CURRICULUM VITAE
Wayne Charles Guida
December, 2006

CURRENT POSITION & ADDRESS:

Professor (Effective Beginning Fall, 2007)
Department of Chemistry
University of South Florida
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Professor
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College of Medicine University of South Florida, Tampa
Professor (Effective Until August, 2007)
Department of Chemistry
Eckerd College
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EDUCATION AND TRAINING:

Sr. Postdoctoral Associate - Columbia University, 1985-86, Computational Chemistry.
Advisor: W. Clark Still
Postdoctoral Associate - Duke University, 1976, Synthetic Organic Chemistry.
Advisors: Steven W. Baldwin and Peter W. Jeffs
Ph.D. - University of South Florida, 1976, Organic Chemistry.
Advisor: Douglas J. Raber (*currently: GreenPoint Science, formerly: Director, BCST, National Research Council, Washington, D.C., formerly: Professor, Department of Chemistry, University of South Florida*).
B. A. - University of South Florida, 1968, Chemistry.

PROFESSIONAL EXPERIENCE:

Professor, Department of Interdisciplinary Oncology, College of Medicine, University of South Florida, Tampa, Florida, September, 2005 - present
Scientific Director, High Throughput Screening & Chemistry Core - H. Lee Moffitt Cancer Center & Research Institute at the University of South Florida; Tampa, Florida; November, 2004 – present.

Professor, Department of Chemistry, Eckerd College;
St. Petersburg, Florida; February, 2003 – present.
Member, Drug Discovery Program - H. Lee Moffitt Cancer Center & Research Institute at the University of South Florida; Tampa, Florida; June, 2001 – present.
Affiliate Assistant Professor - Department of Interdisciplinary Oncology, College of Medicine, University of South Florida, Tampa, Florida, January, 2002 – August, 2005.
Consultant – Celgene, Signal Research Division; San Diego, California, www.signalpharm.com, November, 2002 – August, 2005.
Associate Professor, Department of Chemistry, Eckerd College;
St. Petersburg, Florida; August, 1999 – January, 2003.
Consultant and Member of the Board of Directors - Schrödinger, Inc.; Portland, Oregon and New York, New York, www.schrodinger.com, August, 1999 – present.
Member of the Scientific Advisory Board - Attenuon, L. L. C.; San Diego, California, www.attenuon.com, August, 1999 – present.
CEO and President - Schrödinger, Inc.; One Exchange Place, Jersey City, New Jersey; January, 1999 - July, 1999.
Executive Director - Biomolecular Structure, Lead Finding, and Computing, Novartis Institute for Biomedical Research; Summit, New Jersey; January, 1997-December, 1998.
Executive Director - Core Drug Discovery Technologies, Ciba Pharmaceuticals; Summit, New Jersey; July, 1994 - December, 1996.
Executive Director - Chemical Technologies, Pharmaceuticals Division, Ciba-Geigy Corporation; Summit, New Jersey; May, 1993 - June, 1994.
Director - Drug Discovery Support, Pharmaceuticals Division, Ciba-Geigy Corporation; Summit, New Jersey; May, 1991 - May, 1993.
Manager - Computer Assisted Molecular Modeling and Computational Chemistry, Pharmaceuticals Division, Ciba-Geigy Corporation; Summit, New Jersey; January, 1990 - May, 1991.
Project Team Leader - Purine Nucleoside Phosphorylase Project, Pharmaceuticals Division, Ciba-Geigy Corporation; Summit; New Jersey; January, 1989 - January, 1993.
Senior Staff Scientist - Computer Assisted Molecular Modeling, Pharmaceuticals Division, Ciba-Geigy Corporation; Summit, New Jersey; July, 1988 - December, 1989.
Senior Research Scientist - Computer Assisted Molecular Modeling, Pharmaceuticals Division, Ciba-Geigy Corporation; Summit, New Jersey; September, 1986 - July, 1988.
Senior Postdoctoral Fellow - Department of Chemistry, Columbia University; New York, N. Y.; July, 1985 - Sept., 1986 (*Sr. Postdoctoral Associate with Professor W. Clark Still*).
Visiting Associate Professor - Department of Chemistry, University of South Carolina; Columbia, South Carolina; Aug., 1983 - May, 1984 (*Sabbatical leave from Eckerd College to work with Professor James A. Marshall*).
Associate Professor - Department of Chemistry, Eckerd College; St. Petersburg, Florida; September, 1982 - June, 1986.
Assistant Professor - Department of Chemistry, Eckerd College; St. Petersburg, Florida; June, l977 - September, 1982.
Visiting Assistant Professor - Department of Chemistry, Eckerd College; St. Petersburg, Florida; September, 1976 - June, 1977.

EXPERTISE:

Research - Broad experience doing research with undergraduates, post-doctoral associates, and individually in both academic and industrial settings; experience in computational chemistry and synthetic organic chemistry; co-author of the MacroModel molecular modeling program, which is widely used in academia and industry; recent research has primarily involved computational biochemistry applied to enzyme inhibitor design, protein and peptide conformational studies, and structure-based drug design.

Supervisory - Previously, CEO of a computational chemistry software company (Schrödinger, Inc.); previously supervisor (Novartis) of a group of 36 scientists (mostly at the Ph. D. level) engaged in computer assisted molecular modeling, structural bioinformatics, X-ray crystallography, protein NMR spectroscopy, protein biochemistry, and high throughput screening; previous experience as project team leader of a successful drug discovery project involving structure-based drug design of enzyme inhibitors; previous responsibilities have included managing an analytical sciences group, scale-up (kilo) synthesis lab, and chemical informatics group.

