

Lee G Pedersen

List of Publications by Year in descending order

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155
papers

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times ranked

41975
citing authors

#	ARTICLE	IF	CITATIONS
1	Particle mesh Ewald: An $N^2 \log(N)$ method for Ewald sums in large systems. <i>Journal of Chemical Physics</i> , 1993, 98, 10089-10092.	1.2	24,656
2	A smooth particle mesh Ewald method. <i>Journal of Chemical Physics</i> , 1995, 103, 8577-8593.	1.2	18,266
3	The effect of long-range electrostatic interactions in simulations of macromolecular crystals: A comparison of the Ewald and truncated list methods. <i>Journal of Chemical Physics</i> , 1993, 99, 8345-8348.	1.2	611
4	New tricks for modelers from the crystallography toolkit: the particle mesh Ewald algorithm and its use in nucleic acid simulations. <i>Structure</i> , 1999, 7, R55-R60.	1.6	571
5	Gene selection for sample classification based on gene expression data: study of sensitivity to choice of parameters of the GA/KNN method. <i>Bioinformatics</i> , 2001, 17, 1131-1142.	1.8	560
6	Structure and Function of Sulfotransferases. <i>Archives of Biochemistry and Biophysics</i> , 2001, 390, 149-157.	1.4	306
7	Crystal structure of estrogen sulphotransferase. <i>Nature Structural and Molecular Biology</i> , 1997, 4, 904-908.	3.6	263
8	Molecular Orbital Studies of Hydrogen Bonds. An Ab Initio Calculation for Dimeric H ₂ O. <i>Journal of Chemical Physics</i> , 1968, 48, 3275-3282.	1.2	240
9	Towards an accurate representation of electrostatics in classical force fields: Efficient implementation of multipolar interactions in biomolecular simulations. <i>Journal of Chemical Physics</i> , 2004, 120, 73-87.	1.2	207
10	Atomic-level accuracy in simulations of large protein crystals.. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 1994, 91, 8715-8718.	3.3	183
11	Toward the Accurate Modeling of DNA: The Importance of Long-Range Electrostatics. <i>Journal of the American Chemical Society</i> , 1995, 117, 5001-5002.	6.6	172
12	Gene Assessment and Sample Classification for Gene Expression Data Using a Genetic Algorithm / k-nearest Neighbor Method. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2001, 4, 727-739.	0.6	169
13	Towards accurate solvation dynamics of divalent cations in water using the polarizable amoeba force field: From energetics to structure. <i>Journal of Chemical Physics</i> , 2006, 125, 054511.	1.2	169
14	Phenobarbital Indirectly Activates the Constitutive Active Androstane Receptor (CAR) by Inhibition of Epidermal Growth Factor Receptor Signaling. <i>Science Signaling</i> , 2013, 6, ra31.	1.6	163
15	Influences of solvent water on protein folding: free energies of solvation of cis and trans peptides are nearly identical. <i>Biochemistry</i> , 1988, 27, 4538-4541.	1.2	161
16	Conserved structural motifs in the sulfotransferase family. <i>Trends in Biochemical Sciences</i> , 1998, 23, 129-130.	3.7	158
17	Ab Initio Calculations of the Barriers to Internal Rotation of CH ₃ CH ₃ , CH ₃ NH ₂ , CH ₃ OH, N ₂ H ₄ , H ₂ O ₂ , and NH ₂ OH. <i>Journal of Chemical Physics</i> , 1967, 46, 3941-3947.	1.2	143
18	Ionic charging free energies: Spherical versus periodic boundary conditions. <i>Journal of Chemical Physics</i> , 1998, 109, 10921-10935.	1.2	129

