Lee G Pedersen

List of Publications by Year
in descending order

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155 papers	50,488 citations	66250 44 h-index	9865 146 g-index
157 all docs	157 docs citations	157 times ranked	47074 citing authors

#	Article	IF	Citations
1	From Steroid and Drug Metabolism to Glycobiology, Using Sulfotransferase Structures to Understand and Tailor Function. Drug Metabolism and Disposition, 2022, 50, 1027-1041.	1.7	8
2	Preferential DNA Polymerase Î² Reverse Reaction with Imidodiphosphate. ACS Omega, 2020, 5, 15317-15324.	1.6	0
3	Ligand induced dissociation of the AR homodimer precedes AR monomer translocation to the nucleus. Scientific Reports, 2019, 9, 16734.	1.6	11
4	Warfarin and vitamin K epoxide reductase: a molecular accounting for observed inhibition. Blood, 2018, 132, 647-657.	0.6	32
5	Hiding in Plain Sight: The Bimetallic Magnesium Covalent Bond in Enzyme Active Sites. Inorganic Chemistry, 2017, 56, 313-320.	1.9	10
6	Revealing the role of the product metal in DNA polymerase Î² catalysis. Nucleic Acids Research, 2017, 45, gkw1363.	6.5	27
7	A model for the unique role of factor Va A2 domain extension in the human ternary thrombin-generating complex. Biophysical Chemistry, 2015, 199, 46-50.	1.5	16
8	Do the crystallographic forms of prethrombin-2 revert to a single form in solution?. Biophysical Chemistry, 2015, 203-204, 28-32.	1.5	1
9	Requirement for transient metal ions revealed through computational analysis for DNA polymerase going in reverse. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E5228-36.	3.3	49
10	Applications of Quantum Mechanical/Molecular Mechanical Methods to the Chemical Insertion Step of DNA and RNA Polymerization. Advances in Protein Chemistry and Structural Biology, 2014, 97, 83-113.	1.0	5
11	Structural Comparison of DNA Polymerase Architecture Suggests a Nucleotide Gateway to the Polymerase Active Site. Chemical Reviews, 2014, 114, 2759-2774.	23.0	41
12	Analysis on long-range residue-residue communication using molecular dynamics. Proteins: Structure, Function and Bioinformatics, 2014, 82, 2896-2901.	1.5	6
13	Phenobarbital Indirectly Activates the Constitutive Active Androstane Receptor (CAR) by Inhibition of Epidermal Growth Factor Receptor Signaling. Science Signaling, 2013, 6, ra31.	1.6	163
14	Amino Acid Substitution in the Active Site of DNA Polymerase Î² Explains the Energy Barrier of the Nucleotidyl Transfer Reaction. Journal of the American Chemical Society, 2013, 135, 8078-8088.	6.6	40
15	Weak Antiferromagnetic Coupling via a Superexchange Interaction between Mn(II)â€“Mn(II) Ions: A QM/MM Study of the Active Site of Human Cytosolic X-Propyl Aminopeptidase P. Journal of Physical Chemistry Letters, 2012, 3, 2293-2297.	2.1	5
16	HPAM: Hirshfeld partitioned atomic multipoles. Computer Physics Communications, 2012, 183, 390-397.	3.0	15
17	A revisit to the one-form kinetic model of prothrombinase: A comment on the rebuttal. Biophysical Chemistry, 2012, 160, 77-78.	1.5	1
18	Lee Pedersen s work in theoretical and computational chemistry and biochemistry. World Journal of Biological Chemistry, 2011, 2, 35.	1.7	1

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19	Modeling of the DNA-binding site of yeast Pms1 by mass spectrometry. DNA Repair, 2011, 10, 454-465.	1.3	13
20	A finite field method for calculating molecular polarizability tensors for arbitrary multipole rank. Journal of Computational Chemistry, 2011, 32, 3283-3295.	1.5	24
21	A hetero-dimer model for concerted action of vitamin K carboxylase and vitamin K reductase in vitamin K cycle. Journal of Theoretical Biology, 2011, 279, 143-149.	0.8	15