Teaching – Primary teaching areas are in biochemistry, medicinal chemistry, molecular modeling and organic chemistry.

HONORS, AWARDS, OTHER PROFESSIONAL ACTIVITIES:

Outstanding Alumni Award – selected as the Outstanding Alumnus for 2005, Department of Chemistry, University of South Florida, April, 2005.

Selected to the Governing Board (External Review Panel) of the Hungarian Anýos Jedlik Programme (National R& D Program) to review proposals for the Life Sciences Division of the program, April, 2005.

Member of Chemical Biology Section of Faculty of 1000, September, 2002 - present.

Selected to give one of seven plenary lectures at the first Novartis Pharma Research Conference (an annual internal worldwide research conference for Novartis Pharmaceuticals Division Ph. D. level scientists), held in Barcelona, Spain, September, 1997.

Member of the External Advisory Board for the Center for Advanced Technology, Program in Biotechnology - Cornell University, September, 1994 - September, 1998.

Co-chair of an IUPAC committee to define guidelines for publication of results in computational chemistry, June, 1994 - July, 1998.

Member of National Academy of Sciences/National Research Council Committee to study "Mathematical Challenges from Computational Chemistry", March, 1994 - March, 1995.

Work on structure-based design of inhibitors of the enzyme purine nucleoside phosphorylase was described in *Scientific American* (December, 1993; described in an article by collaborators entitled "Drugs by Design").

Grant application review for: *NSF, Research Corporation, NIH (Teleconference and Mail Reviewer for Myocardial Ischemia and Metabolism Study Section Study Section; Ad Hoc Member of Drug Discovery and Mechanisms of Antimicrobial Resistance Study Section), DoD (Member, CET-4 Peer Review Panel, Breast Cancer Research Program).*

Manuscript review for the following professional journals: *Journal of Computational Chemistry, Journal of Computer Assisted Molecular Design, Nucleosides, Nucleotides & Nucleic Acids, Journal of the American Chemical Society, Journal of Chemical Information and Computer Science, Journal of Medicinal Chemistry, Journal of Molecular Recognition*

PROFESSIONAL AND HONORARY SOCIETIES:

Sigma Xi, Phi Kappa Phi, American Chemical Society.

COURSES TAUGHT:

Organic Chemistry, Biochemistry, Advanced Organic Chemistry, Qualitative Organic Analysis, Introduction to Chemistry, Advanced Inorganic Chemistry, General Chemistry Laboratory, The Chemistry of Color Photography, Computer Algorithms and Programming, Computer Assisted Molecular Modeling, Medicinal Chemistry.

STUDENT B.S. RESEARCH SUPERVISION:

1. ***Mark D. Herbst, 1977***, "Investigation of the Mechanism of Esterification of Aromatic Carboxylic Acids Using Alkyl Chlorosulfites." M.S., USF; M.D., Ph. D. Emory Univ.; Currently Radiologist in the Tampa Bay Area.
2. ***Edward E. Entreken, 1978***, "The Reduction of Organic Compounds using Sodium Borohydride and Ethanedithiol." M.B.A., USF.
3. ***David J. Mathre, 1979***, "The Use of Crown Ethers as Reagents in Organic Synthesis." Ph. D. Caltech, Post-doc Harvard; Currently Group Leader, Merck Research Labs.
4. ***John C. Culberson, 1981***, "The Determination of Structures of Small Molecules Using Molecular Orbital Calculations," Joint Supervision with Professor Reggie L. Hudson; Ph. D., Univ. of Florida, Currently Member of Comp. Chem. Group, Merck Research Labs.
5. ***Peter T. Meinke, 1982***, "Crown Catalyzed Alkali Metal Reductions.", Ph. D., Syracuse Univ., Post-doc, Columbia; Currently Director, Merck Resaerch Labs.
6. ***Glenn S. Smith, 1983***, "The Use of Polymer Supported Polyethers as Catalysts in the N-Alkylation of Heterocycles."
7. ***Jeffrey S. Walters, 1983***, "Phase Transfer Catalysts: A Study of Potential Photochromic Catalysts and Dissolving Metal Reductions." Ph. D., Univ. of Washington; Currently, Manager, National Marine Sanctuary, Dept. of Land and Natural Resources, Hawaii.

8. ***Carlos F. Barbas III, 1985***, "A Semi-empirical MO Investigation of the Nucleophilic Substitution Reaction.", Ph. D. Texas A&M; Post-doc, Penn State and Scripps; Currently, Professor, Scripps Research Institute.
9. ***Tara E. Jackson, 2000***, "Structure-based Inhibitor Design for Purine Nucleoside Phosphorylase and Pyrimidine Phosphorylase." M.D., Duke; Currently, Resident, All Children's Hospital, St. Petersburg, FL.
10. ***Debra J. Roche, 2001,*** "The Analysis of Human Acetylcholinesterase Inhibition Using Molecular Modeling." Currently, Teacher, Jefferson High School, Tampa, FL.
11. ***Justin Crotty, 2002,*** "Applications of the Low-Mode Conformational Search Procedure to the Peptide Dodeca-alanine." Grad. Student, Univ. of Arizona.
12. ***Hank Green, 2002,*** "Partial Purification of and Removal of Inhibitory Compounds from a Pine Cone Extract Through Soxhlet Extraction.", Grad. Student, Univ. of Montana.
13. ***James Kakoullis, 2002,*** "Modeling Zinc Metalloprotease's Active Sites.", Grad. Student, LSU.
14. ***Rebecca Harbach, 2004,*** "A Series of Novel, Copper-Containing Proteasome Inhibitors as Non-Toxic Chemotherapeutic Agents.", Grad. Student, UCSD.

