

CURRICULUM VITAE
WILLIAM F. DEGRADO

Created on 6/11/2013 1:05:00 PM

Home Address: 24 Joy Street
San Francisco, CA 94107

Office Address: William DeGrado
Professor, Department of Pharmaceutical Chemistry
Investigator, Cardiovascular Research Institute
University of California, San Francisco
555 Mission Bay Blvd South
San Francisco, CA 94158-9001

Education:
1973-1975 Northcentral College (Chemistry)
1975-1977 B.A. Kalamazoo College
1977-1981 Ph.D. University of Chicago (Chemistry)

Positions Held:
1981-1990 Research Chemist, DuPont, Central Research & Development Department
1990-1992 Research Leader, DuPont Merck Pharmaceutical Company, Biotechnology
1992-1994 Research Fellow, DuPont Merck Pharmaceutical Company, Structural Biology
1994-1995 Senior Director, DuPont Merck Pharmaceutical Company, Medicinal Chemistry Dept
1996-2011 Professor, Department of Biochemistry and Biophysics, UPenn School of Medicine
2003-2011 Adjunct Professor, Department of Chemistry, University of Pennsylvania
2011-Present Professor, Department of Pharmaceutical Chemistry, UCSF, Investigator, UCSF
Cardiovascular Research Institute.

Visiting Positions:
1986 Instructor: Protein Design Workshop, European Molecular Biology Laboratory, Heidelberg,
Germany.
1987 Sloan Visiting Lecturer. Department of Chemistry, Harvard University.
1987-1989 Adjunct Professor, Department of Biophysics, Johns Hopkins Medical School.
1991 Visiting Professor City University of New York
1991-1996 Adjunct Professor, Department of Biochemistry and Biophysics, University of Pennsylvania.
1994 Wellcome Visiting Professor, Louisiana State University.
2010-2011 University of California, San Francisco

Awards:
1988 Du Vigneaud Award for Young Investigators in Peptide Research.
1989 Protein Society Young Investigator Award.
1992 Eli Lilly Award in Biological Chemistry.
1993 DuPont Merck Summit Award
1995 Fellow, American Association for the Advancement of Science
1998 Fellow, AAAS
1999 Member, National Academy of Sciences (U.S.A.)
2003 Merrifield Award, Peptide Society
2008 Ralph F. Hirschmann Award in Peptide Chemistry (American Chemical Society)
2009 Makineni Award (APS)

Professional Activities:
Protein Society (Program Committee, 3rd American Protein Society, various awards
committees)
1990- Peptide Society (Council 1996-98), Publications Committee 1990-)
1990- ACS (various awards committees, 1990 - ; Search Committee for Editor of Biochemistry)
1991 Organizer, Keystone Meeting on Protein Structure, Folding, and Design
Gordon Research Conference, Council at large

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

1997-2001 Member, Bioorganic Study Section, NIH
2000-2001 President Elect, Protein Society
2001-2003 President, Protein Society

Editorial positions:

1986-1990 Associate editor, *Proteins: Structure, Function, Genetics*.
1998-2000 Associate editor, *Journal of Peptide Research*

Editorial Boards:

1990-2008 Proteins, Structure, Function, Genetics
1988-1995 Journal of the American Chemical Society
1988-2001 Journal of Molecular Recognition
1989-1998 International Journal of Peptide and Protein Research
1998- Journal of Peptide Research
1989- Protein Engineering
1990-1995 Protein Science, Journal of the Protein Society
1994-1997 Biochemistry
1994-1998 Protein and Peptide Letters
1999- Accounts of Chemical Research
1998-2002 Journal of Combinatorial Chemistry
1999- Current Opinion in Chemical Biology
1989 Guest Editor, Emil T. Kaiser Memorial Issue of Biopolymers.
1989 Associate Editor, "Current Research in Protein Chemistry"
1993,95,97,99, 01, 03, 05, 09, 11 Guest Editor "Current Opinion in Structural Biology" (volume on protein engineering)
1999 Guest Editor, Chemical Reviews
2006 Chemical Biology & Drug Design

Bibliography

1. **DeGrado WF** and Kaiser, E. T (1980) Polymer-Bound Oxime Esters as Supports for Solid-Phase Peptide Synthesis. Preparation of Protected Peptide Fragments. *J. Org Chem.* 45, 1295.
2. Bramson, H. N., Thomas, N., **DeGrado WF**, and Kaiser, E. T (1980) Development of a Convenient Spectrophotometric Assay for Peptide Phosphorylation Catalyzed by Adenosine 3', 5' - Monophosphate Dependent Protein Kinase. *J. Amer. Chem. Soc.* 102, 7156.
3. **DeGrado WF**, Kèzdy, F. J., and Kaiser, E. T (1981) Design, Synthesis, and Characterization of a Cytotoxic Peptide with Melittin-Like Activity". *J. Amer. Chem. Soc.* 103, 679.
4. **DeGrado WF**, Musso, G. F., Lieber, M., Kaiser, E. T., and Kèzdy, F. J (1981) Kinetics and Mechanism of Hemolysis Induced by Melittin and a Synthetic Melittin Analogue. *Biophys. J.* 37, 329.
5. **DeGrado WF** and Kaiser, E. T (1982) Solid Phase Synthesis of Protected Peptides on a Polymer-Bound Oxime: Preparation of Segments Comprising the Sequence of a Cytotoxic 26-Peptide. *J. Org. Chem.* 47, 3258.
6. **DeGrado WF**, Wasserman, Z. R. & Chowdhry, V (1982) Sequence and structural homologies among type I and type II interferons. *Nature* 300, 379-81.
7. **DeGrado WF** (1983) "Solution Phase Synthesis of Cecropin A 1-22 and Potent Analogues Thereof", in *Peptides: Structure and Function* (eds. V. J. Hruby and D. H. Rich), 195.
8. Robb, R. J., Kutny, R. M., Panico, M., Morris, H., **DeGrado WF** & Chowdhry, V (1983) Posttranslational modification of human T-cell growth factor. *Biochem Biophys Res Commun* 116, 1049-55.
9. Chow, T. P., **DeGrado WF** & Knight, E., Jr (1984) Antibodies to synthetic peptides of human interferon-beta. Use in biosynthetic studies. *J Biol Chem* 259, 12220-5.
10. Persson, H., Hennighausen, L., Taub, R., DeGrado, W. & Leder, P (1984) Antibodies to human c-myc oncogene product: evidence of an evolutionarily conserved protein induced during cell proliferation. *Science* 225, 687-93.

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

11. Sigal, I. S., **DeGrado WF**, Thomas, B. J. & Petteway, S. R., Jr (1984) Purification and properties of thiol beta-lactamase. A mutant of pBR322 beta-lactamase in which the active site serine has been replaced with cysteine. *J Biol Chem* 259, 5327-32.
12. Briggs, M. S., Gierasch, L. M., Zlotnick, A., Lear, J. D. & **DeGrado WF** (1985) In vivo function and membrane binding properties are correlated for Escherichia coli lamB signal peptides. *Science* 228, 1096-9.
13. Cox, J. A., Comte, M., Fitton, J. E. & **DeGrado WF** (1985) The interaction of calmodulin with amphiphilic peptides. *J Biol Chem* 260, 2527-34.
14. O'Neil, K. T. and **DeGrado WF** (1985) "A Predicted Structure of Calmodulin Suggests an Electrostatic Basis for its Function". *Proc. Natl. Acad. Sci. USA* 82, 4954.
15. **DeGrado WF**, Prendergast, F. G., Wolfe, H. R., Jr., and Cox, J. A (1985) The Design, Synthesis, and Characterization of Tight-Binding Inhibitors of Calmodulin. *J. Cell. Biochem.* 29, 83.
16. **DeGrado WF** and Lear, J. D (1985) Induction of Peptide Conformation at Apolar/Water Interfaces I: A Study with Model Peptides of Defined Hydrophobic Periodicity. *J. Amer. Chem. Soc.* 107, 7684.
17. **DeGrado WF**, Erickson-Viitanen, S., and O'Neil, K. T (1985) Theoretical and Experimental Approaches to the Design of Calmodulin-Binding Peptides, in *Protein Engineering* Chapter 18 (F. Fox and D. Oxender eds.).
18. **DeGrado WF**, O'Neil, K. T., and Erickson-Viitanen, S (1986) Synthetic and Computer Modeling of Calmodulin-Protein Interactions. In *Current Communications in Molecular Biology, Cold Spring Harbor Laboratory*.
19. Kauer, J. C., Viitanen, S., and **DeGrado WF** (1986) p-Benzoyl-phenylalanine, A New Photoprobe That Can Readily Be Incorporated into Synthetic Peptides: Applications to Calmodulin Binding Peptides. *J. Biol. Chem.* 261, 10695.
20. Cheng, Y. E., Becker, M. F., Nguyen, P. D., **DeGrado WF**, and Jonak, G. J (1986) Nonidentical Induction of the Guanylate-Binding Protein and the 56 K Protein by Type-I and Type-II Interferons. *J. Interferon Res.* 6, 417.
21. Eisenberg, D., Wilcox, W., Eshita, S. M., Pryciak, P. M., Ho, S. P., and **DeGrado WF** (1986) The Design Synthesis and Crystallization of an A -Helical Peptide. *Proteins* 1, 16.
22. Erickson-Viitanen S., and DeGrado, W. F (1987) The Interaction of Calmodulin with Amphiphilic Peptides". *Methods in Enzymology* 139, 455.
23. Lear, J. D. & **DeGrado WF** (1987) Membrane binding and conformational properties of peptides representing the NH2 terminus of influenza HA-2. *J Biol Chem* 262, 6500-5.
24. **DeGrado WF**, Regan, L. & Ho, S. P (1987) The design of a four-helix bundle protein. *Cold Spring Harb Symp Quant Biol* 52, 521-6.
25. **DeGrado WF**, Erickson-Viitanen, S., Wolfe, H. R., Jr. & O'Neil, K. T (1987) Predicted calmodulin-binding sequence in the gamma subunit of phosphorylase b kinase. *Proteins* 2, 20-33.
26. Erickson-Viitanen, S. & **DeGrado WF** (1987) Recognition and characterization of calmodulin-binding sequences in peptides and proteins. *Methods Enzymol* 139, 455-78.
27. O'Neil, K. T., Wolfe, H. R., Jr., Erickson-Viitanen, S. & **DeGrado WF** (1987) Fluorescence properties of calmodulin-binding peptides reflect alpha-helical periodicity. *Science* 236, 1454-6.
28. **DeGrado WF** (1988) Design of peptides and proteins. *Adv Protein Chem* 39, 51-124.
29. Lear, J. D., Wasserman, Z. R. & **DeGrado WF** (1988) Synthetic amphiphilic peptide models for protein ion channels. *Science* 240, 1177-81.
30. Regan, L. & **DeGrado WF** (1988) Characterization of a helical protein designed from first principles. *Science* 241, 976-8.

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

31. Regan, L., Ho, S. P., Wasserman, Z., and **DeGrado WF**: "De Novo Design of Helical Proteins." in *The Protein Folding Problem* (J. King and L. Gierasch eds.) based on symposia at the AAAS Annual Meetings 1988 and 1989.
32. Rockwell, A. L., Lear, J. D., and **DeGrado WF** (1989) Minimally Designed Ion Channels. *Proceedings of the Eleventh American Peptide Symposium*.
33. **DeGrado WF**, Wasserman, Z. R. & Lear, J. D (1989) Protein design, a minimalist approach. *Science* 243, 622-8.
34. O'Neil, K. T., Erickson-Viitanen, S. & **DeGrado WF** (1989) Photolabeling of calmodulin with basic, amphiphilic alpha-helical peptides containing p-benzoylphenylalanine. *J Biol Chem* 264, 14571-8.
35. O'Neil, K. T. and **DeGrado WF** (1989) Photolabeling and Fluorescence Studies of Peptide/Calmodulin Complexes; Evidence for Bending of Calmodulin's Central Helix. *Proteins* 6, 284-293.
36. **DeGrado WF** and O'Neil, K. T (1990) How Calmodulin Binds its Targets: Sequence Independent Recognition of Amphiphilic α -helices. *Trends in Biochem. Sci.* 15, 59-64.
37. **DeGrado WF** & Lear, J. D (1990) Conformationally constrained alpha-helical peptide models for protein ion channels. *Biopolymers* 29, 205-13.
38. Rafalski, M., Lear, J. D. & **DeGrado WF** (1990) Phospholipid interactions of synthetic peptides representing the N-terminus of HIV gp41. *Biochemistry* 29, 7917-22.
39. Hill, C. P., Anderson, D. H., Wesson, M., **DeGrado WF**, and Eisenberg, D (1990) Crystal Structure of 1, Implications for Protein Design. *Science* 249, 543.
40. O'Neil, K. T. and **DeGrado WF** (1990) Thermodynamic Parameters for Helix Formation for the Twenty Commonly-Occurring Amino Acids. *Science* 250, 646 .
41. O'Neil, K. T., Hoess, R., and **DeGrado WF** (1990) Design of DNA-Binding Peptides Based on the Leucine Zipper Motif. *Science* 249, 774.
42. Handel, T. and **DeGrado WF** (1990) De Novo Design of a Zn²⁺-Binding Protein *J. Amer. Chem. Soc.* 112, 6710.
43. O'Neil, K. T., Shuman, J. D., Ampe, C., and **DeGrado WF** (1991) DNA-induced increase in the α -helical content of C/EBP and GCN4. *Biochemistry* 30, 9030-9034.
44. Rockwell, A. L., O'Neil, K. T., and **DeGrado WF** (1991) Stabilities of coiled coil dimers as a model for leucine zippers. *Proceedings of the Twelfth American Peptide Symposium*.
45. Live, D., Osterhout, J. J., Jr., Hoch, J. C., Handel, T. and **DeGrado WF** (1991) in *Proceedings of the Twelfth American Peptide Symposium*.
46. **DeGrado WF**, Raleigh, D. P., Handel, T (1991) De Novo protein design: what are we learning?" *Current Opinion in Structural Biology* 1, 984-993.
47. Rafalski, M., Ortiz, A., Rockwell, A., van Ginkel, L. C., Lear, J. D., **DeGrado WF** & Wilschut, J (1991) Membrane fusion activity of the influenza virus hemagglutinin: interaction of HA2 N-terminal peptides with phospholipid vesicles. *Biochemistry* 30, 10211-20.
48. Osterhout, J. J., Jr., Handel, T., Na, G., Toumadje, Z., Long, R. C., Connolly, P. J., Hoch, J. C., Johnson, W. C., Jr., Live, D., and **DeGrado WF** (1992) Characterization of the structural properties of 1B, a peptide designed to form a four-helix bundle. *J. Amer. Chem. Soc.* 114, 331-337.
49. Eband, R. M., Cheetham, J. J., Eband, R., F., Yeagle, P. L., Richardson, C. D., and **DeGrado WF** (1992) Peptide models for the membrane-destabilizing actions of viral fusion proteins. *Biopolymers* 32, 309-314.
50. Anthony-Cahill, S. J., Benfield, P. A., Fairman, R., Wasserman, Z. R., Brenner, S. L., Stafford, W. F., 3rd, Altenbach, C., Hubbell, W. L. & **DeGrado WF** (1992) Molecular characterization of helix-loop-helix peptides. *Science* 255, 979-83.