22	Molecular Insights into DNA Polymerase Deterrents for Ribonucleotide Insertion. Journal of Biological Chemistry, 2011, 286, 31650-31660.	1.6	45
23	Atomic forces for geometryâ€dependent point multipole and Gaussian multipole models. Journal of Computational Chemistry, 2010, 31, 2702-2713.	1.5	18
24	A revisit to the one form kinetic model of prothrombinase. Biophysical Chemistry, 2010, 149, 28-33.	1.5	18
25	Quantum chemical study of the mechanism of action of vitamin K carboxylase in solvent. International Journal of Quantum Chemistry, 2010, 110, 2744-2751.	1.0	3
26	Obligatory role in GTP hydrolysis for the amide carbonyl oxygen of the Mg ²⁺ -coordinating Thr of regulatory GTPases. Proceedings of the National Academy of Sciences of the United States of America, 2010, 107, 9596-9601.	3.3	7
27	Recent Estimates of the Structure of the Factor VIIa (FVIIa)/Tissue Factor (TF) and Factor Xa (FXa) Ternary Complex. Thrombosis Research, 2010, 125, S7-S10.	0.8	15
28	Steric, Quantum, and Electrostatic Effects on S_N2 Reaction Barriers in Gas Phase. Journal of Physical Chemistry A, 2010, 114, 5913-5918.	1.1	80
29	Gaussian Multipole Model (GMM). Journal of Chemical Theory and Computation, 2010, 6, 190-202.	2.3	79
30	Conformational change path between closed and open forms of C2 domain of coagulation factor V on a two-dimensional free-energy surface. Physical Review E, 2009, 79, 041909.	0.8	3
31	Dephosphorylation of Threonine 38 Is Required for Nuclear Translocation and Activation of Human Xenobiotic Receptor CAR (NR1I3). Journal of Biological Chemistry, 2009, 284, 34785-34792.	1.6	117
32	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
33	Reaction Mechanism of the Îµ Subunit of E. coli DNA Polymerase III: Insights into Active Site Metal Coordination and Catalytically Significant Residues. Journal of the American Chemical Society, 2009, 131, 1550-1556.	6.6	64
34	Molecular acidity: A quantitative conceptual density functional theory description. Journal of Chemical Physics, 2009, 131, 164107.	1.2	58
35	Estimation of Molecular Acidity via Electrostatic Potential at the Nucleus and Valence Natural Atomic Orbitals. Journal of Physical Chemistry A, 2009, 113, 3648-3655.	1.1	89
36	Computational study of the putative active form of protein Z (PZa): Sequence design and structural modeling. Protein Science, 2008, 17, 1354-1361.	3.1	6

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37	Catalytic mechanism of human DNA polymerase Î» with Mg2+ and Mn2+ from ab initio quantum mechanical/molecular mechanical studies. DNA Repair, 2008, 7, 1824-1834.	1.3	52
38	Exploring the origin of the internal rotational barrier for molecules with one rotatable dihedral angle. Journal of Chemical Physics, 2008, 129, 094104.	1.2	59
39	Incorrect nucleotide insertion at the active site of a G:A mismatch catalyzed by DNA polymerase Â. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 5670-5674.	3.3	48
40	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
41	A quantum chemical study of the mechanism of action of Vitamin K epoxide reductase (VKOR). Journal of Molecular Graphics and Modelling, 2007, 26, 401-408.	1.3	21
42	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
43	Quantum chemical study of the mechanism of action of vitamin K epoxide reductase (VKOR). International Journal of Quantum Chemistry, 2006, 106, 2944-2952.	1.0	16
44	Searching for the minimum energy path in the sulfuryl transfer reaction catalyzed by human estrogen sulfotransferase: Role of enzyme dynamics. International Journal of Quantum Chemistry, 2006, 106, 2981-2998.	1.0	16