POST-DOCTORAL RESEARCH ASSOCIATE SUPERVISION:

1. ***Regine S. Bohacek, 1987-88***, Topic: Methods for computing molecular volume and surface area.
2. ***Istvan Kolossvary, 1990-93***, Topic: Conformational searching and analysis.
3. ***Bryan Marten, 1995-97***, Topic: Computational methods for predicting binding affinities of enzyme inhibitors.
4. ***Jianling Wang, 1995-1997***, Topic: Application of resonance Raman spectroscopy to protein structure/function.
5. ***Wesley Brooks, 2003-2005,*** Topic: Computational studies on polyamine biosynthetic enzymes.
5. ***Kenyon Daniel, 2005-present,*** Topic: Computational studies on polyamine biosynthetic enzymes.

COMPLETED RESEARCH SUPPORT:

Ventron Corporation. "Borohydride reductions in dichloromethane," PI, 1977.

Research Corporation. "Chiral Crown Ethers in Asymmetric Synthesis," PI, 1979 - 1981.

NSF. "Nuclear Magnetic Resonance Spectroscopy in the Chemistry Laboratory Program at Eckerd College," Co-PI, 1980 - 1982.

Petroleum Research Fund "Dissolving Metal Reductions," PI, 1982 - 1984.

Attenuon, L.L.C. "Structure-based Design of Thymidine Phosphorylase Inhibitors as Anti-Angiogenic Agents," PI, 2000 - 2001.

Attenuon, L.L.C. "Structure-based Design of Superoxide Dismutase Inhibitors as Anti-Cancer Agents," Role: PI, 10% Effort. Research Support for Summer, 2006, Total Costs: $2,900.

CURRENT RESEARCH SUPPORT:

NIH/NCI P01 CA094000-01. "Rational Design of Inhibitors of Polyamine Synthesis," Role: Project Leader for Project III: "Computational studies on polyamine biosynthetic enzymes", 16% Effort. 8/01/03-07/31/08; Total Direct Costs for Project III in the first year: $110,750.

NIH/NCI U19 NCDDG CA067771-11. "Inhibitors of Rho function as novel cancer therapeutics", Role: Co-Project Leader for Core B: "High Throughput Screening and Molecular Modeling", 10% Effort. 05/01/05 – 04/30/10; Total Direct Costs for Core B in the first year: $180,431.

PENDING RESEARCH SUPPORT:

NSF CRIF. "Purchase of a Computational Cluster for Chemical Research and Training at the University of South Florida in Partnership with Eckerd College and the University of Tampa," Role: Co-PI, PI: Mike Zaworotko, Department of Chemistry, University of South Florida.

NIH/NCI P01. "Targeting Signal Transduction Pathways for Cancer Drug Discovery", Role: Core-Leader, Core B: Experimental High Throughput Screening and Virtual Screening/ Molecular Modeling, 15% Effort, Submitted February 1, 2006. PI's: Saïd Sebti and Srikumar Chellappan, Drug Discovery Program, Moffitt Cancer Center.

NIH/NCI R01. "Rb-Raf-1 Disruptors as Anti-Cancer Drugs" Role: Collaborator, 5% effort. PI: Srikumar Chellappan, Drug Discovery Program, Moffitt Cancer Center.

PUBLICATION AND PATENT LIST

Wayne Charles Guida

Starting with the most recent publication; underline denotes senior author or senior co-author.

