Curriculum Vitae 9-29-06

Lee G. Pedersen

EDUCATION:

B.Ch., University of Tulsa, Tulsa, OK 1961
Ph.D., Physical Chemistry, University of Arkansas, Fayetteville, AR 1965

PROFESSIONAL EXPERIENCE:

Undergraduate Teaching Assistant, University of Tulsa, 1960-61
Graduate Research Assistant, University of Arkansas, 1961-65
Postgraduate Research Associate, Columbia University, 1965-66
Postgraduate Research Associate, Harvard University, 1966-67
Assistant Associate, Full Professor, University of North Carolina
1967-present; M.A. Smith Professor Chemistry, 1999-
Visiting Scientist, NIEHS, RTP, 1984-85, 1989-90, Expert, NIEHS
1986-present

AWARDS:

Full Four Year Scholarship, Benedictine Heights College, Tulsa, OK 1956
Full Academic Scholarship, University of Tulsa, 1958-59
NASA Predoctoral Fellowship, University of Arkansas, 1962-65
NSF Postdoctoral Fellowship, Columbia University, 1965-66
NIH Postdoctoral Fellowship, Harvard University, 1966-67
Tanner Award for Excellence in Undergraduate Teaching, UNC 1970

Research Summary:

Current studies involve the development of three dimensional models of blood coagulation proteins and their complexes, quantum mechanical/molecular mechanical studies of DNA beta polymerase and quantum mechanical studies of intermediates and transition states in the vitamin k-dependent pathway.

INVITED TALKS (recent)

March 1996 National ACS Meeting, Computational
Chemistry Symposium "Ionic Forces in Proteins and Nucleic Acids"
April 1996, Beckmann Institute, U. Ill.,
Dist. Speaker Series, "Ionic Forces in Proteins and Nucleic Acids"
April 1996, Virgina PolyTech. Inst., Biochem. Dept.,
"Ionic Forces in Proteins and Nucleic Acids"
Nov. 1996, Regional ACS Meeting, Symposium, "Solution
Structure of Factor IX"

Feb. 1997, UNC/Duke/NYU Computational Structural
Biology Resource Symposium, "Applications of MD/PME to problems
in Coagulation"
July 1997, NIOSH, "Theoretical Treatment of Ionic
Interactions in Macromolecules"
Aug. 1997, FASEB Summer Conference on Vitamim
K-Dependent Proteins, "Theoretical Studies of Vitamin
K-Dependent Proteins"
Jan. 1998, U. Georgia (Chemistry) "Theoretical
Studies of Vit. K. Dependent Proteins)
June 1998, NIEHS "Theoretical Studies of
Vit. K, Dependent Proteins)
Oct. 1999, Emory Univ. "Theoretical Studies of
Vit. K. Dependent Proteins)
Oct. 2000, U. Cal. San Diegeo "Theoretical Studies of
Vit. K. Dependent Proteins"
July 2001 Theoretical Chemistry Conference San Sebaston, Sp.
Theoretical Studies of Vit. K-Dep. Proteins
Aug. 2001 FASEB Vit. K Proteins Vermont "Theoretical Studies of
Vit. K. Dependent Proteins"
Sept. 2001 ACS Regional Meeting (SE, Savannah) "Theoretical
Studies of Vitamin K dependent Proteins"
Jan. 2002 UNC-CH Physical Chemistry Seminar "Modeling/Dynamics
of Vitamin K Dependent Proteins"
March 2002 Workshop of Computational Protein Structure Analysis
"Modeling/Dynamics of Vitamin K Dependent Proteins" RTP,NC
May 2002 Leadership in Drug Discovery: Setting New Standards
in Stucture-based Drug Design, Modeling/Dynamics of Mammalian
P450 enzymes, RTP, NC.
Oct 2002 ISSX Meeting Orlando Fla. Invited Symposium. Modeling
P450 enzymes
March 2003 American Physical Soc. Invited Symposium. Issues in
Modeling Blood Coagulation Complexes
December 2003 Laboratory of Structural Biology NIEHS Issues in modeling Blood
Coagulation Complexes
Jan 2004 UNC-W Symposium Speaker Modeling Blood Coagulation Proteins
Nov 4 Biophysical Symposium RTP Session Chair
Apr 2005 NIEHS Deuterium in Biology
Apr 2005 Session Chair Symposium for MKarplus NIH Washington DC
March 2006 Santa Fe Thom Dunning Appreciation Conference Speaker DNA beta polymerase
March 2006 ACS National Atlanta DNA beta Polymerase
March 2006 ACS National Atlanta Vitamin K Mechanism Q. Mech.
May 2006 FVIIa/TF symp Chapel Hill: Comparison of FVIIa/TF and FVIIa(free).
Sept 2006 NIEHS Energy analysis for correct insertion by DNA Polymerase Beta
Dec 2006 UNC-G Chemistry Energy analysis for correct insertion by DNA Pol Beta
Jan 2006 UNC-CH Chemistry Energy analysis for correct insertion by DNA Pol Beta

