Ulf Ryde

List of Publications by Year
in descending order

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270	18,359	13099	17105
papers	citations	68 h-index	122 g-index

282	282	282	15047
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The MM/PBSA and MM/GBSA methods to estimate ligand-binding affinities. Expert Opinion on Drug Discovery, 2015, 10, 449-461.	5.0	2,907
2	MOLCAS: a program package for computational chemistry. Computational Materials Science, 2003, 28, 222-239.	3.0	1,689
3	Comparison of methods for deriving atomic charges from the electrostatic potential and moments. Journal of Computational Chemistry, 1998, 19, 377-395.	3.3	334
4	Ligand Affinities Predicted with the MM/PBSA Method:Â Dependence on the Simulation Method and the Force Field. Journal of Medicinal Chemistry, 2006, 49, 6596-6606.	6.4	240
5	Structure, strain, and reorganization energy of blue copper models in the protein. International Journal of Quantum Chemistry, 2001, 81, 335-347.	2.0	229
6	Ligand-Binding Affinity Estimates Supported by Quantum-Mechanical Methods. Chemical Reviews, 2016, 116, 5520-5566.	47.7	216
7	Performance of density functionals for first row transition metal systems. Journal of Chemical Physics, 2007, 126, 014103.	3.0	210
8	Protein Flexibility and Conformational Entropy in Ligand Design Targeting the Carbohydrate Recognition Domain of Galectin-3. Journal of the American Chemical Society, 2010, 132, 14577-14589.	13.7	209
9	On the Convergence of QM/MM Energies. Journal of Chemical Theory and Computation, 2011, 7, 761-777.	5.3	185
10	The Cupric Geometry of Blue Copper Proteins is not Strained. Journal of Molecular Biology, 1996, 261, 586-596.	4.2	176
11	On the role of the axial ligand in heme proteins: a theoretical study. Journal of Biological Inorganic Chemistry, 2004, 9, 203-223.	2.6	176
12	The coordination of the catalytic zinc ion in alcohol dehydrogenase studied by combined quantum-chemical and molecular mechanics calculations. Journal of Computer-Aided Molecular Design, 1996, 10, 153-164.	2.9	171
13	How O2 Binds to Heme. Journal of Biological Chemistry, 2004, 279, 14561-14569.	3.4	170
14	Theoretical Prediction of the Coâ^'C Bond Strength in Cobalamins. Journal of Physical Chemistry A, 2003, 107, 7539-7545.	2.5	168
15	How to obtain statistically converged MM/GBSA results. Journal of Computational Chemistry, 2010, 31, 837-846.	3.3	167
16	The Normal-Mode Entropy in the MM/GBSA Method: Effect of System Truncation, Buffer Region, and Dielectric Constant. Journal of Chemical Information and Modeling, 2012, 52, 2079-2088.	5.4	166
17	Relation between the Structure and Spectroscopic Properties of Blue Copper Proteins. Journal of the American Chemical Society, 1998, 120, 13156-13166.	13.7	158
18	Structures of the high-valent metal-ion haemâ€“oxygen intermediates in peroxidases, oxygenases and catalases. Journal of Inorganic Biochemistry, 2006, 100, 460-476.	3.5	152

#	Article	IF	Citations
19	The Carbohydrate-Binding Site in Galectin-3 Is Preorganized To Recognize a Sugarlike Framework of Oxygens: Ultra-High-Resolution Structures and Water Dynamics. Biochemistry, 2012, 51, 296-306.	2.5	137
20	Quantum Mechanical Free Energy Barrier for an Enzymatic Reaction. Physical Review Letters, 2005, 94, 138302.	7.8	136
21	A Comparison of the Inner-Sphere Reorganization Energies of Cytochromes, Ironâ^'Sulfur Clusters, and Blue Copper Proteins. Journal of Physical Chemistry B, 2001, 105, 5546-5552.	2.6	135
