CURRICULUM VITAE
Wayne Charles Guida
June, 2015

CURRENT POSITION & ADDRESS:

Professor, Department of Chemistry
University of South Florida
4202 E. Fowler Avenue, CHE 205
Tampa, FL 33620-5250
Tel: (727) 452-2986
email: wguida@usf.edu

EDUCATION AND TRAINING:

Sr. Research 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:

Current Academic Affiliations:

Professor, Department of Chemistry, College of Arts & Sciences, University of South Florida, Tampa, Florida; August, 2007 – present.
Professor Emeritus, Department of Chemistry, Eckerd College; St. Petersburg, Florida; August, 2007 – present.
Courtesy Professor, Department of Oncologic Sciences, College of Medicine, University of South Florida, Tampa, Florida, January, 2008 – present.

Current Professional Affiliations:

Collaborating Member - H. Lee Moffitt Cancer Center & Research Institute at the University of South Florida; Tampa, Florida; October, 2014 – present.
Consultant – BioMarin Pharmaceutical Co., Navato, CA, www.bmrn.com, June, 2014 – present.
Member of the Scientific Advisory Board - Schrödinger, Inc.; New York, New York, and Portland, Oregon, www.schrodinger.com, March, 2008 – present.

Consultant - Schrödinger, Inc.; New York, New York and Portland, Oregon, www.schrodinger.com, August, 1999 – present.

Prior Experience:

Sr. Member, Drug Discovery Department - H. Lee Moffitt Cancer Center & Research Institute at the University of South Florida; Tampa, Florida; September, 2003 – September, 2014.
Co-Scientific Director, Chemical Biology Core - H. Lee Moffitt Cancer Center & Research Institute at the University of South Florida; Tampa, Florida; November, 2004 – May, 2015.
Member of the Board of Directors - Schrödinger, Inc.; New York, New York and Portland, Oregon, www.schrodinger.com, August, 1999 – December, 2012.
Consultant - Attenuon, L. L. C.; San Diego, California, www.attenuon.com, January, 2008 – December, 2011.
Professor, Department of Chemistry, Eckerd College; St. Petersburg, Florida; February, 2003 – July, 2007.
Consultant – Celgene, Signal Research Division; San Diego, California, www.signalpharm.com, November, 2002 – August, 2005.
Affiliate Assistant Professor - Department of Interdisciplinary Oncology, College of Medicine, University of South Florida, Tampa, Florida, January, 2002 – August, 2005.
Associate Professor, Department of Chemistry, Eckerd College; St. Petersburg, Florida; August, 1999 – January, 2003.
Member of the Scientific Advisory Board - Attenuon, L. L. C.; San Diego, California, www.attenuon.com, August, 1999 – December, 2007.
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 but have taught courses in computer programming, color photography, and Freshman Great Books courses.

HONORS, AWARDS, OTHER PROFESSIONAL ACTIVITIES:

Editorial Board Member, Computational Drug Discovery. 2015-Present

Editorial Advisory Board Member, International Journal of High-Throughput Screening 2014-Present

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 - 2010.

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, and 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; Ad Hoc Member of Drug Discovery and Molecular Pharmacology Study Section; Ad hoc Online Reviewer, Israeli Science Foundation.)*

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 Modeling, Journal of Medicinal Chemistry, Medicinal Chemistry Letters, Journal of Molecular Recognition, Proteins: Structure, Function and Bioinformatics, Journal of Physical Chemistry, Journal of Combinatorial Chemistry.*

PROFESSIONAL AND HONORARY SOCIETIES:

Sigma Xi, Phi Kappa Phi, American Chemical Society.

COURSES TAUGHT:

Organic Chemistry, Biochemistry, Advanced Organic Chemistry, Introduction to Chemistry, Advanced Inorganic Chemistry, General Chemistry Laboratory, The Chemistry of Color

Photography, Computer Algorithms and Programming, Computer Assisted Molecular Modeling, Medicinal Chemistry, Western Heritage in a Global Context.

