Ulf Ryde

List of Publications by Year
in descending order

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270 papers	18,359 citations	15001 68 h-index	19470 122 g-index
282 all docs	282 docs citations	282 times ranked	16842 citing authors

#	Article	IF	Citations
1	Combining crystallography with quantum mechanics. Current Opinion in Structural Biology, 2022, 72, 18-26.	2.6	8
2	Thermodynamically Favourable States in the Reaction of Nitrogenase without Dissociation of any Sulfide Ligand. Chemistry - A European Journal, 2022, , .	1.7	12
3	Comparison of Grand Canonical and Conventional Molecular Dynamics Simulation Methods for Protein-Bound Water Networks. ACS Physical Chemistry Au, 2022, 2, 247-259.	1.9	4
4	Can Water Act as a Nucleophile in CO Oxidation Catalysed by Mo/Cu COâ€Dehydrogenase? Answers from Theory. ChemPhysChem, 2022, 23, .	1.0	5
5	Benchmark Study of Redox Potential Calculations for Ironâ€“Sulfur Clusters in Proteins. Inorganic Chemistry, 2022, 61, 5991-6007.	1.9	8
6	Computationally enhanced X-ray diffraction analysis of a gold(III) complex interacting with the human telomeric DNA G-quadruplex. Unravelling non-unique ligand positioning. International Journal of Biological Macromolecules, 2022, 211, 506-513.	3.6	1
7	Unraveling the Reaction Mechanism of Mo/Cu CO Dehydrogenase Using QM/MM Calculations. ACS Catalysis, 2022, 12, 7336-7343.	5.5	9
8	Two-Substrate Glyoxalase I Mechanism: A Quantum Mechanics/Molecular Mechanics Study. Inorganic Chemistry, 2021, 60, 303-314.	1.9	3
9	QM/MM study of the binding of H2 to MoCu CO dehydrogenase: development and applications of improved H2 van der Waals parameters. Journal of Molecular Modeling, 2021, 27, 68.	0.8	4
10	QM/MM Study of the Catalytic Reaction of Myrosinase; Importance of Assigning Proper Protonation States of Active-Site Residues. Journal of Chemical Theory and Computation, 2021, 17, 1822-1841.	2.3	11
11	Critical evaluation of a crystal structure of nitrogenase with bound N2 ligands. Journal of Biological Inorganic Chemistry, 2021, 26, 341-353.	1.1	24
12	Entropyâ€“Entropy Compensation between the Protein, Ligand, and Solvent Degrees of Freedom Fine-Tunes Affinity in Ligand Binding to Galectin-3C. Jacs Au, 2021, 1, 484-500.	3.6	17
13	Neutron structures of Leishmania mexicana triosephosphate isomerase in complex with reaction-intermediate mimics shed light on the proton-shuttling steps. IUCrJ, 2021, 8, 633-643.	1.0	6
14	Quantum-refinement studies of the bidentate ligand of Vâ€‘nitrogenase and the protonation state of CO-inhibited Moâ€‘nitrogenase. Journal of Inorganic Biochemistry, 2021, 219, 111426.	1.5	7
15	On the Use of Interaction Entropy and Related Methods to Estimate Binding Entropies. Journal of Chemical Theory and Computation, 2021, 17, 5379-5391.	2.3	24
16	Exploring ligand dynamics in protein crystal structures with ensemble refinement. Acta Crystallographica Section D: Structural Biology, 2021, 77, 1099-1115.	1.1	3
17	Hybrids between Rubus idaeus and Rubus sect. Corylifolii and their relation to R. pruinosus and R. rosanthus. Nordic Journal of Botany, 2021, 39, .	0.2	3
18	Comparison of the accuracy of DFT methods for reactions with relevance to nitrogenase. Electronic Structure, 2021, 3, 034005.	1.0	9