22	Metal Ion Enhanced Binding of AMD3100 to Asp262in the CXCR4 Receptorâ€. Biochemistry, 2003, 42, 710-717.	2.5	134
23	Accurate QM/MM Free Energy Calculations of Enzyme Reactions:Â Methylation by CatecholO-Methyltransferase. Journal of Chemical Theory and Computation, 2005, 1, 1240-1251.	5.3	133
24	An MM/3D-RISM Approach for Ligand Binding Affinities. Journal of Physical Chemistry B, 2010, 114, 8505-8516.	2.6	129
25	Molecular dynamics simulations of alcohol dehydrogenase with a four- or five-coordinate catalytic zinc ion. Proteins: Structure, Function and Bioinformatics, 1995, 21, 40-56.	2.6	124
26	Quantum Chemistry Can Locally Improve Protein Crystal Structures. Journal of the American Chemical Society, 2003, 125, 14232-14233.	13.7	124
27	An improved method to predict the entropy term with the MM/PBSA approach. Journal of Computer-Aided Molecular Design, 2009, 23, 63-71.	2.9	122
28	Quantum Refinement Does Not Support Dinuclear Copper Sites in Crystal Structures of Particulate Methane Monooxygenase. Angewandte Chemie - International Edition, 2018, 57, 162-166.	13.8	122
29	Prediction of Activation Energies for Hydrogen Abstraction by Cytochrome P450. Journal of Medicinal Chemistry, 2006, 49, 6489-6499.	6.4	120
30	How the Coâ^'C Bond Is Cleaved in Coenzyme B12Enzymes:Â A Theoretical Study. Journal of the American Chemical Society, 2005, 127, 9117-9128.	13.7	118
31	Theoretical Study of the Electronic Spectrum of Plastocyanin. Journal of the American Chemical Society, 1997, 119, 218-226.	13.7	117
32	Carboxylate Binding Modes in Zinc Proteins: A Theoretical Study. Biophysical Journal, 1999, 77, 2777-2787.	0.5	115
33	A QM/MM Investigation of the Activation and Catalytic Mechanism of Fe-Only Hydrogenases. Inorganic Chemistry, 2007, 46, 5911-5921.	4.0	112
34	Computational modelling of oxygenation processes in enzymes and biomimetic model complexes. Chemical Communications, 2014, 50, 262-282.	4.1	110
35	Comparison of Methods to Obtain Force-Field Parameters for Metal Sites. Journal of Chemical Theory and Computation, 2011, 7, 2452-2463.	5.3	108
36	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	3.3	108

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37	Combined quantum and molecular mechanics calculations on metalloproteins. Current Opinion in Chemical Biology, 2003, 7, 136-142.	6.1	106
38	Quantum chemical geometry optimizations in proteins using crystallographic raw data. Journal of Computational Chemistry, 2002, 23, 1058-1070.	3.3	104
39	On the significance of hydrogen bonds for the discrimination between CO and O2 by myoglobin. Journal of Biological Inorganic Chemistry, 1999, 4, 99-110.	2.6	101
40	How Accurate Can a Force Field Become? A Polarizable Multipole Model Combined with Fragment-wise Quantum-Mechanical Calculations. Journal of Physical Chemistry A, 2009, 113, 617-627.	2.5	99
41	A fundamental view of enthalpyâ€“entropy compensation. MedChemComm, 2014, 5, 1324-1336.	3.4	98
42	Inner-Sphere Reorganization Energy of Ironâ^'Sulfur Clusters Studied with Theoretical Methods. Inorganic Chemistry, 2001, 40, 2509-2519.	4.0	97
43	O-binding to heme: electronic structure and spectrum of oxyheme, studied by multiconfigurational methods. Journal of Inorganic Biochemistry, 2005, 99, 45-54.	3.5	97
44	Geometry, Reduction Potential, and Reorganization Energy of the Binuclear CuASite, Studied by Density Functional Theory. Journal of the American Chemical Society, 2001, 123, 7866-7876.	13.7	96
