CURRICULUM VITAE
Jeffrey M. Blaney

EDUCATION:
1974-1978 Pomona College, Claremont, CA B.A. Chemistry-Zoology
1978-1982 UCSF, San Francisco, CA Ph.D. Pharmaceutical Chemistry
(Principal Advisor: Neal Castagnoli)

PRINCIPAL POSITIONS HELD:
1982-1987 Research Chemist, DuPont Pharmaceuticals, Wilmington, DE
1988-1990 Sr. Research Chemist, DuPont Pharmaceuticals, Wilmington, DE
1990-1992 Sr. Research Scientist, Protos, Emeryville, CA
1992-1997 Director Computational/Biophysical Chemistry, Chiron, Emeryville, CA
1997-2000 Vice President, Computational Chemistry, Metaphorics, Santa Fe, NM
2000-2001 Executive Director, Chemical & Physical Sciences R&D, DuPont Pharmaceuticals Research Laboratories, San Diego, CA
2002-2007 Vice President, Computational Chemistry, SGX Pharmaceuticals, San Diego, CA
2007- Director, Computational Chemistry & Cheminformatics, Small Molecule Drug Discovery, Genentech, South San Francisco, CA

OTHER POSITIONS HELD CONCURRENTLY:
1997-1998 Computational chemistry consultant, Chiron, Emeryville, CA
2001-2005 Computational chemistry and cheminformatics consultant, Kosan Biosciences, Hayward, CA

KEYWORDS/AREAS OF INTEREST:
Structure-activity relationships, QSAR, structure-based drug design, fragment-based drug discovery, hit-to-lead optimization, docking, virtual screening, calculation of protein-ligand binding free energies, library design for parallel and combinatorial synthesis, *de novo* design of ligands to fit a site of known structure, application of computer modeling and experimental design to therapeutic discovery projects, chemical informatics, genetic algorithms, distance geometry, 3D-pharmacophore searching, chemical similarity, and datamining methodology.

PROFESSIONAL ACTIVITIES

2000-2002 Led integration of Combichem (San Diego) computational group and technology into DuPont Pharmaceuticals, following purchase of Combichem by DuPont Pharmaceuticals. Initiated and led project to port entire legacy Combichem software from Windows/NT to Linux, resulting in more robust software that runs on both platforms. Integrated structure-based drug design methods into previously developed Combichem/DuPont Pharma ligand-based drug design software and oversaw their

application to lead discovery projects. Initiated project to develop new subshape matching algorithm for use in 3D-pharmacophore and structure-based design approaches; resulted in successful application to therapeutic target projects and patent application.

2002- Initiated SGX' approach to lead discovery, focusing on a pragmatic approach for fragment screening library design and a computational approach for rank-ordering compounds from virtual libraries for automated parallel synthesis. Lead Computational Chemistry group to develop continuum solvation modification to MM/PBSA free energy calculation which reduced cpu time by 20-fold, while producing similar results. Lead joint team of computational and medicinal chemists to design a ~1500 compound fragment screening library which has provided a 1-5% hit rate on all targets pursued to date in multiple protein families. These hits provided starting points for lead optimization in the majority of SGX projects. Initiated, developed, and led SGX' drug discovery informatics (including comprehensive compound registration, sample request system, sample tracking, biochemical and cell-based assay results, chemical structure searching, datamining approaches, etc.) with combination of commercial and in-house developed software, internal staff, and consultants. I also headed the computational chemistry and crystallography groups and lead their direct participation in SGX' multidisciplinary drug discovery project teams. I provide general scientific oversight and leadership to each of our drug discovery project teams, plus occasional direct computational and datamining project support. I was also responsible for presenting the company's technology and hit-to-lead discovery approach at international scientific conferences and at multiple pharma and biotech companies in the USA, Europe, and Japan.