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19	Can the results of quantum refinement be improved with a continuum-solvation model?. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2021, 77, 906-918.	0.5	0
20	Is density functional theory accurate for lytic polysaccharide monooxygenase enzymes?. Dalton Transactions, 2020, 49, 1501-1512.	1.6	18
21	Importance of the ironâ€“sulfur component and of the siroheme modification in the resting state of sulfite reductase. Journal of Inorganic Biochemistry, 2020, 203, 110928.	1.5	4
22	Putative reaction mechanism of nitrogenase after dissociation of a sulfide ligand. Journal of Catalysis, 2020, 391, 247-259.	3.1	19
23	Does the crystal structure of vanadium nitrogenase contain a reaction intermediate? Evidence from quantum refinement. Journal of Biological Inorganic Chemistry, 2020, 25, 847-861.	1.1	18
24	What Is the Structure of the E₄ Intermediate in Nitrogenase?. Journal of Chemical Theory and Computation, 2020, 16, 1936-1952.	2.3	37
25	Quantum Mechanics/Molecular Mechanics Study of the Reaction Mechanism of Glyoxalase I. Inorganic Chemistry, 2020, 59, 2594-2603.	1.9	6
26	Water structure in solution and crystal molecular dynamics simulations compared to protein crystal structures. RSC Advances, 2020, 10, 8435-8443.	1.7	11
27	N2H2 binding to the nitrogenase FeMo cluster studied by QM/MM methods. Journal of Biological Inorganic Chemistry, 2020, 25, 521-540.	1.1	16
28	fragHAR: towardsab initioquantum-crystallographic X-ray structure refinement for polypeptides and proteins. IUCrJ, 2020, 7, 158-165.	1.0	10
29	Quantum refinement with multiple conformations: application to the P-cluster in nitrogenase. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1145-1156.	1.1	6
30	Automated orientation of water molecules in neutron crystallographic structures of proteins. Acta Crystallographica Section D: Structural Biology, 2020, 76, 1025-1032.	1.1	3
31	Are crystallographic B-factors suitable for calculating protein conformational entropy?. Physical Chemistry Chemical Physics, 2019, 21, 18149-18160.	1.3	16
32	Geometry and Electronic Structure of the P-Cluster in Nitrogenase Studied by Combined Quantum Mechanical and Molecular Mechanical Calculations and Quantum Refinement. Inorganic Chemistry, 2019, 58, 9672-9690.	1.9	20
33	Structure and Energetics of Ligandâ€“Fluorine Interactions with Galectinâ€3 Backbone and Sideâ€Chain Amides: Insight into Solvation Effects and Multipolar Interactions. ChemMedChem, 2019, 14, 1528-1536.	1.6	24
34	Substituted polyfluoroaryl interactions with an arginine side chain in galectin-3 are governed by steric-, desolvation and electronic conjugation effects. Organic and Biomolecular Chemistry, 2019, 17, 1081-1089.	1.5	14
35	Mechanism of hydrogen peroxide formation by lytic polysaccharide monooxygenase. Chemical Science, 2019, 10, 576-586.	3.7	45
36	Extremely large differences in DFT energies for nitrogenase models. Physical Chemistry Chemical Physics, 2019, 21, 2480-2488.	1.3	56

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37	QM/MM study of the conversion of biliverdin into verdoheme by heme oxygenase. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	2
38	A thiocarbonate sink on the enzymatic energy landscape of aerobic CO oxidation? Answers from DFT and QM/MM models of Mo Cu CO-dehydrogenases. Journal of Catalysis, 2019, 372, 201-205.	3.1	11
39	Hostâ€"Guest Relative Binding Affinities at Density-Functional Theory Level from Semiempirical Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2019, 15, 2659-2671.	2.3	19
40	Why does sulfite reductase employ siroheme?. Chemical Communications, 2019, 55, 14047-14049.	2.2	14
41	QM/MM study of the stereospecific proton exchange of glutathiohydroxyacetone by glyoxalase I. Results in Chemistry, 2019, 1, 100011.	0.9	6
42	Theoretical Insights into the Aerobic Hydrogenase Activity of Molybdenumâ€"Copper CO Dehydrogenase. Inorganics, 2019, 7, 135.	1.2	5
43	Interplay between Conformational Entropy and Solvation Entropy in Proteinâ€"Ligand Binding. Journal of the American Chemical Society, 2019, 141, 2012-2026.	6.6	89
44	Refinement of protein structures using a combination of quantum-mechanical calculations with neutron and X-ray crystallographic data. Acta Crystallographica Section D: Structural Biology, 2019, 75, 368-380.	1.1	13
45	Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, 10881-10905.	1.7	108
46	Can MM/GBSA calculations be sped up by system truncation?. Journal of Computational Chemistry, 2018, 39, 361-372.	1.5	6
47	Molecular mechanism of lytic polysaccharide monooxygenases. Chemical Science, 2018, 9, 3866-3880.	3.7	77
48	Assessing the stability of free-energy perturbation calculations by performing variations in the method. Journal of Computer-Aided Molecular Design, 2018, 32, 529-536.	1.3	15
49	Higher Flexibility of Glu-172 Explains the Unusual Stereospecificity of Glyoxalase I. Inorganic Chemistry, 2018, 57, 4944-4958.	1.9	10
50	Quantum Refinement Does Not Support Dinuclear Copper Sites in Crystal Structures of Particulate Methane Monooxygenase. Angewandte Chemie, 2018, 130, 168-172.	1.6	18
51	Influence of the protein and DFT method on the brokenâ€symmetry and spin states in nitrogenase. International Journal of Quantum Chemistry, 2018, 118, e25627.	1.0	42
52	QM/MM study of the reaction mechanism of sulfite oxidase. Scientific Reports, 2018, 8, 4684.	1.6	22
53	Binding affinities of the farnesoid X receptor in the D3R Grand Challenge 2 estimated by free-energy perturbation and docking. Journal of Computer-Aided Molecular Design, 2018, 32, 211-224.	1.3	10
54	Exploration of H2 binding to the [NiFe]-hydrogenase active site with multiconfigurational density functional theory. Physical Chemistry Chemical Physics, 2018, 20, 794-801.	1.3	17