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

51. Chung, L. A., Lear, J. D. & **DeGrado WF** (1992) Fluorescence studies of the secondary structure and orientation of a model ion channel peptide in phospholipid vesicles. *Biochemistry* 31, 6608-16.
52. Lovejoy, B., Åkerfeldt, K. S., **DeGrado WF** & Eisenberg, D (1992) Crystallization of proton channel peptides. *Protein Sci* 1, 1073-7.
53. Fairman, R., Anthony-Cahill, S. J., DeGrado, W. F (1992) The helix-forming propensity of D-Ala in a right-handed α -helix. *J. Amer. Chem. Soc.*, 114, 5458-5459.
54. O'Neil, K. T., Hoess, R. H., Jackson, S. A., Ramachandran, N., Mousa, S. A., **DeGrado WF** (1992) Identification of GPIIb/IIIa-binding peptides using a conformationally constrained phage peptide library" *Proteins*, 14, 509-515.
55. Rao, U., Teeter, M. M., Erickson-Viitanen, S. & **DeGrado WF** (1992) Calmodulin binding to alpha 1-purothionin: solution binding and modeling of the complex. *Proteins* 14, 127-38.
56. Raleigh, D. P., **DeGrado WF** (1992) A de novo designed protein shows a thermally induced transition from a native to a molten globule-like state. *J. Amer. Chem. Soc.* 114, 1079-1081.
57. Lovejoy, B., Le, T. C., Luthy, R., Cascio, D., O'Neil, K. T., **DeGrado WF** & Eisenberg, D (1992) X-ray grade crystals of a designed alpha-helical coiled coil. *Protein Sci* 1, 956-7.
58. Åkerfeldt, K., Kim, R., M., Camac, D., Groves, J. T., Lear, F. D., **DeGrado WF** (1992) Tetraphilin: a four-helix bundle proton channel built on a tetraphenylporphyrin framework. *J. Amer. Chem. Soc.* 114, 9656.
59. Åkerfeldt, K. A., Lear, J. D., Wasserman, Z. R., Chung, L., **DeGrado WF** (1993). Synthetic peptide models for protein ion channels" *Acc. Chem. Res.* 26, 191-197 .
60. Betz, S. F., Raleigh, D. P., **DeGrado WF** (1993) De novo protein design: from molten globules to native-like states. *Current Opinion in Structural Biology*, 3, 601-610.
61. **DeGrado WF**, Matthews, B. W (1993) Engineering and Design. *Current Opinion in Structural Biology*, 3, 547-548.
62. **DeGrado WF** (1993). Catalytically Active Molten Globules, *Nature* 365, 488-489.
63. Handel, T. M., Williams, S. A. & **DeGrado WF** (1993) Metal ion-dependent modulation of the dynamics of a designed protein. *Science* 261, 879-85.
64. Handel, T., Williams, S., Menyhard, D., **DeGrado WF**, (1993) Introduction of a Trp residue into α_4 as a probe of its molten globule character. *J. Amer. Chem. Soc.* 115, 4457-4460.
65. Lovejoy, B., Choe, S., Cascio, D., McRorie, D. K., **DeGrado WF**, Eisenberg, D (1993) Crystal structure of a synthetic triple-stranded leucine zipper. *Science*, 259, 1288-1293.
66. Fairman, R., Beran-Steed, R. K., Anthony-Cahill, S. J., Lear, J. D., Stafford, W. F., 3rd, **DeGrado WF**, Benfield, P. A. & Brenner, S. L (1993) Multiple oligomeric states regulate the DNA binding of helix-loop-helix peptides. *Proc Natl Acad Sci US A* 90, 10429-33.
67. O'Neil, K. T., **DeGrado WF**, Mousa, S. A., Ramachandran, N., Hoess, R., H (1994) Identification of recognition sequences of adhesion molecules using phage display technology. *Methods in Enzymology* 245, 370-385 .
68. O'Neil, K. T., **DeGrado WF**, Hoess, R. H (1994) Phage display of random peptides on a protein scaffold. *Techniques in Protein Chemistry*, 5, 517-524.
69. Lear, J. D., Wasserman, Z. R., **DeGrado WF** (1994). The use of synthetic peptides for the study of protein structure. *Membrane Protein Structure* S. White, ed., Oxford University Press.
70. Choma, C., Lear, J. D., Nelson, M. J., Dutton, P. L., Robertson, D. E., **DeGrado WF** (1994) Design of a heme-binding four-helix bundle. *J. Amer. Chem. Soc.* 116, 856-865.
71. D. E. Robertson, R. S. Farid, C. C. Moser, J. L. Urbauer, S. E. Mulholland, R. Pidikiti, J. D. Lear, A. J. Wand, W. F. DeGrado, P. L. Dutton (1994) Design and synthesis of multi-hem proteins *Nature*, 368 425-432 .

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

72. Mousa, S. A., Bozarth, J. M., Forsythe, M. S., Jackson, S. M., Leamy, A., Diemer, M. M., Kapil, R. P., Knabb, R. M., Mayo, M. C., Pierce, S. K., DeGrado, W. F., Thoolen, M. J., Reilly, T. M (1994) Antiplatelet antothrombotic efficacy of DMP728, a novel platelet GPIIb/IIIa receptor antagonist, *Circulation* 89, 1, 3-12.
73. C. Bach, C. J. Eyermann, J. D. Gross, M. J. Bower, R. L. Harlow, P. C. Weber, W. F. DeGrado (1994) Structural studies of a family of high affinity ligands for IIb/IIIa" *J. Amer. Chem. Soc.* 116, 3207-3219 .
74. Mousa, S.A., Hassell, S., Pierce, S., Lorelli, W., DeGrado, W.F., Thoolen, M., Reilly, T.M (1994) Intravenous antiplatelet efficacy and safety of the platelet GPIIb/IIIa antagonist, DMP728 in anesthetized dogs. *Thrombosis Research*, 76, 109-119.
75. Rabanal, F., **DeGrado WF**, Dutton, P. L (1994) De Novo Design of Peptide Models of Cytochromes: Towards the Synthesis of a Photosynthetic Reaction Center Maquette. *Proceedings 14th Amer. Peptide Symp.*
76. Åkerfeldt, K. S., Lear, J. D., **DeGrado WF** (1994).Synthetic peptides as models for ion channel proteins. *Proceedings of the Tanigushi Symposium, Japan.*
77. Kienker, P.K., **DeGrado, W.F.**, Lear, J.D (1994).A helical-dipole model describes the single-channel rectification of an uncharged peptide ion channel. *Proc. Nat. Acad. Sci.* 91, 4859-4863.
78. Regan, L., Rockwell, A., Wasserman, Z., **DeGrado WF** (1994) Disulfide crosslinks to probe the structure and flexibility of a designed four-helix bundle protein. *Protein Science* , 3, 2419-2427 .
79. Åkerfeldt, K. S., **DeGrado WF** (1994) Synthesis and per-functionalization of heptakis(6-O-carboxymethyl-2,3,-di-O-methyl)cyclomaltoheptaose. *Tetrahedron Letters*, 35, 4489-4492.
80. Jackson, S. A., **DeGrado WF**, Harlow, R., Dwivedi, A., Parthasarathy, A., Higley, A., Krywko, J., Rockwell, A., Markwalder, J., Wells, G., Wexler, R., Mousa, S (1994) Template constrained cyclic peptides: design of high-affinity ligands for GPIIb/IIIa. *J. Amer. Chem. Soc.* 116, 3220-3230.
81. Mousa, S. A., Flint, S. Lorelli, W. Hassell, S., Bozarth, J., **DeGrado WF**, Reilly, T. M (1994) *Thrombosis Research* 76, 109-119.
82. Lear, J. D., Wasserman, Z. R., **DeGrado WF** (1994) Use of Synthetic Peptides for the Study of Membrane Protein Structure, *Membrane Protein Structure, Experimental Approaches*, 190, 1, 335-353.
83. Choma, C. T., Kaestle, K., Åkerfeldt, K. S., Kim, R. M., Groves, J. T., **DeGrado WF** (1994) A general method for coupling unprotected peptides to bromoacetamido porphyrin templates. *Tetrahedron Lett.* 35, 6191-6194.
84. Mousa, S. A., Flint, S., Lorelli, W., Hassell, S., Bozarth, J., **DeGrado WF**, Reilly, T. M (1994) Intravenous Antiplatelet Efficacy and Safety of the Platelet GPIIb/IIIa Antagonist, DMP 728 in Anesthetized Dogs *Thrombosis Research*, 76, 2, 109-119.
85. Mousa, S.A., Bozarth, J. M., Forsythe, M. S., Lorelli, W., Thoolen, M., Ramachandran, N., Jackson, S. A., DeGrado, W.F., Reilly, T.M (1994) Antiplatelet efficacy and specificity of DMP728, a novel platelet GPIIb/IIIa receptor antagonist. *Cardiology* 83, 374-382.
86. Nilsson, Bjorn, **DeGrado WF** (1995) Protein Engineering. *Current Opinion in Structural Biology*, 5, 441-442.
87. O'Neil, K. T., Hoess, R. H., Raleigh, D. P. & **DeGrado WF** (1995) Thermodynamic genetics of the folding of the B1 immunoglobulin-binding domain from streptococcal protein G. *Proteins* 21, 11-21.
88. Betz, S. F., Bryson, J. W. & **DeGrado WF** (1995) Native-like and structurally characterized designed alpha-helical bundles. *Curr Opin Struct Biol* 5, 457-63.
89. Betz, S., Fairman, R., O'Neil, K., Lear, J. & DeGrado, W (1995) Design of two-stranded and three-stranded coiled-coil peptides. *Philos Trans R Soc Lond B Biol Sci* 348, 81-8.
90. Xue, C.-B., DeGrado, W.F (1995) An efficient synthesis of glycoprotein IIb/IIIa inhibitor DMP728. A novel synthesis of N-alpha-methyl-arginine. *J. Org. Chem.* 60, 946-952.
91. Xue, C.-B., DeGrado, W.F (1995) Novel synthesis of Na-methyl arginine and Na-methyl-ornithine derivatives. *Tetrahedron Lett.* 36, 55-58 .

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

92. Raleigh, D. P., Betz, S. F., **DeGrado WF** (1995) A de Novo Designed Protein Mimics the Native State of Natural Proteins. *J. Amer. Chem. Soc.*, 117, 7558-7560.
93. Mousa, S.A., DeGrado, Reilly, T.M (1995) Platelet GPIIb/IIIa antagonists: how safe is this antithrombotic approach? *Am. J. Medicine*, 96, 300.
94. Bryson, J. W., Betz, S. F., Lu, H. S., Suich, D. J., Zhou, H. X., O'Neil, K. T. & **DeGrado WF** (1995) Protein design: a hierarchic approach. *Science* 270, 935-41.
95. Betz, S. F., Raleigh, D. P., **DeGrado WF**, Lovejoy, B., Anderson, D., Ogihara, N. & Eisenberg, D (1995) Crystallization of a designed peptide from a molten globule ensemble. *Fold Des* 1, 57-64.
96. **DeGrado WF** & Sosnick, T. R (1996) Protein minimization: downsizing through mutation. *Proc Natl Acad Sci U S A* 93, 5680-1.
97. **DeGrado WF**, Rabanal, F., Dutton, P. L (1996) Towards the Synthesis of Photosynthetic Reaction Center Maquette: A Cofacial Porphyrin Pair Assembled Between two Subunits of a Synthetic Four-helix Multi-heme Protein. *J. Amer. Chem. Soc.*, 118, 473-474.
98. Bach, A. C., II, Jackson, S. A., Espina, J. R., Stouten, P. F. W., Mousa, S., **DeGrado WF** (1996) Type II' to Type I a-Turn Swap Changes Specificity for Integrins. *J. Amer. Chem. Soc.*, 118, 473-474.
99. Xue, C-B., Rafalski, M., Roderick, J., Eyer mann, C. J., Mousa, S., Olson, R., **DeGrado WF** (1996) Design, Synthesis and in vitro Activities of a Series of Benzimidazole/Benzoxazole Glycoprotein IIb/IIIa Inhibitors. *Bioorg. & Med. Chem. Lett.* 6, 339-344.
100. Betz, S. F., Bryson, J. W., Passador, M. C., Brown, R. J., O'Neil, K. T., **DeGrado WF** (1996) Expression of de novo Designed α -Helical Bundles. *Acta Chim. Scand.*, 50, 688-696.
101. Wityak, J., Fevig, J.M., Jackson, S.A., Mousa, S.A., DeGrado, W.F., Wexler, R. R., "Synthesis and Antiplatelet Activity of DMP 757 Analogs (1996) *Bioorg. Med. Chem. Lett.*" 5, 2097-2100.
102. Mousa, S.A., DeGrado, W.F., Mu, D., Kapil, R., Lucchesi, B., Reilly, T.M (1996) Oral Antiplatelet, Antithrombotic Efficacy of a Novel Orally Active Platelet GPIIb/IIIa Antagonist, DMP728 in Dogs, *Circulation*, 93, 537-543.
103. Mousa, S.A., DeGrado, W.F., Jackson, S.A., Flint, S., Forsythe, M., Reilly, T.M (1996) Intravenous and Oral Antiplatelet/Antithrombotic Efficacy and Specificity DMP757, A Novel Platelet GPIIb/IIIa Antagonist, *Circulation*.
104. Suich, D. J., Ballinger, M. D., Wells, J. A., **DeGrado WF** (1996) Fmoc-based synthesis of glycolate ester peptides for the assembly of de novo designed multimeric proteins using subtiligase. *Tet. Lett.* 37, 6653-6656.
105. Rabanal, F. **DeGrado WF**, Dutton, P. L (1996) Use of 2,2'-dithiobis(5-nitropyridine) for the heterodimerization of cysteine containing peptides. Introduction of the 5-nitro-2-pyridinesulfonyl group. *Tet. Lett.* 37, 13472-1350.
106. Sosnick, T. R., Jackson, S., Wilke, R., Englander, S. W., **DeGrado WF** (1996) The role of helix formation in the folding of a fully α -helical coiled coil. *Proteins* 24, 427-432.
107. Mousa, S.A., Forsythe, M., Lorelli, W., Bozarth, J., Xue, C.-B., Wityak, J., Sielecki, T. M., Olson, R. E., DeGrado, W.F. Wexler, R., Thoolen, M. J., Reilly, T.M (1996) Novel nonpeptide antiplatelet GPIIb/IIIa Receptor Antagonist, DMP754: receptor binding affinity & Specificity. *Coronary Artery Disease*, 7, 767-774.
108. Betz, S. A. and **DeGrado WF** (1996) Controlling topology and native-like behavior of de novo-designed peptides: design and characterization of antiparallel four-stranded coiled coils. *Biochemistry* 35 , 6955-6962.
109. Betz, S. A. and **DeGrado WF** (1996) De novo-design of Native proteins: design and characterization of proteins intended to fold into antiparallel Rop-like, four-helix bundles. *Biochemistry* 36, 2450-2458.
110. Xue, X. B., He, X., Roderick, J., **DeGrado WF** Decicco, C., Copeland, R. A (1996) Potent Matrix Metalloproteinase inhibitors: amino-carboxylate compounds containing modifications of the P1 residue. *Bioorganic & Med. Chem. Lett.* 6, 379-384.