STUDENT COMPLETED B.S. THESIS 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." Ph. D., Univ. of Arizona.
12. ***Hank Green, 2002,*** "Partial Purification of and Removal of Inhibitory Compounds from a Pine Cone Extract Through Soxhlet Extraction.", Ph. D., Univ. of Montana.
13. ***James Kakoullis, 2002,*** "Modeling Zinc Metalloprotease's Active Sites.", M.S., LSU.
14. ***Rebecca Harbach, 2004,*** "A Series of Novel, Copper-Containing Proteasome Inhibitors as Non-Toxic Chemotherapeutic Agents.", M.S., UCSD.

STUDENT COMPLETED PH. D. DISSERTATION RESEARCH SUPERVISION:

1. **Dr. Daniel Santiago, 2012**, "Use and Development of Computational Tools in Drug Discovery: From Small Molecules to Cyclic Peptides." Post-doc., The Scripps Research Institute, La Jolla, CA.

2. **Dr. Divya Ramamoorthy, 2012,** "Design of Novel Inhibitors for Infectious Diseases using Structure-based Drug Design:Virtual Screening, Homology Modeling and Molecular Dynamics." Post-doc, Univ. of Washington, Seattle.

3. **Dr. Sai Vankayala, 2013,** "Computational Approaches for Structure Based Drug Design and Protein Structure-Function Prediction." Post-doc, University of So. FL.

4. **Dr. Courtney DuBoulay, 2013**, "Virtual screening for Inhibitors of Anti-apoptotic Proteins." Assistant Professor, Portland Community College, Portland, OR.

5. **Dr. Katherine Parra**, **2014**, Combination of the Computational Methods: Molecular dynamics, Homology Modeling and Docking to Design Novel Inhibitors and study Structural Changes in Target Proteins for Current Diseases." Laboratory Director Mor-NuCo, Inc., West Lafayette, Indiana.

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.
6. ***Kenyon Daniel, 2005-2009,*** Topic: Computational studies on polyamine biosynthetic enzymes and signal transduction proteins.

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. Total Costs: $5,000.

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

NIH/NCI P01 CA094000. "Rational Design of Inhibitors of Polyamine Synthesis," Role: Project Leader for Project III: "Computational studies on polyamine biosynthetic enzymes", 10% Effort. 8/01/2003-07/31/2009; Total Direct Costs for Project III in the first year: $94,138.

NIH/NCI U19 NCDDG CA067771. "Inhibitors of Rho function as novel cancer therapeutics", Role: Project Leader for Core B: "High Throughput Screening and Molecular Modeling", 7.5% Effort. 05/01/2005 – 04/30/2010; Total Direct Costs for Core B in the first year: $188,431.

Florida Department of Health , James & Esther King Biomedical Research Grant. "Bcl-X_L-templated Assembly of Compounds Modulating Bcl-X_L-protein interactions", Role: Mentor for Roman Manetsch (PI), 3.8% Effort, 07/1/2007-06/30/2010, Total Direct Costs: $375,000 (three years).

NSF MRI 0722887 "Acquisition of a Computational Cluster for Research and Training at the University of South Florida in Partnership with Eckerd College and the University of Tampa," Role: Co-PI, PI: Venkat Bhethanabotla, College of Engineering, University of South Florida, 08/15/2007-08/14/2010, Direct Costs: $500,000 for purchase of a computational cluster.

NIH/NCI R01 CA 71976. "Alkyltransferase Inhibitors for Cancer Chemotherapy" Role: Consultant, 1% Effort, 08/01/2006- 05/31/2011; Total Direct Costs for Guida Lab in first year: $10,116.

NIH/NCI P01 CA118210. "Targeting Signal Transduction Pathways for Cancer Drug Discovery", Role: Project Leader for Core B: Experimental High Throughput Screening and Virtual Screening/ Molecular Modeling, 15% Effort; 02/05/2007-01/31/2012, Total Direct Costs for Core B in the first year: $114,548.

NIH/NCI R01 CA71976 "4'-Substituted Nucleoside Analogs as Anti-cancer Drugs" Role: Consultant, 1% Effort, 08/01/2006-05/31/2012, Total Direct Costs for Guida Lab in first year: $12,450.