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55	Quantum Refinement Does Not Support Dinuclear Copper Sites in Crystal Structures of Particulate Methane Monooxygenase. Angewandte Chemie - International Edition, 2018, 57, 162-166.	7.2	122
56	Reaction Mechanism of [NiFe] Hydrogenase Studied by Computational Methods. Inorganic Chemistry, 2018, 57, 15289-15298.	1.9	19
57	Predicting Relative Binding Affinity Using Nonequilibrium QM/MM Simulations. Journal of Chemical Theory and Computation, 2018, 14, 6613-6622.	2.3	13
58	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.	2.3	52
59	Binding free energies in the SAMPL6 octa-acid hostâ€“guest challenge calculated with MM and QM methods. Journal of Computer-Aided Molecular Design, 2018, 32, 1027-1046.	1.3	15
60	Reaction mechanism of formate dehydrogenase studied by computational methods. Journal of Biological Inorganic Chemistry, 2018, 23, 1243-1254.	1.1	34
61	Relative Ligand-Binding Free Energies Calculated from Multiple Short QM/MM MD Simulations. Journal of Chemical Theory and Computation, 2018, 14, 3228-3237.	2.3	23
62	On the Difference Between Additive and Subtractive QM/MM Calculations. Frontiers in Chemistry, 2018, 6, 89.	1.8	71
63	Insight into the reaction mechanism of lipoyl synthase: a QM/MM study. Journal of Biological Inorganic Chemistry, 2018, 23, 221-229.	1.1	12
64	Frontispiece: Quantum Crystallography: Current Developments and Future Perspectives. Chemistry - A European Journal, 2018, 24, .	1.7	1
65	A novel mechanism of heme degradation to biliverdin studied by QM/MM and QM calculations. Dalton Transactions, 2018, 47, 8283-8291.	1.6	9
66	Effect of the protein ligand in DMSO reductase studied by computational methods. Journal of Inorganic Biochemistry, 2017, 171, 45-51.	1.5	7
67	H₂binding to the active site of [NiFe] hydrogenase studied by multiconfigurational and coupled-cluster methods. Physical Chemistry Chemical Physics, 2017, 19, 10590-10601.	1.3	38
68	Multiscale Modelling of Lytic Polysaccharide Monooxygenases. ACS Omega, 2017, 2, 536-545.	1.6	29
69	Comparison of QM/MM Methods To Obtain Ligand-Binding Free Energies. Journal of Chemical Theory and Computation, 2017, 13, 2245-2253.	2.3	45
70	Can System Truncation Speed up Ligand-Binding Calculations with Periodic Free-Energy Simulations?. Journal of Chemical Information and Modeling, 2017, 57, 2865-2873.	2.5	0
71	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.	2.3	70
72	Targeting the reactive intermediate in polysaccharide monooxygenases. Journal of Biological Inorganic Chemistry, 2017, 22, 1029-1037.	1.1	52

