

## CURRICULUM VITAE

### ELIZABETH A. KOMIVES

Department of Chemistry and Biochemistry  
University of California, San Diego, La Jolla, CA 92093-0378  
Telephone: (858) 534-3058, FAX: (858) 534-6174  
email: [ekomives@ucsd.edu](mailto:ekomives@ucsd.edu), webpage: <http://chem-faculty.ucsd.edu/komives/>

#### Employment

##### **UNIVERSITY OF CALIFORNIA SAN DIEGO**

Assistant Professor of Chemistry and Biochemistry, 1990 - 1996  
Associate Professor of Chemistry and Biochemistry, 1996 - 2000  
Professor of Chemistry and Biochemistry, 2000 - present

#### Education

##### **MASSACHUSETTS INSTITUTE OF TECHNOLOGY**

M.S. in Toxicology, B.S. in Chemistry, 1982

##### **UNIVERSITY OF CALIFORNIA SAN FRANCISCO**

Ph.D. in Pharmaceutical Chemistry with Paul R. Ortiz de Montellano 1982 - 1987  
Research Topic: The Mechanism of  $\pi$ -Bond Oxidation by Cytochrome P-450

##### **HARVARD UNIVERSITY**

NIH Postdoctoral Fellow with Jeremy R. Knowles 1987 - 1990  
Research Topics: Analysis of Triosephosphate Isomerase Mutants using FTIR and X-ray crystallography

#### Academic Honors

Regents Fellowship (1982 - 1983)  
Graduate Opportunity Fellowship (1983 - 1984)  
NIH Graduate Traineeship (1984 - 1986)  
NIH Postdoctoral Traineeship (1987 - 1989)  
Long Award for Excellence in Teaching (1983)  
Rita Allen Scholar (1991 - 1996)  
Searle Scholar (1992 - 1995)  
Kaiser Award for Excellence in Teaching, First Year Medical Students (1999)  
Brown and Williamson Scholar, University of Louisville (2000)  
Barany Award for Outstanding Contributions to Biophysics, Biophysical Society (2000)  
Nominating Committee, Protein Society (2001-2004)  
Council, Biophysical Society (2002-2005)

#### Current Research Funding

National Institute of Health: **R01 HL70999, \$175,000 direct** (07/01/2002-06/30/2008)  
"The Thrombin-Thrombomodulin Interaction" Komives, PI renewal pending  
National Institute of Health: **R01 AG025343, \$205,000 direct** (10/01/2004 - 09/30/2009)  
"Directed Proteomics of Alzheimer's Related Proteins" Komives, PI  
National Institute of Health: : **PO1 GM071862, \$877,000 direct** (04/10/2006 - 03/31/2011)  
" NF-kB-IkB Interaction in silico, in vitro, in vivo" Program Project Grant Komives, PI  
National Institute of Environmental Health and Safety: **P42 ES10337, \$127,000 direct** (2005-2010)  
"Mass Spectrometry Core Facility" for UCSD SUPERFUND Project, R. Tukey PI.

## Graduate Students Trained

Michael J. Hunter, Ph. D. 1995, currently senior scientist, Corvas, International  
Christopher E. White, Ph. D. 1996, currently president and CEO of White Labs Inc. and lecturer, UCSD.  
David P. Meininger, Ph. D. 1997, currently senior scientist, Triad Inc.  
Benedetta A. Sampoli Benitez, Ph. D. 1999, currently assistant professor of Chemistry, Marymount  
Manhattan College  
Jeffrey G. Mandell, Ph. D., 2000, currently postdoctoral fellow with Tom Cech, U. Colorado, Boulder  
Matthew J. Wood, Ph. D., 2000, currently postdoctoral fellow with Gigi Storz, NIH  
Kerney J. Glover, Ph. D. 2001, currently postdoctoral fellow with Barbara Imperiali, MIT  
Jennifer A. Whiles, Ph. D. 2001, currently Assistant Professor at Sonoma State University  
Abel Baerga-Ortiz, Ph. D. 2002, currently Royal Society Fellow with Peter Leadlay,  
Cambridge University  
Carrie A. (Hughes) Croy, Ph. D. 2003, currently American Cancer Society Fellow with Natalie Ahn,  
U. Colorado  
Johnny E. Croy, Ph. D. 2003, currently NIH Postdoctoral Fellow with Deborah Wuttke, U. Colorado  
Judith Helena Prieto, Ph. D. 2005, currently Postdoctoral Fellow with John Yates, III, The Scripps  
Research Institute  
Julia Koepppe, Ph. D. 2006, currently Postdoctoral Fellow with Anthony Watts, Oxford University  
Gina Nubile, Ph. D. 2007, currently Scientist at Invitrogen.  
Current graduate students: Muneera Smith, Miklos Guttman, Carla Cervantes, Ingrid Devries, Amy  
Davenport, Brian Fuglestad, Nicholas Treuheit.