2007- Joined Genentech to head computational chemistry and cheminformatics, plus help start fragment-based discovery operations. I've been responsible for defining the roles for four open positions, recruiting and filling these positions, reorganizing both groups, integrating them more closely into therapeutic project teams, and providing general strategic and scientific guidance for several fragment-based and early leads phase projects. Our first fragment-based discovery went from a weak fragment hit to a low nM compound with cellular activity in less than 6 months. I helped introduce many new software packages to bring physicochemical property calculations and desktop structure-based design to medicinal chemists and other non-specialist scientists. These are now used by the majority of our ~80 chemists and have become a routine part of compound design. I also introduced new software to provide in-house chemistry inventory management, comprehensive searching including a database of ~8 million commercially available chemicals, and streamlined purchasing of commercial compounds. I also help lead our Research IT organization.

PROFESSIONAL ORGANIZATIONS
Memberships
1977-2010, American Chemical Society

SERVICE TO PROFESSIONAL PUBLICATIONS:
Editorial Boards, J. Comp-Aided Mol Design, J. Mol. Graphics, Drug Design and

Discovery (3-5 year periods for each during late 1990s-2001)
Ad hoc referee for J. Med. Chem., J. Chem. Inf. Modeling, miscellaneous others (~5 papers/yr)
ChemMedChem, member Editorial Board through 2009

INVITED PRESENTATIONS
INTERNATIONAL
XVIIth International Symposium on Medicinal Chemistry, Barcelona, Spain, 2002.
SMI Drug Design Conference, London, England, 2003.
SMI Drug Design Conference, London, England, 2004.
World Molecular Engineering Network, Cabo San Lucas, Mexico, 2004.
British Crystallographic Association, Loughborough, England, 2005.
Keystone Symposium, Whistler, BC, 2006.
Merging Chemical and Biological Space, Marburg, Germany, 2007.
Fragment-Based Discovery, York, UK 2009.
Keystone Conference on Computer-Aided Drug Design and New Directions in Small Molecule Drug Discovery, Whistler, CA Apr 2010
UCSF/Scripps Conference, San Jose Del Cabo, MX 2010

NATIONAL
American Chemical Society National Meeting, New York City, 2003.
BIO, New York City, 2003.
SIAM Conference on Life Sciences, Portland, OR, 2004.
Society for Biomolecular Screening National Meeting, Orlando, FL, 2004.
IBC Drug Discovery Technology Symposium, Boston, 2006.
Sanibel Symposium, St. Simons Island, Georgia, 2007.
Roche PPI "BARN" Conference, Cold Spring Harbor, NY, 2009.
Open Eye CUP User Group Meeting, Santa Fe, NM 2010.
American Chemical Society National Meeting, San Diego, 2012.

REGIONAL AND OTHER INVITED PRESENTATIONS
2003 UCSF, Prof. Tack Kuntz' retirement symposium.

CORPORATE PRESENTATIONS
2002-2007 Over 50 seminars presented at pharma/biotech companies in USA, Europe, and Japan.

GOVERNMENT and OTHER PROFESSIONAL SERVICE:
2004 NIH P01 Project Review Team Member, Washington, D.C.
1986-2010 Member of UCSF NIH Program Project Advisory board for Research Resource for Biocomputing, Visualization, and Informatics
2006-2007 NAGMS (NIH) Advisory Committee for 'Drug Docking & Screening Data Resource'
1994-2010 Adjunct Prof., UCSF Dept. Pharmaceutical Chemistry

RESEARCH AND CREATIVE ACTIVITIES

PEER REVIEWED PUBLICATIONS:

1. Buchanan, S. G. *et al.* SGX523 is an exquisitely selective, ATP-competitive inhibitor of the MET receptor tyrosine kinase with antitumor activity in vivo. *Mol Cancer Ther* **8**, 3181–3190 (2009).
2. Antonysamy, S.S.; Aubol, B.; Blaney, J.; Browner, M.F.; Giannetti, A.M; Harris, S.F.; Hébert, N.; Hendle, J.; Hopkins, S.; Jefferson, E.; Kissinger, C.; Leveque, V.; Marciano, D.; McGee, E.; Nájera, I.; Nolan, B.; Tomimoto, M.; Torres, E.; Wright, T. "Fragment-based discovery of hepatitis C virus NS5b RNA polymerase inhibitors", *Bioorg. Medchem. Lett.* **2008,** 18, 2990-2995.
3. Eksterowicz, John E.; Evensen, Erik; Lemmen, Christian; Patrick Brady, G.; Kevin Lanctot, J.; Bradley, Erin K.; Saiah, Eddine; Robinson, Leslie A.; Grootenhuis, Peter D. J.; Blaney, Jeffrey M.. "Coupling structure-based design with combinatorial chemistry: application of active site derived pharmacophores with informative library design." *Journal of Molecular Graphics & Modelling* **2002**, 20, 469-477.
4. Mullenbach G T; Chiu C Y; Gyenes A; Blaney J; Rosenberg S; Marlowe C K; Brown S; Stratton-Thomas J; Montelione G T; George-Nascimento C; Stauber G "Modification of a receptor-binding surface of epidermal growth factor (EGF): analogs with enhanced receptor affinity at low pH or at neutrality", *Protein Engineering* **1998**, 11, 473-80.
5. Martin, E. J., Critchlow, R. E., Spellmeyer, D. C., Rosenberg, S., Spear, K. L., Blaney, J. M. "Diverse Approaches to Combinatorial Library Design", in *Pharmacochemistry Library*; Vol. 29; Elsevier: Amsterdam, **1998**; 133-146.
6. Spellmeyer, D. C., Wong, A. K., Bower, M. J., Blaney, J. M. "Conformational Analysis Using Distance Geometry Methods", *J. Mol. Graph.Modell.* **1997,** 15, 18-36.
7. Bradley, Erin K.; Kerr, Janice M.; Richter, Lutz S.; Figliozzi, Gianine M.; Goff, Dane A.; Zuckermann, Ronald N.; Spellmeyer, David C.; Blaney, Jeffrey M.. "NMR structural characterization of oligo-N-substituted glycine lead compounds from a combinatorial library", *Mol. Diversity* **1997**, *3*, 1-15.
8. Siani, M. A., Weininger, D., James, C. A., Blaney, J. M. "CHORTLES: A Method for Representing Oligomeric and Template-Based Mixtures", *Journal of Chemical Information and Computer Sciences* **1995,** *35,* 1026-1033.
9. Martin, E. J., Blaney, J. M., Siani, M. A., Spellmeyer, D. C., Wong, A. K., Moos, W. H. "Measuring Diversity: Experimental Design of Combinatorial Libraries for Drug Discovery", *J. Med. Chem.* **1995,** *38,* 1431-1436.
10. Moos, W. H., Banville, S. C., Blaney, J. M., Bradley, E. K., Braeckman, R. A., Bray, A. M., Brown, E. G., Desai, M. C., Dollinger, G. D., Doyle, M. V., Gibbons, J. A., Goff, D. A., Goodson, R. J., Huebner, V. D., Jonson, D. E., Kaufman, S. E., McGuire, L. A., Maeji, N. J., Martin, E. J., Min, H. Y., Ng, S., Nuss, J. M., Richter, L. S., Rosenberg, S., Shoemaker, K. R., Spear, K. L., Spellmeyer, D. C., Stauber, G. B., Stratton-Thomas, J. R., Wang, L., Winter, J., Wolfgang, G. H. I., Wong, A. K., Yamamoto, R., Zimmerman, R. J., Zuckermann, R. N. "An integrated approach to exploiting molecular diversity", *Medicinal Chemistry: Today and Tomorrow* **1995,** 137-142.
11. Siani, M. A., Weininger, D., Blaney, J. M. "CHUCKLES: A Method for Representing and Searching Peptide and Peptoid Sequences on Both Monomer and Atomic Levels", *J. Chem. Inf. Comput. Sci.* **1994,** *34,* 588-593.