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73	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.	1.2	62
74	QM/MM Study of the Conversion of Oxophlorin into Verdoheme by Heme Oxygenase. Journal of Physical Chemistry B, 2017, 121, 11427-11436.	1.2	9
75	Binding free energies in the SAMPL5 octa-acid hostâ€"guest challenge calculated with DFT-D3 and CCSD(T). Journal of Computer-Aided Molecular Design, 2017, 31, 87-106.	1.3	21
76	Converging ligandâ€binding free energies obtained with freeâ€energy perturbations at the quantum mechanical level. Journal of Computational Chemistry, 2016, 37, 1589-1600.	1.5	46
77	Catalytic mechanism of human glyoxalase I studied by quantum-mechanical cluster calculations. Journal of Molecular Catalysis B: Enzymatic, 2016, 131, 18-30.	1.8	9
78	Ligand-Binding Affinity Estimates Supported by Quantum-Mechanical Methods. Chemical Reviews, 2016, 116, 5520-5566.	23.0	216
79	QM/MM Calculations on Proteins. Methods in Enzymology, 2016, 577, 119-158.	0.4	75
80	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.	1.3	40
81	Does the DFT Self-Interaction Error Affect Energies Calculated in Proteins with Large QM Systems?. Journal of Chemical Theory and Computation, 2016, 12, 5667-5679.	2.3	14
82	O₂ Activation in Salicylate 1,2-Dioxygenase: A QM/MM Study Reveals the Role of His162. Inorganic Chemistry, 2016, 55, 11727-11735.	1.9	14
83	Protonation states of intermediates in the reaction mechanism of [NiFe] hydrogenase studied by computational methods. Journal of Biological Inorganic Chemistry, 2016, 21, 383-394.	1.1	40
84	A Computational Comparison of Oxygen Atom Transfer Catalyzed by Dimethyl SulfÂoxide Reductase with Mo and W. European Journal of Inorganic Chemistry, 2015, 2015, 3580-3589.	1.0	23
85	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.	1.5	38
86	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.	1.2	24
87	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.	3.3	32
88	The MM/PBSA and MM/GBSA methods to estimate ligand-binding affinities. Expert Opinion on Drug Discovery, 2015, 10, 449-461.	2.5	2,907
89	Multiscale Modeling of the Active Site of [Fe] Hydrogenase: The H₂ Binding Site in Open and Closed Protein Conformations. Angewandte Chemie - International Edition, 2015, 54, 6246-6250.	7.2	22
90	The Neutron Structure of Urate Oxidase Resolves a Long-Standing Mechanistic Conundrum and Reveals Unexpected Changes in Protonation. PLoS ONE, 2014, 9, e86651.	1.1	27

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91	Coupledâ€Cluster Interaction Energies for 200â€Atom Hostâ€“Guest Systems. ChemPhysChem, 2014, 15, 3270-3281.	1.0	18
92	Computational modelling of oxygenation processes in enzymes and biomimetic model complexes. Chemical Communications, 2014, 50, 262-282.	2.2	110
93	Comparison of the Active-Site Design of Molybdenum Oxo-Transfer Enzymes by Quantum Mechanical Calculations. Inorganic Chemistry, 2014, 53, 11913-11924.	1.9	17
94	Theoretical ⁵⁷Fe MÃ¶ssbauer spectroscopy: isomer shifts of [Fe]-hydrogenase intermediates. Physical Chemistry Chemical Physics, 2014, 16, 4853-4863.	1.3	21
95	A Large-Scale Test of Free-Energy Simulation Estimates of Proteinâ€“Ligand Binding Affinities. Journal of Chemical Information and Modeling, 2014, 54, 2794-2806.	2.5	54
96	A fundamental view of enthalpyâ€“entropy compensation. MedChemComm, 2014, 5, 1324-1336.	3.5	98
97	Conformational Entropies and Order Parameters: Convergence, Reproducibility, and Transferability. Journal of Chemical Theory and Computation, 2014, 10, 432-438.	2.3	31
98	A quantum-mechanical study of the reaction mechanism of sulfite oxidase. Journal of Biological Inorganic Chemistry, 2014, 19, 1165-1179.	1.1	23
99	Large Equatorial Ligand Effects on Câ€“H Bond Activation by Nonheme Iron(IV)-oxo Complexes. Journal of Physical Chemistry B, 2014, 118, 1493-1500.	1.2	35
100	Effect of explicit water molecules on ligand-binding affinities calculated with the MM/GBSA approach. Journal of Molecular Modeling, 2014, 20, 2273.	0.8	35
101	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.	1.3	70
102	Accurate calculations of geometries and singletâ€“triplet energy differences for active-site models of [NiFe] hydrogenase. Physical Chemistry Chemical Physics, 2014, 16, 7927-7938.	1.3	58
103	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.	1.0	26
104	Comparison of MM/GBSA calculations based on explicit and implicit solvent simulations. Physical Chemistry Chemical Physics, 2013, 15, 7731.	1.3	76
105	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.	2.3	75
106	Theoretical studies of the active-site structure, spectroscopic and thermodynamic properties, and reaction mechanism of multicopper oxidases. Coordination Chemistry Reviews, 2013, 257, 445-458.	9.5	52
107	Amino Acid Oxidation of Candida antarctica Lipase B Studied by Molecular Dynamics Simulations and Site-Directed Mutagenesis. Biochemistry, 2013, 52, 1280-1289.	1.2	21
108	Accurate Reaction Energies in Proteins Obtained by Combining QM/MM and Large QM Calculations. Journal of Chemical Theory and Computation, 2013, 9, 640-649.	2.3	80