45	On the role of strain in blue copper proteins. Journal of Biological Inorganic Chemistry, 2000, 5, 565-574.	2.6	89
46	Interplay between Conformational Entropy and Solvation Entropy in Proteinâ€“Ligand Binding. Journal of the American Chemical Society, 2019, 141, 2012-2026.	13.7	89
47	Influence of the [2Fe]_H Subcluster Environment on the Properties of Key Intermediates in the Catalytic Cycle of [FeFe] Hydrogenases: Hints for the Rational Design of Synthetic Catalysts. Angewandte Chemie - International Edition, 2009, 48, 3503-3506.	13.8	86
48	Do Quantum Mechanical Energies Calculated for Small Models of Protein-Active Sites Converge?. Journal of Physical Chemistry A, 2009, 113, 11793-11800.	2.5	86
49	Will molecular dynamics simulations of proteins ever reach equilibrium?. Physical Chemistry Chemical Physics, 2012, 14, 8662.	2.8	85
50	On the role of Gluâ€68 in alcohol dehydrogenase. Protein Science, 1995, 4, 1124-1132.	7.6	84
51	Quantum chemical calculations of the reorganization energy of blueâ€copper proteins. Protein Science, 1998, 7, 2659-2668.	7.6	84
52	Sulfoxide, Sulfur, and Nitrogen Oxidation and Dealkylation by Cytochrome P450. Journal of Chemical Theory and Computation, 2008, 4, 1369-1377.	5.3	83
53	Ligand Affinities Estimated by Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2010, 6, 1726-1737.	5.3	81
54	Does DFT-D estimate accurate energies for the binding of ligands to metal complexes?. Dalton Transactions, 2011, 40, 11176.	3.3	81

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55	Redesign of the coenzyme specificity in l-Lactate dehydrogenase from Bacillus stearothermophilus using site-directed mutagenesis and media engineering. Protein Engineering, Design and Selection, 1999, 12, 851-856.	2.1	80
56	Accurate Reaction Energies in Proteins Obtained by Combining QM/MM and Large QM Calculations. Journal of Chemical Theory and Computation, 2013, 9, 640-649.	5.3	80
57	A Combined Quantum and Molecular Mechanical Study of the O2Reductive Cleavage in the Catalytic Cycle of Multicopper Oxidases. Inorganic Chemistry, 2005, 44, 5612-5628.	4.0	79
58	The Structures of Frataxin Oligomers Reveal the Mechanism for the Delivery and Detoxification of Iron. Structure, 2006, 14, 1535-1546.	3.3	78
59	Comparison of endâ€point continuumâ€solvation methods for the calculation of proteinâ€“ligand binding free energies. Proteins: Structure, Function and Bioinformatics, 2012, 80, 1326-1342.	2.6	78
60	Molecular mechanism of lytic polysaccharide monooxygenases. Chemical Science, 2018, 9, 3866-3880.	7.4	77
61	Comparison of MM/GBSA calculations based on explicit and implicit solvent simulations. Physical Chemistry Chemical Physics, 2013, 15, 7731.	2.8	76
62	Conformational entropy changes upon lactose binding to the carbohydrate recognition domain of galectin-3. Journal of Biomolecular NMR, 2009, 45, 157-169.	2.8	75
63	Effect of Geometry Optimizations on QM-Cluster and QM/MM Studies of Reaction Energies in Proteins. Journal of Chemical Theory and Computation, 2013, 9, 4205-4214.	5.3	75
64	QM/MM Calculations on Proteins. Methods in Enzymology, 2016, 577, 119-158.	1.0	75
65	Quantum Refinement of [FeFe] Hydrogenase Indicates a Dithiomethylamine Ligand. Journal of the American Chemical Society, 2010, 132, 4512-4513.	13.7	73
66	The influence of axial ligands on the reduction potential of blue copper proteins. Journal of Biological Inorganic Chemistry, 1999, 4, 654-663.	2.6	72