12. Simon, R. J., Martin, E. J., Miller, S. M., Zuckermann, R. N., Blaney, J. M., Moos, W. H. "Using Peptoid Libraries (Oligo N-Substituted Glycines) for Drug Discovery", in *Techniques in Protein Chemistry*; Vol. 5; Crabb, J. W., Ed.; Academic Press, Inc.: San Diego, **1994**.
13. Bach, A. C., II, Pottorf, R. S., Blaney, J. M., De Lucca, G. V., Ripka, W. C. "Gramicidin S: A general model for β-turn mimics?", in *Peptides: Chemistry and Biology. Proceedings of the 13th American Peptide Symposium.*; Vol. 13; Hodges, R. S., Smith, J. A., Ed.; ESCOM: Leiden, **1994**; 284-286.
14. Blaney, J. M., Dixon, J. S. "A good ligand is hard to find: Automated docking methods", *Persp. Drug Disc. Design* **1993,** *1,* 301-319.
15. Meng, E. C., Gschwend, D. A., Blaney, J. M., Kuntz, I. D. "Orientational Sampling and Rigid-Body Minimization in Molecular Docking", *Proteins* **1993,** *17,* 266-278.
16. Ripka, W. C.; De Lucca, G. V.; Bach, A. C., II; Pottorf, R. S.; Blaney, J. M.. "Protein β-turn mimetics. II. Design, synthesis, and evaluation in the cyclic peptide gramicidin S" *Tetrahedron* **1993**, *49*, 3609-28.
17. Ripka, W. C., Lucca, G. V. D., II, A. C. B., Pottorf, R. S., Blaney, J. M. "Protein β-Turn Mimetics I. Design, Synthesis, and Evaluation in Model Cyclic Peptides.", *Tetrahedron* **1993,** *49,* 3593-3608.
18. Siani, M. A., Marlowe, C. K., Bradley, E. K., Blaney, J. M. "Broccoli: A Systematic Method for Designing Conformationally Constrained Mimics of a Proposed Protein Binding Site", *9th European Symposium on Structure-Activity Relationships: QSAR and Molecular Modelling* **1992,** Strasbourg, France.
19. Cohen, N. C., Blaney, J. M., Humblet, C., Gund, P., Barry, D. C. "Molecular Modeling Software and Methods for Medicinal Chemistry", *J. Med. Chem.* **1990,** *33,* 883-894.
20. Lautz, J., Kessler, H., Blaney, J. M., Scheek, R. M., van Gunsteren, W. F. "Calculating Three-Dimensional Molecular Structure from Atom-Atom Distance Information: Cyclosporin A", *Int. J. Peptide Protein Res.* **1989,** *33,* 281-288.
21. Gund, P., Barry, D. C., Blaney, J. M., Cohen, N. C. "Guidelines for Publications in Molecular Modeling Related to Medicinal Chemistry", *J. Med. Chem.* **1988,** *31,* 2230-2234.
22. Ripka, W. C., Sipio, W. J., Blaney, J. M. "Molecular Modeling and Drug Design: Strategies in the Design and Synthesis of Phospholipase A_2 Inhibitors", *Lectures in Heterocyclic Chemistry* **1987,** *IX,* S95-S104.
23. Kollman, P., Blaney, J. "Simulation of protein-ligand interactions using computer graphics, model building and molecular mechanics: thyroid hormone analogue binding to prealbumin", in *Molecular Graphics and Drug Design*; Vol. 3; Burgen, A. S. V., Roberts, G. C. K., Tute, M. S., Ed.; Elsevier: New York, **1986**; 285-305.
24. Oatley, S. J., Blaney, J. M., Langridge, R., Kollman, P. A. "Molecular Mechanical Studies of Hormone-Protein Interactions: The Interaction of T4 and T3 with Prealbumin", *Biopolymers* **1984,** *23,* 2931.
25. Carotti, A., Hansch, C., Mueller, M. M., Blaney, J. M. "Actinidin Hydrolysis of Substituted-Phenyl Hippurates: A Quantitative Structure-Activity Relationship and Graphics Comparison with Hydrolysis by Papain", *J. Med. Chem.* **1984,** *27,* 1401-1405.
26. Carotti, A., Smith, R. N., Wong, S., Hansch, C., Blaney, J. M., Langridge, R. "Papain Hydrolysis of X-Phenyl-N-Methanesulfonyl Glycinates: A Quantitative Structure-Activity Relationship and Molecular Graphics Analysis", *Arch. Biochem. Biophys.* **1984,** *229,* 112-125.
27. Hansch, C., Hathaway, B. A., Guo, Z., Selassie, C. D., Dietrich, S. W., Blaney, J. M., Langridge, R., Volz, K. W., Kaufman, B. T. "Crystallography, Quantitative Structure-Activity Relationships, and Molecular Graphics in a Comparative Analysis of the Inhibition of Dihydrofolate Reductase from Chicken Liver and Lactobacillus casei by 4, 6-diamino-1, 2-dihydro-2, 2-dimethyl-1-(substituted-phenyl)-s-triazines", *J. Med. Chem.* **1984,** *27,* 129.