## Postdoctoral Fellows Trained

Simon Bergqvist, currently Senior Research Scientist, Pfizer, Inc.  
Current post-doctoral fellows: Diego Ferreiro, Stephanie Truhlar, Francisco Lopez-Lira

## Courses Taught

Freshman Chemistry (Chemistry 6B, undergraduate course) (1992-1996)  
Chemistry of Enzyme Catalyzed Reactions (Chemistry 116/216 upper division undergraduate and core  
graduate course) (1991-present)  
Metabolic Biochemistry (Chemistry 114B, upper division undergraduate course) (1999, 2002-present)  
Structural Biochemistry (MED 211, M. D. students) (1999)  
Pharmaceutical Chemistry (SPPS221, Pharm. D. students) (2002-present)  
Guest lectures on NMR for Chemistry 215, Molecular Modeling (graduate students), SPPS223 (Pharm.  
D. students) and on Proteomics for Cell Biology (Biomedical Sciences graduate  
students)

## National Service

Chair, Molecular Biophysics Subgroup, Biophysical Society  
Editorial Advisory Board, *Biochemistry* (2007-present)  
Council, Biophysical Society (2002 - 2006)  
Nominating Committee, Protein Society, (2001 - present)  
Session Chair, Biophysics of Protein Binding Events, ACS National Meeting (2002)  
Session Chair, Protein Binding and Conformation, ASMS Meeting Montreal (2003)  
Study Section Chair, International and Cooperative Projects (2000 - 2002)  
Session co-Chair, Protein-protein interactions, FASEB Meeting on Signal Transduction (1999)  
Editorial Board, *Molecular and Cellular Proteomics* (2002 - 2008)  
Advisory Committee, UCSF Mass Spectrometry Resource (1999 - present)

NSF standing review panel on Molecular and Cellular Biophysics (2003 - 2007)

Editorial Advisory Board, *Molecular and Cellular Proteomics* (2008)

Manuscript Review: *Proceedings of the National Academy of Sciences*, *Protein Science*, *Journal of Molecular Biology*, *Journal of Biological Chemistry*, *Biochemistry*, *Nature Structural Biology*

### University Service

Principle Investigator: Heme and Blood Proteins Training Program (NIH T32DK07233-26; renewed in 2006; currently funds 5 pre-doctoral and 5 post-doctoral fellows)

Faculty overseeing the Biomolecular Mass Spectrometry Facility, Department of Chemistry and Biochemistry (currently houses four instruments, and has a staff of two Ph. D.-level researchers and serves all of UCSD, including the School of Medicine)

Steering Committee: La Jolla Interfaces in Science funded by Burroughs Wellcome (1998-present)

Steering Committee: Molecular Biophysics Training Program (1995 - present) (representative for Minority recruitment and retention)

Steering Committee: Growth Regulation and Oncogenesis (1994 - present)

Pharmacy School Planning Committee, Admissions Committee, Building Committee

Various committees within the Chemistry and Biochemistry Department including Search Committees, Facilities Committee, Undergraduate Affairs Committee, Biophysics Instrumentation Facility, Biological NMR Instrumentation committee

### Invited Lectures

**Biophysical Society Meeting** "Biophysics of the NF- $\kappa$ B/I $\kappa$ B Interaction" (2008)

**Gordon Research Conference on Biomolecular Interactions** "Biophysics of the NF- $\kappa$ B/I $\kappa$ B Interaction" (2008)

**Gordon Research Conference on Small Integrin Binding Proteins** "Folding and Binding in NF- $\kappa$ B regulation" (2007)

**Gordon Research Conference on Biological Molecules in the Gas Phase** "Folding and Binding of I $\kappa$ B $\alpha$ " (2007)

**University of California, Berkeley** "Biophysics of Protein-Protein interactions" (2006)

**First International Keystone Meeting (Cambridge, England)** (2006)

**National University of Singapore** (2006) "Using Biophysics to unravel NF- $\kappa$ B signaling mechanisms"

**PittCon Conference** (2006) "Mechanisms of Signaling Proteins Probed by H/<sup>2</sup>H Exchange Mass Spectrometry"

**University of Arkansas** (2006) "Biophysics of the Thrombin-Thrombomodulin Interaction"

**University of Washington, Seattle** (2006) "Biophysics of NF- $\kappa$ B /I $\kappa$ B $\alpha$  Signaling"

**ASMS Sanibel Conference on Amide H/D Exchange** (2006)

**Gibbs Conference on Thermodynamics** "Biophysics of NF- $\kappa$ B /I $\kappa$ B $\alpha$  Signaling" (2005)

**Protein Society Meeting** (2005) "Unraveling the Mechanisms of Signaling Proteins by Mass Spectrometry"

**University of Georgia** (2005) "Protein-protein interaction dynamics by amide H/<sup>2</sup>H exchange mass spectrometry"

**IDEC/Biogen Pharmaceuticals** (2004) "Protein-protein interaction dynamics by amide H/<sup>2</sup>H exchange mass spectrometry"

**Duke University** (2004) Molecular Biophysics Students Invited Lecturer "Protein-protein interaction dynamics by amide H/<sup>2</sup>H exchange mass spectrometry"

**University of Wisconsin, Madison** (2004) "Protein-protein interaction dynamics by amide H/<sup>2</sup>H exchange mass spectrometry"