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19	Photochemical reactions in organized assemblies. 37. Photochemistry and photophysics of surfactant trans-stilbenes in supported multilayers and films at the air-water interface. <i>Journal of the American Chemical Society</i> , 1984, 106, 5659-5667.	6.6	128
20	An Atomic Model for the Pleated β -Sheet Structure of $A\beta$ Amyloid Protofilaments. <i>Biophysical Journal</i> , 1999, 76, 2871-2878.	0.2	120
21	Dephosphorylation of Threonine 38 Is Required for Nuclear Translocation and Activation of Human Xenobiotic Receptor CAR (NR113). <i>Journal of Biological Chemistry</i> , 2009, 284, 34785-34792.	1.6	117
22	Crystal Structure of an α 1,4-N-Acetylhexosaminyltransferase (EXTL2), a Member of the Exostosin Gene Family Involved in Heparan Sulfate Biosynthesis. <i>Journal of Biological Chemistry</i> , 2003, 278, 14420-14428.	1.6	95
23	Estimation of Molecular Acidity via Electrostatic Potential at the Nucleus and Valence Natural Atomic Orbitals. <i>Journal of Physical Chemistry A</i> , 2009, 113, 3648-3655.	1.1	89
24	Energy analysis of chemistry for correct insertion by DNA polymerase beta. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 13294-13299.	3.3	88
25	Steric, Quantum, and Electrostatic Effects on S_N2 Reaction Barriers in Gas Phase. <i>Journal of Physical Chemistry A</i> , 2010, 114, 5913-5918.	1.1	80
26	Gaussian Multipole Model (GMM). <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 190-202.	2.3	79
27	Identification of Residues 99, 220, and 221 of Human Cytochrome P450 2C19 as Key Determinants of Omeprazole Hydroxylase Activity. <i>Journal of Biological Chemistry</i> , 1996, 271, 12496-12501.	1.6	77
28	Parallelab initio and molecular mechanics investigation of polycoordinated Zn(II) complexes with model hard and soft ligands: Variations of binding energy and of its components with number and charges of ligands. <i>Journal of Computational Chemistry</i> , 2000, 21, 1011-1039.	1.5	74
29	Structure and Dynamics of Zymogen Human Blood Coagulation Factor X. <i>Biophysical Journal</i> , 2002, 82, 1190-1206.	0.2	73
30	Hydrophobicities of the nucleic acid bases: distribution coefficients from water to cyclohexane 1 1 Edited by I. Tinoco. <i>Journal of Molecular Biology</i> , 1998, 280, 421-430.	2.0	70
31	Structural flexibility and functional versatility of mammalian P450 enzymes. <i>FASEB Journal</i> , 1996, 10, 683-689.	0.2	68
32	Reaction Mechanism of the μ Subunit of E. coli DNA Polymerase III: Insights into Active Site Metal Coordination and Catalytically Significant Residues. <i>Journal of the American Chemical Society</i> , 2009, 131, 1550-1556.	6.6	64
33	Exploring the origin of the internal rotational barrier for molecules with one rotatable dihedral angle. <i>Journal of Chemical Physics</i> , 2008, 129, 094104.	1.2	59
34	Identification of Residues 286 and 289 as Critical for Conferring Substrate Specificity of Human CYP2C9 for Diclofenac and Ibuprofen. <i>Archives of Biochemistry and Biophysics</i> , 1998, 357, 240-248.	1.4	58
35	Molecular acidity: A quantitative conceptual density functional theory description. <i>Journal of Chemical Physics</i> , 2009, 131, 164107.	1.2	58
36	Construction and molecular modeling of phospholipid surfaces. <i>Journal of Computational Chemistry</i> , 1990, 11, 1181-1186.	1.5	56

