

CURRICULUM VITAE

Chaya Rapp
rappc@yu.edu

EDUCATION

1990-1993 Columbia College; Columbia University
B.A. in Biochemistry
1993-1998 Graduate School of Arts and Sciences; Columbia University
M.A in Chemistry, M. Phil, Ph.D. in Theoretical Chemistry

POSITIONS HELD

2006 - Present Stern College for Women, Yeshiva University; Clinical Associate
Professor of Chemistry
1999 - 2006 Stern College for Women, Yeshiva University; Assistant Professor of
Chemistry
1999 - 2006 Department of Chemistry, Columbia University; Adjunct Associate
Research Scientist
2001 Schrödinger Inc., Consultant
1999 Yeshiva College, Yeshiva University; Instructor of Chemistry
1995 - 1996 Manhattan High School for Girls, Instructor of Physics

TEACHING

2010 - Present Advisor to pre-medical and pre-dental students
1999 - Present Teach General Chemistry, Honors General Chemistry and Physical
Chemistry, Stern College for Women
1999 - Present Supervise student research in computational chemistry and mentor honors
thesis projects, Stern College for Women
2002 - Present Faculty advisor to Student Affiliate Chapter of the American
Chemical Society, Stern College for Women
2002 Led joint Senior Seminar in Advanced Chemistry at Stern College for
Women and Yeshiva College
2000, 2002 Taught Biochemistry, Stern College for Women
2000 Set up peer tutoring program for General Chemistry students
2000 Initiated Biochemistry major at Stern College for Women
2000 Developed and taught "Current Topics in Biophysical Chemistry"
1999 Sabbatical Replacement Yeshiva College, General Chemistry,
Physical Chemistry and Senior Seminar
1995 - 1996 High School Physics Instructor, Manhattan High School for Girls
1994 Graduate Instructor Quantum Mechanics, Columbia University
1993 Graduate Instructor General Chemistry, Columbia University

FELLOWSHIPS, HONORS AND AWARDS

2011	Karen Bacon Award to a Senior Faculty Member
2011	Awarded R15 AREA grant (3 years, \$250,000) from National Institutes of Health for proposal entitled "Computational Modeling of Post-translational Modification in Proteins"
2000	Faculty Summer Research Fellowship
1994 - 1997	National Science Foundation Fellow
1993	<i>Phi Beta Kappa</i> Achievement Prize
1993	<i>Summa cum laude</i>
1993	<i>Phi Beta Kappa</i>
1993	Milton Handler Prize for Scholastic Excellence (best academic record in science)
1993	<i>Salutatorian</i> of graduating class; Columbia College Columbia University.
1992	National Science Foundation Summer Research for Undergraduates Fellowship
1990 - 1993	Gruss Life Monument Fund - full tuition award

REVIEWER FOR SCIENTIFIC JOURNALS AND TEXTS

Journal of Chemical Education

Proteins: Structure, Function and Bioinformatics

Journal of Chemical Information and Modeling

Herrington and Dwyer, Chemistry Thompson Brooks/Cole Publishers.

Fine, Bealle and Stuehr, Chemistry for Engineers and Scientists John Wiley and Sons.

ABSTRACTS (Bold face name indicates a student co-author)

Tishbi, N. and Rapp C. The Role of Sulfation in the CCR5 Chemokine Receptor Complex, 58th Annual Meeting of the Biophysical Society, San Francisco, CA.

Laufer, T.S. and Rapp, C. 2013, Effects of tyrosine O-sulfation on binding affinity in CXCR4-SDF-1 complexes, 245th National Meeting of the American Chemical Society, New Orleans, LA.

Snow, S. and Rapp, C., 2013, Role of tyrosine *o*-sulfation in the CXCR4-SDF-1 chemokine receptor complex, 245th National Meeting of the American Chemical Society, New Orleans, LA.

A. Schiffmiller, C. Rapp, C. Kalyanaraman, "Theoretical Ranking of a Series of Protein Kinase Inhibitors", Columbia Undergraduate Research Symposium, April 2009.

R. Eisner, C. Schonbrun, N. Huang and C. Rapp. "Force field based Receptor Ligand Rescoring", 40th American Chemical Society Middle Atlantic Regional Meeting, Ursinus, PA, May 2007.

E. Levine, C.S. Rapp, D.J. Mandell and M.P. Jacobson. “An Implicit Solvent Study of Phosphorylation in Protein Molecules”, 230th American Chemical Society Meeting, Atlanta, Georgia, April 2006.

I. Rienman, D. Benmurgui and C.S. Rapp, “Ligand Stabilization in Fatty Acid Binding Proteins”, 228th American Chemical Society Meeting, Philadelphia, PA, August 2004.

R. Frankel, T. Fischer and C.S. Rapp, “The Effects of Crystal Packing on Protein Loop Structures”, 36th American Chemical Society Middle Atlantic Regional Meeting, Princeton, NJ, June 2003.