28. Havel, T. F., Crippen, G. M., Kuntz, I. D., Blaney, J. M. "The Combinatorial Distance Geometry Method for the Calculation of Molecular Conformation. II. Sample Problems and Computational Statistics", *J. Theor. Biol.* **1983,** *104,* 383.
29. Wipff, G., Dearing, A., Weiner, P. K., Blaney, J. M., Kollman, P. A. "Molecular Mechanics Studies of Enzyme-Substrate Interactions: The Interaction of L- and D-N-acetyltryptophanamide with a-chymotrypsin", *J. Am. Chem. Soc.* **1983,** *105,* 997.
30. Li, R., Hansch, C., Matthews, D., Blaney, J. M., Langridge, R., Delcamp, T. J., Susten, S. S., Freisheim, J. H. "A Comparison by QSAR, Crystallography, and Computer Graphics of the Inhibition of various Dihydrofolate Reductases by 5-(X-benzyl)-2, 4-diaminopyrimidines", *Quant. Struct.-Act. Relat. Pharmacol. Chem. Biol.* **1982,** *1,* 1.
31. Kuntz, I. D., Blaney, J. M., Oatley, S. J., Langridge, R., Ferrin, T. E. "A Geometric Approach to Macromolecule-Ligand Interactions", *J. Mol. Biol.* **1982,** *161,* 269-288.
32. Blaney, J. M., Weiner, P. K., Dearing, A., Kollman, P. A., Jorgensen, E. C., Oatley, S. J., Burridge, J. M., Blake, C. C. F. "Molecular Mechanics Simulation of Protein-Ligand Interactions: Binding of Thyroid Hormone Analogs to Prealbumin", *J. Am. Chem. Soc.* **1982,** *104,* 6424.
33. Weiner, P. K., Langridge, R., Blaney, J. M., Schaefer, R., Kollman, P. A. "Electrostatic Potential Molecular Surfaces", *Proc. Natl. Acad. Sci. USA* **1982,** *79,* 3754.
34. Blaney, J. M., Jorgensen, E. C., Connolly, M. L., Ferrin, T. E., Langridge, R., Oatley, S. J., Burridge, J. M., Blake, C. C. F. "Computer Graphics in Drug Design: Molecular Modeling of Thyroid Hormone-Prealbumin Interactions", *J. Med. Chem.* **1982,** *25,* 785-790.
35. Hansch, C., Li, R., Blaney, J. M., Langridge, R. "Comparison of the Inhibition of Escherichia coli and Lactobacillus casei Dihydrofolate Reductase by 2, 4-diamino-5-(substituted-benzyl)pyrimidines: Quantitative Structure-Activity Relationships, X-Ray Crystallography, and Computer Graphics in Structure-Activity Analysis", *J. Med. Chem.* **1982,** *25,* 777.
36. Smith, R. N., Hansch, C., Kim, K. H., Omiya, B., Fukumura, G., Selassie, C. D., Jow, P. Y. C., Blaney, J. M., Langridge, R. "The Use of Crystallography, Graphics, and Quantitative Structure-Activity Relationships in the Analysis of the Papain Hydrolysis of X-phenylhippurates", *Arch. Biochem. Biophys.* **1982,** *215,* 319.
37. Dietrich, S. W., Blaney, J. M., Reynolds, M. A., Jow, P. Y. C., Hansch, C. "Quantitative Structure-Selectivity Relationships. Comparison of the Inhibition of Escherichia coli and Bovine Liver Dihydrofolate Reductase by 5-(Substituted-benzyl)-2, 4-diaminopyrimidines", *J. Med. Chem.* **1980,** *23,* 1205.
38. Blaney, J. M., Dietrich, S. W., Reynolds, M. A., Hansch, C. "Quantitative Structure-Activity Relationship of 5-(X-Benzyl)-2, 4-diaminopyrimidines Inhibiting Bovine Liver Dihydrofolate Reductase", *J. Med. Chem.* **1979,** *22,* 614.
39. Steinmetz, W. E., Pollard, J. E., Blaney, J. M., Winker, B. K., Mun, I. K., Hickernell, F. J., Hollenberg, S. J. "Conformational Analysis of Conjugated Polyenes by Nuclear Magnetic Resonance and Low Resolution Microwave Spectroscopy", *J. Phys. Chem.* **1979,** *83,* 1540.