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109	Understanding the Chemistry of Lead at a Molecular Level: The Pb(II) 6s6p Lone Pair Can Be Bisdirected in Proteins. Journal of Chemical Theory and Computation, 2013, 9, 2416-2424.	2.3	8
110	How are hydrogen bonds modified by metal binding?. Journal of Biological Inorganic Chemistry, 2013, 18, 499-522.	1.1	8
111	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.	2.3	42
112	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.	2.5	166
113	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.	1.2	137
114	Convergence of QM/MM free-energy perturbations based on molecular-mechanics or semiempirical simulations. Physical Chemistry Chemical Physics, 2012, 14, 12592.	1.3	68
115	Can the protonation state of histidine residues be determined from molecular dynamics simulations?. Computational and Theoretical Chemistry, 2012, 1000, 75-84.	1.1	30
116	Transferability of conformational dependent charges from protein simulations. International Journal of Quantum Chemistry, 2012, 112, 1768-1785.	1.0	10
117	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.	1.5	78
118	On the Possibility of Uphill Intramolecular Electron Transfer in Multicopper Oxidases: Electrochemical and Quantum Chemical Study of Bilirubin Oxidase. Electroanalysis, 2012, 24, 1524-1540.	1.5	49
119	Will molecular dynamics simulations of proteins ever reach equilibrium?. Physical Chemistry Chemical Physics, 2012, 14, 8662.	1.3	85
120	Improving the Efficiency of Proteinâ€“Ligand Binding Free-Energy Calculations by System Truncation. Journal of Chemical Theory and Computation, 2012, 8, 1449-1458.	2.3	18
121	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.	1.3	46
122	A semiempirical approach to ligandâ€binding affinities: Dependence on the Hamiltonian and corrections. Journal of Computational Chemistry, 2012, 33, 1179-1189.	1.5	28
123	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.	1.0	39
124	Targeting Intermediates of [FeFe]-Hydrogenase by CO and CN Vibrational Signatures. Inorganic Chemistry, 2011, 50, 3888-3900.	1.9	51
125	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.	1.3	39
126	On the Convergence of QM/MM Energies. Journal of Chemical Theory and Computation, 2011, 7, 761-777.	2.3	185