MEETINGS ATTENDED

March 1996 ACS National Meeting New Orleans
June 1996 Gordon Conference in Hemostasis

July 1996 Gordon Conf. Computational Chemistry
Nov. 1996 ACS Regional Meeting Greenville SC
Aug. 1997 FASEB Vitamin K Proteins Vermont
Aug. 1998 Gordon Conference in Hemostatsis New Hamp.
Aug. 2001 FASEB Vit. K. Proteins Vermont
Sept. 2001 ACS Regional Savannah. Ga.
Mar. 2002 Workshop on Computational Protein Structure Analysis
RTP, NC
Jul. 2002 Gordon Conf. in Hemostasis, Waterville, Me.
Oct. 2002 ISSX International Meeting, Orlando Fla.
Mar. 2003 APS National Meeting, Austin Tx.
Aug 2003 FASEB Hemostatis Saxon's River Vt.
July 2004 Gordon Conf. in Hemostasis, Waterville Me.
Nov 2004 Triangle Biophysics Symposium
Apr 2005 Martin Karplus 2005 symposium NIH Bethesda Md
July 2005 FASEB meeting Hemostasis Saxon's River Vt
July 2005 International Congress 5th Theoretical Chemical Physics New Orleans
Mar 2006 Dunning Conf. Santa Fe
Mar 2006 ACS National Atlanta Ga
May 2006 FVIIa/TF symposium Chapel Hill
July 2006 Gordon Conference in Hemostasis

Current Support

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Primary Sponsoring Agency/Institution: NIH
Award Number: HL-06350
Title: Modeling Vitamin K-Dependent Proteins and Complexes
Size of Award: 174,764 current year (1/01/06-12/31-06) Direct Cost
Start Date: 01/01/04
Expiration Date: 12/31/08
Role: PI
Research Description: We are developing solution-equilibrated all atom models for coagulation proteins and complexes.

Primary Sponsoring Agency/Institution: NSF
PI(Subcontractor): Lee Pedersen
Award Number: 2001-0759-02 (starting no.)
Size of Award: $143,215 (Total) (2003)
Award Breakdown: per year
Start Date: 10/01/01
Expiration Date: 09/30/07
Title: Methods for Multiscale Biomolecular Simulations
Description: This is a subcontract of a ITR/AP grant to NCSU,
Celeste Sagui Physics NCSU, Overall PI]
Research Description: We are providing applications from a variety of biological systems (coagulation proteins, P450s, HIV-RT and protease, DNA polymerases) for the developed theoretical methodology.