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37	Glucosaminylglycan biosynthesis: what we can learn from the X-ray crystal structures of glycosyltransferases GlcAT1 and EXTL2. <i>Biochemical and Biophysical Research Communications</i> , 2003, 303, 393-398.	1.0	56
38	Role of \hat{I}^3 -Carboxyglutamic Acid in the Calcium-Induced Structural Transition of Conantokin G, a Conotoxin from the Marine Snail <i>Conus geographus</i> . <i>Biochemistry</i> , 1997, 36, 15677-15684.	1.2	54
39	Refinement of the NMR Solution Structure of the \hat{I}^3 -Carboxyglutamic Acid Domain of Coagulation Factor IX Using Molecular Dynamics Simulation with Initial Ca^{2+} Positions Determined by a Genetic Algorithm. <i>Biochemistry</i> , 1997, 36, 2132-2138.	1.2	53
40	Catalytic mechanism of human DNA polymerase \hat{I}^2 with Mg^{2+} and Mn^{2+} from ab initio quantum mechanical/molecular mechanical studies. <i>DNA Repair</i> , 2008, 7, 1824-1834.	1.3	52
41	Molecular Dynamics Simulations of the d(CCAACGTTGG) ₂ Decamer: Influence of the Crystal Environment. <i>Biophysical Journal</i> , 2000, 78, 668-682.	0.2	51
42	Requirement for transient metal ions revealed through computational analysis for DNA polymerase going in reverse. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E5228-36.	3.3	49
43	A role of Lys614 in the sulfotransferase activity of human heparan sulfate N-deacetylase/N-sulfotransferase. <i>FEBS Letters</i> , 1998, 433, 211-214.	1.3	48
44	Incorrect nucleotide insertion at the active site of a G:A mismatch catalyzed by DNA polymerase \hat{I}^2 . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2008, 105, 5670-5674.	3.3	48
45	Accurate crystal molecular dynamics simulations using particle-mesh-Ewald: RNA dinucleotides \hat{I}^2 ApU and CpC. <i>Chemical Physics Letters</i> , 1995, 243, 229-235.	1.2	46
46	Molecular dynamics simulation studies of a high resolution \hat{I}^2 -DNA crystal. <i>Journal of Chemical Physics</i> , 1995, 102, 3830-3834.	1.2	45
47	Molecular Insights into DNA Polymerase Deterrents for Ribonucleotide Insertion. <i>Journal of Biological Chemistry</i> , 2011, 286, 31650-31660.	1.6	45
48	Structural Comparison of DNA Polymerase Architecture Suggests a Nucleotide Gateway to the Polymerase Active Site. <i>Chemical Reviews</i> , 2014, 114, 2759-2774.	23.0	41
49	Amino Acid Substitution in the Active Site of DNA Polymerase \hat{I}^2 Explains the Energy Barrier of the Nucleotidyl Transfer Reaction. <i>Journal of the American Chemical Society</i> , 2013, 135, 8078-8088.	6.6	40
50	An ab Initio Quantum Mechanical Model for the Catalytic Mechanism of HIV-1 Protease. <i>Journal of the American Chemical Society</i> , 1996, 118, 3946-3950.	6.6	38
51	Quantum mechanical calculations on phosphate hydrolysis reactions. <i>Journal of Computational Chemistry</i> , 2000, 21, 43-51.	1.5	37
52	Conformational Changes in Conantokin-G Induced upon Binding of Calcium and Magnesium as Revealed by NMR Structural Analysis. <i>Journal of Biological Chemistry</i> , 1998, 273, 16248-16258.	1.6	36
53	Salt or ion bridges in biological system: A study employing quantum and molecular mechanics. <i>Proteins: Structure, Function and Bioinformatics</i> , 1989, 6, 168-192.	1.5	33
54	Warfarin and vitamin K epoxide reductase: a molecular accounting for observed inhibition. <i>Blood</i> , 2018, 132, 647-657.	0.6	32