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

111. Rockwell, A., Medlen, M., Copeland, R. A., Hardman, K., Decicco, C. P., **DeGrado WF** (1996) Complimentarity of combinatorial chemistry and structure based ligand design: application to the discovery of novel inhibitors of matrix metalloproteinases. *J. Amer. Chem. Soc.* 118, 10337-10338.
112. Boice, J. A., Dieckmann, G. B. **DeGrado WF**, Fairman, R (1996) Thermodynamic analysis of a designed three-stranded coiled coil. *Biochemistry* 35, 14480-14485.
113. Åkerfeldt, K. S., Kienker, P. K., Lear, J. D., **DeGrado WF** (1996) Structure and Conduction Mechanisms of Minimal Ion Channels. *Comprehensive Supramolecular Chemistry vol. 10*, Eds, J.-M. Lehn and D. N. Reinhoudt.
114. Rabanal, F., Lombardi, A., Pavone, V., **DeGrado WF**, Dutton, P. L (1996) Topology of porphyrins linked to four-helix bundle proteins: Towards the design and synthesis of multicofactor redox enzymes. *Proc. of the European Peptide Symposium*.
115. Rabanal, F., Gibney, B. R., **DeGrado WF**, Moser, C. C., Dutton, P. L (1996) Engineering Photosynthesis: Synthetic Redox Protein. *Inorganica Chimica Acta*, 243 213-218.
116. Dieckmann, G., **DeGrado WF** (1997) Modeling oligomeric helical bundles. *Cur. Op. Struct. Biol.* 7, 486-494.
117. **DeGrado WF** (1997) Proteins from scratch. *Science* 278, 80-81.
118. Lear, J. D., Schneider, J. P. Kienker, P. K., and **DeGrado WF** (1997) Electrostatic effects on ion selectivity and rectification in designed ion channel peptides. *J. Amer. Chem. Soc.* 119, 3212-3217.
119. Corbett, J.W., Graciani, N.R., Mousa, S.A., DeGrado, W.F (1997) Solid-phase Synthesis of a Selective $\alpha_1\beta_3$ Integrin Antagonist Library. *Bioorg. Med. Chem. Lett.* 7 1371-1376.
120. Lombardi, A., Bryson, J. W., **DeGrado WF** (1997) De114. 115. Novo Design of Heterotrimeric Coiled Coils. *Biopolymers* 40, 495-504.
121. Bennett, J. S., Chan, C., Vilaire, G., Mousa, S., A., **DeGrado WF** (1997) Agonist-activated $\alpha_v\beta_3$ on platelets and lymphocytes binds to the matrix protein osteopontin. *J. Biol. Chem.* 272, 8137-8140.
122. Ogiwara, N. L., Weiss, M. S., **DeGrado WF**, Eisenberg, D (1997) The structure of the designed trimeric coiled coil coil-Va-Ld: Implications for engineering crystals and supramolecular assemblies. *Protein Science* 6, 78-86.
123. Pinto, L. H., Dieckmann, G. R., Gandhi, C. S., Papworth, C. G., Braman, J., Shaughnessy, M. A., Lear, J. D., Lamb, R. A., **DeGrado WF** (1997) A functionally defined model for the M2 Proton Channel of Influenza A Virus suggests a mechanism for its selectivity. *Proc. Natl. Acad. Sci. U.S.A.* 94, 11301-11306.
124. Lu, H. S. M., Volk, M., Kholodenko, Y., Gooding, E., Hochstrasser, R. M. **DeGrado WF** (1997) Aminothietyrosine disulfide, an optical trigger for initiation of protein folding. *J. Amer. Chem. Soc.* 119, 7173-7180.
125. Volk, M., Kholodenko, Y., Lu, H. S. M., Gooding, E., **DeGrado WF**, Hochstrasser, R. M (1997) Peptide conformational dynamics and vibrational Stark effects following photoinitiated disulfide cleavage. *J. Phy. Chem. B* 101, 8607-8616.
126. Schneider, J. S., Lear, J. D., **DeGrado WF** (1997) A designed buried salt bridge in a heterodimeric coiled coil. *J. Amer. Chem. Soc.* 119, 5742-5743.
127. Lombardi, A., Bryson, Ghirlanda, G., J., **DeGrado WF** (1997) Design of a synthetic receptor for the calmodulin-binding domain of calcineurin. *J. Amer. Chem. Soc.*, 119, 12378-12379.
128. Xue, C-B., Roderick, J., Jackson, S., Rafaksi, M., Rockwell, A., Mousa, S., Olson, R., **DeGrado WF** (1997) Design, Synthesis and In Vitro Activities of a Series of Benzamide-Core Glycoprotein IIb/IIIa Inhibitors: 2,3-Diaminopropionic Acid Derivatives as Surrogates of Aspartic Acid. *Bioorg. & Med. Chem. Lett.* 5, 693-705.
129. Dieckmann, G. R., McRorie, D. K., Tierney, D. L., Utschig, L. M., Singer, C. P., O'Halloran, T. V., Penner-Hahn, J. E., **DeGrado WF** (1997) Pecoraro, V. *J. Amer. Chem. Soc.*, 119, 6195-6196.
130. Xue, C-B., Wityak, J., Sielecki, T. M., Pinto, D. J., Batt, D. G., Cain, G., A., Sworin, M., Rockwell, A. L., Roderick, J. J., Wang, S., Orwat, M., Fritze, W. E., Bostrom, L. L., Liu, J., Higley, C. A., Rankin, F. W., Tobin, A. E., Emmett, G., Lalka, G. K., Sze, J. Y., Di Meo, S. V., Mousa, S. A., Thoolen, M. J., Racanelli, A.

CURRICULUM VITAE
WILLIAM F. DEGRADO

- L., Hausner, E. A., Reilly, T. M., **DeGrado WF**, Wexler, R. R., Olson, R. E (1997) Discovery of an orally active series of isoxazoline glycoprotein IIb/IIIa antagonists. *J. Med. Chem.* 40, 2064-2084.
131. Xue, C.-B., He, X., Roderick, DeGrado, W. F., Hardman, K. D., Nelson, D. J., Copeland, R. A., Jaffee, B. D., DeCicco, C. P (1998) Design and synthesis of cyclic inhibitors of matrix metalloproteinase and TNF- α production. *J. Med. Chem.* 41, 1745-1748.
132. Cherney, R. J., Li, D. T., Xue, C.-B., Wasserman, Z. R., Hardman, K. D., Welch, P. K., Covington, M. B., Copeland, R. A., Amer, E. C., **DeGrado WF**, Decicco, C. P (1998) Macrocyclic amino carboxylates as selective MMP-8 inhibitors. *J. Med. Chem.* 41, 1749-1751.
133. Xue, C.-B., Roderick, J., Mousa, S., Olson, R., DeGrado, W.F (1998) Synthesis and Antiplatelet Effects of an Isoxazole Series of Glycoprotein IIb/IIIa Antagonists. *Bioorg. & Med. Chem. Lett.* 8, 3499-3504.
134. Forrest, L.R., DeGrado, W.F., Dieckmann G.R., Sansom, M.S.P (1998) Two models of the influenza A M2 channel domain: verification by comparison. *Folding and Design* 3, 443-448.
135. Hill, R.B., DeGrado W.F (1998) Solution Structure of α_2D , a Nativelike de Novo Designed Protein. *JACS* 120 1138-1145.
136. Ghirlanda G., Lear J.D., Lombardi, A., DeGrado W.F (1998) From Synthetic Coiled Coils to Functional Proteins: Automated Design of a Receptor for the Calmodulin-binding Domain of Calcineurin. *J. Mol. B.* 281 379-391.
137. Bryson, J.W., Desjarlais, J.R., Handel, T.M., DeGrado, W.F (1998) From coiled coils to small globular proteins: Design of a native-like three-helix bundle. *Prot. Sci.* 7 1404-1414.
138. Lombardi A, Ghirlanda, G. Zaccaro, L. Pavone, P, DeGrado, W.F (1998) A novel class of Calmodulin mimetics: *De Novo* designed proteins in molecular recognition. 94-97 in *Peptides: frontiers of peptide science*, ed. by Tam, J.P., Kaumaya, P.T.P.
139. Dieckmann, G.R., McRorie, D.R., Lear, J.D., Sharp, K.A., DeGrado, W.F., Pecoraro, V.R (1998) The role of protonation and metal chelation preferences in defining the properties of mercury-binding coiled coils. *J. Mol. Biol.* 280, 897-912.
140. Schneider, JP, Lombardi, A & DeGrado, WF (1998) Analysis and Design of Three-Stranded Coiled-Coils and Three-Helix Bundles. *Folding and Design*, 3, R29.
141. Schneider, J. S., **DeGrado WF** (1998) The design of α -helical C-capping auxiliaries. *J. Amer. Chem. Soc.* 2764-2767.
142. Xue, C.-B., Roderick, J., Mousa, S., Olson, R.E., **DeGrado WF** (1998) Synthesis and antiplatelet effects of an isoxazole series of glycoprotein IIb/IIIa antagonists. *Bioorg. Med. Chem. Lett.* 8, 3499-3504.
143. Dieckmann G.R., Lear, J.D., Xhong, Q., Klein, M.L., **DeGrado WF**, Sharp, K.A (1999) Exploration of the Structural Features Defining the Conduction Properties of a Synthetic Ion Channel. *Biophys. J.* 76, 618-630.
144. Gandhi, C.S., Shuck, K., Lear, J.D., Dieckmann, G.R., DeGrado, W.F., Lamb, R.A., Pinto, L.H (1999) Cu(II) Inhibition of the Proton Translocation Machinery of the Influenza A Virus M₂ Protein. *J. Biol. Chem.* 9 5474-5482.
145. Rockwell, A.L., Rafalski, M, Pitts, W.J., Batt, D.G., Petraitis, J.J., DeGrado, W.F., Mousa, S., Jadhav, P.K (1999) Rapid Synthesis of RGD Mimetics with Isoxazoline Scaffolds on Solid Phase: Identification of $\alpha_3\beta_3$ Antagonists Lead Compounds. *Bioorg. & Med. Chem. Lett.* 9 937-942.
146. Kochendoerfer G.D.*, Salom D.*, Lear J.D., Wilk-Orescan R., Kent S.B.H. & DeGrado W.F (1999) Total chemical synthesis of the integral membrane protein Influenza A virus M2: Role of its C-terminal domain in tetramer assembly. *Biochemistry* 38, 11905-11913.
147. Hamm, P., Lim, M., DeGrado, W.F., Hochstrasser, R.M. (1999) The two-dimensional IR nonlinear spectroscopy of a cyclic penta-peptide in relation to its three-dimensional structure. *Proc. Natl. Acad. Sci. USA* 96 2036-2041.

