Jill E Gready

List of Publications by Year
in descending order

78 papers	3,731 citations	218677 26 h-index	133252 59 g-index
79 all docs	79 docs citations	79 times ranked	4668 citing authors

#	Article	IF	Citations
1	Kohnâ€“Sham Density Functional Calculations Reveal Proton Wires in the Enolization and Carboxylase Reactions Catalyzed by Rubisco. Journal of Physical Chemistry B, 2020, 124, 3015-3026.	2.6	7
2	Mechanism of Oxygenase-Pathway Reactions Catalyzed by Rubisco from Large-Scale Kohnâ€“Sham Density Functional Calculations. Journal of Physical Chemistry B, 2019, 123, 2833-2843.	2.6	9
3	Ab Initio Molecular Dynamics Simulation and Energetics of the Ribulose-1,5-biphosphate Carboxylation Reaction Catalyzed by Rubisco: Toward Elucidating the Stereospecific Protonation Mechanism. Journal of Physical Chemistry B, 2019, 123, 2679-2686.	2.6	12
4	Response: Commentary: Directions for Optimization of Photosynthetic Carbon Fixation: RuBisCOâ€™s Efficiency May Not Be So Constrained After All. Frontiers in Plant Science, 2019, 10, 1426.	3.6	8
5	Directions for Optimization of Photosynthetic Carbon Fixation: RuBisCO's Efficiency May Not Be So Constrained After All. Frontiers in Plant Science, 2018, 9, 183.	3.6	46
6	Revised mechanism of carboxylation of ribuloseâ€1,5â€biphosphate by rubisco from large scale quantum chemical calculations. Journal of Computational Chemistry, 2018, 39, 1656-1665.	3.3	17
7	Optimization of parameters for molecular dynamics simulation using smooth particleâ€mesh Ewald in GROMACS 4.5. Journal of Computational Chemistry, 2011, 32, 2031-2040.	3.3	217
8	Methyltetrahydrofolate:corrinoid/ironâ˜sulfur Protein Methyltransferase (MeTr): Protonation State of the Ligand and Active-Site Residues. Journal of Physical Chemistry B, 2009, 113, 14787-14796.	2.6	5
9	Ensuring Mixing Efficiency of Replica-Exchange Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2008, 4, 1119-1128.	5.3	71
10	Redefinition of Rubisco Carboxylase Reaction Reveals Origin of Water for Hydration and New Roles for Active-Site Residues. Journal of the American Chemical Society, 2008, 130, 15063-15080.	13.7	42
11	Calculation of a Complete Enzymic Reaction Surface:â€‰ Reaction and Activation Free Energies for Hydride-Ion Transfer in Dihydrofolate Reductase. Journal of Chemical Theory and Computation, 2007, 3, 1203-1211.	5.3	13
12	Integron-sequestered dihydrofolate reductase: a recently redeployed enzyme. Trends in Microbiology, 2006, 14, 236-242.	7.7	21
13	Defining the Inefficiencies in the Chemical Mechanism of the Photosynthetic Enzyme Rubisco by Computational Simulation. , 2006, , 263-282.		0
14	Combining docking and molecular dynamic simulations in drug design. Medicinal Research Reviews, 2006, 26, 531-568.	10.5	586
15	The Câ€type lectinâ€like domain superfamily. FEBS Journal, 2005, 272, 6179-6217.	4.7	1,162
16	Computational methods for the study of enzymic reaction mechanisms III: A perturbation plus QM/MM approach for calculating relative free energies of protonation. Journal of Computational Chemistry, 2005, 26, 561-568.	3.3	11
17	Multiple ligand-binding modes in bacterial R67 dihydrofolate reductase. Journal of Computer-Aided Molecular Design, 2005, 19, 165-187.	2.9	12
18	Evolution of Vertebrate Genes Related to Prion and Shadoo Proteinsâ€”Clues from Comparative Genomic Analysis. Molecular Biology and Evolution, 2004, 21, 2210-2231.	8.9	50