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127	Binding Affinities of Factor Xa Inhibitors Estimated by Thermodynamic Integration and MM/GBSA. Journal of Chemical Information and Modeling, 2011, 51, 947-958.	2.5	72
128	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.	6.6	38
129	Conformational Dependence of Isotropic Polarizabilities. Journal of Chemical Theory and Computation, 2011, 7, 1404-1414.	2.3	13
130	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.	2.3	71
131	Comparison of Methods to Obtain Force-Field Parameters for Metal Sites. Journal of Chemical Theory and Computation, 2011, 7, 2452-2463.	2.3	108
132	Reductive cleavage of the Oâ€“O bond in multicopper oxidases: a QM/MM and QM study. Faraday Discussions, 2011, 148, 41-53.	1.6	22
133	Reorganization Energy for Internal Electron Transfer in Multicopper Oxidases. Journal of Physical Chemistry B, 2011, 115, 13111-13126.	1.2	55
134	Does DFT-D estimate accurate energies for the binding of ligands to metal complexes?. Dalton Transactions, 2011, 40, 11176.	1.6	81
135	Accurate Predictions of Nonpolar Solvation Free Energies Require Explicit Consideration of Binding-Site Hydration. Journal of the American Chemical Society, 2011, 133, 13081-13092.	6.6	56
136	Arguments for a narrow species concept in Rubus sect. Corylifolii. Nordic Journal of Botany, 2011, 29, 708-721.	0.2	9
137	A QM/MM study of the binding of RAPTA ligands to cathepsin B. Journal of Computer-Aided Molecular Design, 2011, 25, 729-742.	1.3	36
138	Magnetic Properties of [FeFe]â€Hydrogenases: A Theoretical Investigation Based on Extended QM and QM/MM Models of the Hâ€Cluster and Its Surroundings. European Journal of Inorganic Chemistry, 2011, 2011, 1043-1049.	1.0	21
139	Reduction Potentials and Acidity Constants of Mn Superoxide Dismutase Calculated by QM/MM Freeâ€Energy Methods. ChemPhysChem, 2011, 12, 3337-3347.	1.0	38
140	Probing the Effects of Oneâ€Electron Reduction and Protonation on the Electronic Properties of the Feâ€S Clusters in the Activeâ€Ready Form of [FeFe]â€Hydrogenases. A QM/MM Investigation.. ChemPhysChem, 2011, 12, 3376-3382.	1.0	10
141	A comparison of different initialization protocols to obtain statistically independent molecular dynamics simulations. Journal of Computational Chemistry, 2011, 32, 187-195.	1.5	59
142	Isocyanide in Biochemistry? A Theoretical Investigation of the Electronic Effects and Energetics of Cyanide Ligand Protonation in [FeFe]â€Hydrogenases. Chemistry - A European Journal, 2011, 17, 1954-1965.	1.7	16
143	How to obtain statistically converged MM/GBSA results. Journal of Computational Chemistry, 2010, 31, 837-846.	1.5	167
144	A combined computational and experimental investigation of the [2Feâ€“2S] cluster in biotin synthase. Journal of Biological Inorganic Chemistry, 2010, 15, 203-212.	1.1	10

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145	Estimates of ligand-binding affinities supported by quantum mechanical methods. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 21-37.	2.2	21
146	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.	6.6	209
147	Ligand Affinities Estimated by Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2010, 6, 1726-1737.	2.3	81
148	Nonpolar Solvation Free Energies of Proteinâ^'Ligand Complexes. Journal of Chemical Theory and Computation, 2010, 6, 3558-3568.	2.3	26
149	Starting-Condition Dependence of Order Parameters Derived from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2010, 6, 2176-2190.	2.3	38
150	Multireference Ab Initio Calculations of g tensors for Trinuclear Copper Clusters in Multicopper Oxidases. Journal of Physical Chemistry B, 2010, 114, 7692-7702.	1.2	42
151	An MM/3D-RISM Approach for Ligand Binding Affinities. Journal of Physical Chemistry B, 2010, 114, 8505-8516.	1.2	129
152	A Five-Coordinate [2Feâ^'2S] Cluster. Inorganic Chemistry, 2010, 49, 5853-5858.	1.9	16
153	Genetic analysis shows thatRubus vikensisis a distinct species with a disjunct distribution. Nordic Journal of Botany, 2010, 28, 246-250.	0.2	1
154	Quantum Refinement of [FeFe] Hydrogenase Indicates a Dithiomethylamine Ligand. Journal of the American Chemical Society, 2010, 132, 4512-4513.	6.6	73
155	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.	6.6	34
156	Conformational dependence of charges in protein simulations. Journal of Computational Chemistry, 2009, 30, 750-760.	1.5	23
157	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.	7.2	86
158	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.	1.2	72
159	Which functional groups of the molybdopterin ligand should be considered when modeling the active sites of the molybdenum and tungsten cofactors? A density functional theory study. Journal of Biological Inorganic Chemistry, 2009, 14, 1053-1064.	1.1	23
160	An improved method to predict the entropy term with the MM/PBSA approach. Journal of Computer-Aided Molecular Design, 2009, 23, 63-71.	1.3	122
161	How accurate are continuum solvation models for drug-like molecules?. Journal of Computer-Aided Molecular Design, 2009, 23, 395-409.	1.3	68
162	Conformational entropy changes upon lactose binding to the carbohydrate recognition domain of galectin-3. Journal of Biomolecular NMR, 2009, 45, 157-169.	1.6	75

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