisite Using Effective Core Potentials," 208th National Meeting of the American Chemical Society, Anaheim, CA, 3 April, 1995

20. 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.

21. 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

22. 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.

23. Urban, J. J. “Molecular Modeling in Aqueous Solution” 1993 Summit for Scientific Computing and Automation, Washington, DC, October 1993.

24. 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.

25. 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

26. 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.

27. 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

28. 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

29. Urban, J. J. “Molecular Modeling in Aqueous Solution: Free Energy Calculations” invited seminar at Villanova University, April, 1992

30. 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

31. 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