CURRENT RESEARCH SUPPORT:

NIH/NCI 3P30 CA76292. "Moffitt Cancer Center Support Grant", Role: Scientific Co-Director for the Chemical Biology Core, 5% Effort, 02/01/2012-01/31/2017. Total Direct Costs for the HTS & Chemistry Core in first year: $65,666.

NIH/NCI R01 CA140681 "Targeting STAT3 as a novel approach to cancer therapy" Role: Co-Investigator, 4% Effort, 07/01/2009 - 05/31/2015. Total Direct Costs for Guida Lab in first year: $5,387. On No Cost Extension.

Florida Bank-head Coley Biomedical Research Program. "Design, synthesis, and evaluation of γ-AApeptide-based protein tyrosine phosphatase inhibitors as novel anticancer agents", Role: Mentor for J. Cai (PI), 07/01/12-06/30/2015.

Univ. of So. Fl., Proposal Enhancement Grant (Internal Award). "Discovery and Design of Copper Activated Proteasome Inhibitors", 06/01/2014- 10/31/2015.

PUBLICATION AND PATENT LIST

Wayne Charles Guida

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

1. "A computational design approach for virtual sreening of peptide interactions across K(+) channel families. Doupnik CA, Parra KC, **Guida WC**. *Comput Struct Biotechnol J.*, 2014, *13*, 85.
2. Orally bioavailable 6-chloro-7-methoxy-4(1H)-quinolones efficacious against multiple stages of Plasmodium. 2: Cross RM, Flanigan DL, Monastyrskyi A, LaCrue AN, Sáenz FE, Maignan JR, Mutka TS, White KL, Shackleford DM, Bathurst I, Fronczek FR, Wojtas L, **Guida WC**, Charman SA, Burrows JN, Kyle DE, Manetsch R. *J Med Chem*. 2014, 57, 8860.
3. "Plasmodium vivax 1-deoxy-D-xylulose-5-phosphate synthase: Homology Modeling, Domain Swapping, and Virtual Screening." Ramamoorthy D, Handa S, Merkler DJ, **Guida WC.** *J Data Mining Genomics Proteomics*, 2014, S1:003. doi:10.4172/2153-0602.S1-003.
4. "Virtual target screening to rapidly identify potential protein targets of natural products in drug discovery." Pevzner Y, Santiago DN, Salm JL, Metcalf RS, Daniel KG, Calcul Woodcock HL, Baker BJ, **Guida WC**, Brooks WH. *AIMS Molecular Science*, 2014, *1*, 81.
5. "Orally bioavailable 6-chloro-7-methoxy-4(1H)-quinolones efficacious against multiple stages of Plasmodium." Cross RM, Flanigan DL, Monastyrskyi A, LaCrue AN, Sáenz FE, Maignan JR, Mutka TS, White KL, Shackleford DM, Bathurst I, Fronczek FR, Wojtas L, **Guida WC**, Charman SA, Burrows JN, Kyle DE, Manetsch R. *J Med Chem.*, 2014, *57*, 8860.
6. "*In silico* characterization of an atypical MAPK phosphatase of Plasmodium falciparum as a suitable target for drug discovery." Campbell CO, Santiago DN, **Guida WC**, Manetsch R, Adams JH. *Chem Biol Drug Des.*, 2014, *84*, 158.
7. "Production of recombinant 1-deoxy-d-xylulose-5-phosphate synthase from Plasmodium vivax in Escherichia coli." Handa S, Ramamoorthy D, Spradling TJ, **Guida WC**, Adams JH, Bendinskas KG, Merkler DJ. FEBS *Open Bio.*, 2013, *3*, 124.
8. "Development of new N-Arylbenzamides as STAT3 Dimerization Inhibitors." Urlam MK, Pireddu R, Ge Y, Zhang X, Sun Y, Lawrence HR, **Guida WC**, Sebti SM, Lawrence NJ. *Medchemcomm.*, 2013, *4*, 932.
9. "Identification of a New Binding Site in E. coli FabH using Molecular Dynamics Simulations: Validation by Computational Alanine Mutagenesis and Docking Studies." Ramamoorthy D, Turos E, **Guida WC.** *J Chem Inf Model.*, 2013, *53*,1138.
10. "Oxadiazole-isopropylamides as Potent and Noncovalent Proteasome Inhibitors." Ozcan S, Kazi A, Marsilio F, Fang B, **Guida WC**, Koomen J, Lawrence HR, Sebti SM. *J Med Chem.*, 2013, *56*, 3783-3805.
11. "A novel inhibitor of STAT3 homodimerization selectively suppresses STAT3 activity and malignant transformation." Zhang X, Sun Y, Pireddu R, Yang H, Urlam MK, Lawrence HR, **Guida WC**, Lawrence NJ, Sebti SM. *Cancer Res.*, 2013,*73*,1922.