67	Review: Studies of ferric heme proteins with highly anisotropic/highly axial low spin (S = 1/2) electron paramagnetic resonance signals with bisâ€Histidine and histidineâ€methionine axial iron coordination. Biopolymers, 2009, 91, 1064-1082.	2.4	72
68	Binding Affinities of Factor Xa Inhibitors Estimated by Thermodynamic Integration and MM/GBSA. Journal of Chemical Information and Modeling, 2011, 51, 947-958.	5.4	72
69	Comparison of the Efficiency of the LIE and MM/GBSA Methods to Calculate Ligand-Binding Energies. Journal of Chemical Theory and Computation, 2011, 7, 3768-3778.	5.3	71
70	On the Difference Between Additive and Subtractive QM/MM Calculations. Frontiers in Chemistry, 2018, 6, 89.	3.6	71
71	Free-energy perturbation and quantum mechanical study of SAMPL4 octa-acid hostâ€“guest binding energies. Journal of Computer-Aided Molecular Design, 2014, 28, 375-400.	2.9	70
72	How Many Conformations Need To Be Sampled To Obtain Converged QM/MM Energies? The Curse of Exponential Averaging. Journal of Chemical Theory and Computation, 2017, 13, 5745-5752.	5.3	70

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73	Theoretical study of the discrimination between O2 and CO by myoglobin. Journal of Inorganic Biochemistry, 2002, 91, 101-115.	3.5	69
74	The importance of porphyrin distortions for the ferrochelatase reaction. Journal of Biological Inorganic Chemistry, 2003, 8, 273-282.	2.6	68
75	How accurate are continuum solvation models for drug-like molecules?. Journal of Computer-Aided Molecular Design, 2009, 23, 395-409.	2.9	68
76	Convergence of QM/MM free-energy perturbations based on molecular-mechanics or semiempirical simulations. Physical Chemistry Chemical Physics, 2012, 14, 12592.	2.8	68
77	Protein Influence on Electronic Spectra Modeled by Multipoles and Polarizabilities. Journal of Chemical Theory and Computation, 2009, 5, 649-658.	5.3	67
78	Comparison of the Chemical Properties of Iron and Cobalt Porphyrins and Corrins. ChemBioChem, 2003, 4, 413-424.	2.6	66
79	The axial N -base has minor influence on Coâ€“C bond cleavage in cobalamins. Computational and Theoretical Chemistry, 2002, 585, 239-255.	1.5	64
80	Protonation States of Homocitrate and Nearby Residues in Nitrogenase Studied by Computational Methods and Quantum Refinement. Journal of Physical Chemistry B, 2017, 121, 8242-8262.	2.6	62
81	Cobalamins uncovered by modern electronic structure calculations. Coordination Chemistry Reviews, 2009, 253, 769-778.	18.8	61
82	An automatic method to generate force-field parameters for hetero-compounds. Acta Crystallographica Section D: Biological Crystallography, 2003, 59, 274-289.	2.5	60
83	The role of axial ligands for the structure and function of chlorophylls. Journal of Biological Inorganic Chemistry, 2006, 12, 49-61.	2.6	59
84	A comparison of different initialization protocols to obtain statistically independent molecular dynamics simulations. Journal of Computational Chemistry, 2011, 32, 187-195.	3.3	59
85	A theoretical study of the copper-cysteine bond in blue copper proteins. Theoretical Chemistry Accounts, 2001, 105, 452-462.	1.4	58
86	Accurate calculations of geometries and singletâ€“triplet energy differences for active-site models of [NiFe] hydrogenase. Physical Chemistry Chemical Physics, 2014, 16, 7927-7938.	2.8	58
87	The Protonation Status of Compound II in Myoglobin, Studied by a Combination of Experimental Data and Quantum Chemical Calculations: Quantum Refinement. Biophysical Journal, 2004, 87, 3437-3447.	0.5	56