L. Blau, C. Dobin, D. Estes, and C.S. Rapp, "Nontraditional Experiments in an Honors Biochemistry Laboratory Course", 225th American Chemical Society Meeting, New Orleans, LA, March 2003.

M.P. Jacobson, Y. An, T. Day, V. Eylich, R. Farid, J. Gunn, S. Harrington, X. Li, D.L. Pincus, C.S. Rapp, D. Standley and R.A. Friesner, “Bridging the Gap Between Physical Chemistry and Bioinformatics”, CASP5, Community Wide Assessment of Techniques for Protein Structure Meeting, Asimolar, CA, December 2002.

C.S. Rapp, M.P. Jacobson and R.A. Friesner, “Prediction of Geometries for Short and Medium Size Protein Loops”, 35th American Chemical Society Middle Atlantic Regional Meeting, Fairfax, VA, May 2002.

INVITED TALKS

“Protein Structure Prediction”, Department of Chemistry, Yeshiva College, December 2003.

“High Resolution Structure Prediction Using All Atom Models”, Department of Chemistry and Biochemistry, Vassar College, April 2002.

“The Prediction of Protein Loop Geometries; The State of the Art”, Department of Chemistry, St. John’s University, January 2002.

“The Use of the Internet in Teaching Biochemistry”, Yeshiva College, November 1999.

“Homology Modeling in Proteins; Implications for Loop Structures”, Department of Chemistry and Department of Biochemistry and Molecular Biophysics, Columbia University, June 1997.

“A Rigid Body Dynamics Approach to the Simulation of Large Scale Domain Motions in Receptor Proteins”, Department of Chemistry, Columbia University, November 1996

PUBLICATIONS (Bold face name indicates a student co-author)

C. Rapp, **E. Goldberger**, **N. Tishbi**, and **R. Kirshenbaum**. "Cation- π Interactions of Methylated Ammonium Ions: A Quantum Mechanical Study" (2014) *Proteins: Structure, Function, and Bioinformatics*, *in press*.

C. Rapp, **S. Snow**, **T. Laufer**, and C.L. McClendon. "The role of tyrosine sulfation in the dimerization of the CXCR4:SDF-1 complex" (2013) *Protein Science* 22:1025–1036.

C. Rapp, **H. Klerman**, **E. Levine**, and C.L. McClendon. "Hydrogen Bond Strengths in Phosphorylated and Sulfated Amino Acid Residues" (2013). *PLoS ONE* 8(3): e57804. doi:10.1371/journal.pone.0057804

C. Rapp, C. Kalyanaraman, **A. Schiffmiller**, **E.L. Schoenbrun**, and M.P. Jacobson. "A Molecular Mechanics Approach to Modeling Protein-Ligand Interactions: Relative Binding Affinities in Congeneric Series" (2011) *Journal of Chemical Information and Modeling* 51(9), 2082–2089.

C. Rapp, **C. Schonbrun**, M.P. Jacobson, C. Kalyanaraman and N. Huang. "Automated Site Preparation in Physics-Based Rescoring of Receptor Ligand Complexes" (2009) *Proteins: Structure, Function, and Bioinformatics* 77(1), 52-61.

C. Rapp, **T. Strauss**, G. Fuentes and A. Nederveen. "Prediction of Protein Loops in Solution" (2007) *Proteins: Structure, Function, and Bioinformatics* 69(1), 69-74.

D.J. Mandell, I. Chorny, E.S. Groban, S. Wong, **E. Levine**, C.S. Rapp, and M.P. Jacobson. "The strengths of hydrogen bonds involving phosphorylated amino acid side chains" (2007) *Journal of the American Chemical Society*, 129(4), 820-827.

C. Rapp and **R.M. Pollack**. "Crystal Packing Effects on Protein Loops" (2005) *Proteins: Structure, Function, and Bioinformatics* 60(1), 103-109.

M.P. Jacobson, D.L. Pincus, C.S. Rapp, T. Day, B. Honig, D.E. Shaw and R.A. Friesner. "A Hierarchical Approach to All-Atom Loop Prediction" (2004) *Proteins: Structure, Function, and Bioinformatics* 55(2), 351-367.

Z. Yu, M.P. Jacobson, **J. Josovitz**, C.S. Rapp and R.A. Friesner. "First Shell Solvation of Ion Pairs: Correction of Systematic Errors in Implicit Solvent Models" (2004) *Journal of Physical Chemistry B*, 108, 6643-6654.

M.P. Jacobson, G.A. Kaminski, R.A. Friesner and C.S. Rapp. "Force Field Validation Using Protein Side Chain Prediction" (2002) *Journal of Physical Chemistry B*, 106, 11673-11680.

C.S. Rapp and R.A. Friesner. "Prediction of Loop Geometries using a Generalized Born model of Solvation Effects" (1999) *Proteins: Structure, Function, and Bioinformatics* 35(2), 173-183.

A. Ghosh, C.S. Rapp and R.A. Friesner. "A Generalized Born Model based on a Surface Integral Formulation" (1998) *Journal of Physical Chemistry B*, 102, 10983-10990.