Lee Pedersen: Most Cited Papers (>40) as of 2-23-07 (part. update) (* might increase significantly with time) [papers under l g pedersen, l pedersen, l Pederson]

*1495	J. Chem. Phys. 98:10089-10092	1993	PME (w. darden, cites growing exp.)
*1298	J. Chem. Phys. 103:8577-8593	1995	PME (w. darden, cites growing exp.)
218	J. Chem. Phys. 48:3275-	1968	water dimer(1^{st}) (w. morokuma 1968)
201	J. Chem. Phys. 46:3941-	1967	rotational barriers (as l. Pederson)
*159	Nat-Stru.Biol. 4:904-908	1997	sulfotransferases (w. lars)
155	J. Chem. Phys. 99:8345-48	1993	PME (w.darden)
132	JACS 106:5659-	1984	photochem (w. whitten)
125	JACS 117:5001-2	1995	PME (w.darden)
90	Biochem. 27:4538-4541	1988	hydrophobicity (wolfenden)
85	PNAS 91:8715-8	1994	PME (w. darden)
*82	TIBS 23:129-130	1998	sulfotransferase (w. lars)
76	J. Chem. Phys. 48:4801-	1968	radicals (km,mk)
78	J. Chem. Phys. 96:7321-32	1992	spectroscopy of cluster (miller)
*90	Bioinformatics 17:1131-42 (2001)		DNA microarray analysis (leping)
*72	Biophys J. 76:2871- (1999)		amyloid (leping, bartolotti)
62	Biochem. 33:3237-	1994	P21 hras (marshall Anderson)
*69	Arch. Biochem. Biophys. 390:149-2001		sulfotransferases (lars and negishi)
54	J. Biol. Chem. 268:759-762	1993	P450 (negishi
55	J. Chem. Phys. 99:8585-8598	1993	spectroscopy of cluster (miller)
52	J. Med. Chem 30:79-86	1987	PCBs (mckinney)
50	J. Biol. Chem. 263:14216-14223	1988	PL binding assay (hiskey, weber)
49	J. Biol. Chem. 271:12496- (1996)		2C19 P450 (goldstein)
49	Biochem. 32:1443-53	1993	HIV protease (m. anderson)
48	FASEB J 683-9 (1996)	1996	P450 (negishi)
49	Chem. Phys. 139:15-30 (1989)		spectroscopy of cluster (miller)
49	J. Biol. Chem. 273:16248- (1998)		Conatokin (castellino)
44	J. Chem. Phys. 47:4751-	1967	thesis on PESs (l. Pederson)
43	J. Comp. Chem. 11:1181-6 (1990)		PL surfaces (charifson)
39	J. Biol Chem. 262 4017-23 (1987)		Mg binding to proteins (dwd,olson,rgh)
38	J. Am. Chem. Soc. 89 5064 (1967)		vib active. (karplus, morokuma)
43	Quant. Struc.-Act. Rel. 4, 166-172) (1985)		PCB/Ah recp. (mckinney)
36	FEBS Letts 433 211-214 (1998)		Sult Trans. (negishi, lars)
40	J. Am. Chem. Soc. 93 6330 (1971)		stilbenes (w. whitten)

BIBLIOGRAPHY (~250 publications)

The equivalent conductance of electrolytes," E.S. Amis, L. Pedersen, Z. Physik. Chem. Neue. Folge 36, 205 (1963).

"Ab initio calculations of the barriers to internal rotation of CH3-CH3 etc.," L. Pedersen, K. Morokuma, J. Chem. Phys. 46, 3941 (1967).

"Vibrational vs. translational activation in the (H2, H2) and (H2, D2) exchange reactions," K. Morokuma, L. Pedersen, M. Karplus, J. Am. Chem. Soc. 89, 5064(1967).

"A modified semiempirical approach to the H3 potential energy surface, L. Pedersen, R.N. Porter, J. Chem. Phys. 47, 4751 (1967).

"Molecular orbital studies of hydrogen bonds: an ab initio calculation for dimeric H2O," K. Morokuma, L. Pedersen, J. Chem. Phys. 48, 3275 (1968).

"The structure of CH3 and CF3," K. Morokuma, L. Pedersen, M. Karplus, J. Chem. Phys. 48, 4081 (1968).