**University of Pennsylvania** (2004) Molecular Biophysics Students Invited Lecturer "Protein-protein interaction dynamics by amide H/<sup>2</sup>H exchange mass spectrometry"

**University of California, Riverside** (2004) “Protein-protein interaction dynamics by amide H<sup>2</sup>H exchange mass spectrometry”

**University of Texas, Galveston** (2004) “Protein-protein interaction dynamics by amide H<sup>2</sup>H exchange mass spectrometry”

**Notre Dame University** (2004) Plenary Lecture, Department of Chemistry and Biochemistry Annual Retreat “Protein-protein interaction dynamics by amide H<sup>2</sup>H exchange mass spectrometry”

**Protein Society Meeting** (2003) “Protein-protein interaction dynamics by amide H<sup>2</sup>H exchange mass spectrometry”

**Proteins Gordon Conference** (2003) “Probing protein-protein interfaces and allostery by amide H<sup>2</sup>H exchange “

**American Society of Mass Spectrometry Meeting** (2003) “From epitope mapping to structures of protein-protein complexes using amide H<sup>2</sup>H exchange and protein docking” and Session chair-Protein: Conformations and Dynamics

**University of California, San Francisco** (2002) “Biophysics of Protein-Protein Interactions”

**NIH Wednesday Afternoon Lecture** (2002) “Biophysics of Protein-Protein Interactions”

**Oklahoma Medical Research Foundation** (2002) “The Thrombin-Thrombomodulin Interaction”

**American Chemical Society National Meeting** (2002) Physical Chemistry Division Session “Biophysical Chemistry of Protein Binding Events” Session co-Chair

**Discovery Proteomics Meeting**, La Jolla (2002) “Biophysical Studies of Protein-Protein Interfaces”

**University of Colorado, Boulder** (2001) “Biophysical Studies of Protein-Protein Interfaces Using Biacore, NMR, and H<sup>2</sup>H Exchange”

**“Energy Landscapes” Symposium, San Diego Super Computer Center** (2001) “Measurement of electrostatic and solvation effects in protein-protein interactions”

**Royal Chemical Society of Sweden, Stockholm** (2001) “Mass Spectrometry in the Post-genomic Era”

**Karolinska Institute, Stockholm, Sweden** (2001) Invited Lecture

**Uppsala University, Sweden** (2001) Invited Lecture

**National Institutes of Health** (2001) “Mapping Protein-protein Interactions

**University of North Carolina, Chapel Hill** (2001) Electrostatics and Dynamics of the Thrombin-Thrombomodulin Interaction

**St. Louis, University** (2001) “Biophysics of the Thrombin-Thrombomodulin Interaction”

**University of California, San Diego** (2001) “Mapping Protein-Protein Interfaces Thrombomodulin-Thrombin LRP-apoE”

**The Scripps Research Institute** (2001) “What can we learn from Amide Hydrogen/Deuterium Exchange Mass Spectrometry”

**FASEB Workshop on Signal Transduction**, Taos, NM (2001) “Biophysical Studies of Protein-protein interfaces”

**Barany Award Lecture, Biophysical Society National Meeting**, New Orleans, LA (2000) “Biophysics of Protein-protein Interactions”

**UC Riverside** (2000) “Biophysics of Protein-protein Interactions”

**UC San Diego** (2000) “Biophysics of Protein-protein Interactions”

**Vanderbilt University** (1999) “Biophysical Studies of the Thrombin-Thrombomodulin Interaction”

**Cal State Los Angeles** (1999) “Mapping Protein-protein Interfaces by Amide Exchange and MALDI Mass Spectrometry”

**International Society of Mass Spectrometry**, San Francisco, CA (1999) “Mapping Protein-protein Interfaces by Amide Exchange and MALDI Mass Spectrometry”