88	Accurate Predictions of Nonpolar Solvation Free Energies Require Explicit Consideration of Binding-Site Hydration. Journal of the American Chemical Society, 2011, 133, 13081-13092.	13.7	56
89	Extremely large differences in DFT energies for nitrogenase models. Physical Chemistry Chemical Physics, 2019, 21, 2480-2488.	2.8	56
90	Reaction Mechanism of Porphyrin Metallation Studied by Theoretical Methods. Chemistry - A European Journal, 2005, 11, 1549-1564.	3.3	55

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91	Accurate metal-site structures in proteins obtained by combining experimental data and quantum chemistry. Dalton Transactions, 2007, , 607-625.	3.3	55
92	A Synthetic Analogue of Rieskeâ€Type [2Feâ€2S] Clusters. Angewandte Chemie - International Edition, 2008, 47, 9537-9541.	13.8	55
93	Prediction of Activation Energies for Aromatic Oxidation by Cytochrome P450. Journal of Physical Chemistry A, 2008, 112, 13058-13065.	2.5	55
94	QM/MMâ˜PBSA Method To Estimate Free Energies for Reactions in Proteins. Journal of Physical Chemistry B, 2008, 112, 12537-12548.	2.6	55
95	Reorganization Energy for Internal Electron Transfer in Multicopper Oxidases. Journal of Physical Chemistry B, 2011, 115, 13111-13126.	2.6	55
96	General Transition-State Force Field for Cytochrome P450 Hydroxylation. Journal of Chemical Theory and Computation, 2007, 3, 1765-1773.	5.3	54
97	A Large-Scale Test of Free-Energy Simulation Estimates of Proteinâ€“Ligand Binding Affinities. Journal of Chemical Information and Modeling, 2014, 54, 2794-2806.	5.4	54
98	Quantum refinementâ€”a combination of quantum chemistry and protein crystallography. Computational and Theoretical Chemistry, 2003, 632, 259-275.	1.5	52
99	Combined computational and crystallographic study of the oxidised states of [NiFe] hydrogenase. Computational and Theoretical Chemistry, 2006, 770, 199-219.	1.5	52
100	Theoretical studies of the active-site structure, spectroscopic and thermodynamic properties, and reaction mechanism of multicopper oxidases. Coordination Chemistry Reviews, 2013, 257, 445-458.	18.8	52
101	Targeting the reactive intermediate in polysaccharide monooxygenases. Journal of Biological Inorganic Chemistry, 2017, 22, 1029-1037.	2.6	52
102	Protonation and Reduction of the FeMo Cluster in Nitrogenase Studied by Quantum Mechanics/Molecular Mechanics (QM/MM) Calculations. Journal of Chemical Theory and Computation, 2018, 14, 6653-6678.	5.3	52
103	Calculation of Proteinâ˜Ligand Interaction Energies by a Fragmentation Approach Combining High-Level Quantum Chemistry with Classical Many-Body Effects. Journal of Physical Chemistry B, 2009, 113, 11085-11094.	2.6	51
104	Targeting Intermediates of [FeFe]-Hydrogenase by CO and CN Vibrational Signatures. Inorganic Chemistry, 2011, 50, 3888-3900.	4.0	51
105	Conversion of Homocysteine to Methionine by Methionine Synthase: A Density Functional Study. Journal of the American Chemical Society, 2003, 125, 13970-13971.	13.7	50
106	The crystal structure of peroxymyoglobin generated through cryoradiolytic reduction of myoglobin compound III during data collection. Biochemical Journal, 2008, 412, 257-264.	3.7	50
107	On the Possibility of Uphill Intramolecular Electron Transfer in Multicopper Oxidases: Electrochemical and Quantum Chemical Study of Bilirubin Oxidase. Electroanalysis, 2012, 24, 1524-1540.	2.9	49
108	The coordination chemistry of the structural zinc ion in alcohol dehydrogenase studied by ab initio quantum chemical calculations. European Biophysics Journal, 1996, 24, 213.	2.2	48