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55	Modeling Zymogen Protein C. <i>Biophysical Journal</i> , 2000, 79, 2925-2943.	0.2	31
56	Consequences of charge reversal of gaseous formate and acetate ions. Acyloxy ions. <i>Journal of the American Chemical Society</i> , 1979, 101, 5489-5493.	6.6	30
57	Models for protein-zinc ion binding sites. II. The catalytic sites. <i>International Journal of Quantum Chemistry</i> , 2001, 83, 150-165.	1.0	30
58	Molecular dynamics simulation of bovine prothrombin fragment 1 in the presence of calcium ions. <i>Biochemistry</i> , 1992, 31, 8840-8848.	1.2	27
59	The Roles of Individual \hat{I}^3 -Carboxyglutamate Residues in the Solution Structure and Cation-dependent Properties of Conantokin-T. <i>Journal of Biological Chemistry</i> , 1998, 273, 7512-7522.	1.6	27
60	Revealing the role of the product metal in DNA polymerase \hat{I}^2 catalysis. <i>Nucleic Acids Research</i> , 2017, 45, gkw1363.	6.5	27
61	Europium ion coordination with .gamma.-carboxyglutamic acid containing ligand systems. <i>Journal of the American Chemical Society</i> , 1980, 102, 3404-3412.	6.6	26
62	Structural flexibility and functional versatility of cytochrome P450 and rapid evolution. <i>Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis</i> , 1996, 350, 43-50.	0.4	25
63	Long range nonbonded attractive constants for some charged atoms. <i>Journal of Computational Chemistry</i> , 1991, 12, 1125-1128.	1.5	24
64	A finite field method for calculating molecular polarizability tensors for arbitrary multipole rank. <i>Journal of Computational Chemistry</i> , 2011, 32, 3283-3295.	1.5	24
65	Molecular orbital studies of the protonation of the methylanisoles. <i>Journal of the American Chemical Society</i> , 1976, 98, 4061-4064.	6.6	23
66	Altering the Regiospecificity of Androstenedione Hydroxylase Activity in P450s 2a-4/5 by a Mutation of the Residue at Position 481. <i>Biochemistry</i> , 1995, 34, 5054-5059.	1.2	23
67	Modeling Human Zymogen Factor IX. <i>Thrombosis and Haemostasis</i> , 2001, 85, 596-603.	1.8	22
68	Heparan Sulfate Biosynthesis: A Theoretical Study of the Initial Sulfation Step by N-Deacetylase/N-Sulfotransferase. <i>Biophysical Journal</i> , 2000, 79, 2909-2917.	0.2	21
69	A quantum chemical study of the mechanism of action of Vitamin K epoxide reductase (VKOR). <i>Journal of Molecular Graphics and Modelling</i> , 2007, 26, 401-408.	1.3	21
70	Do residue levels of polychlorinated biphenyls (PCBs) in human blood produce mild hypothyroidism?. <i>Journal of Theoretical Biology</i> , 1987, 129, 231-241.	0.8	20
71	Four loops of the catalytic domain of factor VIIa mediate the effect of the first EGF-like domain substitution on factor VIIa catalytic activity ¹¹ Edited by R. Huber. <i>Journal of Molecular Biology</i> , 2001, 307, 1503-1517.	2.0	20
72	Relative affinity of Ca(II) and Mg(II) ions for human and bovine prothrombin and fragment 1. <i>Biochemical and Biophysical Research Communications</i> , 1987, 144, 520-527.	1.0	19

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73	Reciprocal Size-Effect Relationship of the Key Residues in Determining Regio- and Stereospecificities of DHEA Hydroxylase Activity in P450 2a5. <i>Biochemistry</i> , 1997, 36, 3193-3198.	1.2	19
74	Trans-Cis Isomerization of Proline 22 in Bovine Prothrombin Fragment 1: A Surprising Result of Structural Characterization. <i>Biochemistry</i> , 1998, 37, 10920-10927.	1.2	19
75	Homology modeling and molecular dynamics simulation of human prothrombin fragment 1. <i>Protein Science</i> , 1995, 4, 2341-2348.	3.1	18
76	Atomic forces for geometry-dependent point multipole and Gaussian multipole models. <i>Journal of Computational Chemistry</i> , 2010, 31, 2702-2713.	1.5	18
77	A revisit to the one form kinetic model of prothrombinase. <i>Biophysical Chemistry</i> , 2010, 149, 28-33.	1.5	18
78	The first solvation shell of magnesium ion in a model protein environment with formate, water, and X-NH ₃ , H ₂ S, imidazole, formaldehyde, and chloride as ligands: An ab initio study. <i>Proteins: Structure, Function and Bioinformatics</i> , 1995, 21, 244-255.	1.5	17
79	The Role of Hydrated Divalent Metal Ions in the Bridging of Two Anionic Groups. An ab initio Quantum Chemical and Molecular Mechanics Study of Dimethyl Phosphate and Formate Bridged by Calcium and Magnesium Ions. <i>Journal of Biomolecular Structure and Dynamics</i> , 1989, 6, 1077-1091.	2.0	16
80	Interaction of calcium and magnesium ions with malonate and the role of the waters of hydration: a quantum mechanical study. <i>Journal of the American Chemical Society</i> , 1991, 113, 1892-1899.	6.6	16
81	The interaction of Na(I), Ca(II), and Mg(II) metal ions with duplex DNA: A theoretical modeling study. <i>International Journal of Quantum Chemistry</i> , 1992, 44, 145-166.	1.0	16
82	Quantum chemical study of the mechanism of action of vitamin K epoxide reductase (VKOR). <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2944-2952.	1.0	16
83	Searching for the minimum energy path in the sulfuryl transfer reaction catalyzed by human estrogen sulfotransferase: Role of enzyme dynamics. <i>International Journal of Quantum Chemistry</i> , 2006, 106, 2981-2998.	1.0	16
84	Deuterium and its role in the machinery of evolution. <i>Journal of Theoretical Biology</i> , 2006, 238, 914-918.	0.8	16
85	A model for the unique role of factor Va A2 domain extension in the human ternary thrombin-generating complex. <i>Biophysical Chemistry</i> , 2015, 199, 46-50.	1.5	16
86	An ab initio quantum mechanical study of thioesters. <i>Computational and Theoretical Chemistry</i> , 1995, 358, 99-106.	1.5	15
87	Predicted solution structure of zymogen human coagulation FVII. <i>Journal of Computational Chemistry</i> , 2002, 23, 35-47.	1.5	15
88	Recent Estimates of the Structure of the Factor VIIa (FVIIa)/Tissue Factor (TF) and Factor Xa (FXa) Ternary Complex. <i>Thrombosis Research</i> , 2010, 125, S7-S10.	0.8	15
89	A hetero-dimer model for concerted action of vitamin K carboxylase and vitamin K reductase in vitamin K cycle. <i>Journal of Theoretical Biology</i> , 2011, 279, 143-149.	0.8	15
90	HPAM: Hirshfeld partitioned atomic multipoles. <i>Computer Physics Communications</i> , 2012, 183, 390-397.	3.0	15