12. "Virtual target screening: validation using kinase inhibitors." Santiago DN, Pevzner Y, Durand AA, Tran M, Scheerer RR, Daniel K, Sung SS, Woodcock HL, **Guida WC**, Brooks WH. *J Chem Inf Model.* 2012, *52*, 2192.
13. "Fragment-Based and Structure-Guided Discovery and Optimization of Rho Kinase Inhibitors" Li R, Martin MP, Liu Y, Wang B, Patel RA, Zhu JY, Sun N, Pireddu R, Lawrence NJ, Li J, Haura EB, Sung SS, **Guida WC**, Schonbrunn E, Sebti SM. *J Med Chem.* 2012, *55*, 2474.
14. "Pyridylthiazole-based ureas as inhibitors of Rho associated protein kinases (ROCK1 and 2)." Pireddu R, Forinash KD, Sun NN, Martin MP, Sung SS, Alexander B, Zhu JY, **Guida WC**, Schönbrunn E, Sebti SM, Lawrence NJ. *Medchemcomm.*, 2012, *3*, 699.
15. "Discovery and Synthesis of Hydronaphthoquinonesas Novel Proteasome Inhibitors" Ge Y, Kazi A, Marsilio F, Luo Y, Jain S, Brooks W, Daniel KG, **Guida WC**, Sebti SM, Lawrence HR. *J Med Chem.* 2012, *55*, 1978.
16. "Synthesis and evaluation of substituted hexahydronaphthalenes as novel inhibitors of the Mcl-1/BimBH3 interaction." Kim YB, Balasis ME, Doi K, Berndt N, DuBoulay C, Hu CC, **Guida W**, Wang HG, Sebti SM, Del Valle JR. *Bioorg Med Chem Lett.*, 2012 *22*, 5961.
17. "Shp2 protein tyrosine phosphatase inhibitor activity of estramustine phosphate and its triterpenoid analogs" Scott L.M.; Chen L.; Daniel K.G.; Brooks W.H.; **Guida W.C.**; Lawrence H.R.; Sebti S.M.; Lawrence N.J.; Wu J. *Bioorg Med Chem Lett*. 2011, *21*,730.
18. "The significance of chirality in drug design and development" Brooks W.H.; **Guida W.C.**; Daniel K.G. *Curr Top Med Chem.* 2011, *11*, 760.
19. "Synthesis and biological evaluation of naphthoquinone analogs as a novel class of proteasome inhibitors" Lawrence H.R.; Kazi, A.; Luo, Y.; Kendig, R.; Ge, Y.; Jain, S.; Daniel, K.; Santiago, D.; **Guida, W.C.**; Sebti, S.M. *Bioorg. Med. Chem.* 2010, *18*, 5576.
20. "Facile iterative synthesis of 2,5-terpyrimidinylenes as nonpeptidic alpha-helical mimics" Anderson, L.; Zhou, M.; Sharma, V.; McLaughlin, J.M.; Santiago, D.N.; Fronczek, F.R.; **Guida, W.C.**; McLaughlin, M.L. *J. Org. Chem.*, 2010, *75*, 4288.
21. "Inhibition of cellular Shp2 activity by a methyl ester analog of SPI-112" Chen, L; Pernazza, D.; Scott, L.M.; Lawrence, H.R.; Ren, Y.; Luo, Y.; Wu, X.; Sung, S-S.; **Guida, W.C.**; Sebti, S.M.; Lawrence, N.J.; Wu. *J. Biochem Pharmacol.*, 2010, *80*, 801.
22. "Structure-based design of high affinity peptides inhibiting the interaction of p53 with MDM2 and MDMX" Phan J.; Li, Z.; Kasprzak, A.; Li, B.; Sebti, S.; **Guida, W.**; Schönbrunn, E; Chen, J. *J. Biol. Chem.* 2010, *285*, 2174.
23. "Role of the sulfonium center in determining the ligand specificity of human S-adenosylmethionine decarboxylase" Bale, S.; Brooks, W.; Hanes, J.W.; Mahesan, A.M.; **Guida, W.C.**; Ealick, S.E. *Biochemistry*, 2009, *48*, 6423.
24. "Discovery of a novel proteasome inhibitor selective for cancer cells over non-transformed cells" Kazi, A.; Lawrence, H.; **Guida, W.C.**; McLaughlin, M.L.; Springett, G.M.; Berndt, N.; Yip, R.M.; Sebti, S.M.; *Cell Cycle*, 2009, *8*,1940.
25. "Identification of a disruptor of the MDM2-p53 protein-protein interaction facilitated by high-throughput in silico docking" Lawrence, H.R.; Li Z.; Yip, M.L.; Sung, S-S.; Lawrence, N.J.; McLaughlin, M.L; McManus, G.J.; Zaworotko, M.J.; Sebti, S.M.; Chen, J.; **Guida, W.C.** *Bioorg Med Chem Lett.*, 2009,*19*, 3756.
26. "New Insights into the Design of Inhibitors of Human S-Adenosylmethionine Decarboxylase: Studies of Adenine C(8) Substitution in Structural Analogues of S-