45	Deuterium and its role in the machinery of evolution. Journal of Theoretical Biology, 2006, 238, 914-918.	0.8	16
46	Towards accurate solvation dynamics of divalent cations in water using the polarizable amoeba force field: From energetics to structure. Journal of Chemical Physics, 2006, 125, 054511.	1.2	169
47	New Distributed Multipole Metdhods for Accurate Electrostatics in Large-Scale Biomolecular Simulations. , 2006, , 297-312.		1
48	Energy analysis of chemistry for correct insertion by DNA polymerase beta. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 13294-13299.	3.3	88
49	Early Unfolding Response of a Stable Protein Domain to Environmental Changesâ€. Journal of Physical Chemistry A, 2004, 108, 9834-9840.	1.1	0
50	Towards an accurate representation of electrostatics in classical force fields: Efficient implementation of multipolar interactions in biomolecular simulations. Journal of Chemical Physics, 2004, 120, 73-87.	1.2	207
51	Glucosaminylglycan biosynthesis: what we can learn from the X-ray crystal structures of glycosyltransferases GlcAT1 and EXTL2. Biochemical and Biophysical Research Communications, 2003, 303, 393-398.	1.0	56
52	Explicit Water Near the Catalytic I Helix Thr in the Predicted Solution Structure of CYP2A4. Biophysical Journal, 2003, 84, 57-68.	0.2	14
53	Crystal Structure of an Î±1,4-N-Acetylhexosaminyltransferase (EXTL2), a Member of the Exostosin Gene Family Involved in Heparan Sulfate Biosynthesis. Journal of Biological Chemistry, 2003, 278, 14420-14428.	1.6	95
54	Structure and Dynamics of Zymogen Human Blood Coagulation Factor X. Biophysical Journal, 2002, 82, 1190-1206.	0.2	73

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55	Predicted solution structure of zymogen human coagulation FVII. Journal of Computational Chemistry, 2002, 23, 35-47.	1.5	15
56	Three-dimensional solution structure of Tropidechis carinatus venom extract trocarin: a structural homologue of Xa and prothrombin activator. Journal of Molecular Modeling, 2002, 8, 302-313.	0.8	6
57	Structure and Function of Sulfotransferases. Archives of Biochemistry and Biophysics, 2001, 390, 149-157.	1.4	306
58	Four loops of the catalytic domain of factor VIIa mediate the effect of the first EGF-like domain substitution on factor VIIa catalytic activity11Edited by R. Huber. Journal of Molecular Biology, 2001, 307, 1503-1517.	2.0	20
59	Modeling Human Zymogen Factor IX. Thrombosis and Haemostasis, 2001, 85, 596-603.	1.8	22
60	Models for protein-zinc ion binding sites. II. The catalytic sites. International Journal of Quantum Chemistry, 2001, 83, 150-165.	1.0	30
61	Gene selection for sample classification based on gene expression data: study of sensitivity to choice of parameters of the GA/KNN method. Bioinformatics, 2001, 17, 1131-1142.	1.8	560
62	Gene Assessment and Sample Classification for Gene Expression Data Using a Genetic Algorithm / k-nearest Neighbor Method. Combinatorial Chemistry and High Throughput Screening, 2001, 4, 727-739.	0.6	169
63	Quantum mechanical calculations on phosphate hydrolysis reactions. Journal of Computational Chemistry, 2000, 21, 43-51.	1.5	37
64	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. Journal of Computational Chemistry, 2000, 21, 1011-1039.	1.5	74
65	A Molecular Dynamics Model of HIV-1 Reverse Transcriptase Complexed with DNA: Comparison with Experimental Structures. Journal of Molecular Modeling, 2000, 6, 575-586.	0.8	9