## PUBLICATIONS

## ELIZABETH A. KOMIVES

1. Penman, B. W.; Crespi, C. L.; Liber, H. L.; **Komives, E. A.** and Thilly, W. G. (1983) "Mutation of Human Lymphoblasts Exposed to Low Concentrations of Chemical Mutagens for Long Periods of Time". *Mutat. Res.* 108: 417 - 436.
2. DeLuca, J. G.; Kaden, D. A.; **Komives, E. A.** and Thilly, W.G. (1984) "Mutation of Xeroderma Pigmentosum Lymphoblasts by Far-ultraviolet Light". *Mutat. Res.* 128: 47 - 57.
3. Kaden, D. A.; Call, K. M.; Leong, P. M.; **Komives, E. A.** and Thilly, W.G. (1987) "Killing and Mutation of Human Lymphoblast Cells by Aflatoxin B1: Evidence for an Inducible Repair Response". *Can. Res.* 47: 1993 - 2001.
4. Ortiz de Montellano, P. R. and **Komives, E. A.** (1985) "Branchpoint for Heme Alkylation and Metabolite Formation in the Oxidation of Arylacetylenes by Cytochrome P-450". *J. Biol. Chem.* 260: 3330 - 3336.
5. **Komives, E. A.** and Ortiz de Montellano, P. R. (1987) "Mechanism of Oxidation of  $\pi$ -Bonds by Cytochrome P-450: Electronic Requirements of the Transition State in the Turnover of Phenylacetylenes". *J. Biol. Chem.* 262: 9793 - 9802.
6. **Komives, E. A.**, Tew, D., Olmstead, M. M. and Ortiz de Montellano, P. R. (1988) "Models for Cytochrome P-450 Prosthetic Heme Alkylation. Reaction of Diazoacetophenone with (Tetraphenylporphyrinato)iron(II) Chloride" *Inorganic Chem.* 27: 3112 - 3117.
7. **Komives, E. A.**, Chang, L. C., Lolis, E., Tilton, R. F., Petsko, G. and Knowles, J. R. (1991) "Electrophilic Catalysis in Triosephosphate Isomerase: The Role of Histidine-95" *Biochemistry* 30, 3011 - 3019.
8. Warn-Cramer, B. J., Broze, G. J. and **Komives, E. A.** (1992) "cDNA Sequence of Rabbit Tissue Factor Pathway Inhibitor" *Nucleic Acids Research* 20: 3548. Corrigendum.
9. Fanuel, L., Granier, B., Wilkin, J.M., Bellefroid-Bourguignon, C., Joris, B., Knowles, J., **Komives, E.**, Van Beeumen, J., Ghuysen, J.M., Frere, J. M. (1994) "The precursor of the Streptomyces R61 DD-peptidase containing a C-terminal extension is inactive" *Febs Letters* 351: 49-52.
10. Lodi, P. J., Chang, L. C., Knowles, J. R. and **Komives, E. A.** (1994) "Triosephosphate Isomerase Requires a Positively Charged Active Site: The Role of Lysine-12" *Biochemistry* 33: 2809 - 2814.
11. Joseph-McCarthy, D., Rost, L. E., **Komives, E. A.** and Petsko, G. A. (1994) "Crystal Structure of the Mutant Yeast Triosephosphate Isomerase in which the Catalytic Base Glu-165 is Changed to Asp" *Biochemistry* 33: 2824 - 2830.
12. Joseph-McCarthy, D., Lolis, E., **Komives, E. A.** and Petsko, G. A. (1994) "Crystal Structure of the K12M/G15A Triosephosphate Isomerase Double Mutant and Electrostatic Analysis of the Active Site" *Biochemistry* 33: 2815 - 2823.
13. Zhang, Z., Sugio, S., **Komives, E. A.**, Liu, K. D., Knowles, J. R., Petsko, G. A. and Ringe, D. (1994) "Crystal Structure of Recombinant Chicken Triosephosphate Isomerase-Phosphoglycolohydroxamate Complex at 1.8-Å Resolution" *Biochemistry* 33: 2830 - 2837.
14. White, C. E., Kempf, N. M. and **Komives, E. A.** (1994) "Expression of Highly Disulfide-Bonded Proteins in *Pichia Pastoris*" *Structure* 2: 1003 - 1005.
15. Srinivasan, J., Hu, S., Hrabal, R., Zhu, Y., **Komives, E. A.** and Ni, F. (1994) "Thrombin-Bound Structure of an EGF Subdomain from Thrombomodulin Determined by Transferred Nuclear Overhauser Effects" *Biochemistry* 33: 13553 - 13560.
16. Loughheed, J. L., Bowman, C. A. Meininger, D. P. and **Komives, E. A.** (1995) "Thrombin Inhibition by Cyclic Peptides from Thrombomodulin" *Protein Science.* 4:773-780.
17. Hunter, M. J. and **Komives, E. A.** (1995) "Deprotection of S-Acetamidomethyl Cysteine Containing Peptides by Silver Trifluoromethanesulfonate Avoids the Oxidation of Methionines" *Anal. Biochem.* 228:173 - 177.