1. "Discovery of a Novel Shp2 Protein Tyrosine Phosphatase Inhibitor." Chen, L.; Sung, S-S.; Yip, M. L. R.; Lawrence, H. R.; Ren, Y.; **Guida, W. C.**; Sebti, S. M.; Lawrence, N. J.; Wu, J. *Mol. Pharm.*, 2006, *70*, 562.
2. "Protein Farnesyltransferase: Flexible Docking Studies on Inhibitors Using Computational Modeling", **Guida, W. C.**; Hamilton, A.D.; Crotty, J.W.; and Sebti, S. M. *J. Comp. Aided Mol. Des.*, 2005, *19*, 871.
3. "IL-8/CXC ligand 8 survives neonatal gastric digestion as a result of intrinsic aspartyl proteinase resistance", Maheshwari A.; Lu, W.; **Guida, W. C.**; Christensen, R. D.; Calhoun, D. A. *Pediatric Res.* 2005, *57*, 438.
4. "Copper storage diseases: Menkes, Wilsons, and cancer", Daniel, K. G.; Harbach, R. H.; **Guida, W. C.**; Dou, Q. P. *Front. Biosci.* 2004, *9*, 2652.
5. "Organic Copper Complexes as a New Class of Proteasome Inhibitors and Apoptosis Inducers in Human Cancer Cells", Daniel, K. G.; Gupta, P.; Harbach, R. H.; **Guida, W. C.**; Dou, Q. P. *Biochem. Pharm.* 2004, *67*, 1139.
6. "Docking Studies and Model Development of Tea Polyphenol Proteasome Inhibitors: Applications to Rational Drug Design", Smith, D. M.; Daniel, K. G.; Wang, Z.; **Guida, W. C.**; Chan, T-H.; Dou, Q. P. *Proteins: Structure Function and Genetics* 2004, 54, 58.
7. "Circular Permutation of 5-Aminolevulinate Synthase", Cheltsov, A. V., **Guida, W. C.**; Ferreira, G. C. *J. Biol. Chem.* 2003, *278*, 27945.
8. "Design of Novel N-(2,4-Dioxo-1,2,3,4-tetrahydro-thieno[3,2-d] pyrimidin-7-yl)-guanidines as Thymidine Phosphorylase Inhibitors, and Flexible Docking to a Homology Model", Price, M. L. P.; **Guida, W. C.**; Jackson, T. E.; Nydick, J. A.; Gladstone, P. L.; Juarez, J. C.; Donate, F.; Ternansky, R. J. *Bioorg. Med. Chem. Lett.* 2003, *13*, 107.
9. "Chemosensors for the Marine Toxin Saxitoxin", Gawley, R.E; Pinet, S., Cardona, C. M; Probal, D. K; Tong, R.; **Guida, W. C.**; Nydick, J.; Leblanc, R. M. *J. Am. Chem. Soc.* 2002, *124*, 13448.
10. "Accurate Prediction of the Acidity Constant by *ab-initio* Methods", Klicic, J. A.; Friesner, R. A.; Liu, S-Y.; **Guida, W. C.** *J. Phys. Chem.* 2002, *106*, 1327.
11. "Low-mode Conformational Search Elucidated. Application to $C_{39}H_{80}$ and Flexible Docking of 9-Deazaguanine Inhibitors to PNP" Kolossvary, I.; **Guida, W. C.** *J. Comp. Chem.* 1999, *20*, 1671.
12. "Guidelines for Publication of Research Results from Force Field Calculations" Raber, D. J; **Guida, W. C.** *Pure and Applied Chemistry* 1998, *70*, 2047.
13. "Conformational Analysis: 1" Kolossvary, I.; **Guida, W.C.**, in *The Encyclopedia of Computational Chemistry*, Schleyer, Allinger, Clark, Gasteiger, Kollman, Schaefer & Schreiner, Eds., John Wiley & Sons: New York, 1998.
14. "Purine Nucleoside Phosphorylase. Catalytic Mechanism" Erion, M. D.; Stoeckler, J. D.; **Guida, W. C.**; Walter, R. L.; Ealick, S. E. *Biochemistry* 1997, *36*,11735.
15. Babu, Y. S.; Montgomery, J. A.; Bugg, C. E.; Carson, W. M.; Narayana, S. V. L.; Cook, W. J.; Ealick, S. E.; **Guida, W. C.**; Erion, M. D.; Secrist, J. A. "Design of Purine

Nucleoside Phosphorylase Inhibitors" in *Structure-Base Drug Design*, Veerapandian, P., Ed., Marcel Dekker, Inc.: New York, 1997.

16. "Low Mode Search. An Efficient, Automated Computational Method for Conformational Analysis: Application to Cyclic and Acyclic Alkanes and Cyclic Peptides" Kolossvary, I.; **Guida, W. C.** *J . Am. Chem. Soc.* 1996, *118*, 5011.
17. "The Art and Practice of Structure-Based Drug Design: A Molecular Modeling Perspective" Bohacek, R. S.; McMartin, C.; **Guida, W. C.** *Medicinal Research Reviews*, 1996, *16*, 3.
18. Stillinger, F. H.; Andersen, H. C.; Auslander, L.; Beveridge, D. L.; Davidson, E. R.; **Guida, W. C.**; Kollman, P. A.; Lester, W. A.; Martin, Y. C.; Schatz, G. C.; Schlick, T.; Scott, L. R.; Sumners, D. L.; Wolynes, P. G.; Houk, K. N.; Weidman, S. T. *Mathematical Challenges from Computational Chemistry*; National Academy Press: Washington, D. C., 1995.
19. "Tetra-n-butylammonium Borohydride" Raber, D. J.; **Guida, W. C.** *in Encyclopedia of Reagents for Organic Synthesis*, Paquette, L. A., Ed., John Wiley & Sons, New York, 1995, p. 4722.
20. "Structure-Based Design of Inhibitors of Purine Nucleoside Phosphorylase" Babu, Y. S.; Ealick, S. E.; Bugg, C. E.; Erion, M. D.; **Guida, W. C.**; Montgomery, J. A.; Secrist, J. A.; *Acta Cryst.* 1995, *D51*, 529.
21. "The biochemical and pharmacological activity of 9-benzyl-9-deazaguanine, a potent purine nucleoside phosphorylase (PNP) inhibitor" Kimble,. E.; Hadala, J.; Ludewig, R.; Peters, P.; Greenberg, G.; Xiao, G.; **Guida, W.**; McQuire, L.; Simon, P. *Inflamm. Res.* 1995, *44*, *Supplement 2*,S182.
22. "On searching the conformational space of cyclic molecules. Conformational interconversion pathways in trans-cycloalkenes" Kolossvary, I.; **Guida, W. C.** *J. Molecular Structure (Theochem)* 1994, *308*, 91-102.
23. "Solvent Effects on the Conformation of Cyclo-(-D-Trp-D-Asp-Pro-D-Val-Leu-). An NMR Spectroscopy and Molecular Modeling Study" Gonnella, N. C.; Zhang, X.; Jin, J.; Prakash, O.; Paris, C. G.; Kolossvary, I.; **Guida, W. C.**; Bohacek, R. S.; Vlattas, I.; Sytwu, T. *Int. J. Peptide Protein Res.* 1994, *43*, 454.
24. "Software for Structure-based Drug Design" **Guida, W. C.** *Current Opinion in Struct. Biol.* 1994, 777-781.
25. "Structure-Based Design of Inhibitors of Purine Nucleoside Phosphorylase. 4. A Study of Phosphate Mimics" **Guida, W. C.**; Elliott, R. D.; Thomas, H. J.; Secrist, J. A.; Babu, Y. S.; Bugg, C. E.; Erion, M. D.; Ealick, S. E.; Montgomery, J. A. *J. Med. Chem.* 1994, *37*, 1109.
26. "Application of X-ray Crystallographic Methods in the Design of Purine Nucleoside Phosphorylase Inhibitors" Ealick, S. E.; Babu, Y. S.; Bugg, C. E.; Erion, M. D.; **Guida, W. C.**; Montgomery, J. A.; Secrist, J. A. III *Annals of the New York Acad. of Sci.* 1993, *685*, 237.
27. "Structure-Based Design of Inhibitors of Purine Nucleoside Phosphorylase. 3. 9- Aryl-methyl Derivatives of 9-Deazaguanine Substituted on the Methylene Group" Erion, M. D.; Niwas, S.; Rose, J. D.; Anathan, S.; Allen, M.; Secrist, J. A.; Babu, Y. S.; Bugg, C. E.; **Guida, W. C.**; Ealick, S. E.; Montgomery, J. A. *J. Med. Chem.* 1993, *36*, 3771.
28. "Structure-Based Design of Inhibitors of Purine Nucleoside Phosphorylase. 2. 9-Alicyclic and 9-Heteroalicyclic Derivatives of 9-Deazaguanine" Secrist, J. A.; Niwas, S.;