66	Heparan Sulfate Biosynthesis: A Theoretical Study of the Initial Sulfation Step by N-Deacetylase/N-Sulfotransferase. Biophysical Journal, 2000, 79, 2909-2917.	0.2	21
67	Modeling Zymogen Protein C. Biophysical Journal, 2000, 79, 2925-2943.	0.2	31
68	Molecular Dynamics Simulations of the d(CCAACGTTGG)2 Decamer: Influence of the Crystal Environment. Biophysical Journal, 2000, 78, 668-682.	0.2	51
69	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. Journal of Computational Chemistry, 2000, 21, 1011.	1.5	3
70	A quantum mechanical study of the transfer of biological sulfate. Computational and Theoretical Chemistry, 1999, 461-462, 105-111.	1.5	11
71	New tricks for modelers from the crystallography toolkit: the particle mesh Ewald algorithm and its use in nucleic acid simulations. Structure, 1999, 7, R55-R60.	1.6	571
72	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

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73	An Atomic Model for the Pleated Î²-Sheet Structure of AÎ² Amyloid Protofilaments. Biophysical Journal, 1999, 76, 2871-2878.	0.2	120
74	Conserved structural motifs in the sulfotransferase family. Trends in Biochemical Sciences, 1998, 23, 129-130.	3.7	158
75	A role of Lys614in the sulfotransferase activity of human heparan sulfateN-deacetylase/N-sulfotransferase. FEBS Letters, 1998, 433, 211-214.	1.3	48
76	Transâ^'CisIsomerization of Proline 22 in Bovine Prothrombin Fragment 1:Â A Surprising Result of Structural Characterizationâ€. Biochemistry, 1998, 37, 10920-10927.	1.2	19
77	Identification of Residues 286 and 289 as Critical for Conferring Substrate Specificity of Human CYP2C9 for Diclofenac and Ibuprofen. Archives of Biochemistry and Biophysics, 1998, 357, 240-248.	1.4	58
78	Hydrophobicities of the nucleic acid bases: distribution coefficients from water to cyclohexane 1 1Edited by I. Tinoco. Journal of Molecular Biology, 1998, 280, 421-430.	2.0	70
79	Ionic charging free energies: Spherical versus periodic boundary conditions. Journal of Chemical Physics, 1998, 109, 10921-10935.	1.2	129
80	The Roles of Individual Î³-Carboxyglutamate Residues in the Solution Structure and Cation-dependent Properties of Conantokin-T. Journal of Biological Chemistry, 1998, 273, 7512-7522.	1.6	27
81	Conformational Changes in Conantokin-G Induced upon Binding of Calcium and Magnesium as Revealed by NMR Structural Analysis. Journal of Biological Chemistry, 1998, 273, 16248-16258.	1.6	36
82	Role of Î³-Carboxyglutamic Acid in the Calcium-Induced Structural Transition of Conantokin G, a Conotoxin from the Marine SnailConus geographusâ€,â€¡. Biochemistry, 1997, 36, 15677-15684.	1.2	54
83	Reciprocal Sizeâ^'Effect Relationship of the Key Residues in Determining Regio- and Stereospecificities of DHEA Hydroxylase Activity in P450 2a5. Biochemistry, 1997, 36, 3193-3198.	1.2	19
84	Refinement of the NMR Solution Structure of the Î³-Carboxyglutamic Acid Domain of Coagulation Factor IX Using Molecular Dynamics Simulation with Initial Ca2+Positions Determined by a Genetic Algorithmâ€. Biochemistry, 1997, 36, 2132-2138.	1.2	53
85	Crystal structure of estrogen sulphotransferase. Nature Structural and Molecular Biology, 1997, 4, 904-908.	3.6	263
86	Structure and relative acidity for a model zinc finger. Computational and Theoretical Chemistry, 1997, 419, 221-226.	1.5	11
87	Studies on the peptide corresponding to residues 34â€“47 of bovine factor X. Chemical Biology and Drug Design, 1997, 50, 34-38.	1.2	0
88	Selected New Developments in Computational Chemistry. Environmental Health Perspectives, 1996, 104, 69.	2.8	0