NON-PEER REVIEWED PUBLICATIONS AND OTHER CREATIVE ACTIVITIES:

Review Articles

1. Blaney, J. A very short history of structure-based design: how did we get here and where do we need to go? *J Comput Aided Mol Des* **26**, 13–14 (2012).
2. Blaney, J. M., Martin, E. J. "Computational Approaches for combinatorial library design and molecular diversity analysis", *Curr. Opin. Chem. Biol.* **1997,** *1,* 54-59.

3. Blaney, J. M., Dixon, J. S. "Receptor Modeling by Distance Geometry", in *Ann. Rept. Med. Chem.*; Vol. 26; Bristol, J. A., Ed.; Academic Press: New York, **1991**; 281-285.
4. Blaney, J. M., Hansch, C., Silipo, C., Vittoria, A. "Structure-Activity Relationships of Dihydrofolate Reductase Inhibitors", *Chem. Rev.* **1984,** *84,* 333.

Books and Chapters

1. Blaney, Jeff; Nienaber, Vicki; Burley, Stephen K. "Fragment-Based Lead Discovery and Optimization Using X-Ray Crystallography, Computational Chemistry, and High-Throughput Organic Synthesis" in *Fragment-based Approaches in Drug Discovery*, Jahnke, W., Erlanson, D., Ed., Wiley-VCH, Weinheim, Germany, **2006**; 215-248.
2. Oprea, Tudor I.; Blaney, Jeffrey M. "Cheminformatics approaches to fragment-based lead discovery" in *Fragment-based Approaches in Drug Discovery*, Jahnke, W., Erlanson, D., Ed., Wiley-VCH, Weinheim, Germany, **2006**; 91-110.
3. Truhlar, Donald G.; Howe, W. Jeffrey; Hopfinger, Anthony J.; Blaney, Jeff; Dammkoehler, Richard A. "Rational Drug Design" in: IMA Vol. Math. Its Appl., 1999; 108.
4. Dixon, J. S., Blaney, J. M. "Docking: Predicting the Structure and Binding Affinity of Ligand-Receptor Complexes", in *Designing Bioactive Molecules: Three-Dimensional Techniques and Applications*; Martin, Y. C., Willett, P., Ed.; American Chemical Society: Washington, D.C., **1998**; 175-197.
5. Martin, E. J., Spellmeyer, D. C., Roger E. Critchlow, J., Blaney, J. M. "Does Combinatorial Chemistry Obviate Computer-Aided Drug Design?", in *Reviews in Computational Chemistry*; Vol. 10; Lipkowitz, K. B., Boyd, D. B., Ed.; VCH Publishers: New York, NY, **1997**; 75-100.
6. Spellmeyer, D. C., Blaney, J. M., Martin, E. M. "Computational Approaches to Chemical Libraries", in *Practical Application of Computer-Aided Drug Design*; Charifson, P. S., Ed.; Marcel Dekker, Inc.: NY, **1997**; 165-193.
7. Blaney, J. M., Dixon, J. S. "Distance Geometry in Molecular Modeling", in *Reviews in Computational Chemistry*; Vol. 5; Lipkowitz, K. B., Boyd, D. B., Ed.; VCH: New York, **1994**; 299-335.
8. Ripka, W. C., Blaney, J. M. "Computer Graphics and Molecular Modeling in the Analysis of Synthetic Targets", in *Topics in Stereochemistry*; Vol. 20; Eliel, E. L., Wilen, S. H., Ed.; Wiley: New York, **1991**; 1-85.
9. Blaney, J. M., Hansch, C. "The Application of Molecular Graphics to the Analysis of Macromolecular Structures", in *Comprehensive Medicinal Chemistry: The Rational Design, Mechanistic Study and Therapeutic Application of Chemical Compounds*; Vol. 4; Ramsden, C., Ed.; Pergamon Press: Oxford, **1990**; 459-489.
10. Hansch, C., Blaney, J. M. "The New Look to QSAR", in *Drug Design: Fact or Fantasy?*; Jolles, G., Wooldridge, K. R. H., Ed.; Academic Press: New York, **1984**; 185-208.