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19	C-type lectin-like domains in Fugu rubripes. BMC Genomics, 2004, 5, 51.	2.8	59
20	Conformation of Prion Protein Repeat Peptides Probed by FRET Measurements and Molecular Dynamics Simulations. Biophysical Journal, 2004, 86, 2467-2483.	0.5	60
21	Synthesis of quaternised 2-aminopyrimido[4,5-d]pyrimidin-4(3H)-ones and their biological activity with dihydrofolate reductase. European Journal of Medicinal Chemistry, 2003, 38, 719-728.	5.5	67
22	Computational methods for the study of enzymic reaction mechanisms. II. An overlapping mechanically embedded method for hybrid semi-empirical-QM/MM calculations. Computational and Theoretical Chemistry, 2003, 632, 247-257.	1.5	5
23	Comparative analysis of structural properties of the C-type-lectin-like domain (CTLD). Proteins: Structure, Function and Bioinformatics, 2003, 52, 466-477.	2.6	104
24	Comparison of electrostatic potential around proteins calculated from Amber and AM1 charges: application to mutants of prion protein. Molecular Physics, 2003, 101, 2437-2450.	1.7	12
25	Solvent Simulation. , 2003, , .		0
26	Computational Methods for the Study of Enzymic Reaction Mechanisms. 1. Application to the Hydride Transfer Step in the Catalysis of Dihydrofolate Reductase. Journal of Physical Chemistry B, 2002, 106, 9934-9944.	2.6	26
27	Copper-induced conformational change in a marsupial prion protein repeat peptide probed using FTIR spectroscopy. FEBS Letters, 2002, 512, 38-42.	2.8	22
28	Comparison of linear-scaling semiempirical methods and combined quantum mechanical/molecular mechanical methods for enzymic reactions. II. An energy decomposition analysis. Journal of Computational Chemistry, 2002, 23, 1314-1322.	3.3	26
29	Comparison of semiempirical and ab initio QM decomposition analyses for the interaction energy between molecules. Chemical Physics Letters, 2002, 352, 245-251.	2.6	17
30	Energetically Most Likely Substrate and Active-Site Protonation Sites and Pathways in the Catalytic Mechanism of Dihydrofolate Reductase. Journal of the American Chemical Society, 2001, 123, 3418-3428.	13.7	52
31	CO2Fixation by Rubisco:Â Computational Dissection of the Key Steps of Carboxylation, Hydration, and Câ'C Bond Cleavage. Journal of the American Chemical Society, 2001, 123, 10821-10829.	13.7	64
32	Comparison of enzyme polarization of ligands and charge-transfer effects for dihydrofolate reductase using point-charge embeddedab initio quantum mechanical and linear-scaling semiempirical quantum mechanical methods. Journal of Computational Chemistry, 2000, 21, 788-811.	3.3	35
33	Comparison of linear-scaling semiempirical methods and combined quantum mechanical/molecular mechanical methods applied to enzyme reactions. Chemical Physics Letters, 2000, 320, 169-176.	2.6	35
34	QM/MM and SCRF studies of the ionization state of 8-methylpterin substrate bound to dihydrofolate reductase: existence of a low-barrier hydrogen bond. Journal of Molecular Graphics and Modelling, 2000, 18, 42-49.	2.4	10
35	Combined Quantum and Molecular Mechanics (QM/MM) Study of the Ionization State of 8-Methylpterin Substrate Bound to Dihydrofolate Reductase. Journal of Physical Chemistry B, 2000, 104, 4503-4510.	2.6	26
36	Molecular Dynamics Simulations of L-Lactate Dehydrogenase: Conformation of a Mobile Loop and Influence of the Tetrameric Protein Environment. Journal of Molecular Modeling, 1999, 5, 153-168.	1.8	12