89	Anab InitioQuantum Mechanical Model for the Catalytic Mechanism of HIV-1 Protease. Journal of the American Chemical Society, 1996, 118, 3946-3950.	6.6	38
90	Characterization of Î³-Carboxyglutamic Acid Residue 21 of Human Factor IXâ€. Biochemistry, 1996, 35, 10321-10327.	1.2	9

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91	Structural flexibility and functional versatility of mammalian P450 enzymes. FASEB Journal, 1996, 10, 683-689.	0.2	68
92	Structural flexibility and functional versatility of cytochrome P450 and rapid evolution. Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis, 1996, 350, 43-50.	0.4	25
93	Enol and deprotonated forms of acetic and malonic acid. Computational and Theoretical Chemistry, 1996, 368, 163-171.	1.5	14
94	Identification of Residues 99, 220, and 221 of Human Cytochrome P450 2C19 as Key Determinants of Omeprazole Hydroxylase Activity. Journal of Biological Chemistry, 1996, 271, 12496-12501.	1.6	77
95	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
96	Computational Studies of Human Prothrombin Fragment 1 the Gla Domain of Factor IX and Several Biological Interesting Mutants. Pathophysiology of Haemostasis and Thrombosis: International Journal on Haemostasis and Thrombosis Research, 1996, 26, 54-59.	0.5	2
97	Accurate crystal molecular dynamics simulations using particle-mesh-Ewald: RNA dinucleotides â€" ApU and GpC. Chemical Physics Letters, 1995, 243, 229-235.	1.2	46
98	The first solvation shell of magnesium ion in a model protein environment with formate, water, and X-NH3, H2S, imidazole, formaldehyde, and chloride as ligands: An ab initio study. Proteins: Structure, Function and Bioinformatics, 1995, 21, 244-255.	1.5	17
99	Homology modeling and molecular dynamics simulation of human prothrombin fragment 1. Protein Science, 1995, 4, 2341-2348.	3.1	18
100	An ab initio quantum mechanical study of thioesters. Computational and Theoretical Chemistry, 1995, 358, 99-106.	1.5	15
101	Molecular dynamics simulation studies of a high resolution Zâ€ĐNA crystal. Journal of Chemical Physics, 1995, 102, 3830-3834.	1.2	45
102	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
103	Altering the Regiospecificity of Androstenedione Hydroxylase Activity in P450s 2a-4/5 by a Mutation of the Residue at Position 481. Biochemistry, 1995, 34, 5054-5059.	1.2	23
104	A smooth particle mesh Ewald method. Journal of Chemical Physics, 1995, 103, 8577-8593.	1.2	18,266
105	Toward the Accurate Modeling of DNA: The Importance of Long-Range Electrostatics. Journal of the American Chemical Society, 1995, 117, 5001-5002.	6.6	172
106	The Effect of Hydrostatic Pressure on Protein Crystals Investigated by Molecular Simulation. Jerusalem Symposia on Quantum Chemistry and Biochemistry, 1995, , 203-215.	0.2	0
107	Atomic-level accuracy in simulations of large protein crystals.. Proceedings of the National Academy of Sciences of the United States of America, 1994, 91, 8715-8718.	3.3	183
108	Particle mesh Ewald: AnNâ‹…log(N) method for Ewald sums in large systems. Journal of Chemical Physics, 1993, 98, 10089-10092.	1.2	24,656

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109	The effect of longâ€range electrostatic interactions in simulations of macromolecular crystals: A comparison of the Ewald and truncated list methods. Journal of Chemical Physics, 1993, 99, 8345-8348.	1.2	611
110	Molecular dynamics simulation of bovine prothrombin fragment 1 in the presence of calcium ions. Biochemistry, 1992, 31, 8840-8848.	1.2	27
111	The interaction of Na(I), Ca(II), and Mg(II) metal ions with duplex DNA: A theoretical modeling study. International Journal of Quantum Chemistry, 1992, 44, 145-166.	1.0	16