Rose, J. D.; Babu, Y. S.; Bugg, C. E.; Erion, M. D.; **Guida, W. C.**; Ealick, S. E.; Montgomery, J. A. *J. Med. Chem.* 1993, *36*, 1847.

29. "Torsional Flexing: Conformational Searching of Cyclic Molecules in Biased Internal Coordinate Space" Kolossvary, I.; **Guida, W. C.** *J. Comp. Chem.* 1993, *14*, 691.
30. "Comprehensive Conformational Analysis of the Four- to Twelve-Membered Ring Cycloalkanes: Identification of the Complete Set of Interconversion Pathways on the MM2 Potential Energy Hypersurface" Kolossvary, I.; **Guida, W. C.** *J. Am. Chem. Soc.* 1993, *115*, 2107.
31. "Structure-Based Design of Inhibitors of Purine Nucleoside Phosphorylase. 1. 9-(Arylmethyl) Derivatives of 9-Deazaguanine" Montgomery, J. A.; Niwas, S.; Rose, J. D.; Secrist, J. A.; Babu, Y. S.; Bugg, C. E.; Erion, M. D.; **Guida, W. C.**; Ealick, S. E. *J. Med. Chem.* 1993, *36*, 55.
32. "Compare_Conformer: A Program for the Rapid Comparison of Molecular Conformers Based on Interatomic Distances and Torsion Angles" Kolossvary, I.; **Guida, W. C.** *J. Chem. Inform. and Computer Sciences* 1992, *32*, 191.
33. "Probing the Conformational Space Available to Inhibitors in the Thermolysin Active Site Using Monte Carlo / Energy Minimization Techniques" **Guida, W. C.**; Bohacek, R. S.; Erion, M. D. *J. Comp. Chem.* 1992, *13*, 214.
34. "Application of Crystallographic and Modeling Methods in the Design of Novel Purine Nucleoside Phosphorylase Inhibitors" Ealick, S. E.; Babu, S.; Bugg, C.E.; Erion, M. D.; **Guida, W. C.**; Montgomery. J. A.; Secrist. J. A. *Proc. Nat. Acad. Sci.* 1991, *88*, 11540.
35. "MacroModel - An Integrated Software System for Modeling Organic and Bioorganic Molecules Using Molecular Mechanics" Mohamadi, F.; Richards, N. G. J.; **Guida, W. C.**; Liskamp, R.; Lipton, M.; Caufield, C.; Chang, G.; Hendrickson T.; Still, W. C. *J. Comp. Chem.* 1990, *11*, 440.
36. "Conformations of Cycloheptadecane. A Comparison of Methods for Conformational Searching" Saunders, M.; Houk, K. N.; Wu Y-D; Still, W. C.; Lipton, M.; Chang, G.; **Guida, W. C.** *J. Am. Chem. Soc.* 1990, *112*, 1419.
37. "An Internal Coordinate Monte Carlo Method for Searching Conformational Space" Chang, G.; **Guida, W. C.**; Still, W. C. *J. Am. Chem. Soc.* 1989, *111*, 4379.
38. "A Rapid Method for the Computation, Comparison and Display of Molecular Volumes" Bohacek, R. S.; **Guida, W. C.** *J. Mol. Graph.* 1989, *7*, 113.
39. "4-(Phosphonoalkyl)- and 4-(Phosphonoalkenyl)-2-piperidinecarboxylic Acids: Synthesis, Activity at the N-Methyl-*D*-aspartic Acid Receptors, and Anticonvulsant Activity," Hutchison, A. J.; Williams, M.; Angst, C.; de Jesus, R.; Blanchard, L.; Jackson, R. H.; Wilusz, E. J.; Murphy, D. E.; Bernard, P. S., Schneider, J., Campbell, T, **Guida, W.**, Sills, M. A. *J. Med. Chem.* 1989, *32*, 2171.
40. "Jump Rope Rotation in *trans*-Cycloalkenes," Marshall, J. A.; Audia, V. H.; Jenson, T. M.; **Guida, W. C.** *Tetrahedron* 1985, *42*, 1703.
41. "Reduction of Esters and Other Carboxylates by Sodium Borohydride/Ethanedithiol: Improved Procedures and an Investigation into the Nature of the Reducing Species," **Guida, W. C.**; Entreken, E. E.; Guida, A. R. *J. Org. Chem.* 1984, *49*, 3024.
42. "A Pocket Calculator Program for the solution of pH Problems via the Method of Successive Approximations," **Guida, W. C.** in *Computer Series, 37, Bits and Pieces, 14, J. Chem. Educ.* 1983, *60*, 101.