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37	Simple method for locating possible ligand binding sites on protein surfaces. Journal of Computational Chemistry, 1999, 20, 983-988.	3.3	38
38	Coupled semiempirical quantum mechanics and molecular mechanics (QM/MM) calculations on the aqueous solvation free energies of ionized molecules. Journal of Computational Chemistry, 1999, 20, 1028-1038.	3.3	26
39	Enzyme polarization of substrates of dihydrofolate reductase by different theoretical methods. , 1999, 37, 157-165.		23
40	31P and1H NMR spectroscopic studies of liver extracts of carbon tetrachloride-treated rats. NMR in Biomedicine, 1999, 12, 395-401.	2.8	31
41	Enzyme polarization of substrates of dihydrofolate reductase by different theoretical methods. Proteins: Structure, Function and Bioinformatics, 1999, 37, 157-165.	2.6	1
42	Identification and energetic ranking of possible docking sites for pterin on dihydrofolate reductase. , 1998, 12, 325-333.		15
43	Molecular dynamics and free energy perturbation study of hydride-ion transfer step in dihydrofolate reductase using combined quantum and molecular mechanical model. Journal of Computational Chemistry, 1998, 19, 977-988.	3.3	40
44	Investigating Enzyme Reaction Mechanisms with Quantum Mechanical-Molecular Mechanical Plus Molecular Dynamics Calculations. ACS Symposium Series, 1998, , 250-263.	0.5	9
45	Quantum Chemical Analysis of the Enolization of Ribulose Bisphosphate:â€‰ The First Hurdle in the Fixation of CO2 by Rubisco. Biochemistry, 1998, 37, 15414-15422.	2.5	39
46	Hybrid Quantum and Molecular Mechanical (QM/MM) Studies on the Pyruvate to l-Lactate Interconversion in l-Lactate Dehydrogenase. Journal of Physical Chemistry B, 1997, 101, 5614-5618.	2.6	60
47	Predicted structure of the extracellular region of ligandâ€gated ionâ€channel receptors shows SH2â€like and SH3â€like domains forming the ligandâ€binding site. Protein Science, 1997, 6, 983-998.	7.6	33
48	Coupled semiempirical molecular orbital and molecular mechanics model (QM/MM) for organic molecules in aqueous solution. Journal of Computational Chemistry, 1997, 18, 1496-1512.	3.3	67
49	Numerical calculation of molecular surface area. I. Assessment of errors. Journal of Computational Chemistry, 1996, 17, 962-969.	3.3	13
50	Numerical calculation of molecular surface area. II. Speed of calculation. Journal of Computational Chemistry, 1996, 17, 970-975.	3.3	6
51	Solvent effects in active-site molecular dynamics simulations on the binding of 8-methyl-N5-deazapterin and 8-methylpterin to dihydrofolate reductase. Journal of Computational Chemistry, 1996, 17, 1598-1611.	3.3	11
52	A New Approach to Estimation of the Electrostatic Component of the Solvation Energy in Molecular Mechanics Calculations. The Journal of Physical Chemistry, 1995, 99, 14506-14513.	2.9	5
53	Structure-Activity Relationships for the 8-Alkylpterins: A New Class of Mechanism-Based Substrates for Dihydrofolate Reductase (DHFR). Biochemistry, 1995, 34, 3724-3733.	2.5	9
54	The Influence of Starting Coordinates in Free Energy Simulations of Ligand Binding to Dihydrofolate Reductase. Molecular Simulation, 1995, 15, 155-175.	2.0	4