18. **Komives, E. A.**, Loughheed, J. C., Liu, K., Zhang, Z., Petsko, G. A. and Ringe, D. (1995) "The Structural Basis for Pseudoreversion of the E165D Lesion by the Secondary S96P Mutation in Triosephosphate Isomerase Depends on the Position of Bound Water Molecules" *Biochemistry* 34: 13612-21.
19. Meininger, D. P., Hunter, M. J. and **Komives, E. A.** (1995) "Synthesis and Preliminary Structure of the Fourth EGF-like Domain of Thrombomodulin" *Protein Science* 4, 1683 - 1695 .
20. Hunter, M. J. and **Komives, E. A.** (1995) "Thrombin-Binding Affinities of Different Disulfide Bonding Isomers of the Fifth EGF-like Domain of Thrombomodulin" *Protein Science* 4: 2129 - 2137.
21. Blackmar, C., Healy, V. L., Narendra, U., Hrabal, R., Ni, F. and **Komives, E. A.** (1995) "Structure/Activity of the Region of Thrombomodulin that binds to Thrombin" *Bioorganic Chemistry* 23, 519 - 527.
22. White, C. E., Hunter, M. J., Meininger, D. P., White, L. R. and **Komives, E. A.** (1995) "Large Scale Expression, Purification and Characterization of the Smallest Active Fragment of Thrombomodulin: The Roles of the Sixth Domain and of Methionine-388" *Protein Engineering* 8, 1177 - 1187.
23. **Komives, E. A.**, Hunter, M. J., Meininger, D. P., White, L. R. and White, C. E. (1995) "Structure/Function of the Fourth and Fifth EGF Domains of Thrombomodulin" *Techniques in Protein Chemistry VII* 391 - 400.
24. Hrabal, R., **Komives, E. A.** and Ni, F. (1996) "Structural Resiliency of an EGF-like Subdomain Bound to its Target Protein, Thrombin" *Protein Science* 5, 195 - 203.
25. Chen, Y. L., Cino, J., White, C. E. and **Komives, E. A.** (1996) "Continuous Production of Thrombomodulin from a *Pichia pastoris* in Fermentation" *Journal of Chemical Technology and Biotechnology* 67, 143 - 148.
26. White, C. E., Hunter, M. J., Meininger, D. P., Garrod, S. and **Komives, E. A.** (1996) "The Fifth EGF-like domain of Thrombomodulin Does Not Have An EGF-like Disulfide Bonding Pattern" *Proc. Nat. Acad. Sci. U. S. A.* 93, 10177 - 82.
27. **Komives, E. A.**, Loughheed, J. C., Zhang, Z., Sugio, S., Narayana, N., Xuong, N. H., Petsko, G. and Ringe, D. (1996) "The Structural Basis for Pseudoreversion of the H95N Lesion by the Secondary S96P Mutation in Triosephosphate Isomerase" *Biochemistry* 35, 15474-484.
28. Chen, Y. L., Cino, J., Hart, G., Freedman, D., White, C. E. and **Komives, E. A.** (1997) "High Protein Expression in Fermentation of Recombinant *Pichia Pastoris* by Fed Batch Process" *Process Biochemistry* 32, 107 - 111.
29. Gleeson, M.A. G., White. C. E., Meininger, D. P. and **Komives, E. A.** (1997) "Generation of Protease Deficient Strains of *Pichia pastoris* and Their Use in Heterologous Protein Expression" *Methods in Molecular Biology* 103, 81 - 94.
30. Sampoli Benitez B., Hunter, M. J., Meininger D. P. and **Komives, E. A.** (1997) "Structure of the Fifth EGF-like Domain of Thrombomodulin: An EGF-like Domain with a Novel Disulfide Bonding Pattern" (1997) *J. Mol. Biol.* 273, 913 - 926.
31. Vindigni, A., White, C. E., **Komives, E. A.** and Di Cera, E. (1997) "Energetics of Thrombin-Thrombomodulin Interaction" *Biochemistry* 36, 6674 - 6681.
32. Mandell, J. G., Falick, A. M. and **Komives, E. A.** (1998) "Measurement of Amide Hydrogen Exchange by MALDI-TOF Mass Spectrometry" *Analytical Chemistry* 70, 3987 - 3995.
33. Mandell, J. G., Falick, A. M. and **Komives, E. A.** (1998) "Identification of Protein-Protein Interfaces by Decreased Amide Proton Solvent Accessibility" *Proc. Nat. Acad. Sci. U. S. A.* 95, 14705 - 14710.
34. Struppe, J., **Komives, E. A.**, Taylor, S. S. and Vold, R. R. (1998) "<sup>2</sup>H NMR Studies of a Myristoylated Peptide in Neutral and Acidic Phospholipid Bicelles." *Biochemistry* 37, 15523 - 15527.