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

148. Jia, Y., Talaga, D.S., Lau, W.L., Lu, H.S.M., DeGrado, W.F., Hochstrasser, R.M (1999) Folding Dynamics of Single GCN4 Peptides by Fluorescence Resonant Energy Transfer Confocal Microscopy. *J. Chem. Phys.* 247 69-83.
149. Walsh, S.T.R., Chang, H. Bryson, J. W., Roder, H., **DeGrado WF** (1999) Solution structure and dynamics of a de novo designed 3-helix bundle protein. *Proc. Natl. Acad. Sci.* 96, 5486-5491.
150. Patterson, W. R., Anderson, D. H., **DeGrado WF**, Cascio, D., Eisenberg, D (1999) Centrosymmetric bilayers in the 0.75 resolution structure of a designed alpha-helical peptide, D,L-Alpha-1. *Protein Science* 8, 1410-1422.
151. DeGrado, W.F., Schneider, J.P., Hamuro, Y (1999) The Twists and turns of β -peptides. *J. Peptide Res.* 54 206-217.
152. Hamuro, Y, Scialdone, M.A., DeGrado, W.F (1999) Resin-to-resin acyl- and aminoacyl-transfer reactions using oxime supports. *J. Am. Chem. Soc.* 121 1636-44.
153. Summa, C.M., Lombardi, A., Lewis, M., DeGrado, W.F (1999) Tertiary templates for the design of diiron proteins. *Curr Opin Struct Biol.* 9, 500-508.
154. DeGrado, W.F., Summa, C.M., Pavone, V., Natri, F., Lombardi, A (1999) De novo design and structural characterization of proteins and metalloproteins. *Ann. Rev. Biochem.* 68 779-819.
155. Hamm, P., Lim M., DeGrado, W.F., Hochstrasser, R. M (1999) Stimulated Photon Echoes from Amide I Vibrations. *J. Phys. Chem.* 103, 10049-10053.
156. Hamuro, Y., Schneider, J. P., **DeGrado WF** (1999) De novo design of antibacterial β -peptides. *J. Amer. Chem. Soc.* 121, 12200-12201.
157. Hamm, P., Lim M., DeGrado, W.F., Hochstrasser, R. M (2000) Pump/probe self heterodyned 2D spectroscopy of vibrational transitions of a small globular peptide. *J. Phys. Chem.* 112, 1907-1916
158. Hill, R. B., Hong, J.-K., **DeGrado WF** (2000) Hydrogen-bonded cluster can specify the native state of a protein. *J. Amer. Chem. Soc.* 122, 746-747.
159. Hill, R. B., **DeGrado WF** (2000) A polar, solvent-exposed residue can be essential for native protein structure. *Structure*, 8, 471-479.
160. Lombardi, A., Summa, C. M., Geremia, S., Randaccio, L., Pavone, V., **DeGrado WF** (2000) Retrostrutural analysis of metalloproteins: Application to the design of a minimal model for diiron proteins. *Proc. Natl. Acad. Sci.* 97, 6298-6305.
161. Choma, C., Gratkowski, H., Lear, J. D., **DeGrado WF** (2000) Asparagine-mediated self-association of a model transmembrane helix. *Nature, Structural Biology*, 7, 161-166.
162. Talaga, D. S. Lau, W. L., Roder, H., Tang J., Jia, Y, **DeGrado WF**, Hochstrasser, R (2000) Dynamics and folding of single two-stranded coiled-coil peptides studied by fluorescent energy transfer confocal microscopy. *Proc Natl Acad Sci U S A* 97, 13021-13026.
163. O'Neil, K. T. ; Bach, A. C.; DeGrado, W.F (2000) Structural Consequences of an Amino Acid Deletion in the B1 Domain of Protein G. *Proteins: Structure, Function, Genetics* 41, 323-333.
164. Salom D., Hill B.R., Lear J.D., DeGrado W.F (2000) pH-Dependent tetramerization and amantadine binding of the transmembrane helix of M2 from influenza A virus. *Biochemistry* 39, 14160-14170.
165. Hill, R. B., Bracken, C., **DeGrado WF**, Palmer, A. G., III (2000) Molecular motions and protein folding: Characterization of the backbone dynamics and folding equilibrium of a2D using ^{13}C NMR Spin Relaxation. *J. Amer. Chem. Soc.* 122, 11610-19.
166. Mannes, E. S., Getahun, Z., Wright, W. W., **DeGrado WF**, Vanderkooi, J. M (2000) Infrared spectra of amide groups in α -helical proteins: evidence for hydrogen bonding between helices and water. *J. Amer. Chem. Soc.* 122, 9883-90.
167. Hill, R. B., Raleigh, D. P., Lombardi, A., **DeGrado WF** (2000) De novo design of helical bundles as models for understanding protein folding and function. *Acc. Chem. Res.* 33, 745-754.

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

168. Changenet-Barret, P., Choma, C. T., Gooding, E. F., **DeGrado WF**, Hochstrasser, R. M (2000) *J. Phys. Chem. B.* 104, 9322-9329.
169. Dalby, P. A., Hoess, R. H., **DeGrado WF** (2000) Evolution of binding affinity in a WW domain probed by phage display. *Protein Science* 9, 2366.
170. Helluin, O., Chan, C., Vilaire, G., Mousa, S., **DeGrado WF**, Bennett, J. S (2000) The activation state of α 5 β 3 regulates platelet and lymphocyte adhesion to intact and thrombin-cleaved osteopontin. *J. Biol. Chem.* 275, 18337-343.
171. Ogihara, N. L., Ghirlanda, G., Bryson, J. W., Gingery, M., DeGrado, W.F., Eisenberg, D (2000) Design of three-dimensional domain-swapped dimers and fibrous oligomers. *Proc. Natl. Acad. Sci. USA* 98: 1404-1409.
172. Suich, D.J., Mousa, S. A., Singh, G., Liapakis, G., Reisine, T., DeGrado, W.F (2000) Novel template-constrained cyclic peptide analogs of somatostatin: Subtype-selective binding to somatostatin receptors and antiangiogenic activity. *Med. Chem. Lett.*, 8, 2229-41.
173. Gratkowski, H., Lear, J. D., DeGrado, W.F (2001) Polar side chains drive the association of model transmembrane peptides. *Proc. Natl. Acad. Sci. USA* 98, 880-885.
174. Ogihara, N. L.; Ghirlanda, G., Bryson, J.W., Gingery, M., DeGrado, W.F., Eisenberg, D (2001) Design of three-dimensional domain-swapped dimers and fibrous oligomers. *Proc. Natl. Acad. Sci. USA* 98, 1404-1409.
175. Pasternak, A., Kaplan, J., Lear, J. D. & **DeGrado WF** (2001) Proton and metal ion-dependent assembly of a model diiron protein. *Protein Sci* 10, 958-69.
176. Tang, Y., Ghirlanda, G., Vaidehi, N., Kua, J., Mainz, D. T., Goddard, I. W., **DeGrado WF** & Tirrell, D. A (2001) Stabilization of coiled-coil peptide domains by introduction of trifluoroleucine. *Biochemistry* 40, 2790-6.
177. Walsh, S. T., Sukharev, V. I., Betz, S. F., Vekshin, N. L. & **DeGrado WF** (2001) Hydrophobic core malleability of a de novo designed three-helix bundle protein. *J Mol Biol* 305, 361-73.
178. Cheng, R. P. **DeGrado WF** (2001) De novo design of a monomeric beta-peptide stabilized by electrostatic interactions. *J. Amer. Chem. Soc.* 123, 5162-63.
179. Tang, Y., Ghirlanda, G., Petka, W. A., Nakajima, T., **DeGrado WF** & Tirrell, D. A (2001) Fluorinated coiled-coil proteins prepared in vivo display enhanced thermal and chemical stability *Angew. Chem.* 113, 1542-44.
180. Liu, D., DeGrado, W.F (2001) De Novo Design, Synthesis, and Characterization of Antimicrobial β -Peptides. *J. Am. Chem. Soc.* 123, 7553-7559.
181. Xue, C.-B.; Voss, M. E.; Nelson, D. J.; Duan, J.-W.; Cherney, R. J.; Jacobson, I. C.; He, X.; Roderick, J.; Chen, L.; Corbett, R. L.; Wang, L.; Meyer, D. T.; Kennedy, K.; **DeGrado WF**; Hardman, K. D.; Teleha, C. A.; Jaffee, B. D.; Liu, R.-Q.; Copeland, R. A.; Covington, M. B.; Christ, D. D.; Trzaskos, James M.; Newton, R. C.; Magolda, R. L.; Wexler, R. R.; Decicco, C. P (2001) Design, Synthesis, and Structure-Activity Relationships of Macrocyclic Hydroxamic Acids That Inhibit Tumor Necrosis Factor α Release in Vitro and in Vivo *J. Med. Chem.* 44(16), 2636-2660.
182. Lear, J. D., Gratkowski, H., **DeGrado WF** (2001) De novo design, synthesis, and characterization of membrane-active peptides. *Biochem. Soc. Transactions*, 29, 559-564.
183. Walsh, S. T. R., Lee, A. L., **DeGrado WF**, Wand, J. A (2001) Dynamics of a de novo designed three-helix bundle protein studied by ^{15}N , ^{13}C , and ^2H NMR Relaxation methods. *Biochemistry* 40, 9560-9569.
184. Huang, C.Y., Klemke, J., Getahun, Z., **DeGrado WF**, Gai, F (2001) Temperature-dependent helix-coil transition of an alanine-based peptide. *J. Amer. Chem. Soc.* 123, 9235-38.
185. Cheng, R. P., Gellman, S. H., **DeGrado WF** (2001) β -Peptides: From Structure to Function. *Chem. Rev.* 101, 3219-32.
186. Di Costanzo, L. Wade, H., Geremia, S., Randaccio, L., Pavone, V., **DeGrado WF**, Lombardi, A (2001) Toward the de novo design of a catalytically active helix bundle: a substrate-accessible carboxylate-bridged dinuclear metal center. *J Am Chem Soc* 123, 12749-12757.

CURRICULUM VITAE
WILLIAM F. DEGRADO

187. Huang, C. Y., Getahun, Z., Wang, T., **DeGrado WF** & Gai, F (2001) Time-resolved infrared study of the helix-coil transition using (13)C- labeled helical peptides. *J Am Chem Soc* 123, 12111-12112.
188. Li, R., Babu, C. R., Lear, J. D., Wand, A. J., Bennett, J. S., **DeGrado WF** (2001) Oligomerization of the integrin alphaIIb beta3: roles of the transmembrane and cytoplasmic domains. *Proc Natl Acad Sci U S A* 98, 12462-12467.
189. North, B., Summa, C. M., Ghirlanda, G., **DeGrado WF** (2001) D_n-symmetrical tertiary templates for the design of tubular proteins. *J. Mol. Biol.* 311, 1081-1090.
190. Cheng, R.P., Suich, D.J., Cheng, H., Roder, H. & DeGrado, W.F (2001) Template-constrained somatostatin analogues: a biphenyl linker induces a type-V' turn. *J Am Chem Soc* 123, 12710-12711.
191. DeGrado, W.F (2001) Introduction: protein design. *Chem Rev* 101, 3025-3026.
192. Huang, C. Y., Getahun, Z., Zhu, Y., Klemke, J. W., **DeGrado WF** & Gai, F (2002) Helix formation via conformation diffusion search. *Proc Natl Acad Sci U S A* 99, 2788-2793.
193. Marsh, E. N. G., **DeGrado WF** (2002) Noncovalent self-assembly of a heterotetrameric diiron protein. *Proc. Natl. Acad. Sci. USA* 99 5150-5154.
194. Tew, G.N, Liu, D, Chen, B, Doerksen, RJ, Kaplan, J, Carroll, PJ, Klein, ML, DeGrado, WF (2002) Supramolecular Chemistry And Self-assembly Special Feature: De novo design of biomimetic antimicrobial polymers. *Proc Natl Acad Sci U S A* 99, 5110-5114.
195. Ghirlanda, G., Lear, J.D., Ogihara, N.L., Eisenberg, D. & DeGrado, W.F (2002) A hierarchic approach to the design of hexameric helical barrels. *J Mol Biol* 319, 243-253.
196. Huang, C.Y., He, S., DeGrado, W.F., McCafferty, D.G. & Gai, F (2002) Light-induced helix formation. *J Am Chem Soc* 124, 12674-12675.
197. Howard, K.P., Lear, J.D. & DeGrado, W.F (2002) Sequence determinants of the energetics of folding of a transmembrane four-helix-bundle protein. *Proc Natl Acad Sci U S A* 99, 8568-8572.
198. Gratkowski, H., Dai, Q.H., Wand, A.J., DeGrado, W.F. & Lear, J.D (2002) Cooperativity and specificity of association of a designed transmembrane peptide. *Biophys J* 83, 1613-1619.
199. Summa, C.M., Rosenblatt, M.M., Hong, J.K., Lear, J.D. & DeGrado, W.F (2002) Computational de novo design, and characterization of an A(2)B(2) diiron protein. *J Mol Biol* 321, 923-938.
200. Cheng, R.P. & DeGrado, W.F (2002) Long-range interactions stabilize the fold of a non-natural oligomer. *J Am Chem Soc* 124, 11564-11565.
201. Li R., Hoess RH, Bennett JS, **DeGrado WF** (2003) Use of phage display to probe the evolution of binding specificity and affinity in integrins. *Protein Engineering* 16, 65-72.
202. Li, R., Babu, CR, Valetine, K, Lear, JD, Wand, AJ, Bennett, JS, DeGrado, WF (2003) Characterization of the monomeric form of the transmembrane and cytoplasmic domains of the integrin b3 subunit by NMR spectroscopy. *Biochem* 41, 52. 15618-15624.
203. Maglio O, Nastro F, Pavone V, Lombardi A, **DeGrado WF** (2003) Preorganization of molecular binding sites in designed diiron proteins. *Proc.Natl. Acad. Sci. USA* 100, 3772-3777.
204. Getahun Z, Huang C-Y, Wang T, De Leon B, **DeGrado WF**, Gai F (2003) Using nitrile-derivitized amino acids as infrared probes of local environment. *J Am Chem Soc* 125, 405-411.
205. **DeGrado WF**, Gratkowski H, Lear JD (2003) How do helix-helix interactions help determine the folds of membrane proteins? Perspectives from the study of homo-oligomeric bundles. *Prot. Sci.* 12, 647-665.
206. Papoian GA. **DeGrado WF**. Klein ML (2003) Probing the configurational space of a metalloprotein core: an ab initio molecular dynamics study of Duo Ferro 1 binuclear Zn cofactor. *Journal of the American Chemical Society.* 125, 560-9.
207. Slovic AM. Summa CM. Lear JD. **DeGrado WF** (2003) Computational design of a water-soluble analog of phospholamban *Protein Science.* 12, 337-48.