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109	Metal binding to Bacillus subtilis ferrochelatase and interaction between metal sites. Journal of Biological Inorganic Chemistry, 2003, 8, 452-458.	2.6	48
110	Protonation status of metal-bound ligands can be determined by quantum refinement. Journal of Inorganic Biochemistry, 2004, 98, 1539-1546.	3.5	47
111	Reaction Mechanism of Manganese Superoxide Dismutase Studied by Combined Quantum and Molecular Mechanical Calculations and Multiconfigurational Methods. Journal of Physical Chemistry B, 2009, 113, 6074-6086.	2.6	47
112	Binding affinities in the SAMPL3 trypsin and hostâ€“guest blind tests estimated with the MM/PBSA and LIE methods. Journal of Computer-Aided Molecular Design, 2012, 26, 527-541.	2.9	46
113	Converging ligandâ€binding free energies obtained with freeâ€energy perturbations at the quantum mechanical level. Journal of Computational Chemistry, 2016, 37, 1589-1600.	3.3	46
114	Comparison of QM/MM Methods To Obtain Ligand-Binding Free Energies. Journal of Chemical Theory and Computation, 2017, 13, 2245-2253.	5.3	45
115	Mechanism of hydrogen peroxide formation by lytic polysaccharide monooxygenase. Chemical Science, 2019, 10, 576-586.	7.4	45
116	Structural Insights into the Active-Ready Form of [FeFe]-Hydrogenase and Mechanistic Details of Its Inhibition by Carbon Monoxide. Inorganic Chemistry, 2007, 46, 7256-7258.	4.0	44
117	Structure of Reduced and Oxidized Manganese Superoxide Dismutase:Â A Combined Computational and Experimental Approach. Journal of Physical Chemistry B, 2006, 110, 11511-11518.	2.6	43
118	Dynamics of Water Molecules in the Active-Site Cavity of Human Cytochromes P450. Journal of Physical Chemistry B, 2007, 111, 5445-5457.	2.6	43
119	Protein strain in blue copper proteins studied by free energy perturbations. , 1999, 36, 157-174.		42
120	Multireference Ab Initio Calculations on Reaction Intermediates of the Multicopper Oxidases. Inorganic Chemistry, 2006, 45, 11051-11059.	4.0	42
121	The reaction mechanism of iron and manganese superoxide dismutases studied by theoretical calculations. Journal of Computational Chemistry, 2006, 27, 1398-1414.	3.3	42
122	Multireference Ab Initio Calculations of g tensors for Trinuclear Copper Clusters in Multicopper Oxidases. Journal of Physical Chemistry B, 2010, 114, 7692-7702.	2.6	42
123	Large Density-Functional and Basis-Set Effects for the DMSO Reductase Catalyzed Oxo-Transfer Reaction. Journal of Chemical Theory and Computation, 2013, 9, 1799-1807.	5.3	42
124	Influence of the protein and DFT method on the brokenâ€symmetry and spin states in nitrogenase. International Journal of Quantum Chemistry, 2018, 118, e25627.	2.0	42
125	Proton Transfer at Metal Sites in Proteins Studied by Quantum Mechanical Free-Energy Perturbations. Journal of Chemical Theory and Computation, 2008, 4, 985-1001.	5.3	40
126	Binding-affinity predictions of HSP90 in the D3R Grand Challenge 2015 with docking, MM/GBSA, QM/MM, and free-energy simulations. Journal of Computer-Aided Molecular Design, 2016, 30, 707-730.	2.9	40

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127	Protonation states of intermediates in the reaction mechanism of [NiFe] hydrogenase studied by computational methods. Journal of Biological Inorganic Chemistry, 2016, 21, 383-394.	2.6	40