"The barrier to internal rotation of O2F2," L. Pedersen, J. Mol. Structure 3, 510 (1969).

"Excited states of N-hetero molecules," L. Pedersen, D.G. Whitten, T. McCall, Chem. Phys. Lett. 3, 569 (1969).

"Possible contributing structures in polywater," L. Pedersen, Chem. Phys. Lett. 4, 280 (1969).

"On the struct. of the li-napthalenide anion," L. Pedersen, R. Griffin, Chem. Phys. 5, 373 (1970).

"The structure of the triatomic free radicals HCO, HCN-, FCO," L. Pedersen, J. Mol. Structure 5, 21 (1970).

"The preferred conformation of noradrenaline," L. Pedersen, H. Cable, D. Hoskins, J. Pharmacol. 23, 46 (1971).

"Importance of 1n,ã* states in N-heterocycles, Y.J. Lee, D.G. Whitten, L. Pedersen, J. Am. Chem. Soc. 93, 6330 (1971).

"Rotational relaxation in the H2, Ar system. A Monte Carlo trajectory calculation," L. Pedersen, K. Gammon, D. Hoskins, Chem. Phys. Lett. 11, 407 (1971).

"The preferred conformation of noradrenaline," L. Pedersen, R.G. Hoskins, H.Cable, J. Pharm. Pharmacol. 23, 216 (1971).

"Scrambling in ethane molecular ion: an indo model for hydrogen exchange before mass spectral fragmentation," C. Parker, M.M. Bursey, L. Pedersen, Org. Mass. Spect. 7, 1077 (1973).

"The preferred conformation of cyclophosphamide," H. Cable, A. Rauch, L.

Pedersen, J. Pharm. Pharmacol. 25, 509-510 (1973).

"The ortho effect in mass spectra, insight into the tightening of activted complexes for the loss of ketene from phenyl acetates and ethylene from phenetoles from indo molecular orbital calculations," C. Parker, J.R.Haas, M.M. Bursey, L. Pedersen, Org. Mass. Spect. 7, 1189 (1973).

"Chemistry c11. A correspondence course," L. Pedersen, W.E. Hatfield, University of North Carolina (1973).

"Chemistry c21. A correspondence course," W.E. Hatfield, L. Pedersen, University of North Carolina (1973).

"Problems in quantum chemistry and physics," C.S. Johnson, L. Pedersen, Addison-Wesley (1974).

"Internal rotation in the molecular ions of benzoic acid and salicyclic acid. An indo molecular orbital approach," C. Parker, M.M. Bursey, L. Pedersen, Org.Mass. Spect. 7, 204 (1974).

"The lowest electronic states of the benzoyl ion. A molecular orbital study with configuration interaction," J.L. Kao, M.M. Bursey, L. Pedersen, Org. Mass. Spect. 10, 38 (1975).

"Extension of GAUSSIAN70 to any number of atomic orbitals," G. Carlson, L. Pedersen, J. Comp. Phys. 17, 38 (1975).

"The planarity of hexachlorobenzene: an ab initio investigation," L. Pedersen, G. Carlson, J. Chem. Phys. 62, 2009 (1975).

An ab initio investigation of S8," G. Carlson, L. Pedersen, J. Chem. Phys. 62, 4567 (1975).

"The correlation of partial and total scores of the SAT of the CEEB with grades in freshman chemistry," L. Pedersen, Ed. Psychol. Meas. 35, 509 (1975).

"Position of protonation of the cresols: Semi-empirical and ab initio calculations," M.M. Bursey, R.S. Greenberg, L. Pedersen, Chem. Phys. Lett. 36, 470 (1975).

"Discovery of a cyclic 3'-5'guanosine monophosphate simulating factor in amoebae of dictyostelium discoideum," J.B. Putnam, L. Pedersen, Biochem. Biophys. Acta. 411, 168 (1975).

"An ab initio investigation of ascorbic acid," G.L. Carlson, H. Cable,

L. Pedersen, Chem. Phys. lett. 38, 75 (1976).

"Molecular fragment transfer in ab initio calculations," L. Pedersen, G. Carlson, Computers & Chem. 1, 137 (1976).

