

NAME		POSITION TITLE	
Pedersen, Lee G.		Professor of Chemistry	
EDUCATION/TRAINING <i>(Begin with baccalaureate or other initial professional education, such as nursing, and include postdoctoral training.)</i>			
INSTITUTION AND LOCATION	DEGREE <i>(if applicable)</i>	YEAR(s)	FIELD OF STUDY
University of Tulsa	B.Ch.	1961	Chemistry
University of Arkansas	Ph.D.	1965	Physical Chemistry
Columbia University	Postdoc	1965-66	Theoretical Chem.
Harvard University	Postdoc	1966-67	Theoretical Chem.

A. Positions and Honors

1960-61 Undergraduate Teaching Assistant, University of Tulsa
 1961-5 Graduate Research Assistant, University of Arkansas
 1965-6 Postgraduate Research Associate, Columbia University, 1965-66
 1966-7 Postgraduate Research Associate, Harvard University, 1966-67
 1967- Assistant, Associate, Full Professor, University of North Carolina-CH 1967-present,
 1999-2006 M. A. Smith Professor. Adjunct Professor Chemistry 2006-.

Other Experience and Professional Memberships:

1984- Visiting Scientist, NIEHS, RTP, 1984-85, 1989-90, Expert, NIEHS 1986- present
 1987-95 Member Academic Affiliate Board, Pittsburgh Supercomputing Center
 1988-02 Member Advisory Board, North Carolina Supercomputing Center
 1992- Reviewer for many NIH, NSF, EPA and NIOSH study sections and promotion proposals

Honors:

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-CH 1970
 Lee G. Pedersen Professor of Psychology created UNC-CH 2008

B. Publications (of ~250 total peer reviewed publications)

Perera L, Darden T and Pedersen L. Modeling human factor IX. *Thrombosis and Hemostasis*. 2001 85:596-603.

Venkateswarlu D, Duke RE, Perera L, Darden TA, Pedersen LG. An all-atom solution-equilibrated model for human extrinsic blood coagulation complex (sTF-VIIa-Xa): a protein docking and molecular dynamics refinement study. *J. Throm. Haem.* 1:2577-88 (2003)

Sagui C., Pedersen LG, Darden TA. Towards an accurate representation of electrostatics in classical force fields: efficient implementation of multipolar interactions in biomolecular simulations. *J. Chem. Phys.* 120:73-87 (2004).

Perera L, Darden T, Duke R, Venkateswarlu D, Pedersen L. Early unfolding response of a stable protein domain to environmental changes. *J. Phys. Chem. A.* (2004) 108:9834-9840

Perera L and Pedersen LG. A reconsideration of the evidence for structural reorganization of FVII zymogen. *J. Thromb. Haemost.* (2005) 3:1543-5.

Deerfield DW, Wymore T, Stafford DW, Davis CH, Pedersen LG. A quantum chemical study of action of Vitamin K Epoxide Reductase (VKOR) (2006) *Inter. J. Q. Chem.* 106:2944-52.

Lin P, Yang WT, Pedersen LC, Negishi M, Pedersen LG. Searching for the minimum energy path in the sulfuryl transfer reaction catalyzed by estrogen sulfotransferase: the role of enzyme dynamics. (2006) *Inter. J. Q. Chem.* 106:2981-98.

Lin P, Pedersen LC, Batra VK, Beard WA, Wilson SH, Pedersen LG. Energy analysis of chemistry for correct insertion by DNA polymerase β . (2006) *Proc. Nat. Acad. Sci.* 103:13294-99

Sagui C., Roland C, Pedersen LG, Darden TA. New distributed multipole methods for accurate electrostatics in large-scale biomolecular simulations in (New Algorithms for Macromolecular Simulation, Springer Berlin 2006, Eds B. Leimkuhler, et al.) pp. 2997-312.

Piquemal JP, Perera L, Cisneros GA, Ren PY, Pedersen LG, Darden TA. Towards accurate solvation dynamics of divalent cations in water using the polarizable amoeba force field: From energetics to structure. (2006). *J. Chem. Phys.* 125:054511.

Colina C, Venkateswarlu D, Perera L., Pedersen LG, A detailed comparison of Factor VIIa bound and unbound (w. Tissue Factor). *J. Thromb. Haem.* (2006) 4:2726-2729

Hoffman M, Colina C, McDonald A, Arepally G, Pedersen L. Monroe, M. Tissue factor around dermal vessels has bound factor VII in the absence of injury. *J. Thrombosis and Haemostasis* 2007 5:1403-1408.

Davis C, Deerfield D, Stafford D, Pedersen L. A Quantum Chemical study of the mechanism of action of Vitamin K Carboxylase (VKC). IV. Intermediates and Transition States. *J. Phys. Chem. A.* 2007 111:7257-7261

Davis C, Deerfield D, Wymore T, Stafford D, Pedersen L. A quantum chemical study of the mechanism of Vitamin K epoxide reductase (VKOR). II. Transition States. *J. Molecular Graphics and Modelling* 2007 26:401-408

Davis C, Deerfield D, Wymore T, Stafford D A quantum chemical study of the mechanism of action of Vitamin K carboxylase (VKC) III. Intermediates and transition states. *J. Molecular Graphics and Modelling* 2007 26:409-414

Lee C, Chandrasekaran V, Duke R, Perera, L, Pedersen L A proposed model of human Protein Z (PZ) *J. Thrombosis and Haemostasis* 2007 5:1558-61

Lee CJ, Lin P, Chandrasekaran V, Duke RE, Everse, SJ, Perera L and Pedersen LG. Proposed structural models of human factor Va and prothrombinase. *J. Thrombosis and Haemostasis.* 2008 6:83-89.

Lin P, Batra VK, Pedersen LC, Beard W, Wilson S, Pedersen LG Incorrect nucleotide insertion at the active site of G:A mismatch catalyzed by DNA polymerase beta. Proc. Nat. Acad. Sci. 2008 105:5670-5674

Liu SB, Perera L, Pedersen LG. Binuclear manganese (II) complexes in biological systems. Mol. Phys. 105:2893-2898.

Chandrasekaran V, Lee CJ, Duke RE, Perera L, Pedersen LG Computational study of the putative active form of protein Z (PZa): Sequence design and structural modeling. Prot. Sci. 17:1354-1361.

Liu SB, Govind N, Pedersen LG. Exploring the origin of the internal rotational barriers for molecules with one rotatable dihedral angle. J. Chem. Phys. 2008 129:094104

Cisneros GA, Perera L, Garcia-Diaz M, Bebenek K, Kunkel TA, Pedersen LG. Catalytic mechanism of human DNA polymerase lambda with Mg²⁺ and Mn²⁺ from ab initio quantum mechanical/ molecular molecular studies. DNA Repair 2008 7:1824-34.