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91	The n .fwdarw. 3s Rydberg transition of jet-cooled tetrahydropyran, 1,4-dioxane, and 1,4-dioxane-d8 studied by 2 + 1 resonance-enhanced multiphoton ionization. The Journal of Physical Chemistry, 1989, 93, 6064-6069.	2.9	14
92	Enol and deprotonated forms of acetic and malonic acid. Computational and Theoretical Chemistry, 1996, 368, 163-171.	1.5	14
93	Explicit Water Near the Catalytic I Helix Thr in the Predicted Solution Structure of CYP2A4. Biophysical Journal, 2003, 84, 57-68.	0.2	14
94	The barrier to proton transfer from multiply protonated molecules: A quantum mechanical approach. Organic Mass Spectrometry, 1992, 27, 974-975.	1.3	13
95	Probing the Structural Changes in the Light Chain of Human Coagulation Factor VIIa Due to Tissue Factor Association. Biophysical Journal, 1999, 77, 99-113.	0.2	13
96	Quantum Chemical Study of the Mechanism of Action of Vitamin K Carboxylase (VKC). IV. Intermediates and Transition Statesâ€. Journal of Physical Chemistry A, 2007, 111, 7257-7261.	1.1	13
97	A computational modeling and molecular dynamics study of the Michaelis complex of human protein Z-dependent protease inhibitor (ZPI) and factor Xa (FXa). Journal of Molecular Modeling, 2009, 15, 897-911.	0.8	13
98	Modeling of the DNA-binding site of yeast Pms1 by mass spectrometry. DNA Repair, 2011, 10, 454-465.	1.3	13
99	Structure and relative acidity for a model zinc finger. Computational and Theoretical Chemistry, 1997, 419, 221-226.	1.5	11
100	A quantum mechanical study of the transfer of biological sulfate. Computational and Theoretical Chemistry, 1999, 461-462, 105-111.	1.5	11
101	Ligand induced dissociation of the AR homodimer precedes AR monomer translocation to the nucleus. Scientific Reports, 2019, 9, 16734.	1.6	11
102	OXYGEN-17 NMR STUDIES OF HETEROCYCLIC SULFONES AND<i>trans</i>-2-(ALKYLSULFONYL)CYCLOHEXANOLS UTILIZING THE LANTHANIDE SHIFT REAGENT, Eu(fod)₃. Phosphorus, Sulfur and Silicon and the Related Elements, 1991, 59, 205-210.	0.8	10
103	Determination of strontium binding to macromolecules. Analytical Biochemistry, 1991, 198, 391-393.	1.1	10
104	The First Solvation Shell of Magnesium and Calcium Ions in a Model Nucleic Acid Environment: An ab initio Study. Journal of Biomolecular Structure and Dynamics, 1995, 13, 167-180.	2.0	10
105	A quantum chemical study of the mechanism of action of Vitamin K carboxylase (VKC). Journal of Molecular Graphics and Modelling, 2007, 26, 409-414.	1.3	10
106	Hiding in Plain Sight: The Bimetallic Magnesium Covalent Bond in Enzyme Active Sites. Inorganic Chemistry, 2017, 56, 313-320.	1.9	10
107	Characterization of \hat{I}^3 -Carboxyglutamic Acid Residue 21 of Human Factor IXâ€. Biochemistry, 1996, 35, 10321-10327.	1.2	9
108	Homology Modeling and Molecular Dynamics Simulations of the Gla Domains of Human Coagulation Factor IX and Its G[12]A Mutant. The Journal of Physical Chemistry, 1996, 100, 2475-2479.	2.9	9