"Experimental and theoretical studies on M2X+ (M=Li, Na; X=F, C1)," C. Rechnsteiner, R.P. Buck, L. Pedersen, J. Chem. Phys. 65, 1659 (1976).

"Lower level freshman chemistry: how to choose the audience," L. Pedersen, J. Chem. Ed. 53, 418 (1976).

"Alkyl-metal surface complexes: methyl and lithium," W. McLean, L. Pedersen, R. Jarnagin, J. Chem. Phys. 65, 2491 (1976).

"Molecular orbital studies of the protonation of the methylanisoles," R.S. Greenberg, M.M. Bursey, L. Pedersen, J. Am. Chem. Soc. 98, 4061 (1976).

"Massive body collisions with the solar system," W. Peacock, J.B. Putnam, L. Pedersen, The Astronomy Quarterly 1, 201 (1977).

"An ab initio investigation of molecules with a disulfide bond: (HS)2, (CH3S)2' and cystine," A. Eslava, J.B. Putnam, L. Pedersen, Int. J. Peptide Prot. Res. 11, 149 (1978).

"Rotational barriers in the guanidinium ion: an ab initio study," J.F. Capitani, L. Pedersen, Chem. Phys. Lett. 54, 547 (1978).

"The interaction of charged disks in a dielectric medium," Sr. M.E. Adamson, L. Pedersen, J. Chem. Phys. 68, 4333 (1978).

"A simple and inexpensive solar energy expt.," J. Evans, L. Pedersen, J. Chem. Ed. 56, 339 (1979).

"Surface complexes between O2'H2O, and lithium," J. Schultz, W. McLean, L. Pedersen, Sur. Sci. 83, 354 (1979).

"The structure and formation of methyllithium ionic fragments," W. McLean, J. Schultz, L. Pedersen, R.C. Jarnagin, J. Organometallic Chem. 175, 1 (1979).

"H2O on Lin clusters: a theoretical study," J.A. Schultz, W. McLean, L. Pedersen, R.C. Jarnagin, Chem. Phys. Lett. 64, 230 (1979).

"Consequences of charge reversal of gaseous formate ions. Acyloxy ion," M.M. Bursey, J. Hass, D. Harvan, C. Parker, L. Pedersen, J. Hass, J. Am. Chem. Soc. 101, 5489 (1979).

"Chemistry 11. A correspondence course," W.E. Hatfield, L. Pedersen, University of North Carolina (1979).

"Chemistry 21. A correspondence course," L. Pedersen, W.E. Hatfield, University of North Carolina (1979).

"Chemistry of peptides containing þ-carboxyglutamic acid residues," H.C.

Marsh, N.T. Boggs, III, P. Robertson, M.M. Sarasua, M.E. Scott, P.B.W. Ten Kortenaar, J.A. Helpern, K. Koehler, R.G. Hiskey, L. Pedersen, International Workshop on Regulation of Coagulation. Elsevier North Holland, 1979. F. Taylor and K.G. Mann, eds.

"Europium ion coordination w. g-arboxyglutamic acid-containing ligand systems,"M.M. Sarasua, M.E. Scott, J.A. Helpern, P.B.W. Ten Kortenaar, N.T. Boggs, III, K. Koehler, R.G. Hiskey, L. Pedersen, J. Am. Chem. Soc. 102, 3404 (1980).

"Methoxide surface complexes on lithium," J.A. Schultz, S.M. Gates, L. Pedersen, R.C. Jarnagin, Chem. Phys. Lett. 72, 156 (1980).

"Chemical field ionization. Effect of chemically bonded surface groups in field ionization spectrometry," T.L. Youngless, M.M. Bursey, L. Pedersen,
J. Am. Chem. Soc. 102, 6881 (1980).

"Chemistry 10. A correspondence course," T.L. Isenhour, L. Pedersen, U. of North Carolina (1980).