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55	Electronic spectra of some pterins and deazapterins. Chemical Physics, 1994, 179, 55-69.	1.9	21
56	The electrostatic potential in the semiempirical molecular orbital approximation. Chemical Physics Letters, 1994, 225, 11-17.	2.6	18
57	Thermodynamic integration calculations on the relative free energies of complex ions in aqueous solution: Application to ligands of dihydrofolate reductase. Journal of Computational Chemistry, 1994, 15, 704-718.	3.3	13
58	An improved procedure for the preparation of 2â€aminoâ€8â€alkylpyridoâ€[2,3â€d]pyrimidinâ€4(3H)â€ones (8â€alkylâ€N5â€deazapterins). Journal of Heterocyclic Chemistry, 1994, 31, 1385-1397.	2.6	6
59	Ionization state and pKa of pterin-analogue ligands bound to dihydrofolate reductase. FEBS Journal, 1994, 221, 1055-1062.	0.2	9
60	Structure-Activity Relationships and pH Dependence of Binding of 8-Alkyl-N5-Deazapterins to Dihydrofolate Reductase. Journal of Medicinal Chemistry, 1994, 37, 4211-4221.	6.4	6
61	Theoretical study of â€œprotonated pyruvateâ€: A methylhydroxycarbene-carbon dioxide complex-implications for the decarboxylation of pyruvic acid. Journal of Computational Chemistry, 1993, 14, 699-714.	3.3	12
62	Novel mechanism-based substrates of dihydrofolate reductase and the thermodynamics of ligand binding: A comparison of theory and experiment for 8-methylpterin and 6,8-dimethylpterin. Proteins: Structure, Function and Bioinformatics, 1993, 15, 426-435.	2.6	8
63	Investigation of Spectra and Ionization Constants of 8-Alkyl Pterins by Fluorimetry. Pteridines, 1993, 4, 32-38.	0.5	5
64	NMR studies of bond orders in heteroaromatic systems. Journal of Heterocyclic Chemistry, 1992, 29, 935-946.	2.6	22
65	Progress on the Unambiguous Synthesis of S-Methyl-7,8-dihydropterin. Pteridines, 1991, 3, 113-114.	0.5	0
66	Isomer Distributions and Separation of 6- and 7- Methyl-8-Alkyl Pterins. Pteridines, 1991, 3, 105-107.	0.5	5
67	Use of SCX HPLC in the Study of 8-Alkyl-Pterins and their Reduced Derivatives. Pteridines, 1991, 3, 115-117.	0.5	4
68	Prediction of Relative Binding Constants of Cofactors and Designed Ligands to Dihydrofolate Reductase by Computer Simulation. Pteridines, 1991, 3, 137-139.	0.5	1
69	NMR Studies of the Structures and Degradation of 8-(2â€™-Hydroxyethyl)Pterins. Pteridines, 1991, 3, 109-111.	0.5	2
70	Mechanistic aspects of biological redox reactions involving NADH 2: A combined semiempirical andab initio study of hydride-ion transfer between the NADH analogue, 1-methyl-dihydronicotinamide, and folate and dihydrofolate analogue substrates of dihydrofolate reductase. Journal of Computational Chemistry, 1990, 11, 791-804.	3.3	31
71	Guanidinium-Type resonance stabilization and its biological implications. I. the guanidine and extended-guanidine series. Journal of Computational Chemistry, 1989, 10, 35-54.	3.3	39
72	Guanidinium-Type resonance stabilization and its biological implications. 2. The doubly-extended-guanidine series. Journal of Computational Chemistry, 1989, 10, 186-202.	3.3	8

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73	Computational strategies for the optimization of equilibrium geometries and transition-state structures at the semiempirical level. Journal of Computational Chemistry, 1989, 10, 939-950.	3.3	22
74	Enzymic properties of a new mechanism-based substrate for dihydrofolate reductase. Biochemistry, 1989, 28, 6042-6049.	2.5	25
75	Prediction and experimental comparison of deuterium quadrupole coupling constants in some bifluoride salts: An extreme example of symmetric hydrogen bonding in different crystalline environments. Journal of Chemical Physics, 1988, 88, 2526-2539.	3.0	16
76	Analysis of inter-ring coupling effects inN-heterobicyclic ?-systems using a structural definition of aromaticity. International Journal of Quantum Chemistry, 1987, 31, 369-382.	2.0	12
77	Theoretical studies on pteridines. 2. Geometries, tautomer, ionization and reduction energies of substrates and inhibitors of dihydrofolate reductase. Journal of Computational Chemistry, 1985, 6, 377-400.	3.3	25
78	Theoretical studies on the activation of the pterin cofactor in the catalytic mechanism of dihydrofolate reductase. Biochemistry, 1985, 24, 4761-4766.	2.5	68