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

208. Lear JD, Gratkowski H, Adamian L, Liang J, **DeGrado WF** (2003) Position-dependence of stabilizing polar interactions of asparagine in transmembrane helical bundles. *Biochemistry*. 42, 6400-7.
209. Walsh ST, Cheng RP, Wright WW, Alonso DO, Daggett V, Vanderkooi JM, **DeGrado WF** (2003) The hydration of amides in helices; a comprehensive picture from molecular dynamics, IR, and NMR. *Protein Science*. 12, 520-31.
210. **DeGrado WF**, Di Costanzo L, Geremia S, Lombardi A, Pavone V, Randaccio L (2003) Sliding helix and change of coordination geometry in a model di-MnII protein. *Angewandte Chemie. International Ed.* 42, 417-20.
211. Li R, Mitra N, Gratkowski H, Vilaire G, Litvinov R, Nagasami C, Weisel JW, Lear JD, **DeGrado WF**, Bennett JS (2003) Activation of integrin alphaIIb beta3 by modulation of transmembrane helix associations. *Science*. 300, 795-8.
212. **DeGrado WF** (2003) Computational biology: Biosensor design. *Nature*. 423(6936):132-3.
213. R. S. Signarvic, W. F. DeGrado (2003) De novo design of a molecular switch: phosphorylation-dependent association of designed peptides. *J. Mol. Biol.* 334, 1-12.
214. Cristian, L., Lear, J. D. & **DeGrado WF** (2003) Use of thiol-disulfide equilibria to measure the energetics of assembly of transmembrane helices in phospholipid bilayers. *Proc Natl Acad Sci U S A* 100, 14772-7.
215. Cristian, L., Lear, J. D. & **DeGrado WF** (2003) Determination of membrane protein stability via thermodynamic coupling of folding to thiol-disulfide interchange. *Protein Sci* 12, 1732-40.
216. Calhoun, J. R., Kono, H., Lahr, S., Wang, W., **DeGrado WF** & Saven, J. G (2003) Computational design and characterization of a monomeric helical dinuclear metalloprotein. *J Mol Biol* 334, 1101-15.
217. Zhu, Y., Alonso, D. O., Maki, K., Huang, C. Y., Lahr, S. J., Daggett, V., Roder, H., **DeGrado WF** & Gai, F (2003) Ultrafast folding of alpha3D: a de novo designed three-helix bundle protein. *Proc Natl Acad Sci U S A* 100, 15486-91.
218. Slovic, A. M., Kono, H., Lear, J. D., Saven, J. G. & **DeGrado WF** (2004) Computational design of water-soluble analogues of the potassium channel KcsA. *Proc Natl Acad Sci U S A* 101, 1828-33.
219. Lau, W. L., Ege, D. S., Lear, J. D., Hammer, D. A. & **DeGrado WF** (2004) Oligomerization of fusogenic peptides promotes membrane fusion by enhancing membrane destabilization. *Biophys J* 86, 272-84.
220. Summa, C., **DeGrado WF** (2004) A multibody atomic potential for use in *de novo* protein design. to be submitted to *J. Mol. Biol.*
221. Liu, D., Choi, S., Chen, B., Doerksen, R. J., Clements, D. J., Winkler, J. D., Klein, M. L. & **DeGrado WF** (2004) Nontoxic membrane-active antimicrobial arylamide oligomers. *Angew Chem Int Ed Engl* 43, 1158-62.
222. Tucker, M. J., Getahun, Z., Nanda, V., **DeGrado WF** & Gai, F (2004) A new method for determining the local environment and orientation of individual side chains of membrane-binding peptides. *J Am Chem Soc* 126, 5078-9.
223. Li, R., Gorelik, R., Nanda, V., Law, P. B., Lear, J. D., **DeGrado WF** & Bennett, J. S (2004) Dimerization of the transmembrane domain of integrin alpha IIb subunit in cell membranes. *J Biol Chem*. 279, 26666-26673.
224. Engel, D. E. & **DeGrado WF** (2004) Amino acid propensities are position-dependent throughout the length of alpha-helices. *J Mol Biol* 337, 1195-205.
225. Magistrato, A., **DeGrado WF**, Laio, A., Rothlisberger, U., VandeVondele, J. & Klein, M. L (2003) Characterization of the dizinc analogue of the synthetic diiron protein DF1 using ab initio and hybrid quantum/classical molecular dynamics simulations. *J. Phys. Chem. B* 107, 4182-8.
226. Doerksen, R. J., Chen, B., Liu, D., Tew, G. N., **DeGrado WF** & Klein, M. L (2004) Controlling the Conformation of Arylamides: Computational Studies of Intramolecular Hydrogen Bonds between Amides and Ethers or Thioethers. *Chemistry, A European Journal* 10, 5008-5016.
227. Lear, J. D., Stouffer, A. L., Gratkowski, H., Nanda, V. & **DeGrado WF** (2004) Association of a model transmembrane Peptide containing gly in a heptad sequence motif. *Biophys J* 87, 3421-9.

CURRICULUM VITAE
WILLIAM F. DEGRADO

228. Kaplan, J. & **DeGrado WF** (2004) De novo design of catalytic proteins. *Proc Natl Acad Sci U S A* 101, 11566-70.
229. Baltzer, L. & **DeGrado WF** (2004) Engineering and design Expanding the protein world. *Curr Opin Struct Biol* 14, 455-7.
230. Ghirlanda, G., Osyczka, A., Liu, W., Antolovich, M., Smith, K. M., Dutton, P. L., Wand, A. J. & **DeGrado WF** (2004) De Novo Design of a D(2)-Symmetrical Protein that Reproduces the Diheme Four-Helix Bundle in Cytochrome bc(1) *J Am Chem Soc* 126, 8141-8147.
231. Li, R., Bennett, J. S. & **DeGrado WF** (2004) Structural basis for integrin alphaIIb beta3 clustering. *Biochem Soc Trans* 32, 412-5.
232. Wang, T., Zhu, Y., Getahun, Z., Du, D., Huang, C., DeGrado, W. & Gai, F (2004) Length dependent helix-coil transition kinetics of nine alanine-based peptides. *J. Phys. Chem. B* 108, 15301-10.
233. Ghirlanda, G., Hilcove, S. A., Pidikiti, R., Johansson, J. S., Lear, J. D., **DeGrado WF** & Eckenhoff, R. G (2004) Volatile anesthetic modulation of oligomerization equilibria in a hexameric model peptide. *FEBS Lett* 578, 140-4.
234. Nanda, V. & **DeGrado WF** (2004) Simulated evolution of emergent chiral structures in polyalanine. *J Am Chem Soc* 126, 14459-67.
235. Senes, A., Engel, D. E. & **DeGrado WF** (2004) Folding of helical membrane proteins: the role of polar, GxxxG-like and proline motifs. *Curr Opin Struct Biol* 14, 465-79.
236. Kovalenko OV, Metcalf DG, **DeGrado WF**, Hemler ME. Structural organization and interactions of transmembrane domains in tetraspanin proteins. *BMC Struct Biol*. 2005 Jun 28;5:11.
237. Engel DE, **DeGrado WF**. Alpha-alpha linking motifs and interhelical orientations. *Proteins*. 2005 Nov 1;61(2):325-37.
238. Choi S, Clements DJ, Pophristic V, Ivanov I, Vemparala S, Bennett JS, Klein ML, Winkler JD, **DeGrado WF**. The design and evaluation of heparin-binding foldamers. *Angew Chem Int Ed Engl*. 2005 Oct 21;44(41):6685-9.
239. Howard, K. P., Liu, W., Crocker, E., Nanda, V., Lear, J. D., DeGrado, W. & Smith, S. O (2005) Rotational orientation of monomers within a designed homo-oligomer transmembrane helical bundle. *Protein Science* 14, 1019 – 1024.
240. Li, W., Metcalf, D. G., Gorelik, R., Li, R., Mitra, N., Nanda, V., Law, P. B., Lear, J. D., **DeGrado WF** & Bennett, J. S (2005) A push-pull mechanism for regulating integrin function. *Proc Natl Acad Sci U S A* 102, 1424-9.
241. Cochran FV, Wu SP, Wang W, Nanda V, Saven JG, Therien MJ, **DeGrado WF**. Computational de novo design and characterization of a four-helix bundle protein that selectively binds a nonbiological cofactor. *J Am Chem Soc*. 2005 Feb 9;127(5):1346-7. Erratum in: *J Am Chem Soc*. 2006 Jan 18;128(2):663.
242. Calhoun, J. R., Natri, F., Maglio, O., Pavone, V., Lombardi, A. & **DeGrado WF** (2005) Artificial diiron proteins: From structure to function. *Biopolymers* 80, 264-278.
243. Lahr, S. J., Engel, D. E., Stayrook, S. E., Maglio, O., North, B., Geremia, S., Lombardi, A. & **DeGrado WF** (2005) Analysis and design of turns in alpha-helical hairpins. *J Mol Biol* 346, 1441-54.
244. Stouffer, A. L., Nanda, V., Lear, J. D. & **DeGrado WF** (2005) Sequence determinants of a transmembrane proton channel: an inverse relationship between stability and function. *J Mol Biol* 347, 169-79.
245. Duong-Ly, K. C., Nanda, V., **DeGrado WF** & Howard, K. P (2005) The conformation of the pore region of the M2 proton channel depends on lipid bilayer environment. *Protein Sci* 14, 856-61.
246. Nanda, V. & **DeGrado WF** (2005) Automated use of mutagenesis data in structure prediction. *Proteins* 59, 454-66.
247. Kuroda, K. & **DeGrado WF** (2005) Amphiphilic polymethacrylate derivatives as antimicrobial agents. *J Am Chem Soc* 127, 4128-9.

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

248. Slovic, A. M., Lear, J. D. & **DeGrado WF** (2005) De novo design of a pentameric coiled-coil: decoding the motif for tetramer versus pentamer formation in water-soluble phospholamban. *J Pept Res* 65, 312-21.
249. Adamian, L., Nanda, V., **DeGrado WF** & Liang, J (2005) Empirical lipid propensities of amino acid residues in multispan alpha helical membrane proteins. *Proteins* 59, 496-509.
250. Maglio, O, Natri, F, Calhoun, J, Lahr, S, Wade, H, Pavone, V, DeGrado, WF, Lombardi, A (2005) Artificial di-iron proteins: solution characterization of four helix bundles containing two distinct types of inter-helical loops. *J Biol Inorg Chem*, 10, 539-549.
251. Summa, C. M., Levitt, M. & **DeGrado WF** (2005) An Atomic Environment Potential for use in Protein Structure Prediction. *J Mol Biol* 352, 986-1001.
252. Slovic, A. M., Stayrook, S. E., North, B. & **DeGrado WF** (2005) X-ray structure of a water-soluble analog of the membrane protein phospholamban: sequence determinants defining the topology of tetrameric and pentameric coiled coils. *J Mol Biol* 348, 777-87.
253. Nanda, V., Rosenblatt, M. M., Osyczka, A., Kono, H., Getahun, Z., Dutton, P. L., Saven, J. G. & **DeGrado WF** (2005) De novo design of a redox-active minimal rubredoxin mimic. *J Am Chem Soc* 127, 5804-5.
254. Willcox, P. J., Reinhart-King, C. A., Lahr, S. J., **DeGrado WF** & Hammer, D. A (2005) Dynamic heterodimer-functionalized surfaces for endothelial cell adhesion. *Biomaterials* 26, 4757-66.
255. Cristian, L., Nanda, V., Lear, J. D. & **DeGrado WF** (2005) Synergistic Interactions between Aqueous and Membrane Domains of a Designed Protein Determine its Fold and Stability. *J Mol Biol* 348, 1225-1233.
256. Wei, P. P., Skulan, A. J., Wade, H., **DeGrado WF** & Solomon, E. I (2005) Spectroscopic and computational studies of the de novo designed protein DF2t: correlation to the biferrous active site of ribonucleotide reductase and factors that affect O₂ reactivity. *J Am Chem Soc* 127, 16098-106.
257. Wang, T., Lau, W. L., **DeGrado WF** & Gai, F (2005) T-jump Infrared Study of the Folding Mechanism of Coiled-coil GCN4-p1. *Biophys J*, 89, 4180-7.
258. Geremia S, Di Costanzo L, Randaccio L, Engel DE, Lombardi A, Natri F, **DeGrado WF**. Response of a designed metalloprotein to changes in metal ion coordination, exogenous ligands, and active site volume determined by X-ray crystallography. *J Am Chem Soc*. 2005 Dec 14;127(49):17266-76.
259. Yin, H, Frederick, K. K., Liu, D., Wand, A. J. & **DeGrado WF** (2006) Arylamide derivatives as peptidomimetic inhibitors of calmodulin. *Org Lett* 8, 223-5.
260. Nanda, V. & **DeGrado WF** (2006) Computational design of heterochiral peptides against a helical target. *J Am Chem Soc* 128, 809-16.
261. Ivanov, I., Vemparala, S., Pophristic, V., Kuroda, K., **DeGrado WF**, McCammon, J. A. & Klein, M. L (2006) Characterization of nonbiological antimicrobial polymers in aqueous solution and at water-lipid interfaces from all-atom molecular dynamics. *J Am Chem Soc* 128, 1778-9.
262. Pophristic, V., Vemparala, S., Ivanov, I., Liu, Z., Klein, M. L. & **DeGrado WF** (2006) Controlling the Shape and Flexibility of Arylamides: A Combined ab Initio, ab Initio Molecular Dynamics, and Classical Molecular Dynamics Study. *J Phys Chem B Condens Matter Mater Surf Interfaces Biophys* 110, 3517-3526.
263. Stouffer, A.L., DeGrado, W.F. & Lear, J.D (2006) Analytical Ultracentrifugation Studies of the Influenza M2 Homotetramerization Equilibrium in Detergent Solutions. *Progr Colloid Polym Sci* 131: 108-115.
264. Tatko, C.D., Nanda, V., Lear, J.D., DeGrado, W.F (2006) Polar networks control oligomeric assembly in membranes, *J Am Chem Soc* 128, 4170-1.
265. Litvinov, R.I., Vilaire, G., Li, W., DeGrado, W.F., Weisel, J.W., & Bennett, J.S (2006) Activation of individual alphaIIb beta3 integrin molecules by disruption of transmembrane domain interactions in the absence of clustering. *Biochemistry* 45, 4957-64.
266. Lopez, C., Nielsen, S., Srinivas, G., WF, D. & MK, K (2006) Probing membrane insertion activity of antimicrobial polymers via coarse-grain molecular dynamics. *J Chem Theory Comp* 2, 649-655.