"A theoretical study of the interaction of Mg2+ and two malonate ions," K. Gottschalk, R.G. Hiskey, L. Pedersen, K. Koehler, J. Mol. Struc. 85, 337 (1981).

"A theoretical study of malonate ion and its metal binding by ab initio and semiempirical techniques," K. Gottschalk, R.G. Hiskey, L. Pedersen, J. Mol. Structure 76, 197 (1981).

"A theoretical study of the interaction of magnesium(II) and two malonate ions," L.G. Pedersen, K.E. Gottschalk, R.G. Hiskey, K.A. Koehler, J. Mol. Structure 85, 337 (1981).

"Field ionization at a surface modified by chem. bound carboxylic acidgroups,"
T.L. Youngless, M.M. Bursey, L. Pedersen, Int. J. Mass Spect. and Ion Phys. 38, 223 (1981).

"Conformational transitions of gcarboxyglutamic acid-containing peptides," H.C. Marsh, M. Sarasua, D. Madar, N.T. Boggs, III, L.G. Pedersen, Proc. Am. Peptide Symposium, 227 (1981).

"Passing freshman chemistry: prerequisite skills and concepts," L.G. Pedersen, T.L. Isenhour, Harcourt Brace Jovanovich (1981).

"A theoretical study of malonate and formate calcium binding by ab initio techniques," K. Gottschalk, R.G. Hiskey, L. Pedersen, K. Koehler, J. Mol. Strutcture 87, 155 (1982).

"The relationship betw. protein-protein and protein-lipid interactions and the immunological properties of bov. prothrombin and several of its fragments," D.Madar, M. Sarasua, M. Marsh, L.G. Pedersen, K. Gottschalk, R.G. Hiskey, K. Koehler, J. Biol. Chem. 257, 1836 (1982).

"Surface complexes formed by nonohydric alcohols on lithium," J.A. Schultz, S.M. Gates, L. Pedersen, R.C. Jarnagin, Sur. Sci. 118, 634 (1982).

"A theoretical study of the chelation complex comprising formate ions, calcium ion and water of hydration," K. Gottschalk, R.G. Hiskey, L. Pedersen, K. Koehler, J. Mol. Structure 90, 265 (1982).

"Resistive heating of emitter wires for field desorption and ionization: a theory," D. Fraley, L. Pedersen, M. Bursey, Inter. J. Mass Spect. and Ion Phys.43, 99 (1982).

"Detailed structure of acetylide carbon on the surface of lithium," S.M. Gates, L. Pedersen, R.C. Jarnagin, Summary Abs., J. Vac. Sci. Technol. A 1, 1216 (1983).

"Direct observation of the H2NO2- ion," L. Pedersen, M.M. Bursey, R.L. Cerny, K.E. Gottschalk, K.B. Tamer,T. Lehman, J. Chem. Soc. Chem. Commun., 517 (1983).

"A theoretical investigation of molecular NaOH," G.A. Long, J.F. Capitani, L.Pedersen, J. Mol. Structure 105, 229 (1983).

"A theoretical investigation of the conformation of polychlorinated biphenyls (PCB's)," J.D. McKinney, K.E. Gottschalk, L. Pedersen, J. Mol. Struc. 104, 445(1983).

"The polarizability of planar aromatic systems. An appli. to polychlorinated biphenyls (PCB's), dioxins and polyaromatic hydrocarbons," J.D. McKinney, K.E. Gottschalk, L. Pedersen, J. Mol. Structure 105, 427 (1983).

"The role of g-carboxyglutamic acid (Gla) in blood clotting proteins: a theor. study of Mg-malonate complexes," G.A. Long, R.G. Hiskey, L. Pedersen, K. Koehler, J. Mol. Structure 108, 173 (1984).

"PCB and dioxin binding to cytosol receptors: a theoretical model based onmolecular parameters," J.D. McKinney, G.A. Long, L. Pedersen, J. QuantitativeStructure Activity Relationships 3, 99 (1984).