43. "Tetraalkylammonium Borohydrides: Versatile Reagents for Reductions in Aprotic Solvents," **Guida, W. C.**; Raber, D. J. *Ventron Alembic* 1982, Issue *25*.
44. "Reduction of Aldehydes and Ketones with Tetraalkylammonium Borohydrides," Raber, D. J.; **Guida, W. C.**; Shoenberger, D. C. *Tetrahedron Lett.* 1981, 5107.
45. "Dissolving Metal Reductions with Sodium Potassium Alloy in the Presence of 18-Crown-6," Mathre, D. J.; **Guida, W. C.** *Tetrahedron Lett.* 1980, 4773.
46. "An Inexpensive Kugelrohr Still," **Guida, W. C.**; Gawley, R. E. *J. Chem. Educ.* 1980, *57*, 554.
47. "Phase Transfer Alkylation of Heterocycles in the Presence of 18-Crown-6 and Potassium *tert*-Butoxide," **Guida, W. C.**; Mathre, D. J. *J. Org. Chem.* 1980, *45*, 3172.
48. "Esterification of Carboxylic Acids with Trialkyloxonium Salts," Raber, D. J.; Gariano, P.; Brod, A. O.; Gariano, A.; **Guida, W. C.**; Guida, A. R.; Herbst, M. D. *J. Org. Chem.* 1979, *44*, 1149.
49. "Esterification of Carboxylic Acids with Trialkyloxonium Salts," Raber, D. J.; Gariano, P; **Guida, W. C.** *Organic Syntheses* 1977, *56*, 59.
50. "Borohydride Reductions in Dichloromethane: Tetrabutylammonium Borohydride," Raber, D. J.; **Guida, W. C.** *J. Org. Chem.* 1976, *41*, 690.
51. "The Chemistry of Color Photography," **Guida, W. C.**; Raber, D. J. *J. Chem. Educ.* 1975, *52*, 622.
52. "Preparation of Ethylene Acetals from 2-Methoxyethylcarboxylates via 1,3-Dioxolanium Ions," Raber, D. J.; **Guida, W. C.** *Synthesis* 1974, 808.
53. "The Molecular Adduct Between 2,2-Dichloro-4,4,6,6-tetra-phenylcyclotriphosphazatriene and Acetonitrile," Whitaker, R. D.; **Guida, W. C.** *J. Inorg. and Nucl. Chem.* 1969, *31* ,875.
54. "A study of the Molecular Adduct Between Hexaphenylcyclotriphosphazatriene and 1,1,2,2-Tetrachoro-ethane," Whitaker, R. D.; Bario, A. J.; Furman, P. A.; Stallings, E. S.; **Guida, W. C.** *J. Inorg. and Nucl. Chem.* 1968, *30*, 2921.

Patents:

1. "2-Amino-7-(Pyridinylmethyl)-3H, 5H, -Pyrrolo [3,2-D] Pyrimidin-4-ones and Pharmaceutical Uses and Compositions Containing the Same" Secrist, J. A.; Montgomery, J. A.; Ealick, S. E.; Erion, M. D.; **Guida, W. C.**, United States Patent, Number 4,985,433, January 15, 1991.
Patent describing inhibitors of Purine Nucleoside Phosphorylase.

2. "7-Substituted Derivatives of 2-Amino-3H,5H -Pyrrolo [3,2-D] Pyrimidin-4-ones and Pharmaceutical Uses and Compositions Containing the Same" Secrist, J. A.; Montgomery, J. A.; Ealick, S. E.; Erion, M. D.; **Guida, W. C.**, United States Patent, Number 4,985,434, January 15, 1991.
Patent describing inhibitors of Purine Nucleoside Phosphorylase.

3. "2-Amino-7-(alicyclomethyl)-3H, 5H, -Pyrrolo [3,2-D] Pyrimidin-4-ones and Pharmaceutical Uses and Compositions Containing the Same" Secrist, J. A.; Montgomery, J. A.; Ealick, S. E.; Erion, M. D.; **Guida, W. C.**, United States Patent, Number 5,008,265, April 16, 1991.
Patent describing inhibitors of Purine Nucleoside Phosphorylase.

4. "2-Amino-7-(heterocyclomethyl)-3H, 5H, -Pyrrolo [3,2-D] Pyrimidin-4-ones and Pharmaceutical Uses and Compositions Containing the Same" Secrist, J. A.; Montgomery, J. A.; Ealick, S. E.; Erion, M. D.; **Guida, W. C.**, United States Patent, Number 5,008,270, April 16, 1991.
Patent describing inhibitors of Purine Nucleoside Phosphorylase.