35. Greenwald, J., Le, V., Corrigan, A., Fischer, W., **Komives, E.**, Vale, W., Choe, S. (1998) Characterization of the extracellular ligand-binding domain of the type II activin receptor. *Biochemistry* 37, 16711 - 16718.
36. Mentz, S., DeLacalle, S. Baerga-Ortiz, A. J., Knauer, M. F., Knauer, D. J. and **Komives, E. A.** (1999) "Binding and Internalization of Thrombin by Human Astrocyte Cells" *J. Neurochemistry* 72, 980 – 987.
37. Wood, M. J. and **Komives, E. A.** (1999) "Production of Large Quantities of Isotopically-Labeled Protein in *Pichia pastoris* by Fermentation" *J. Biomolecular NMR* 13, 149 - 159.
38. Zhang, Z., **Komives, E. A.** Sugio, S., Blacklow, S. C., Narayana, N., Xuong, N. H., Stock, A. M., Petsko, G. and Ringe, D. (1999) "The role of water in the catalytic efficiency of triosephosphate isomerase". *Biochemistry* 38, 4389 – 4397.
39. Mandell, J. G., Falick, A. M. and **Komives, E. A.** (1999) "Identification of Protein-Protein Interfaces by Amide Proton Exchange Coupled to MALDI-TOF Mass Spectrometry" in Mass Spectrometry in Biology and Medicine, A. L. Burlingame, ed. Humana Press pgs 91 - 109.
40. Glover, K. J., Martini, P. M., Vold, R. R. and **Komives, E. A.** (1999) "Preparation of insoluble transmembrane peptides: *Glycophorin-A*, *Prion (110-137)*, *FGFR (368-397)*. *Anal. Biochem.* 272, 270 - 4.
41. Baerga-Ortiz, A. J., Rezaie, A. R. and **Komives, E. A.** (2000) "Electrostatic Dependence of the Thrombin-Thrombomodulin interaction" *J. Mol. Biol.* 296: 651 - 658.
42. Wood, M. J., Sampoli Benitez, B., **Komives, E. A.** (2000) "Solution structure of the smallest cofactor-active fragment of thrombomodulin" *Nature Structural Biology* 7: 200 - 204.
43. Sampoli Benitez, B. and **Komives, E. A.** (2000) Disulfide bond plasticity in EGF" *Proteins, Structure, Function and Genetics* 40, 168 - 174.
44. Whiles, J. A., Brasseur, R., Glover, K. J., Melacini, G., **Komives, E. A.** and Vold, R. R. (2001) "The Orientation and the Effects of Mastoparan X on Phospholipid Bicelles." *Biophys. J.* 80, 280 - 293.
45. Mandell, J. G. Baerga-Ortiz, A., Akashi, S., Takio, K. and **Komives, E. A.** (2001) "Solvent Accessibility of the Thrombin-Thrombomodulin Interface" *J. Mol. Biol.* 306, 575-589.
46. Hughes, C. A., Mandell, J. G., Anand, G. S., Stock, A. M. and **Komives, E. A.** (2001) "Phosphorylation Causes Subtle Changes in Solvent Accessibility at the Interdomain Interface of Methylesterase CheB" *J. Mol. Biol.* 307, 967-976.
47. Glover, K. J., Whiles, J. A., Wu, G., Yu, N., Deems, R., Struppe, J. O., Stark, R. E., **Komives, E. A.** and Vold, R. R. (2001) "Structural Evaluation of Phospholipid Bicelles for Solution-State Studies of Membrane Associated Biomolecules" *Biophys. J.* 81, 2163 - 2171.
48. Glover, K. J., Whiles, J. A., Wood, M. J., Melacini, G., **Komives, E. A.** and Vold, R. R. (2001) "Conformational dimorphism and transmembrane orientation of Prion protein residues 110-136 in bicelles" *Biochemistry* 40, 13137-13142.
49. Baerga-Ortiz, A., Hughes, C. A., Mandell, J. G. and **Komives, E. A.** (2002) "Epitope Mapping of a monoclonal antibody against human thrombin by H/D exchange mass spectrometry reveals selection of a diverse sequence in a highly conserved protein" *Protein Science* 11, 1300-1308.
50. Anand, G. S., Hughes, C. A., Jones, J. M., Taylor, S. S. and **Komives, E. A.** (2002) "Amide H<sup>2</sup>H exchange reveals communication between the cAMP- and catalytic subunit-binding sites in the regulatory subunit of protein kinase A" *Journal of Molecular Biology* 323, 377-386.
51. Whiles, J. A. Glover, K. J., Vold, R. R. and **Komives, E. A.** (2002) "Methods for studying transmembrane peptides in bicelles: Consequences of hydrophobic mismatch and peptide sequence." *Journal of Magnetic Resonance* 158, 149-156.
52. Huxford, T. Mischler, D., Reeves, R. Sengchanthalangsy, L. L. Huang, D.-B., Phelps, C. B., Hughes, C. A., **Komives, E. A.** and Ghosh, G. (2002) "Solvent exposed non-contacting amino acids play a critical role in the NF-kB/IkBa complex formation" *Journal of Molecular Biology* 324, 587-597.