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109	A Molecular Dynamics Model of HIV-1 Reverse Transcriptase Complexed with DNA: Comparison with Experimental Structures. <i>Journal of Molecular Modeling</i> , 2000, 6, 575-586.	0.8	9
110	UTILIZATION OF HEAVY ATOM EFFECT QUENCHING OF PYRENE FLUORESCENCE TO DETERMINE THE INTRAMEMBRANE DISTRIBUTION OF HALOTHANE. <i>Photochemistry and Photobiology</i> , 1984, 40, 693-702.	1.3	8
111	Free energy calculations on calcium and magnesium complexes: Protein and phospholipid model systems. <i>Journal of Computational Chemistry</i> , 1991, 12, 899-908.	1.5	8
112	From Steroid and Drug Metabolism to Glycobiology, Using Sulfotransferase Structures to Understand and Tailor Function. <i>Drug Metabolism and Disposition</i> , 2022, 50, 1027-1041.	1.7	8
113	The determination of a calcium-dependent binding constant of the bovine prothrombin GLA domain (residues 1-45) to phospholipid vesicles. <i>Biochemical and Biophysical Research Communications</i> , 1988, 155, 230-235.	1.0	7
114	Generation of potential structures for the G-domain of chloroplast EF-Tu using comparative molecular modeling. <i>Proteins: Structure, Function and Bioinformatics</i> , 1990, 8, 237-250.	1.5	7
115	Obligatory role in GTP hydrolysis for the amide carbonyl oxygen of the Mg ²⁺ -coordinating Thr of regulatory GTPases. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2010, 107, 9596-9601.	3.3	7
116	Chemical field ionization. Effect of chemically bonded surface groups in field ionization mass spectrometry. <i>Journal of the American Chemical Society</i> , 1980, 102, 6881-6882.	6.6	6
117	Three-dimensional solution structure of Tropidechis carinatus venom extract trocarin: a structural homologue of Xa and prothrombin activator. <i>Journal of Molecular Modeling</i> , 2002, 8, 302-313.	0.8	6
118	Computational study of the putative active form of protein Z (PZa): Sequence design and structural modeling. <i>Protein Science</i> , 2008, 17, 1354-1361.	3.1	6
119	Analysis on long-range residue-residue communication using molecular dynamics. <i>Proteins: Structure, Function and Bioinformatics</i> , 2014, 82, 2896-2901.	1.5	6
120	Field ionization at a surface modified by chemically bound carboxylic acid groups. <i>International Journal of Mass Spectrometry and Ion Physics</i> , 1981, 38, 223-239.	1.3	5
121	Estimation of apparent quadrupolar coupling constants for complexes of magnesium ions with mono- and dicarboxylic acid ligands. applications to magnesium ion: protein interactions. <i>Journal of Inorganic Biochemistry</i> , 1987, 29, 153-164.	1.5	5
122	Weak Antiferromagnetic Coupling via a Superexchange Interaction between Mn(II)-Mn(II) Ions: A QM/MM Study of the Active Site of Human Cytosolic X-Propyl Aminopeptidase P. <i>Journal of Physical Chemistry Letters</i> , 2012, 3, 2293-2297.	2.1	5
123	Applications of Quantum Mechanical/Molecular Mechanical Methods to the Chemical Insertion Step of DNA and RNA Polymerization. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014, 97, 83-113.	1.0	5
124	Position of protonation of the cresols: Semi-empirical and ab initio calculations. <i>Chemical Physics Letters</i> , 1975, 36, 470-474.	1.2	4
125	Direct observation of the hydrogen metatitanate (HTiO ₃ ⁻) ion. <i>Inorganic Chemistry</i> , 1985, 24, 4748-4749.	1.9	4
126	Relative spectral response as a function of sequential ligand binding. <i>Biochemical and Biophysical Research Communications</i> , 1986, 141, 1207-1212.	1.0	4