112	The barrier to proton transfer from multiply protonated molecules: A quantum mechanical approach. Organic Mass Spectrometry, 1992, 27, 974-975.	1.3	13
113	Predicted secondary structure of bovine prothrombin fragment 1 and related proteins in different environments by circular dichroism spectroscopy. International Journal of Peptide and Protein Research, 1992, 40, 127-133.	0.1	0
114	Structural properties of a Gla-domain peptide of prothrombin fragment I. , 1992, , 285-286.		0
115	Interaction of calcium and magnesium ions with malonate and the role of the waters of hydration: a quantum mechanical study. Journal of the American Chemical Society, 1991, 113, 1892-1899.	6.6	16
116	OXYGEN-17 NMR STUDIES OF HETEROCYCLIC SULFONES ANDtrans-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
117	Determination of strontium binding to macromolecules. Analytical Biochemistry, 1991, 198, 391-393.	1.1	10
118	Free energy calculations on calcium and magnesium complexes: Protein and phospholipid model systems. Journal of Computational Chemistry, 1991, 12, 899-908.	1.5	8
119	Long range nonbonded attractive constants for some charged atoms. Journal of Computational Chemistry, 1991, 12, 1125-1128.	1.5	24
120	Proton, calcium, and magnesium binding by peptides containing Î³â€carboxyglutamic acid. International Journal of Peptide and Protein Research, 1991, 37, 33-38.	0.1	4
121	Generation of potential structures for the G-domain of chloroplast EF-Tu using comparative molecular modeling. Proteins: Structure, Function and Bioinformatics, 1990, 8, 237-250.	1.5	7
122	Construction and molecular modeling of phospholipid surfaces. Journal of Computational Chemistry, 1990, 11, 1181-1186.	1.5	56
123	The Role of Hydrated Divalent Metal Ions in the Bridging of Two Anionic Groups. Anab initioQuantum Chemical and Molecular Mechanics Study of Dimethyl Phosphate and Formate Bridged by Calcium and Magnesium Ions. Journal of Biomolecular Structure and Dynamics, 1989, 6, 1077-1091.	2.0	16
124	Salt or ion bridges in biological system: A study employing quantum and molecular mechanics. Proteins: Structure, Function and Bioinformatics, 1989, 6, 168-192.	1.5	33
125	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
126	Influences of solvent water on protein folding: free energies of solvation of cis and trans peptides are nearly identical. Biochemistry, 1988, 27, 4538-4541.	1.2	161

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127	The determination of a calcium-dependent binding constant of the bovine prothrombin GLA domain (residues 1â€“45) to phospholipid vesicles. Biochemical and Biophysical Research Communications, 1988, 155, 230-235.	1.0	7
128	Relative affinity of Ca(II) and Mg(II) ions for human and bovine prothrombin and fragment 1. Biochemical and Biophysical Research Communications, 1987, 144, 520-527.	1.0	19
129	Determination of magnesium binding to macromolecules. Analytical Biochemistry, 1987, 160, 468-470.	1.1	4
130	Estimation of apparent quadrupolar coupling constants for complexes of magnesium ions with mono- and dicarboxylic acid ligands. applications to magnesium ion: protein interactions. Journal of Inorganic Biochemistry, 1987, 29, 153-164.	1.5	5
131	Do residue levels of polychlorinated biphenyls (PCBs) in human blood produce mild hypothyroidism?. Journal of Theoretical Biology, 1987, 129, 231-241.	0.8	20
132	Relative spectral response as a function of sequential ligand binding. Biochemical and Biophysical Research Communications, 1986, 141, 1207-1212.	1.0	4