53. Wood, M. J., Becvar, L. A., Prieto, J. H., Melacini, G., and **Komives, E. A.** (2003) "NMR Structures Reveal How Oxidation Inactivates Thrombomodulin" *Biochemistry* 42, 11932-42.
54. Jennings, L. L., Malecki, M., **Komives, E. A.** and Taylor, P. (2003) "Direct Analysis of the Kinetic Profiles of Organophosphate-Acetylcholinesterase Adducts by MALDI-TOF Mass Spectrometry" *Biochemistry* 42, 11083-91.
55. Croy, J. E., Shin, W. D., Knauer, M. F., Knauer, D. J., and **Komives, E. A.** (2003) "All three LDL receptor homology regions of the LDL receptor-related protein (LRP) bind multiple ligands" *Biochemistry* 42, 13049-57.
56. Anand, G. S., Law, D., Mandell, J. G., Snead, A. N., Tsigelny, I., Taylor, S. S., Ten Eyck, L., and **Komives, E. A.** (2003) "Identification of the Protein Kinase A Regulatory RI $\alpha$ -Catalytic Subunit Interface by Amide H<sup>2</sup>H Exchange and Protein Docking" *Proc. Nat. Acad. Sci. U. S. A.* 100, 13264-13269.
57. Baerga-Ortiz, A., Bergqvist, S. P., Mandell, J. G. and **Komives, E. A.** (2004) "Two different proteins that compete for binding to thrombin have opposite kinetic and thermodynamic profiles". *Protein Science* 13, 166-176.
58. Croy, C. H., Koeppe, J. R., Bergqvist, S. P. and **Komives, E. A.** (2004) "Allosteric Changes in Solvent Accessibility Observed in Thrombin upon Active Site Occupation" *Biochemistry* 43, 5346-55.
59. Croy, J. E., Brandon, T. and **Komives, E. A.** (2004) "Two apolipoprotein E mimetic peptides, apoE(130-149) and apoE(141-155)<sup>2</sup>, bind to LRP1" *Biochemistry* 43, 7328-35.
60. Croy, C. H., Bergqvist, S. P., Huxford, T., Ghosh, G. and **Komives, E. A.** (2004) "Biophysical Characterization of Free I $\kappa$ B $\alpha$  in Solution" *Protein Science* 13, 1767-77.
61. Prieto, J. H., Sampoli Benitez, B. A., Melacini, G., Johnson, D. A., Wood M. A. and **Komives, E. A.** (2005) "Dynamics of the Fragment of Thrombomodulin containing the fourth and fifth EGF-like domains correlate with function" *Biochemistry* 44, 1225-1233.
62. **Komives, E. A.** (2005) "Protein-protein interaction dynamics by amide H<sup>2</sup>H exchange mass spectrometry", *International Journal of Mass Spectrometry* 240, 285-290.
63. Wood, M. J., Prieto, J. H. and **Komives, E. A.** (2005) "Structural and functional consequences of methionine oxidation in thrombomodulin" *Biochim. Biophys. Acta* 1703, 141-147.
64. Mandell, J. G., Baerga-Ortiz, A., Falick, A. H. and **Komives, E. A.** (2005) "Measurement of Solvent Accessibility at Protein-protein Interfaces". *Methods in Molecular Biology*, vol. 305 "Protein-Ligand Interactions", Chapter 4, pgs 65-80, G. U. Nienhaus, Ed.
65. Mandell, J. G., Baerga-Ortiz, A., Croy, C. H., Falick, A. H. and **Komives, E. A.** (2005) "Application of Hydrogen-Exchange- Mass Spectrometry for the Study of Protein-Protein Interactions" *Current Protocols in Protein Science* vol. 20.
66. Koeppe, J. R., Seitova, A., Mather, T. and **Komives, E. A.** (2005) "Thrombomodulin tightens the thrombin active site loops to promote protein C activation" *Biochemistry* 44, 14784-91.
67. Ferreiro, D. U., Cho, S. S. **Komives, E. A.** and Wolynes, P. G. (2005) "The energy landscape of modular repeat proteins: Topology determines folding mechanism in the ankyrin family" *J. Mol. Biol.* 354, 679-92.
68. Hotchko, M., Anand, G., **Komives, E. A.**, and Ten Eyck, L. (2006) "Automated extraction of backbone deuteration levels from amide H<sup>2</sup>H exchange mass spectrometry experiments" *Protein Science* 15, 583 - 601.
69. Shi, J., Koeppe, J. R., **Komives, E. A.** and Taylor, P. (2006) Ligand-induced conformational changes in the acetylcholine binding protein analyzed by hydrogen-deuterium exchange mass spectrometry. *J Biol Chem.* 281, 12170-7.
70. Chen, A., **Komives, E. A.** and Schroeder, J. I. (2006) An improved grafting technique for mature Arabidopsis plants demonstrates long-distance shoot-to-root transport of phytochelatin in Arabidopsis. *Plant Physiol.* 141, 108-20.