5. "7-Disubstituted-Methyl-4-Oxo-3H, 5H, -Pyrrolo [3,2-D] Pyrimidine and Pharmaceutical Uses and Compositions Containing the Same" Niwas, S. Secrist, J. A.; Montgomery, J. A.; Erion, M. D.; **Guida, W. C.** ;Ealick, S. E., United States Patent, Number 5,189,039, February 23, 1993.
Patent describing inhibitors of Purine Nucleoside Phosphorylase.

6. "7-Disubstituted-Methyl-4-Oxo-3H, 5H, -Pyrrolo [3,2-D] Pyrimidine and Pharmaceutical Uses and Compositions Containing the Same" Niwas, S. Secrist, J. A.; Montgomery, J. A.; Erion, M. D.; **Guida, W. C.** ;Ealick, S. E., United States Patent, Number 5,726,311, March 10, 1998.
Patent describing inhibitors of Purine Nucleoside Phosphorylase.

Papers Presented at Professional Meetings over the past 15 years:

1. "Computational Techniques for Determining the Conformational Preferences of Inhibitors Bound to Thermolysin and Purine Nucleoside Phosphorylase" Third Biennial *Workshop on Molecular Mechanics and Molecular Dynamics*, Florida State University, April, 1992 - **Invited Lecture.**
2. "Structure-Based Drug Design: Computational Approaches for Determining the Binding Geometry of Inhibitors of Thermolysin and Purine Nucleoside Phosphorylase" *Drug Information Association Meeting on Research Perspectives in Structural Biology and Chemistry*, Orlando, Florida, January, 1993 - **Invited Lecture.**
3. "Ligands and Receptors: Computational Techniques for Determining Binding Geometries" *Gordon Research Conference on Mycotoxins and Phycotoxins* Plymouth State College, New Hampshire, July, 1993 - **Invited Lecture.**
4. "Structure-Based Drug Design: A Multidisciplinary Approach Employing Protein Crystallography, Molecular Modeling and Site Directed Mutagenesis for the Design of Inhibitors of Purine Nucleoside Phosphorylase" *Conference on Rational Drug Design: Advances in Technology & Therapeutic Applications,* San Diego, California, December, 1993 - **Invited Lecture.**
5. "Structure-Based Drug Design: Computational Approaches for Determining the Binding Geometry of Inhibitors of the Enzyme Purine Nucleoside Phosphorylase", *Symposium on Molecular Modeling, 1994 Annual Meeting of the Florida Section - American Chemical Society,* Orlando; Florida, May, 1994 - **Invited Lecture.**
6. "Structure-Based Drug Design: A Multidisciplinary Approach Employing Protein Crystallography and Molecular Modeling for the Design of Inhibitors of Purine Nucleoside Phosphorylase", *Symposium on Macromolecular Interactions and Drug*

Design, Inflammation, Research Association Meeting, Poconos, PA, September, 1994 - **Invited Lecture.**

7. "How Protein Conformation has Influenced the Design of Inhibitors of Purine Nucleoside Phosphorylase", *Banbury Conference on Protein Design/Folding, The Banbury Center of Cold Spring Harbor Laboratory*, Long Island, NY, October, 1994 - **Invited Lecture.**

8. "Strategies for Conformational Searching in Gas Phase, in Solution and in Enzyme Binding Sites", *Symposium on Conformational Analysis: Methods and Applications, sponsored by the Division on Computers in Chemistry, 209th National Meeting of the American Chemical Society*, Anaheim, CA, April, 1995 - **Invited Lecture**.

9. "Dealing with Flexible Molecules: How Effective are Conformational Search Strategies Coupled with Molecular Mechanics at Reproducing Reality?" *Symposium on the Performance of Quantum Chemical and Molecular Modeling Codes for Complex Chemical Systems: How Applicable is Current Simulation Technology to Real World Problems - Biological Simulations , sponsored by the Division of Physical Chemistry, 212th National Meeting of the American Chemical Society*, Orlando, FL, August, 1996 **Invited Lecture.**

10. "L-Arginine-Based Inhibitors Perturb the Structure of the Heme Active Site of Human Inducible NOS: Evidence of Hydrogen-Bonding in the L-Arg Complex" J. Wang, W. C. Boyar, S.-I. Hu, D. T. Parker, D. J. Stuehr, J. Liebman, J. Strassman , **W. C. Guida**, Selected Lecture in "Hot Topics" section, 5th International. Meeting on the Biology of Nitric Oxide, September, 1997, Kyoto, Japan. – Lecture Presented by J. Wang.

11. "Structure-based Drug Design: Dealing with Flexible Proteins and Their Ligands" *Conference on Computational Chemistry and the Living World,* Chambery, France, April, 1998 – **Invited Lecture.**

12. "Structure-based Drug Design: Dealing with Flexible Proteins and Their Ligands*" 15th International Symposium on Medicinal Chemistry*, Edinburgh, Scotland, September, 1998 - **Invited Lecture**.

13. "Structure-based Design of Pyrimidine and Purine Nucleoside Phosphorylase Inhibitors as Novel Therapeutic Agents", *Florida Annual Meeting and Exposition 2000,* Orlando, Florida, May, 2000 - **Invited Lecture.**

14. "Next Generation Flexible Docking: Low Mode Search" *2nd Annual Computational Drug Design Conference,* San Francisco, California, July, 2000 - **Invited Lecture.**

15. "Nitric oxide synthase: searching for isoform-selective inhibitory drugs using resonance Raman spectroscopy" J. Wang, W. C. Boyar, S.-I. Hu, D. T. Parker, D. J. Stuehr, J. Liebman, J. Strassman and **W. C. Guida**, *17th International Conference on Raman Spectroscopy*", August, 2000, Beijing, China - Lecture Presented by J. Wang.