128	Structural and Photoluminescence Properties of Excited State Intramolecular Proton Transfer Capable CompoundsPotential Emissive and Electron Transport Materials. Journal of Physical Chemistry A, 2006, 110, 7935-7942.	2.5	39
129	Fast generation of brokenâ€symmetry states in a large system including multiple ironâ€“sulfur assemblies: Investigation of QM/MM energies, clusters charges, and spin populations. International Journal of Quantum Chemistry, 2011, 111, 3949-3960.	2.0	39
130	Unraveling the similarity of the photoabsorption of deprotonated p-coumaric acid in the gas phase and within the photoactive yellow protein. Physical Chemistry Chemical Physics, 2011, 13, 1585-1589.	2.8	39
131	Identification of the Peroxy Adduct in Multicopper Oxidases by a Combination of Computational Chemistry and Extended X-ray Absorption Fine-Structure Measurements. Journal of the American Chemical Society, 2007, 129, 726-727.	13.7	38
132	Starting-Condition Dependence of Order Parameters Derived from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2010, 6, 2176-2190.	5.3	38
133	Mechanistic and Physiological Implications of the Interplay among Ironâ€“Sulfur Clusters in [FeFe]-Hydrogenases. A QM/MM Perspective. Journal of the American Chemical Society, 2011, 133, 18742-18749.	13.7	38
134	Reduction Potentials and Acidity Constants of Mn Superoxide Dismutase Calculated by QM/MM Freeâ€Energy Methods. ChemPhysChem, 2011, 12, 3337-3347.	2.1	38
135	Binding affinities by alchemical perturbation using <scp>QM/MM</scp> with a large <scp>QM</scp> system and polarizable <scp>MM</scp> model. Journal of Computational Chemistry, 2015, 36, 2114-2124.	3.3	38
136	H₂binding to the active site of [NiFe] hydrogenase studied by multiconfigurational and coupled-cluster methods. Physical Chemistry Chemical Physics, 2017, 19, 10590-10601.	2.8	38
137	Theoretical Study of the Structural and Spectroscopic Properties of Stellacyanin. Journal of Physical Chemistry B, 1998, 102, 4638-4647.	2.6	37
138	The structure of sitting-atop complexes of metalloporphyrins studied by theoretical methods. Journal of Inorganic Biochemistry, 2004, 98, 878-895.	3.5	37
139	What Is the Structure of the E₄ Intermediate in Nitrogenase?. Journal of Chemical Theory and Computation, 2020, 16, 1936-1952.	5.3	37
140	A QM/MM study of the binding of RAPTA ligands to cathepsin B. Journal of Computer-Aided Molecular Design, 2011, 25, 729-742.	2.9	36
141	Large Equatorial Ligand Effects on Câ€“H Bond Activation by Nonheme Iron(IV)-oxo Complexes. Journal of Physical Chemistry B, 2014, 118, 1493-1500.	2.6	35
142	Effect of explicit water molecules on ligand-binding affinities calculated with the MM/GBSA approach. Journal of Molecular Modeling, 2014, 20, 2273.	1.8	35
143	Functionally Relevant Interplay between the Fe₄S₄ Cluster and CN^â Ligands in the Active Site of [FeFe]-Hydrogenases. Journal of the American Chemical Society, 2010, 132, 4992-4993.	13.7	34
144	Reaction mechanism of formate dehydrogenase studied by computational methods. Journal of Biological Inorganic Chemistry, 2018, 23, 1243-1254.	2.6	34

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145	Comparison of overlap-based models for approximating the exchange-repulsion energy. Journal of Chemical Physics, 2006, 124, 244101.	3.0	33
146	Simulation of the isotropic EXAFS spectra for the S ₂ and S ₃ structures of the oxygen evolving complex in photosystem II. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 3979-3984.	7.1	32