Adenosylmethionine", McCloskey, D.E.; Bale, S.; Secrist, J.A.; Tiwari, A.; Moss, T.H.; Valiyaveettil, J.; Brooks, W.H.; **Guida, W.C.**; Pegg, A.E.; Ealick, S.E. *J Med. Chem.*, 2009, *51*, 7144.

27. "Substitution of Aminomethyl at the Meta-Position Enhances the Inactivation of O(6)-Alkylguanine-DNA Alkyltransferase by O(6)-Benzylguanine.", Pauly, G. T.; Loktionova, N. A.; Fang, Q.; Vankayala, S. L.; **Guida W. C.**; Pegg, A. E. *J. Med. Chem.*, 2008, *51*, 7144.
28. "Inhibitors of Src homology-2 domain containing protein tyrosine phosphatase-2 (Shp2) based on oxindole scaffolds", Lawrence, H.R.; Pireddu R.; Chen, L.; Luo, Y; Sung, S-S; Szymanski, A.M.; Yip, M.L.; **Guida W. C.**; Sebti, S.M.; Wu, J; Lawrence, N.J. *J. Med. Chem.*, 2008, *51*, 4948.
29. "A small-molecule E2F inhibitor blocks growth in a melanoma culture model", Ma, Y.; Kurtyka, C. A.; Boyapalle, S.; Sung, S-S; Lawrence, H.; **Guida, W.**; Cress, W.D.; Cancer Res., 2008, *68*, 6292.
30. "Computational validation of the importance of absolute stereochemistry in virtual screening", Brooks, W.H.; Daniel, K.G.;Sung, S-S; **Guida, W.C.** *J Chem. Inf. Model.*, 2008, *48*, 639.
31. "In Silico Chemical Library Screening and Experimental Validation of a Novel 9-Aminoacridine Based Lead-Inhibitor of Human S-Adenosylmethionine Decarboxylase", Brooks, W.H.; McCloskey, D.E.; Daniel, K.G.; Ealick, S.E., Secrist, J.A.3rd, Waud, W.R.; Pegg, A.E.; **Guida, W.C.** *J. Chem. Inf. Model.* 2007, *47*,1897.
32. "Selective chemical probe inhibitor of Stat3, identified through structure-based virtual screening, induces antitumor activity", Siddiquee, K.; Zhang, S.; **Guida, W. C.**; Blaskovich, M. A.; Greedy, B.; Lawrence, H. R.; Yip, M. L.; Jove, R.; McLaughlin, M. M.; Lawrence, N. J.; Sebti, S. M.; Turkson, J. *Proc. Natl. Acad. Sci. USA* 2007, *104*, 7391.
33. "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.
34. "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.
35. "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.
36. "Copper storage diseases: Menkes, Wilsons, and cancer", Daniel, K. G.; Harbach, R. H.; **Guida, W. C.**; Dou, Q. P. *Front. Biosci.* 2004, *9*, 2652.
37. "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.
38. "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.
39. "Circular Permutation of 5-Aminolevulinate Synthase", Cheltsov, A. V., **Guida, W. C.**; Ferreira, G. C. *J. Biol. Chem.* 2003, *278*, 27945.