"Electronic and geometric structure of acetylide carbon on the surface oflithium," S.M. Gates, H.M. Meyer, L. Pedersen, R.C. Jarnagin, Sur. Sci. 140, 455 (1984).

"Photochemistry and photophysics of surfactant trans-stilbenes in supported multilayers and films at the air-water interface," W.F. Mooney, III, P.E. Brown , J.C. Russell, S.B. Costa, L. Pedersen, D.G. Whitten, J. Am. Chem. Soc. 106, 5659 (1984).

"Utilization of heavy-atom effect quenching of pyrene fluorescence to determine intramembrane distribution of halothane," K. Washington, M.M. Sarasua, L.S. Koehler, K.A. Koehler, J.A. Schultz, L. Pedersen, R.G. Hiskey, Photochem. Photobiol. 40, 693 (1984).

"A kinetic model describ. the interaction of bovine prothrombin fragment 1 with calcium ions," C.W. Kabis, M.M. Sarasua, K.E. Gottschalk, C.D. Bourne, L.G. Pedersen, C.M. Jackson, R.G. Hiskey, K.A. Koehler, Thromb. Haemostasis 15, 19-23(1985).

"An ab initio MO study of calcium and magnesium complexes with malonate andformate," A.T. Maynard, R.G. Hiskey, L. Pedersen, K.A. Koehler, Mol. Structure 124, 213 (1985).

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"Direct obser. of the HTiO3-Ion," M.M. Bursey, D.J. Harvan, L. Pedersen, A.T. Maynard, Inorg. Chem. 24, 4748 (1985).

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"Conformation of the 18-23 loop region of bovine prothrombin in the absence and presence of a model Ca2+ ion: an energy minimization study," L. Pedersen, M.A. Eastman, R.G. Hiskey, M. Pique, K.A. Koehler, K.E. Gottschalk, G.

Nemethy, H.A.Scheraga, Int. J. Peptide Protein Res. 27, 530-553 (1986).

"A theoretical study of the minimum energy structures of diethylstilbestrol and its analogs by molecular mechanics (MM2p), MNDO and ab initio calcns.," T.Darden, J.D. McKinney, K. Gottschalk, A.T. Maynard, L. Pedersen, J. Am. Chem.Soc. 108, 207 (1986).

"Isotope effects in collision-activated dissociations of simple ions," T.A. Lehman, J.R. Hass, F.W. Crow, K.B. Turner, L. Pedersen, Int. J. Mass. Spect.and Ion Process, 69, 85-96 (1986).

"The effect of divalent metal ions on the electrophoretic mobility of bovine prothrombin and bovine prothrombin fragment 1," D. Deerfield, P. Berkowitz, D.Olson, S. Wells, R. Hoke, K. Koehler, L. Pedersen, R. Hiskey, J. Biol. Chem. 261,4833-4839 (1986).

"An ab initio study of the relationship between nitroarene mutagenicity and electron affinity," A.T. Maynard, L.G. Pedersen, H.S. Posner, J.D. McKinney, Mol. Pharmacol. 29, 629-636 (1986).

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"Relative spectral response as a function of sequential ligand binding," D.W.Deerfield, II, R.A. Hoke, L.G. Pedersen, T. Darden, R.G. Hiskey, Biochem. Biophys. Res. Comm. 141, 1207-1212 (1986).

"A theoretical study of the binding of polychlorinated biphenyls (PCB's),dibenzodioxins and dibenzofuran to human plasma prealbumin," L.Pedersen, T. Darden, S. Oatley, J. McKinney, J. Med. Chem. 26, 2451-2457 (1986).

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"Synthesis of a g-carboxyglutamic acid containing heptapeptide

corresponding tobovine prothrombin residues 17-23," R.A. Hoke, D.W. Deerfield II, L.G. Pedersen,K.A. Koehler, R.G. Hiskey, Int. J. Peptide Res. 28, 569-578 (1986).

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