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

267. North B, Cristian L, Fu Stowell X, Lear JD, Saven JG, **DeGrado WF**. Characterization of a membrane protein folding motif, the Ser zipper, using designed peptides. *J Mol Biol*. 2006 Jun 16;359(4):930-9. Epub 2006 Apr 19. PubMed PMID: 16697010.
268. **DeGrado WF** & Woolfson, D. N (2006) Engineering and design. *Curr Opin Struct Biol* **16**, 505-7.
269. Yin, H., Gerlach, L.O., Miller, M.W., Moore, D.T., Liu, D., Vilaire, G., Bennett, J.S. & DeGrado, W.F (2006) Arylamide derivatives as allosteric inhibitors of the integrin alpha(2)beta(1)/type 1 collagen interaction. *Bioorg Med Chem Lett* **16** (13) 3380-82.
270. Wade, H., Stayrook, S. E. & **DeGrado WF** (2006) The structure of a designed diiron(III) protein: implications for cofactor stabilization and catalysis. *Angew Chem Int Ed Engl* **45**, 4951-4.
271. Walters, R. F. & **DeGrado WF** (2006) Helix-packing motifs in membrane proteins. *Proc Natl Acad Sci US A* **103**, 13658-63.
272. Bunagan, M. R., Cristian, L., **DeGrado WF** & Gai, F (2006) Truncation of a cross-linked GCN4-p1 coiled coil leads to ultrafast folding. *Biochemistry* **45**, 10981-6.
273. Fang, C., Senes, A., Cristian, L., **DeGrado WF** & Hochstrasser, R. M (2006) Amide vibrations are delocalized across the hydrophobic interface of a transmembrane helix dimer. *Proc Natl Acad Sci US A* **103**, 16740-5.
274. Yin, H., Litvinov, R. I., Vilaire, G., Zhu, H., Li, W., Caputo, G. A., Moore, D. T., Lear, J. D., Weisel, J. W., **DeGrado WF** & Bennett, J. S (2006) Activation of platelet alphaIIb beta3 by an exogenous peptide corresponding to the transmembrane domain of alphaIIb. *J Biol Chem* **281**, 36732-41.
275. Senes, A., Chadi, D. C., Law, P. B., Walters, R. F., Nanda, V. & **DeGrado WF** (2007) E(z), a depth-dependent potential for assessing the energies of insertion of amino acid side-chains into membranes: derivation and applications to determining the orientation of transmembrane and interfacial helices. *J Mol Biol* **366**, 436-48.
276. Dal Peraro, M., Spiegel, K., Lamoureux, G., Vivo, M. D., **DeGrado WF** & Klein, M. L (2007) Modeling the charge distribution at metal sites in proteins for molecular dynamics simulations. *J Struct Biol* **157**, 444-53.
277. White, T. C., Berny, M. A., Robinson, D. K., Yin, H., **DeGrado WF**, Hanson, S. R. & McCarty, O. J (2007) The leech product saratin is a potent inhibitor of platelet integrin alpha2beta1 and von Willebrand factor binding to collagen. *Febs J* **274**, 1481-91.
278. Yin, H., Slusky, J. S., Berger, B. W., Walters, R. S., Vilaire, G., Litvinov, R. I., Lear, J. D., Caputo, G. A., Bennett, J. S. & **DeGrado WF** (2007) Computational design of peptides that target transmembrane helices. *Science* **315**, 1817-22.
279. Lee MH, Adams CS, Boettiger D, **DeGrado WF**, Shapiro IM, Composto RJ, Ducheyne P. Adhesion of MC3T3-E1 cells to RGD peptides of different flanking residues: detachment strength and correlation with long-term cellular function. *J Biomed Mater Res A*. 2007 Apr;81(1):150-60.
280. Metcalf, D. G., Law, P. B. & **DeGrado WF** (2007) Mutagenesis data in the automated prediction of transmembrane helix dimers. *Proteins* **67**, 375-84.
281. Goodman, C. M., Choi, S., Shandler, S. & **DeGrado WF** (2007) Foldamers as versatile frameworks for the design and evolution of function. *Nat Chem Biol* **3**, 252-262.
282. Cady, S. D., Goodman, C., Tatko, C. D., **DeGrado WF** & Hong, M (2007) Determining the orientation of uniaxially rotating membrane proteins using unoriented samples: a (2)h, (13)c, and (15)n solid-state NMR investigation of the dynamics and orientation of a transmembrane helical bundle. *J Am Chem Soc* **129**, 5719-29.
283. Wang PC, Vilaire, G., **DeGrado WF** & Bennett, J. S (2007) Interactions of ADP-stimulated human platelets with PEGylated polystyrene substrates prepared by surface amidation. *Colloids Surf B Biointerfaces* **58**:225-230.
284. Finikova OS, Troxler T, Senes A, **DeGrado WF**, Hochstrasser RM, Vinogradov SA (2007) Energy and electron transfer in enhanced two-photon-absorbing systems with triplet cores. *J Phys Chem A* **111**:6977-6990.

CURRICULUM VITAE
WILLIAM F. DEGRADO

285. Bender GM, Lehmann A, Zou H, Cheng H, Fry HC, Engel D, Therien MJ, Blasie JK, Roder H, Saven JG, **DeGrado WF** (2007) De novo design of a single-chain diphenylporphyrin metalloprotein. *J Am Chem Soc* 129, 10732-10740.
286. Mukherjee S, Chowdhury P, **DeGrado WF**, Gai F (2007) Site-specific hydration status of an amphipathic peptide in AOT reverse micelles. *Langmuir* 23:11174-11179.
287. Balakrishnan G, Hu Y, Bender GM, Getahun Z, **DeGrado WF**, Spiro TG (2007) Enthalpic and entropic stages in alpha-helical peptide unfolding, from laser T-jump/UV Raman spectroscopy. *J Am Chem Soc* 129:12801-12808.
288. Choi S, Vilaire G, Marcinkiewicz C, Winkler JD, Bennett JS, **DeGrado WF** (2007) Small molecule inhibitors of integrin alpha2beta1. *J Med Chem* 50:5457-5462.
289. Tang J, Signarvic RS, **DeGrado WF**, & Gai F (2007) Role of helix nucleation in the kinetics of binding of mastoparan X to phospholipid bilayers. *Biochemistry* 46:13856-13863.
290. Stouffer AL, Acharya R, Salom D, Levine AS, Di Costanzo L, Soto CS, Tereshko V, Nanda V, Stayrook S, **DeGrado WF** (2008) Structural basis for the function and inhibition of an influenza virus proton channel. *Nature* 451:596-599.
291. Fadeev Alexander Y. **DeGrado William F.**, (2008) COLL 23-Lipid-bilayers supported on nanosilicas: Optically transparent systems for model biochemical studies. *Abstracts of Papers of the American Chemical Society* 236.
292. Calhoun JR, Liu W, Spiegel K, Dal Peraro M, Klein ML, Valentine KG, Wand AJ, **DeGrado WF** (2008) Solution NMR structure of a designed metalloprotein and complementary molecular dynamics refinement. *Structure* 16, 210-215.
293. Ma C, Soto CS, Ohigashi Y, Taylor A, Bournas V, Glawe B, Udo MK, **DeGrado WF**, Lamb RA, Pinto LH (2008) Identification of the Pore-lining Residues of the BM2 Ion Channel Protein of Influenza B Virus. *J Biol Chem* 283:15921-15931.
294. Goldberg SD, Soto CS, Waldburger CD, **DeGrado WF** (2008) Determination of the physiological dimer interface of the PhoQ sensor domain. *J Mol Biol* 379:656-665.
295. Moore DT, Berger BW, **DeGrado WF** (2008) Protein-protein interactions in the membrane: sequence, structural, and biological motifs. *Structure* 16:991-1001.
296. Stouffer AL, Ma C, Cristian L, Ohigashi Y, Lamb RA, Lear JD, Pinto LH, **DeGrado WF** (2008) The interplay of functional tuning, drug resistance, and thermodynamic stability in the evolution of the M2 proton channel from the influenza A virus. *Structure*. 16:1067-1076.
297. Grigoryan G, **DeGrado WF** (2008) Modest membrane hydrogen bonds deliver rich results. *Nat Chem Biol* 4:393-394.
298. Calhoun JR, Bell CB 3rd, Smith TJ, Thamann TJ, **DeGrado WF**, Solomon EI (2008) Oxygen reactivity of the biferrrous site in the de novo designed four helix bundle peptide DFsc: nature of the "intermediate" and reaction mechanism. *J Am Chem Soc* 130:9188-9189.
299. Shu JY, Tan C, **DeGrado WF**, Xu T (2008) New design of helix bundle peptide-polymer conjugates. *Biomacromolecules* 9:2111-2117.
300. Caputo GA, Litvinov RI, Li W, Bennett JS, **DeGrado WF** & Yin, H (2008) Computationally designed peptide inhibitors of protein-protein interactions in membranes. *Biochemistry* 47:8600-8606.
301. McAllister KA, Zou H, Cochran FV, Bender GM, Senes A, Fry HC, Nanda V, Keenan PA, Lear JD, Saven JG, Therien MJ, Blasie JK, **DeGrado WF** (2008) Using alpha-helical coiled-coils to design nanostructured metalloporphyrin arrays. *J Am Chem Soc* 130:11921-11927.
302. Nguyen PA, Soto CS, Polishchuk A, Caputo GA, Tatko CD, Ma C, Ohigashi Y, Pinto LH, **DeGrado WF**, Howard KP (2008) pH-Induced Conformational Change of the Influenza M2 Protein C-Terminal Domain. *Biochemistry* 47:9934-9936.

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

303. Scott RW, **DeGrado WF**, Tew GN (2008) De novo designed synthetic mimics of antimicrobial peptides. *Curr Opin Biotechnol* 19:620-627.
304. Goldberg SD, Derr P, **DeGrado WF**, Goulian M (2009) Engineered single- and multi-cell chemotaxis pathways in *E. coli*. *Mol Syst Biol* 5:283.
305. Kuroda K, Caputo GA, **DeGrado WF** (2009) The role of hydrophobicity in the antimicrobial and hemolytic activities of polymethacrylate derivatives. *Chemistry* 15:1123-1133.
306. Bell CB, Calhoun JR, Bobyr E, Wei PP, Hedman B, Hodgson KO, **DeGrado WF**, Solomon EI (2009) Spectroscopic definition of the biferrous and biferric sites in de novo designed four-helix bundle DFsc peptides: implications for O₂ reactivity of binuclear non-heme iron enzymes. *Biochemistry* 48:59-73.
307. Miller MW, Basra S, Kulp DW, Billings PC, Choi S, Beavers MP, McCarty OJ, Zou Z, Kahn ML, Bennett JS & **DeGrado WF** (2009) Small-molecule inhibitors of integrin alpha2beta1 that prevent pathological thrombus formation via an allosteric mechanism. *Proc Natl Acad Sci U S A* 106:719-724.
308. Basani RB, Zhu H, Thornton MA, Soto CS, **DeGrado WF**, Kowalska MA, Bennett JS, Poncz M (2009) Species differences in small molecule binding to alpha IIb beta 3 are the result of sequence differences in 2 loops of the alpha IIb beta propeller. *Blood* 113, 902-10.
309. Khurana E, Dal Peraro M, DeVane R, Vemparala S, **DeGrado WF**, Klein ML (2009) Molecular dynamics calculations suggest a conduction mechanism for the M2 proton channel from influenza A virus. *Proc Natl Acad Sci U S A* 106:1069-1074.
310. Signarvic RS, **DeGrado WF** (2009) Metal-Binding Dependent Disruption of Membranes by Designed Helices. *J Am Chem Soc.* 131:3377-3384.
311. Bissonnette ML, Donald JE, **DeGrado WF**, Jardetzky TS, Lamb, R. A (2009) Functional analysis of the transmembrane domain in paramyxovirus F protein-mediated membrane fusion. *J Mol Biol* 386:14-36.
312. Liu F, Dumont C, Zhu Y, **DeGrado WF**, Gai F, Gruebele M (2009) A one-dimensional free energy surface does not account for two-probe folding kinetics of protein alpha(3)D. *J Chem Phys.* 130:061101.
313. Tang J, Yin H, Qiu J, Tucker MJ, **DeGrado WF**, Gai F (2009) Using two fluorescent probes to dissect the binding, insertion, and dimerization kinetics of a model membrane peptide. *J Am Chem Soc.* 131:3816-3817.
314. Choi S, Isaacs A, Clements D, Liu D, Kim H, Scott RW, Winkler JD, **DeGrado WF** (2009) De novo design and in vivo activity of conformationally restrained antimicrobial arylamide foldamers. *Proc Natl Acad Sci U S A.* 106:6968-6973.
315. Wang J, Cady SD, Balannik V, Pinto LH, **DeGrado WF**, Hong M (2009) Discovery of spiro-piperidine inhibitors and their modulation of the dynamics of the M2 proton channel from influenza A virus. *J Am Chem Soc.* 131:8066-8076.
316. Ma C, Polishchuk AL, Ohigashi Y, Stouffer AL, Schön A, Magavern E, Jing X, Lear JD, Freire E, Lamb RA, **DeGrado WF**, Pinto LH (2009) Identification of the functional core of the influenza A virus A/M2 proton-selective ion channel. *Proc Natl Acad Sci U S A.* 106:12283-12288.
317. Kuhlman B, DeGrado WF (2009) Engineering and design: editorial overview. *Curr Opin Struct Biol* 19:440-441.
318. Zhang Y, Kulp DW, Lear JD, **DeGrado WF** (2009) Experimental and computational evaluation of forces directing the association of transmembrane helices. *J Am Chem* 131:11341-11343.
319. He F, Nair GR, Soto CS, Chang Y, Hsu L, Ronzone E, **DeGrado WF**, Binns AN (2009) Molecular basis of ChvE function in sugar binding, sugar utilization, and virulence in *Agrobacterium tumefaciens*. *J Bacteriol.* 191:5802-5813.
320. San Antonio JD, Zoeller JJ, Habursky K, Turner K, Pimpong W, Burrows M, Choi S, Basra S, Bennett JS, **DeGrado WF**, Iozzo RV (2009) A key role for the integrin alpha2beta1 in experimental and developmental angiogenesis. *Am J Pathol* 175:1338-1347.