40. "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.
41. "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.
42. "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.
43. "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.
44. "Guidelines for Publication of Research Results from Force Field Calculations" Raber, D. J; **Guida, W. C.** *Pure and Applied Chemistry* 1998, *70*, 2047.
45. "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.
46. "Purine Nucleoside Phosphorylase. Catalytic Mechanism" Erion, M. D.; Stoeckler, J. D.; **Guida, W. C.**; Walter, R. L.; Ealick, S. E. *Biochemistry* 1997, *36*,11735.
47. 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.
48. "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.
49. "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.
50. 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.
51. "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.
52. "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.
53. "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.

54. "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.
55. "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.
56. "Software for Structure-based Drug Design" **Guida, W. C.** *Current Opinion in Struct. Biol.* 1994, 777-781.
57. "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.
58. "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.
59. "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.
60. "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.
61. "Torsional Flexing: Conformational Searching of Cyclic Molecules in Biased Internal Coordinate Space" Kolossvary, I.; **Guida, W. C.** *J. Comp. Chem.* 1993, *14*, 691.
62. "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.
63. "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.
64. "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.
65. "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.
66. "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.
67. "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.

68. "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.
69. "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.
70. "A Rapid Method for the Computation, Comparison and Display of Molecular Volumes" Bohacek, R. S.; **Guida, W. C.** *J. Mol. Graph.* 1989, *7*, 113.
71. "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.
72. "Jump Rope Rotation in *trans*-Cycloalkenes," Marshall, J. A.; Audia, V. H.; Jenson, T. M.; **Guida, W. C.** *Tetrahedron* 1985, *42*, 1703.
73. "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.
74. "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.
75. "Tetraalkylammonium Borohydrides: Versatile Reagents for Reductions in Aprotic Solvents," **Guida, W. C.**; Raber, D. J. *Ventron Alembic* 1982, Issue *25*.
76. "Reduction of Aldehydes and Ketones with Tetraalkylammonium Borohydrides," Raber, D. J.; **Guida, W. C.**; Shoenberger, D. C. *Tetrahedron Lett.* 1981, 5107.
77. "Dissolving Metal Reductions with Sodium Potassium Alloy in the Presence of 18-Crown-6," Mathre, D. J.; **Guida, W. C.** *Tetrahedron Lett.* 1980, 4773.
78. "An Inexpensive Kugelrohr Still," **Guida, W. C.**; Gawley, R. E. *J. Chem. Educ.* 1980, *57*, 554.
79. "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.
80. "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.
81. "Esterification of Carboxylic Acids with Trialkyloxonium Salts," Raber, D. J.; Gariano, P; **Guida, W. C.** *Organic Syntheses* 1977, *56*, 59.
82. "Borohydride Reductions in Dichloromethane: Tetrabutylammonium Borohydride," Raber, D. J.; **Guida, W. C.** *J. Org. Chem.* 1976, *41*, 690.
83. "The Chemistry of Color Photography," **Guida, W. C.**; Raber, D. J. *J. Chem. Educ.* 1975, *52*, 622.
84. "Preparation of Ethylene Acetals from 2-Methoxyethylcarboxylates via 1,3-Dioxolanium Ions," Raber, D. J.; **Guida, W. C.** *Synthesis* 1974, 808.
85. "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.