71. Koeppe, J. R. and **Komives, E. A.** (2006) Amide H<sup>2</sup>H Exchange Reveals a Mechanism of Thrombin Activation. *Biochemistry* 45, 7724-32.
72. Bergqvist, S., Croy, C. H., Kjaergaard, M., Huxford, T., Ghosh, G. and **Komives, E. A.** (2006) Thermodynamics reveal that helix four in the NLS of NF-kappaB p65 anchors IkappaBalpha, forming a very stable complex. *J. Mol. Biol.* 360, 421-34.
73. Truhlar, S. M. E., Croy, C. H., Torpey, J. W., Koeppe, J. R. and **Komives, E. A.** (2006) Solvent Accessibility of Protein Surfaces by Amide H<sup>2</sup>H Exchange MALDI-TOF Mass Spectrometry. *J. Am. Soc. Mass Spectrom.* 17, 1490 - 97.
74. Truhlar, S. M. E., Torpey, J. W., and **Komives, E. A.** (2006) Regions of IkBα that are critical for its inhibition of NF-κB•DNA interaction fold upon binding to NF-κB. *Proc. Nat. Acad. Sci. U. S. A.* 103, 18951-6.
75. Ferreira, D. U., Cervantes, C. F., Truhlar, S. M. E., Cho, S. S., Wolynes, P. G., and **Komives, E. A.** (2007) Stabilizing IkBα by 'consensus' design. *J. Mol. Biol.* 365, 1201-16.
76. Latzer, J., Papoian, G. A., Prentiss, M. C., **Komives, E. A.**, Wolynes, P. G. (2007) Induced fit, folding, and recognition of the NF-kappaB-nuclear localization signals by IkappaBalpha and IkappaBbeta. *J Mol Biol.* 367, 262-74.
77. Wu, X., Li, Z. F., Brooks, R., **Komives, E. A.**, Torpey, J. W., Engvall, E., Gonias, S. L. and Shelton, G. D. (2007) Autoantibodies in canine masticatory muscle myositis recognize a novel myosin binding protein-C family member. *J. Immunol.* 179, 4939-44.
78. Sung, D. Y., Lee, D., Harris, H., Raab, A., Feldmann, J., Meharg, A., Kumabe, B., **Komives, E. A.** and Schroeder, J. I. (2007) Identification of an arsenic tolerant double mutant with a thiol-mediated component and increased arsenic tolerance in phyA mutants. *Plant J.* 49, 1064-75.
79. Ferreira, D. U. and **Komives, E. A.** (2007) The plastic landscape of repeat proteins. *Proc Natl Acad Sci U S A.* 104, 7735-6.
80. Anand, G. S., Hotchko, M., Brown, S. H., Ten Eyck, L. F., **Komives, E. A.** and Taylor, S. S. (2007) R-subunit Isoform Specificity in Protein Kinase A: Distinct Features of Protein Interfaces in PKA Types I and II by Amide H/(2)H Exchange Mass Spectrometry. *J Mol Biol.* 374, 487-99. .
81. Ferreira, D. U., Hegler, J. A., Komives, E. A. and Wolynes, P. G. (2007) Localizing Frustration in native proteins and protein assemblies. *Proc. Nat. Acad. Sci. U. S. A.* 104, 19819-24.
82. Barrick, D., Ferreira, D. U., **Komives, E. A.** (2008) Folding landscapes of ankyrin repeat proteins: experiments meet theory. *Curr. Opp. Struct. Biol.* 18, 27-34.
83. Truhlar, S. M. E., Mathes, E., Cervantes, C. F., Ghosh, G., **Komives, E. A.** (2008) Pre-folding IkBα alters control of NF-κB signaling. *J. Mol. Biol.* 380, 67-82.
84. Huang CM, Torpey JW, Liu YT, Chen YR, Williams KE, **Komives EA**, Gallo RL. (2008) A Peptide with ProGln C-terminus in the Human Saliva Peptidome Exerts Bactericidal Activity Against Propionibacterium acnes. *Antimicrob Agents Chemother.* 52, 1834-6.
85. Betts, G. N, van der Geer, P., and **Komives, E. A.** (2008) Structural and Functional Consequences of Tyrosine Phosphorylation in the LRP1 Cytoplasmic Domain. *J Biol Chem.* 283, 15656-64.
86. Mendoza-Cózatl DG, Butko E, Springer F, Torpey JW, **Komives EA**, Kehr J, Schroeder JI. (2008) Identification of high levels of phytochelatins, glutathione and cadmium in the phloem sap of Brassica napus. A role for thiol-peptides in the long-distance transport of cadmium and the effect of cadmium on iron translocation. *Plant J.* 54, 249-59.
87. Stephanie M. E. Truhlar, Erika Mathes, Carla F. Cervantes, Gourisankar Ghosh, and **Elizabeth A. Komives.** (2008) Pre-folding IkBα alters control of NF-κB signaling. *J. Mol. Biol.* (in press).
88. Ferreira, D.U., Walczak, A. M., **Komives, E. A.** and Wolynes, P. G. (2008) The energy landscapes of repeat-containing proteins: topology, cooperativity, and the folding funnels of one-dimensional architectures. *PLoS Comput Biol.* 16, 4(5):e1000070.
89. Truhlar, S. M., **Komives, E. A.** (2008) LRR Domain Folding: Just Put a Cap on It! *Structure.* 16, 655-7.



## Doctoral Theses Completed under my supervision

1996 Michael J. Hunter

The structure and function of the fifth EGF-like domain of thrombomodulin

1997 David P. Meininger

The solution structure and function of the fourth and fifth EGF-like domains of thrombomodulin

1997 Christopher E. White

Expression and characterization of small fragments of thrombomodulin

1999 Benedetta Sampoli Benitez

Structure and dynamics of EGF-like domains of thrombomodulin

2000 Matthew J. Wood

Solution structure and backbone dynamics of the thrombomodulin fragments TMEGF45 and TMEGF45ox

2000 Jeffrey G. Mandell

Protein protein interactions studied by hydrogen-deuterium exchange and computer-aided docking

2001 Kerney J. Glover

Interactions of transmembrane domains with lipid bilayers in phospholipid bicelles

2001 Jennifer Whiles-Lillig

Bicelles: a new system for studying membrane associated peptides and proteins

2002 Abel Baerga-Ortiz

The energetics of the thrombin-thrombomodulin interaction

2003 Carrie A. Hughes

Protein-protein interactions and dynamics probed by H/<sup>2</sup>H exchange

2003 Johnny E. Croy

Characterization of ligands binding to the low density lipoprotein receptor-related protein (LRP1)

2005 Judith Helena Prieto

Correlations between dynamic motions and function in modular proteins

2006 Julia R. Koeppe

The Thrombin-Thrombomodulin Interaction

2008 Muneera Beach

Thermodynamics and the Role of Allostery in the Thrombin-Thrombomodulin Interaction