CURRICULUM VITAE
WILLIAM F. DEGRADO

321. Metcalf DG, Kulp DW, Bennett JS, **DeGrado WF** (2009) Multiple approaches converge on the structure of the integrin α IIb/ β 3 transmembrane heterodimer. *J Mol Biol* 392:1087-1101.
322. Faiella M, Andreozzi C, de Rosales RT, Pavone V, Maglio O, Natri F, **DeGrado WF** & Lombardi A (2009) An artificial di-iron oxo-protein with phenol oxidase activity. *Nat Chem Biol* 5:882-884.
323. Balannik V, Wang J, Ohigashi Y, Jing X, Magavern E, Lamb RA, **DeGrado WF**, Pinto LH (2009) Design and pharmacological characterization of inhibitors of amantadine-resistant mutants of the M2 ion channel of influenza A virus. *Biochemistry*. 48:11872-11882.
324. Berger BW, Kulp DW, Span LM, DeGrado JL, Billings PC, Senes A, Bennett JS, **DeGrado WF** (2010) Consensus motif for integrin transmembrane helix association. *Proc Natl Acad Sci U S A* 107:703-8.
325. Tew GN, Scott RW, Klein ML, **DeGrado WF** (2010) De novo design of antimicrobial polymers, foldamers, and small molecules: from discovery to practical applications. *Acc Chem Res* 43:30-39.
326. Balannik V, Obrdlik P, Inayat S, Steensen C, Wang J, Rausch JM, **DeGrado WF**, Kelety B, Pinto LH (2010) Solid-supported membrane technology for the investigation of the influenza A virus M2 channel activity. *Pflugers Arch* 459:593-605.
327. Cady SD, Schmidt-Rohr K, Wang J, Soto CS, **DeGrado WF**, Hong M (2010) Structure of the amantadine binding site of influenza M2 proton channels in lipid bilayers. *Nature* 463:689-692.
328. Balannik V, Carnevale V, Fiorin G, Levine BG, Lamb RA, Klein ML, **DeGrado WF**, Pinto LH (2010) Functional studies and modeling of pore-lining residue mutants of the influenza a virus M2 ion channel. *Biochemistry* 49:696-708.
329. Fry HC, Lehmann A, Saven JG, **DeGrado WF**, Therien MJ (2010) Computational design and elaboration of a de novo heterotetrameric alpha-helical protein that selectively binds an emissive abiological (porphinato)zinc chromophore. *J Am Chem Soc* 132:3997-4005.
330. Lucumi, E., Darling, C., Jo, H., Napper, A. D., Chandramohanadas, R., Fisher, N., Shone, A. E., Jing, H., Ward, S. A., Biagini, G. A., DeGrado, W. F., Diamond, S. L. & Greenbaum, D. C. Discovery of potent small-molecule inhibitors of multidrug-resistant Plasmodium falciparum using a novel miniaturized high-throughput luciferase-based assay. *Antimicrob Agents Chemother* **54**, 3597-604.
331. Shandler SJ, Shapovalov MV, Dunbrack RL, Jr., **DeGrado WF** (2010) Development of a rotamer library for use in beta-peptide foldamer computational design. *J Am Chem Soc* 132:7312-7320.
332. Goldberg SD, Clinthorne GD, Goulian M, **DeGrado WF** (2010) Transmembrane polar interactions are required for signaling in the Escherichia coli sensor kinase PhoQ. *Proc Natl Acad Sci U S A* 107:8141-8146.
333. Montalvo G, Waegel MM, Shandler S, Gai F, **DeGrado WF** (2010) Infrared signature and folding dynamics of a helical beta-peptide. *J Am Chem Soc* 132:5616-5618.
334. Balannik, V., Obrdlik, P., Inayat, S., Steensen, C., Wang, J., Rausch, J. M., DeGrado, W. F., Kelety, B. & Pinto, L. H. (2010). Solid-supported membrane technology for the investigation of the influenza A virus M2 channel activity. *Pflugers Arch* **459**, 593-605.
335. Carnevale, V., Fiorin, G., Levine, B. G., DeGrado, W. F. & Klein, M. L. (2010). Multiple Proton Confinement in the M2 Channel from the Influenza A Virus. *J Phys Chem C Nanomater Interfaces* **114**, 20856-20863.
336. Donald, J. E., Zhu, H., Litvinov, R. I., DeGrado, W. F. & Bennett, J. S. (2010). Identification of interacting hot spots in the beta3 integrin stalk using comprehensive interface design. *J Biol Chem* **285**, 38658-65.
337. Fiorin, G., Carnevale, V. & DeGrado, W. F. (2010). The Flu's Proton Escort. *Science* **330**, 456-8.
338. Jo, H., Culik, R. M., Korendovych, I. V., DeGrado, W. F. & Gai, F. (2010). Selective incorporation of nitrile-based infrared probes into proteins via cysteine alkylation. *Biochemistry* **49**, 10354-6.
339. Korendovych, I. V., Kim, Y. H., Ryan, A. H., Lear, J. D., DeGrado, W. F. & Shandler, S. J. (2010). Computational design of a self-assembling beta-peptide oligomer. *Org Lett* **12**, 5142-5.

CURRICULUM VITAE
WILLIAM F. DEGRADO

340. Korendovych, I. V., Senes, A., Kim, Y. H., Lear, J. D., Fry, H. C., Therien, M. J., Blasie, J. K., Walker, F. A. & DeGrado, W. F. (2010). De novo design and molecular assembly of a transmembrane diporphyrin-binding protein complex. *J Am Chem Soc* **132**, 15516-8.
341. Lau, W. L., DeGrado, W. F. & Roder, H. (2010). The effects of pK(a) tuning on the thermodynamics and kinetics of folding: design of a solvent-shielded carboxylate pair at the α -position of a coiled-coil. *Biophys J* **99**, 2299-308.
342. Su Yongchao, DeGrado William F., Hong Mei. (2010). Orientation, Dynamics, and Lipid Interaction of an Antimicrobial Arylamide Investigated by (19)F and (31)P Solid-State NMR Spectroscopy, *J Am Chem Soc* **132**, 9197-9205.
343. Ivankin A, Livne L, Mor A, Caputo GA, DeGrado WF, Meron M, Lin B, Gidalevitz D (2010) Role of the conformational rigidity in the design of biomimetic antimicrobial compounds. *Angew Chem Int Ed Engl* **49**:8462-8465.
344. Leiding Thom; Martinsson Jonas; DeGrado William. (2010) Proton/ion co-transport by protein M2 of influenza virus A. *Biochemica ET Biophysica Acta-Bioenergetics* **1797**, 45-45.
345. Leiding, T., Wang, J., Martinsson, J., DeGrado, W. F. & Arskold, S. P. (2010). Proton and cation transport activity of the M2 proton channel from influenza A virus. *Proc Natl Acad Sci U S A* **107**, 15409-14.
346. Metcalf, D. G., Moore, D. T., Wu, Y., Kielec, J. M., Molnar, K., Valentine, K. G., Wand, A. J., Bennett, J. S. & DeGrado, W. F. (2010). NMR analysis of the α 11b β 3 cytoplasmic interaction suggests a mechanism for integrin regulation. *Proc Natl Acad Sci U S A* **107**, 22481-6.
347. Polishchuk, A. L., Lear, J. D., Ma, C., Lamb, R. A., Pinto, L. H. & DeGrado, W. F. (2010). A pH-dependent conformational ensemble mediates proton transport through the influenza A/M2 protein. *Biochemistry* **49**, 10061-71.
348. Zhu, H., Metcalf, D. G., Streu, C. N., Billings, P. C., DeGrado, W. F. & Bennett, J. S. (2010). Specificity for homooligomer versus heterooligomer formation in integrin transmembrane helices. *J Mol Biol* **401**, 882-91.
349. Acharya, R., Carnevale, V., Fiorin, G., Levine, B. G., Polishchuk, A. L., Balannik, V., Samish, I., Lamb, R. A., Pinto, L. H., DeGrado, W. F. & Klein, M. L. (2010). Structure and mechanism of proton transport through the transmembrane tetrameric M2 protein bundle of the influenza A virus. *Proc Natl Acad Sci U S A* **107**, 15075-80.
350. DeGrado W. F., (2010). From peptides to proteins: Analysis of the hierarchic organization of proteins and de novo design of protein-like architectures. *Journal of Peptide Science* **16**, 23-23.
351. Wang, J., Qiu, J. X., Soto, C. & DeGrado, W. F. (2011). Structural and dynamic mechanisms for the function and inhibition of the M2 proton channel from influenza A virus. *Curr Opin Struct Biol* **21**, 68-80.
352. Fadeev, A. Y. & DeGrado, W. F. (2011). Lipid membranes supported on optically transparent nanosilicas: synthesis and application in characterization of protein-membrane interactions. *J Colloid Interface Sci* **355**, 265-8.
353. Chakraborty, S., Yudenfreund Kravitz, J., Thulstrup, P. W., Hemmingsen, L., DeGrado, W. F. & Pecoraro, V. L. (2011). Design of a three-helix bundle capable of binding heavy metals in a triscysteine environment. *Angew Chem Int Ed Engl* **50**, 2049-53.
354. Rogers, J. M., Polishchuk, A. L., Guo, L., Wang, J., DeGrado, W. F. & Gai, F. (2011). Photoinduced Electron Transfer and Fluorophore Motion as a Probe of the Conformational Dynamics of Membrane Proteins: Application to the Influenza A M2 Proton Channel. *Langmuir*.
355. Cady, S. D., Wang, J., Wu, Y., DeGrado, W. F. & Hong, M. (2011). Specific Binding of Adamantane Drugs and Direction of Their Polar Amines in the Pore of the Influenza M2 Transmembrane Domain in Lipid Bilayers and Dodecylphosphocholine Micelles Determined by NMR Spectroscopy. *J Am Chem Soc.* ``
356. Donald, J. E., Zhang, Y., Fiorin, G., Carnevale, V., Slochower, D. R., Gai, F., Klein, M. L. & DeGrado, W. F. (2011). From the Cover: Transmembrane orientation and possible role of the fusogenic peptide from parainfluenza virus 5 (PIV5) in promoting fusion. *Proc Natl Acad Sci U S A* **108**, 3958-63.

CURRICULUM VITAE
WILLIAM F. DEGRADO

357. Donald, J. E., Kulp, D. W. & DeGrado, W. F. (2011). Salt bridges: geometrically specific, designable interactions. *Proteins* **79**, 898-915.
358. Grigoryan, G. & DeGrado, W. F. (2011). Probing designability via a generalized model of helical bundle geometry. *J Mol Biol* **405**, 1079-100.
359. Grigoryan, G., Kim, Y.H. Acharya, R., Axelrod, K., Jain, R. M., Willis, L., Drndic, R., Kikkawa, J.M., **DeGrado, W.F.** (2011) Computational Design of Virus-like Protein Assemblies on Carbon Nanotube Surfaces. *Science* **332**, 1071-6.
360. Remorino, A., Korendovych, I., Wu, Y, **DeGrado, W.F.**, Hochstrasser, R.M. (2011) Three dimensional structures of transmembrane proteins from residue specific vibrational photon echoes. *Science* **332**, 1206-9.
361. Grigoryan, G., Moore, D. T. & DeGrado, W. F. (2011). Transmembrane communication: general principles and lessons from the structure and function of the M2 proton channel, K channels, and integrin receptors. *Annu Rev Biochem* **80**, 211-37.
362. Korendovych, I. V., Shandler, S. J., Montalvo, G. L. & DeGrado, W. F. (2011). Environment- and sequence-dependence of helical type in membrane-spanning peptides composed of beta3-amino acids. *Org Lett* **13**, 3474-7.
363. Wang, J., Ma, C., Balannik, V., Pinto, L. H., Lamb, R. A. & DeGrado, W. F. (2011). Exploring the Requirements for the Hydrophobic Scaffold and Polar Amine in inhibitors of M2 from Influenza A Virus. *ACS Med Chem Lett* **2**, 307-312.
364. Wang, J., Ma, C., Fiorin, G., Carnevale, V., Wang, T., Hu, F., Lamb, R. A., Pinto, L. H., Hong, M., Klein, M. L. & DeGrado, W. F. (2011). Molecular dynamics simulation directed rational design of inhibitors targeting drug-resistant mutants of influenza A virus M2. *J Am Chem Soc* **133**, 12834-41.
365. Shandler, S. J., Korendovych, I. V., Moore, D. T., Smith-Dupont, K. B., Streu, C. N., Litvinov, R. I., Billings, P. C., Gai, F., Bennett, J. S. & DeGrado, W. F. (2011). Computational design of a beta-peptide that targets transmembrane helices. *J Am Chem Soc* **133**, 12378-81.
366. Wang, J., Ma, C., Wu, Y., Lamb, R. A., Pinto, L. H. & DeGrado, W. F. (2011). Exploring organosilane amines as potent inhibitors and structural probes of influenza a virus M2 proton channel. *J Am Chem Soc* **133**, 13844-7.
367. Mensa, B., Kim, Y. H., Choi, S., Scott, R., Caputo, G. A. & DeGrado, W. F. (2011). Antibacterial mechanism of action of arylamide foldamers. *Antimicrob Agents Chemother* **55**, 5043-53.
368. Soto, C. S., Hannigan, B. T. & DeGrado, W. F. (2011). A photon-free approach to transmembrane protein structure determination. *J Mol Biol* **414**, 596-610.
369. Kim, Y. H., Donald, J. E., Grigoryan, G., Leser, G. P., Fadeev, A. Y., Lamb, R. A. & DeGrado, W. F. (2011). Capture and imaging of a prehairpin fusion intermediate of the paramyxovirus PIV5. *Proc Natl Acad Sci U S A* **108**, 20992-7.
370. Moore, D. T., Nygren, P., Jo, H., Boesze-Battaglia, K., Bennett, J. S. & DeGrado, W. F. (2012). Affinity of talin-1 for the beta3-integrin cytosolic domain is modulated by its phospholipid bilayer environment. *Proc Natl Acad Sci U S A* **109**, 793-8.
371. Montero, M., Gulzar N., Klaric K., A. Donald, J. E. Lepik, C. Wu, S. Tsai, S, Julien, J. P. Hessel, A. J., Wang, S. Lu S., Burton D. R., Pai, E. F., DeGrado, W. F. Scott, J. K., (2012) Neutralizing Epitopes in the Membrane-Proximal External Region of HIV-1 gp41 Are Influenced by the Transmembrane Domain and the Plasma Membrane. *J Virol.* **86**, 2930-41.
372. Borza, C. M., Su, Y., Chen, X., Yu, L., Mont, S., Chetyrkin, S., Voziyan, P., Hudson, B. G., Billings, P. C., Jo, H., Bennett, J. S., DeGrado, W. F., Eckes, B., Zent, R. & Pozzi, A. (2012). Inhibition of integrin alpha2beta1 ameliorates glomerular injury. *J Am Soc Nephrol* **23**, 1027-38.
373. Culik, R. M., Jo, H., DeGrado, W. F. & Gai, F. (2012). Using thioamides to site-specifically interrogate the dynamics of hydrogen bond formation in beta-sheet folding. *J Am Chem Soc* **134**, 8026-9.
374. Hong, M. & DeGrado, W. F. (2012). Structural basis for proton conduction and inhibition by the influenza M2 protein. *Protein Sci* **21**, 1620-33.