Other Publications

PATENTS ISSUED OR PENDING (ALLOWED)

1. Blaney, J.M., Cohen, F. "Method and compositions for increasing the serum half-life of pharmacologically active agents by binding to transthyretin-selective ligands", **1998,** US5714142.
2. Wernette-Hammond, Mary Ellen; Shyamala, Venkatakrishna; Siani, Michael; Blaney, Jeff; Tekamp Olson, Patrica. "Polypeptides with interleukin-8 receptor-binding properties", PCT Int. Appl. **1997**, 39 pp. CODEN: PIXXD2 WO 9700601
3. Wernette-Hammond, Mary Ellen; Shyamala, Venkatakrishna; Siani, Michael; Blaney, Jeff; Tekamp-Olson, Patricia. "Interleukin-8 receptor-binding compounds", PCT Int. Appl. **1997**, 38 pp. CODEN: PIXXD2 WO 9700893

4. Blaney, J.M., Siani, M.A. “Method and apparatus for mimicking protein active sites”, **1997,** US5680331.
5. Mullenbach, G.T., Blaney, J.M., Rosenberg, S. “Muteins of human epidermal growth factor exhibiting enhanced binding at low PH”, **1996,** US5547935.
6. Kompis, Ivan; Blaney, Jeffrey M.; Marlow, Charles K. “Specific inhibition of Pneumocystis carinii dihydrofolate reductase and antifungal pyrimidine-derived compounds”, PCT Int. Appl. **1992**, 23 pp. CODEN: PIXXD2 WO 9208461.

OTHER CREATIVE ACTIVITIES

Computer Programs

1. Blaney, J. M., Crippen, G. M., Dearing, A., Dixon, J. S. *DGEOM, #590*, Quantum Chemistry Program Exchange, Indiana University: Bloomington, **1990**.
2. Blaney, J.M., Dixon, J.S., DOCKIT, Metaphorics, Santa Fe, NM, **2002**. (Commercial software product for protein-ligand docking in drug discovery)

RESEARCH PROGRAM (SEPARATE SUMMARY)

My major research focus during 2002-2007 was to lead the development of fragment-based lead discovery at SGX. The approach combined high-throughput X-ray crystallographic screening of a fragment library of approximately 1500 small molecules to identify weak hits (IC50 = 10uM -- 10mM) bound at a specific active or allosteric site on a target enzyme, computational chemistry to select 50-100 members from 10,000 -- 20,000 compound virtual libraries of analogs of the fragment hits, parallel synthesis and purification of ~5-50 compounds per library, followed by biochemical assay for all library members and cocrystal structure determination of selected active compounds. This has continued since coming to Genentech in Oct 2007. My specific research interests include: improvement and application of computational approaches for predicting the free energy of binding of ligands to proteins, development of improved interactive medicinal chemistry-driven SBDD tools, criteria for selecting compounds for a fragment screening library, criteria for selecting fragment hits for hit-to-lead optimization, predicting fragment binding sites, analog and library design for fragment hit-to-lead optimization, new chemical informatics approaches to integrate three-dimensional X-ray cocrystal structure data with conventional drug discovery data, correlation and prediction of *in vitro/in vivo* ADMET/PK.