16. "Application of Computational Techniques to the Understanding of Enzyme/Substrate and Enzyme/Inhibitor Interactions Involved in Cancer", *National Cancer Institute Workshop on the Application of Structural Biology in Cancer Biology*, Bethesda, Maryland, December, 2000 – **Invited Lecture.**

17. "The Analysis of Human Acetylcholinesterase Inhibition Using Molecular Modeling", D. J. Roche and **W. C. Guida**, *Florida Annual Meeting and Exposition 2001*, Orlando, Florida, May, 2001 – **Lecture Presented by D. J. Roche.**

18. "Application of Computational Techniques to the Flexible Docking of Enzyme Inhibitors", *Structure-based Drug Design Workshop, sponsored by Schrödinger, Inc*., Princeton, New Jersey, June, 2001 - **Invited Lecture.**
19. "Zinc Metalloprotease Model Systems", D. Delo, J. Kakoullis, R. C. Schnabel and **W. C. Guida**, *American Chemical Society National Meeting*, Orlando, Florida, March, 2002 Poster Presented by D. Delo and J. Kakoullis.
20. "Protein farnesyltransferase: Flexible docking studies on inhibitors using computational modeling", **W. C. Guida**, A. D. Hamilton, J. W. Crotty and Saïd Sebti, *American Association for Cancer Research Meeting*, Anaheim, California, April, 2005. Poster presented by Saïd Sebti.

Seminars Presented at Colleges and Universities or to Professional Organizations over the past 15 years:

1. "Structure-Based Drug Design: Computational Techniques for Determining the Binding Geometry of Inhibitors of Thermolysin and Purine Nucleoside Phosphorylase", *NIEHS Marine/Freshwater Biomedical Research Center, University of Miami*; Miami; November, 1992.
2. "Protein Modeling and X-ray Crystallography in Drug Design", *Current Topics in Medicinal Chemistry - A Distinguished Lecture Series, Boston University*; Boston; April, 1994.
3. "Structure-Based Drug Design: Application of Crystallography and Molecular Modeling for the Design of Inhibitors of Purine Nucleoside Phosphorylase", *Biotechnology Research Institute of the National Research Council of Canada*, Montreal, September, 1994.
4. "Structure-Based Drug Design: A Multidisciplinary Approach Employing Protein Crystallography and Molecular Modeling for the Design of Inhibitors of Purine Nucleoside Phosphorylase", *Department of Pharmacology, University of California at Santa Barbara*, April, 1995.
5. "Structure-Based Drug Design: Is it Worth the Effort?", *Department of Pharmacology, University of Pennsylvania*, Philadelphia, March, 1997.
6. "Dealing with Flexible Molecules: How Effective are Conformational Search Strategies Coupled with Molecular Mechanics at Reproducing Reality?", *Department of Chemistry, Hunter College*, New York, N. Y., April, 1997.
7. "From Here to There and Back: Reflections of an Academic and Industrial Chemist", *Department of Chemistry, University of Florida,* Gainesville, Florida, March, 2000.
8. "Structure-based Design of Pyrimidine and Purine Nucleoside Phosphorylase Inhibitors as Novel Therapeutic Agents", *Department of Chemistry, University of South Florida,* Tampa, Florida, September, 2000.
9. "Structure-based Design of Thymidine Phosphorylase and Purine Nucleoside Phosphorylase Inhibitors as Potential Therapeutic Agents for Cancer", *H. Lee Moffitt Cancer Center & Research Institute,* Tampa, Florida, January, 2001.
10. "Structure-based Design of Thymidine Phosphorylase and Purine Nucleoside Phosphorylase Inhibitors as Potential Therapeutic Agents", *Department of Chemistry Florida International University,* Miami, Florida, January, 2001.

11. “Structure-based Drug Design Employing Structural Bioinformatics and Molecular Simulation Techniques”, *Department of Biochemistry and Molecular Biology, University of South Florida College of Medicine,* Tampa, Florida, January, 2002.
12. “Structure-based Drug Design Employing Structural Bioinformatics and Computer Assisted Molecular Modeling”, *Information Technology Department, H. Lee Moffitt Cancer Center & Research Institute,* Tampa, Florida, March, 2002.
13. “The Application of Computer Simulation and Structural Bioinformatics to Structure-based Drug Design”, *Department of Chemical Engineering, University of South Florida,* Tampa, Florida, March, 2003.
14. "Application of Computational Modeling to the Structure-based Design of Cancer Drugs", *Department of Chemistry and Biochemistry, University of Arkansas,* Fayetteville, Arkansas, April, 2004.
15. "The Application of Computational Modeling to the Structure-based Design of Drugs for the Treatment of Cancer", *Lexicon Pharmaceuticals,* Princeton, New Jersey, December, 2004.
16. “The Use of Computational Modeling in the Structure-based Discovery and Design of Drugs for the Treatment of Cancer”, *Gideon Richter Pharmaceuticals,* Budapest, Hungary, July, 2005.
17. “Structure-based Discovery and Design of Drugs for the Treatment of Cancer Guided by Computational Modeling”, Department of Biochemistry & Molecular Biology, *Hershey Medical Center, Penn State University,* Hershey, PA, August, 2006.