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

375. Jo, H., Meinhardt, N., Wu, Y., Kulkarni, S., Hu, X., Low, K. E., Davies, P. L., DeGrado, W. F. & Greenbaum, D. C. (2012). Development of alpha-helical calpain probes by mimicking a natural protein-protein interaction. *J Am Chem Soc* **134**, 17704-13.
376. Lanci, C. J., MacDermaid, C. M., Kang, S. G., Acharya, R., North, B., Yang, X., Qiu, X. J., DeGrado, W. F. & Saven, J. G. (2012). Computational design of a protein crystal. *Proc Natl Acad Sci U S A* **109**, 7304-9.
377. Love, M. S., Millholland, M. G., Mishra, S., Kulkarni, S., Freeman, K. B., Pan, W., Kavash, R. W., Costanzo, M. J., Jo, H., Daly, T. M., Williams, D. R., Kowalska, M. A., Bergman, L. W., Poncz, M., DeGrado, W. F., Sinnis, P., Scott, R. W. & Greenbaum, D. C. (2012). Platelet Factor 4 Activity against *P. falciparum* and Its Translation to Nonpeptidic Mimics as Antimalarials. *Cell Host Microbe* **12**, 815-23.
378. Reig, A. J., Pires, M. M., Snyder, R. A., Wu, Y., Jo, H., Kulp, D. W., Butch, S. E., Calhoun, J. R., Szyperki, T. G., Solomon, E. I. & DeGrado, W. F. (2012). Alteration of the oxygen-dependent reactivity of de novo DUE Ferri proteins. *Nat Chem* **4**, 900-6.
379. Schramm, C. A., Hannigan, B. T., Donald, J. E., Keasar, C., Saven, J. G., DeGrado, W. F. & Samish, I. (2012). Knowledge-based potential for positioning membrane-associated structures and assessing residue-specific energetic contributions. *Structure* **20**, 924-35.
380. Balgi, A. D., Wang, J., Cheng, D. Y., Ma, C., Pfeifer, T. A., Shimizu, Y., Anderson, H. J., Pinto, L. H., Lamb, R. A., DeGrado, W. F. & Roberge, M. (2013). Inhibitors of the influenza A virus M2 proton channel discovered using a high-throughput yeast growth restoration assay. *PLoS One* **8**, e55271.
381. Hu, X., Zhao, J., DeGrado, W. F. & Binns, A. N. (2013). *Agrobacterium tumefaciens* recognizes its host environment using ChvE to bind diverse plant sugars as virulence signals. *Proc Natl Acad Sci U S A* **110**, 678-83.
382. Lemmin, T., Soto, C. S., Clinthorne, G., DeGrado, W. F. & Dal Peraro, M. (2013). Assembly of the Transmembrane Domain of *E. coli* PhoQ Histidine Kinase: Implications for Signal Transduction from Molecular Simulations. *PLoS Comput Biol* **9**, e1002878.
383. Mao, L., Wang, J., DeGrado, W. F. & Inouye, M. (2013). An assay suitable for high throughput screening of anti-influenza drugs. *PLoS One* **8**, e54070.
384. Thomaston, J. L., Nguyen, P. A., Brown, E. C., Upshur, M. A., Wang, J., DeGrado, W. F. & Howard, K. P. (2013). Detection of drug-induced conformational change of a transmembrane protein in lipid bilayers using site-directed spin labeling. *Protein Sci* **22**, 65-73.
385. Wang, J., Wu, Y., Ma, C., Fiorin, G., Wang, J., Pinto, L. H., Lamb, R. A., Klein, M. L. & DeGrado, W. F. (2013). Structure and inhibition of the drug-resistant S31N mutant of the M2 ion channel of influenza A virus. *Proc Natl Acad Sci U S A* **110**, 1315-20.
386. Wang J, *et al.* (2013) Discovery of novel dual inhibitors of the wild-type and the most prevalent drug-resistant mutant, S31N, of the M2 proton channel from influenza A virus. *J Med Chem* **56**(7):2804-2812.

U.S. Patents (Issued)

1. DeGrado, William Frank; Jackson, Sharon Anne; Mousa, Shaker Ahmed; Parthasarathy, Anju; Sworin, Michael. Preparation of cyclopeptides useful as inhibitors of platelet glycoprotein IIb/IIIa. PCT Int. Appl. (1993), 211 pp. CODEN: PIXXD2 WO 9307170 A1 19930415 CAN 120:164903 AN 1994:164903 CAPLUS
2. Robertson, Dan E.; Farid, Ramy S.; DeGrado, William F.; Dutton, P. Leslie. Electrically conducting synthetic peptide complexes. PCT Int. Appl. (1994), 34 pp. CODEN: PIXXD2 WO 9415628 A1 19940721 CAN 121:200396 AN 1994:600396 CAPLUS
3. DeGrado, William Frank; Dorow, Roberta Louise; Ward, Randall Kay; Xue, Chu-Biao. Process for the preparation of cyclopeptide platelet glycoprotein IIb/IIIa inhibitors containing N^ε-methylarginine. PCT Int. Appl. (1994), 161 pp. CODEN: PIXXD2 WO 9422911 A2 19941013 CAN 122:133860 AN 1995:350562 CAPLUS
4. Wells, Gregory James; Wityak, John; Parthasarathy, Anju; DeGrado, William Frank; Jackson, Sharon Anne; Mousa, Shaker Ahmed. Preparation of peptides cyclocondensed to heterocyclic rings useful as antagonists of platelet glycoprotein IIb/IIIa. PCT Int. Appl. (1994), 179 pp. CODEN: PIXXD2 WO 9411398 A1 19940526 CAN 122:133849 AN 1995:356700 CAPLUS
5. Zhang, Lin Hua; Ma, Philip; DeGrado, William Frank. Process for the preparation of cyclopeptide platelet

CURRICULUM VITAE
WILLIAM F. DEGRADO

- glycoprotein IIb/IIIa inhibitors. PCT Int. Appl. (1994), 93 pp. CODEN: PIXXD2 WO 9422909 A1 19941013 CAN 122:133862 AN 1995:358758 CAPLUS
6. DeGrado, William Frank; Jackson, Sharon Anne; Mousa, Shaker Ahmed; Parthasarathy, Anju; Sworin, Michael; Rafalski, Maria. Preparation of cyclic peptides as inhibitors of platelet glycoprotein IIb/IIIa. PCT Int. Appl. (1994), 254 pp. CODEN: PIXXD2 WO 9422910 A1 19941013 CAN 123:144642 AN 1995:723128 CAPLUS
 7. DeGrado, William Frank; Mousa, Shaker Ahmed; Sworin, Michael; Barrett, John Andrew; Edwards, David Scott; Harris, Thomas David; Rajopadhye, Milind; Liu, Shuang. Preparation of radiolabeled platelet GPIIb/IIIa receptor antagonists as imaging agents for the diagnosis of thromboembolic disorders. PCT Int. Appl. (1994), 459 pp. CODEN: PIXXD2 WO 9422494 A1 19941013 CAN 123:199405 AN 1995:767392 CAPLUS
 8. DeGrado, William Frank; Xue, Chu-Biao. Preparation of compounds containing basic and acidic termini useful as fibrinogen receptor antagonists. PCT Int. Appl. (1995), 201 pp. CODEN: PIXXD2 WO 9518111 A1 19950706 CAN 123:285548 AN 1995:890154 CAPLUS
 9. Wityak, John; Xue, Chu-Biao; Sielecki-Dzurdz, Thais Motria; Olson, Richard Eric; DeGrado, William Frank; Cain, Gary Avonn. Preparation of isoxazolinealkanoates and analogs as fibrinogen receptor antagonists. PCT Int. Appl. (1995), 376 pp. CODEN: PIXXD2 WO 9514683 A1 19950601 CAN 124:8795 AN 1995:943445 CAPLUS
 10. DeGrado, William F.; Xue, Chu-biao. Aromatic compounds containing basic and acidic termini useful as fibrinogen receptor antagonists. U.S. (1996), 83 pp., Cont.-in-part of U.S. Ser. No. 174,552, abandoned. CODEN: USXXAM US 5563158 A 19961008 CAN 125:329475 AN 1996:653632 CAPLUS
 11. Xue, Chu-Biao; DeGrado, William F.; Decicco, Carl Peter. Preparation of novel hydroxamic acid and amino-carboxylate compounds as metalloprotease and TNF inhibitors. PCT Int. Appl. (1996), 100 pp. CODEN: PIXXD2 WO 9633176 A1 19961024 CAN 126:31664 AN 1997:4165 CAPLUS
 12. Wityak, John; Cain, Gary Avonn; Batt, Douglas Guy; Pinto, Donald; Hussain, Munir Alwan; Xue, Chu-Biao; Sielecki-Dzurdz, Thais Motria; Olson, Richard Eric; DeGrado, William Frank; Mousa, Shaker Ahmed. Preparation of novel isoxazoline and isoxazole fibrinogen receptor antagonists. PCT Int. Appl. (1996), 412 pp. CODEN: PIXXD2 WO 9638426 A1 19961205 CAN 126:117965 AN 1997:105201 CAPLUS
 13. Xue, C.-B., **DeGrado WF**, DeCicco, C. P., Jacobson, I. C. "Hydroxamic acid compounds as metalloprotease and TNF inhibitors" US Patent # 5,703,092 (Dec. 1997).
 14. **DeGrado WF**, Jackson, S. A., Mousa, S. A., Parthasarathy, A., Sworin, M., Rafalski, M. "Cyclic compounds useful as inhibitors of glycoprotein IIb/IIIa" US Patent number 5,635,477 (June 3, 1997).
 15. Xue, Chu-Biao; Cherney, Robert Joseph; Decicco, Carl Peter; DeGrado, William Frank; He, Xiaohua; Hodge, Carl Nicolas; Jacobson, Irina Cipora; Magolda, Ronald Louis; Arner, Elizabeth Catherine; Duan, Jingwu; Nelson, David J. Novel macrocyclic compounds as metalloprotease inhibitors. PCT Int. Appl. (1997), 351 pp. CODEN: PIXXD2 WO 9718207 A2 19970522 CAN 127:81789 AN 1997:443298 CAPLUS
 16. Xue, Chu-biao; DeGrado, William F.; Decicco, Carl Peter; Jacobson, Irina Cipora. Preparation of peptidyl hydroxamic acid derivatives as metalloprotease and tumor necrosis factor inhibitors. U.S. (1997), 26 pp., Cont.-in-part of U.S. Ser. No. 423,197, abandoned. CODEN: USXXAM US 5703092 A 19971230 CAN 128:102393 AN 1998:28238 CAPLUS
 17. Wells, G. J., Wityak, J., Parthasarathy, A., DeGrado, W., Jackson, S. A., Mousa, S. A. Cyclic compounds linked by a heterocyclic ring useful as inhibitors of platelet glycoprotein IIB/IIIA US Patent #5,773,411 (June 30, 1998).
 18. Xue, Chu-Bio; Decicco, Carl P.; Cherney, Robert J.; Arner, Elizabeth; DeGrado, William F.; Duan, Jingwu; He, Xiaohua; Jacobson, Irina Cipora; Magolda, Ronald L.; Nelson, David. Novel macrocyclic compounds as metalloprotease inhibitors. PCT Int. Appl. (1998), 80 pp. CODEN: PIXXD2 WO 9851665 A2 19981119 CAN 130:14260 AN 1998:761877 CAPLUS
 19. Wityak, John; Xue, Chu-Biao; Sielecki-Dzurdz, Thais Motria; Olson, Richard Eric; DeGrado, William Frank; Cain, Gary Avonn; Batt, Douglas Guy; Pinto, Donald; Hussain, Munir Alwan; Mousa, Shaker Ahmed. Preparation of isoxazoline and isoxazole fibrinogen receptor antagonists. U.S. (1998), 153 pp., Cont.-in-part of U.S. Ser. No. 337,920, abandoned. CODEN: USXXAM US 5849736 A 19981215 CAN 130:66484 AN 1998:816104 CAPLUS
 20. DeGrado, William Frank; Mousa, Shaker Ahmed; Sworin, Michael; Barrett, John Andrew; Edwards, Scott David; Harris, Thomas David; Rajopadhye, Milind; Liu, Shuang. Preparation of radiolabeled platelet GPIIb/IIIa receptor antagonists as imaging agents for the diagnosis of thromboembolic disorders. U.S. (1999), 135 pp., Cont.-in-part of U.S. Ser. No. 40,336, abandoned. CODEN: USXXAM US 5879657 A 19990309 CAN 130:237883 AN 1999:181611 CAPLUS
 21. W. F. DeGrado "Design, Preparation & Properties of Antibacterial beta-Peptides" (Submitted, U.S. Patent, 11

**CURRICULUM VITAE
WILLIAM F. DEGRADO**

- Dec. 2000).
22. Xue, Chu-bio; Decicco, Carl P.; Cherney, Robert J.; Arner, Elizabeth; DeGrado, William F.; Duan, Jingwu; He, Xiaohua; Jacobson, Irina Cipora; Magolda, Ronald L.; Nelson, David. Novel macrocyclic compounds as metalloprotease inhibitors. U.S. (2001), 118 pp., Cont.-in-part of U.S. Ser. No. 743,439, abandoned. CODEN: USXXAM US 6281352 B1 20010828 CAN 135:195793 AN 2001:630906 CAPLUS
 23. DeGrado, William F.; Tew, Gregory N.; Klein, Michael L. Facially amphiphilic polymers as anti-infective agents, articles, and attaching facially amphiphilic polymers to a solid support. PCT Int. Appl. (2002), 48 pp. CODEN: PIXXD2 WO 2002072007 A2 20020919 CAN 137:233786 AN 2002:716014 CAPLUS
 24. DeGrado, William F.; Hamuro, Yoshimoto; Liu, Dahui. Design, preparation, and properties of antibacterial peptides. U.S. Pat. Appl. Publ. (2002), 22 pp. CODEN: USXXCO US 2002132766 A1 20020919 CAN 137:232921 AN 2002:717050 CAPLUS
 25. Doerksen, Robert J.; Chen, Bin; Klein, Michael L.; DeGrado, William F.. Methods, systems, and computer program products for computational analysis and design of amphiphilic polymers. PCT Int. Appl. (2003), 31 pp. CODEN: PIXXD2 WO 2003100701 A1 20031204 CAN 139:396387 AN 2003:951325 CAPLUS
 26. Saven, Jeffery G.; DeGrado, William F.; Slovic, Avram M.; Summa, Christopher M.; Kono, Hidetoshi. Computational design of a water-soluble analog of a protein, such as phospholamban and potassium channel KcsA. PCT Int. Appl. (2004), 73 pp. CODEN: PIXXD2 WO 2004065363 A2 20040805 CAN 141:169771 AN 2004:633910 CAPLUS
 27. DeGrado, William F.; Liu, Dahui; Tew, Gregory N.; Klein, Michael L.; Yuan, Jing; Choi, Sungwook. Facially amphiphilic polymers and oligomers and uses. PCT Int. Appl. (2004), 211 pp. CODEN: PIXXD2 WO 2004082634 A2 20040930 CAN 141:314809 AN 2004:802698 CAPLUS
 28. DeGrado, William F.; Liu, Dahui; Tew, Gregory N.; Klein, Michael L. Facially amphiphilic polyaryl and polyaryalkynyl polymers and oligomers and uses thereof. PCT Int. Appl. (2005), 105 pp. CODEN: PIXXD2 WO 2005072246 A2 20050811 CAN 143:186694 AN 2005:732525 CAPLUS
 29. Kuroda, Kenichi; DeGrado, William F. Antimicrobial copolymers, preparation and uses in pharmaceuticals. U.S. Pat. Appl. Publ. (2006), 44 pp. CODEN: USXXCO US 2006024264 A1 20060202 CAN 144:171858 AN 2006:103691 CAPLUS