133	Terbium ion binding to a synthetic .gamma.-carboxyglutamic acid containing heptapeptide corresponding to bovine prothrombin residues 17-23. Inorganic Chemistry, 1986, 25, 4503-4506.	1.9	2
134	Direct observation of new antimony-containing anions: SbH2Oâ^', Sb3â^', and monomeric Sb3O5â^'. Inorganica Chimica Acta, 1986, 115, 203-205.	1.2	3
135	Synthesis of a Î³â€carboxyglutamic acid containing heptapeptide corresponding to bovine prothrombin residues 17â€“23. International Journal of Peptide and Protein Research, 1986, 28, 569-578.	0.1	2
136	Direct observation of the hydrogen metatitanate (HTiO3-) ion. Inorganic Chemistry, 1985, 24, 4748-4749.	1.9	4
137	A Kinetic Model Describing the Interaction of Bovine Prothrombin Fragment 1 with Calcium Ions. Thrombosis and Haemostasis, 1985, 53, 019-023.	1.8	2
138	UTILIZATION OF HEAVYâ€ATOM EFFECT QUENCHING OF PYRENE FLUORESCENCE TO DETERMINE THE INTRAMEMBRANE DISTRIBUTION OF HALOTHANE. Photochemistry and Photobiology, 1984, 40, 693-702.	1.3	8
139	Photochemical reactions in organized assemblies. 37. Photochemistry and photophysics of surfactant trans-stilbenes in supported multilayers and films at the air-water interface. Journal of the American Chemical Society, 1984, 106, 5659-5667.	6.6	128
140	Direct observation of the H2NO2 ? ion. Journal of the Chemical Society Chemical Communications, 1983, , 517.	2.0	2
141	Resistive heating of emitter wires for field desorption and ionization: A theory. International Journal of Mass Spectrometry and Ion Physics, 1982, 43, 99-129.	1.3	3
142	Field ionization at a surface modified by chemically bound carboxylic acid groups. International Journal of Mass Spectrometry and Ion Physics, 1981, 38, 223-239.	1.3	5
143	Chemical field ionization. Effect of chemically bonded surface groups in field ionization mass spectrometry. Journal of the American Chemical Society, 1980, 102, 6881-6882.	6.6	6
144	Europium ion coordination with .gamma.-carboxyglutamic acid containing ligand systems. Journal of the American Chemical Society, 1980, 102, 3404-3412.	6.6	26

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145	Consequences of charge reversal of gaseous formate and acetate ions. Acyloxy ions. Journal of the American Chemical Society, 1979, 101, 5489-5493.	6.6	30
146	The interaction of charged disks in a dielectric medium. Journal of Chemical Physics, 1978, 68, 4333-4337.	1.2	1
147	Molecular orbital studies of the protonation of the methylanisoles. Journal of the American Chemical Society, 1976, 98, 4061-4064.	6.6	23
148	Position of protonation of the cresols: Semi-empirical and ab initio calculations. Chemical Physics Letters, 1975, 36, 470-474.	1.2	4
149	Extension of GAUSSIAN70 to any number of atomic orbitals. Journal of Computational Physics, 1975, 17, 415-419.	1.9	1
150	Internal rotation in the molecular ions of benzoic acid and salicylic acid. An INDO molecular orbital approach. Organic Mass Spectrometry, 1974, 9, 204-210.	1.3	3
151	Scrambling in ethane molecular ion: An INDO model for hydrogen exchange before mass spectral fragmentation. Organic Mass Spectrometry, 1973, 7, 1077-1081.	1.3	3
152	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. Organic Mass Spectrometry, 1973, 7, 1189-1195.	1.3	3
153	Molecularâ€Orbital Studies of Hydrogen Bonds. An Ab Initio Calculation for Dimeric H2O. Journal of Chemical Physics, 1968, 48, 3275-3282.	1.2	240
154	Ab InitioCalculations of the Barriers to Internal Rotation of CH3CH3, CH3NH2, CH3OH, N2H4, H2O2, and NH2OH. Journal of Chemical Physics, 1967, 46, 3941-3947.	1.2	143
155	A smooth particle mesh Ewald method. , 0, .		1