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127	Determination of magnesium binding to macromolecules. <i>Analytical Biochemistry</i> , 1987, 160, 468-470.	1.1	4
128	Proton, calcium, and magnesium binding by peptides containing γ -carboxyglutamic acid. <i>International Journal of Peptide and Protein Research</i> , 1991, 37, 33-38.	0.1	4
129	Scrambling in ethane molecular ion: An INDO model for hydrogen exchange before mass spectral fragmentation. <i>Organic Mass Spectrometry</i> , 1973, 7, 1077-1081.	1.3	3
130	Theortho effect in mass spectra. Insight into the tightening of activated complexes for the loss of ketene from phenyl acetates and ethylene from phenetoles from INDO molecular orbital calculations. <i>Organic Mass Spectrometry</i> , 1973, 7, 1189-1195.	1.3	3
131	Internal rotation in the molecular ions of benzoic acid and salicylic acid. An INDO molecular orbital approach. <i>Organic Mass Spectrometry</i> , 1974, 9, 204-210.	1.3	3
132	Resistive heating of emitter wires for field desorption and ionization: A theory. <i>International Journal of Mass Spectrometry and Ion Physics</i> , 1982, 43, 99-129.	1.3	3
133	Direct observation of new antimony-containing anions: SbH_2O^- , Sb_3^- , and monomeric Sb_3O_5^- . <i>Inorganica Chimica Acta</i> , 1986, 115, 203-205.	1.2	3
134	Conformational change path between closed and open forms of C2 domain of coagulation factor V on a two-dimensional free-energy surface. <i>Physical Review E</i> , 2009, 79, 041909.	0.8	3
135	Quantum chemical study of the mechanism of action of vitamin K carboxylase in solvent. <i>International Journal of Quantum Chemistry</i> , 2010, 110, 2744-2751.	1.0	3
136	Parallel ab initio and molecular mechanics investigation of polycoordinated Zn(II) complexes with model hard and soft ligands: Variations of binding energy and of its components with number and charges of ligands. <i>Journal of Computational Chemistry</i> , 2000, 21, 1011.	1.5	3
137	Direct observation of the H_2NO_2^- ion. <i>Journal of the Chemical Society Chemical Communications</i> , 1983, , 517.	2.0	2
138	Terbium ion binding to a synthetic γ -carboxyglutamic acid containing heptapeptide corresponding to bovine prothrombin residues 17-23. <i>Inorganic Chemistry</i> , 1986, 25, 4503-4506.	1.9	2
139	Computational Studies of Human Prothrombin Fragment 1 the Gla Domain of Factor IX and Several Biological Interesting Mutants. <i>Pathophysiology of Haemostasis and Thrombosis: International Journal on Haemostasis and Thrombosis Research</i> , 1996, 26, 54-59.	0.5	2
140	Synthesis of a γ -carboxyglutamic acid containing heptapeptide corresponding to bovine prothrombin residues 17-23. <i>International Journal of Peptide and Protein Research</i> , 1986, 28, 569-578.	0.1	2
141	A Kinetic Model Describing the Interaction of Bovine Prothrombin Fragment 1 with Calcium Ions. <i>Thrombosis and Haemostasis</i> , 1985, 53, 019-023.	1.8	2
142	Extension of GAUSSIAN70 to any number of atomic orbitals. <i>Journal of Computational Physics</i> , 1975, 17, 415-419.	1.9	1
143	The interaction of charged disks in a dielectric medium. <i>Journal of Chemical Physics</i> , 1978, 68, 4333-4337.	1.2	1
144	New Distributed Multipole Methods for Accurate Electrostatics in Large-Scale Biomolecular Simulations. , 2006, , 297-312.		1

#	ARTICLE	IF	CITATIONS
145	Lee Pedersen s work in theoretical and computational chemistry and biochemistry. World Journal of Biological Chemistry, 2011, 2, 35.	1.7	1
146	A revisit to the one-form kinetic model of prothrombinase: A comment on the rebuttal. Biophysical Chemistry, 2012, 160, 77-78.	1.5	1
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154	Structural properties of a Gla-domain peptide of prothrombin fragment I. , 1992, , 285-286.		0
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