86. "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.

7. "Small Molecule Inhibitors of Stat3 with Anti-tumor Activity" Turkson, J.; Sebti, S.M.; **Guida, W.C.**; Yip, M. L.; Lawrence, N.; Lawrence, H.; Greedy, B. United States Patent, Number 7,960,434 B2, June 14, 2011.

8. "Proteasome inhibitors for selectively inducing apoptosis in cancer cells Lawrence H, Ge Y, Sebti SM, **Guida W.**, US Patent 8,673,910, 2014

9. "5′,-Substituted adenosynes preparation thereof and use as inhibitors of S-adenosylmethionine decarboxylase" Secrist III, JA; Ealick, S.; Bale, S.; AE Pegg, AE.; Mccloskey, DE; **Guida**, **W.C.** US Patent 8,637,485, 2014

Papers Presented at Professional Meetings over the past 20 years:

1. "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.
2. "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.**
3. "Structure-based Drug Design: Dealing with Flexible Proteins and Their Ligands*" 15th International Symposium on Medicinal Chemistry*, Edinburgh, Scotland, September, 1998 - **Invited Lecture**.
4. "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.**
5. "Next Generation Flexible Docking: Low Mode Search" *2nd Annual Computational Drug Design Conference,* San Francisco, California, July, 2000 - **Invited Lecture.**
6. "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.
7. "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.**
8. "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.**
9. "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.**
10. "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.
11. "Protein farnesyltransferase: Flexible docking studies on inhibitors using computational modeling", **W. C. Guida**, A. D. Hamilton, J. W. Crotty and S. Sebti,

American Association for Cancer Research Meeting, Anaheim, California, April, 2005. Poster presented by Saïd Sebti.
12. "Structure-based Discovery and Design of Drugs for the Treatment of Cancer Guided by Computational Modeling", W. C. Guida, *Schrödinger Users Symposium*, New York City, May, 2006 – **Invited Lecture**.
13. "Virtual Counter Screening: New targets for old molecules", W. C. Guida, D. Santiago and W. Brooks, *Schrödinger Users Symposium*, New York City, April, 2007-**Invited Lecture**

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

1. "From Here to There and Back: Reflections of an Academic and Industrial Chemist", *Department of Chemistry, University of Florida,* Gainesville, Florida, March, 2000.
2. "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.
3. "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.
4. "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.
5. "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.
6. "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.
7. "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.
8. "Application of Computational Modeling to the Structure-based Design of Cancer Drugs", *Department of Chemistry and Biochemistry, University of Arkansas,* Fayetteville, Arkansas, April, 2004.
9. "The Application of Computational Modeling to the Structure-based Design of Drugs for the Treatment of Cancer", *Lexicon Pharmaceuticals,* Princeton, New Jersey, December, 2004.
10. "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.
11. "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.

12. "Structure-based Discovery and Design of Drugs for the Treatment of Cancer Guided by Computational Modeling, City of Hope Cancer Center and Beckman Research Institute, Duarte, CA, January, 2007.
13. "Structure-based Discovery and Design of Drugs for the Treatment of Cancer Guided by Computational Modeling", Department of Chemistry, University of Florida, Gainesville, FL, November, 2007.
14. "Structure-based Discovery and Design of Drugs for the Treatment of Cancer Guided by Computational Modeling", Research Grand Rounds Lecture, H. Lee Moffitt Cancer Center & Research Institute, Tampa, FL, March, 2008.
15. "Computation in the Health Sciences", First Annual Symposium on Computational Science & Engineering, University of South Florida, Tampa, FL, January, 2009.
16. "In Silico Structure-based Drug Design: Virtual Reality or Virtual Fantasy?", Department of Molecular Medicine, College of Medicine, University of South Florida, September, 2010.
17. "In Silico Docking and Medicinal Chemistry: A Marriage made in Heaven or a Shotgun Wedding?" Research in Progress, H. Lee Moffitt Cancer Center & Research Institute, October, 2010.