147	Conformational Entropies and Order Parameters: Convergence, Reproducibility, and Transferability. Journal of Chemical Theory and Computation, 2014, 10, 432-438.	5.3	31
148	The coordination chemistry of the catalytic zinc ion in alcohol dehydrogenase studied by ab initio quantum chemical calculations. International Journal of Quantum Chemistry, 1994, 52, 1229-1243.	2.0	30
149	Ab Initio Calculations of Electric Field Gradients in Cadmium Complexes. The Journal of Physical Chemistry, 1996, 100, 4803-4809.	2.9	30
150	Can the protonation state of histidine residues be determined from molecular dynamics simulations?. Computational and Theoretical Chemistry, 2012, 1000, 75-84.	2.5	30
151	Lactam Hydrolysis Catalyzed by Mononuclear Metallo-Î²-lactamases:Â A Density Functional Study. Journal of Physical Chemistry B, 2003, 107, 2366-2375.	2.6	29
152	Importance of proximal hydrogen bonds in haem proteins. Molecular Physics, 2003, 101, 2003-2018.	1.7	29
153	Interpretation of EXAFS spectra for sitting-atop complexes with the help of computational methods. Inorganica Chimica Acta, 2006, 359, 1081-1092.	2.4	29
154	Protonation of the Proximal Histidine Ligand in Heme Peroxidases. Journal of Physical Chemistry B, 2008, 112, 2501-2510.	2.6	29
155	Multiscale Modelling of Lytic Polysaccharide Monooxygenases. ACS Omega, 2017, 2, 536-545.	3.5	29
156	A semiempirical approach to ligandâ€binding affinities: Dependence on the Hamiltonian and corrections. Journal of Computational Chemistry, 2012, 33, 1179-1189.	3.3	28
157	Geometric and Electronic Structure of Co(II)-Substituted Azurin. Journal of Physical Chemistry B, 1999, 103, 8375-8382.	2.6	27
158	Erratum to â€œO2-binding to heme: electronic structure and spectrum of oxyheme, studied by multiconfigurational methodsâ€•[J. Inorg. Biochem. 99(1) (2004) 45â€“54]. Journal of Inorganic Biochemistry, 2005, 99, 978.	3.5	27
159	The Neutron Structure of Urate Oxidase Resolves a Long-Standing Mechanistic Conundrum and Reveals Unexpected Changes in Protonation. PLoS ONE, 2014, 9, e86651.	2.5	27
160	Transition-State Docking of Flunitrazepam and Progesterone in Cytochrome P450. Journal of Chemical Theory and Computation, 2008, 4, 673-681.	5.3	26
161	Nonpolar Solvation Free Energies of Proteinâ^'Ligand Complexes. Journal of Chemical Theory and Computation, 2010, 6, 3558-3568.	5.3	26
162	Theoretical EXAFS studies of a model of the oxygenâ€evolving complex of photosystem II obtained with the quantum cluster approach. International Journal of Quantum Chemistry, 2013, 113, 474-478.	2.0	26

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163	The structure and function of blue copper proteins. Theoretical and Computational Chemistry, 2001, 9, 1-55.	0.4	24
164	Theoretical study of structure of catalytic copper site in nitrite reductase. International Journal of Quantum Chemistry, 2005, 102, 520-541.	2.0	24
165	EXAFS structure refinement supplemented by computational chemistry. Physical Review B, 2006, 74, .	3.2	24
166	Prediction and Rationalization of the pH Dependence of the Activity and Stability of Family 11 Xylanases. Biochemistry, 2007, 46, 13581-13592.	2.5	24
167	Secondary Bonding Interactions in Biomimetic [2Feâ^'2S] Clusters. Inorganic Chemistry, 2008, 47, 1586-1596.	4.0	24
168	Catalytic Cycle of Multicopper Oxidases Studied by Combined Quantum- and Molecular-Mechanical Free-Energy Perturbation Methods. Journal of Physical Chemistry B, 2015, 119, 8268-8284.	2.6	24
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