

Alessandra Magistrato

List of Publications by Year in descending order

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120
papers

3,587
citations

126907

33
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182427

51
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133
all docs

133
docs citations

133
times ranked

4236
citing authors

#	ARTICLE	IF	CITATIONS
1	An oomycete NLP cytolysin forms transient small pores in lipid membranes. <i>Science Advances</i> , 2022, 8, eabj9406.	10.3	11
2	Dynamical interplay between the human high-affinity copper transporter hCtr1 and its cognate metal ion. <i>Biophysical Journal</i> , 2022, 121, 1194-1204.	0.5	6
3	All-atom simulations to studying metallodrugs/target interactions. <i>Current Opinion in Chemical Biology</i> , 2021, 61, 1-8.	6.1	23
4	Atomic-Level Mechanism of Pre-mRNA Splicing in Health and Disease. <i>Accounts of Chemical Research</i> , 2021, 54, 144-154.	15.6	23
5	An Expanded Two-Zn ²⁺ -Ion Motif Orchestrates Pre-mRNA Maturation in the 5'-End Processing Endonuclease Machinery. <i>ACS Catalysis</i> , 2021, 11, 4319-4326.	11.2	6
6	Nep1-like proteins as a target for plant pathogen control. <i>PLoS Pathogens</i> , 2021, 17, e1009477.	4.7	9
7	Computing Metal-Binding Proteins for Therapeutic Benefit. <i>ChemMedChem</i> , 2021, 16, 2034-2049.	3.2	12
8	Molecular Mechanisms of the Blockage of Glioblastoma Motility. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2967-2980.	5.4	7
9	Discovery of a natural cyan blue: A unique food-sourced anthocyanin could replace synthetic brilliant blue. <i>Science Advances</i> , 2021, 7, .	10.3	34
10	Allosteric Cross-Talk among Spike's Receptor-Binding Domain Mutations of the SARS-CoV-2 South African Variant Triggers an Effective Hijacking of Human Cell Receptor. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5987-5993.	4.6	33
11	Deciphering the Molecular Terms of Arp2/3 Allosteric Regulation from All-Atom Simulations and Dynamical Network Theory. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 5384-5389.	4.6	8
12	All-Atom Simulations Uncover the Molecular Terms of the NKCC1 Transport Mechanism. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3649-3658.	5.4	9
13	Spontaneous Production of Ultrastable Reactive Oxygen Species on Titanium Oxide Surfaces Modified with Organic Ligands. <i>Advanced Materials Interfaces</i> , 2021, 8, 2100629.	3.7	11
14	Balanced dual acting compounds targeting aromatase and estrogen receptor α as an emerging therapeutic opportunity to counteract estrogen responsive breast cancer. <i>European Journal of Medicinal Chemistry</i> , 2021, 224, 113733.	5.5	11
15	Investigating the Molecular Mechanism of H3B-8800: A Splicing Modulator Inducing Preferential Lethality in Spliceosome-Mutant Cancers. <i>International Journal of Molecular Sciences</i> , 2021, 22, 11222.	4.1	9
16	Frontiers of metal-coordinating drug design. <i>Expert Opinion on Drug Discovery</i> , 2021, 16, 497-511.	5.0	28
17	Molecular Basis of SARS-CoV-2 Nsp1-Induced Immune Translational Shutdown as Revealed by All-Atom Simulations. <i>Journal of Physical Chemistry Letters</i> , 2021, 12, 11745-11750.	4.6	7
18	Exploiting Cryo-EM Structural Information and All-Atom Simulations To Decrypt the Molecular Mechanism of Splicing Modulators. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2510-2521.	5.4	24

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19	Peptide Inhibitors of Bacterial Protein Synthesis with Broad Spectrum and SbmA-Independent Bactericidal Activity against Clinical Pathogens. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 9590-9602.	6.4	24
20	Molecular Basis for Endocrine Disruption by Pesticides Targeting Aromatase and Estrogen Receptor. <i>International Journal of Environmental Research and Public Health</i> , 2020, 17, 5664.	2.6	29
21	Cu(I) Controls Conformational States in Human Atox1 Metallochaperone: An EPR and Multiscale Simulation Study. <i>Journal of Physical Chemistry B</i> , 2020, 124, 4399-4411.	2.6	10
22	Is the Rigidity of SARS-CoV-2 Spike Receptor-Binding Motif the Hallmark for Its Enhanced Infectivity? Insights from All-Atom Simulations. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 4785-4790.	4.6	147
23	Targeting Orthosteric and Allosteric Pockets of Aromatase via Dual-Mode Novel Azole Inhibitors. <i>ACS Medicinal Chemistry Letters</i> , 2020, 11, 732-739.	2.8	18
24	All-Atom Simulations Disclose How Cytochrome Reductase Reshapes the Substrate Access/Egress Routes of Its Partner CYP450s. <i>Journal of Physical Chemistry Letters</i> , 2020, 11, 1189-1193.	4.6	18
25	All-Atom Simulations Decrypt the Molecular Terms of RNA Catalysis in the Exon-Ligation Step of the Spliceosome. <i>ACS Catalysis</i> , 2020, 10, 5328-5334.	11.2	26
26	Decrypting the Information Exchange Pathways across the Spliceosome Machinery. <i>Journal of the American Chemical Society</i> , 2020, 142, 8403-8411.	13.7	35
27	Recent advances in computational design of potent aromatase inhibitors: open-eye on endocrine-resistant breast cancers. <i>Expert Opinion on Drug Discovery</i> , 2019, 14, 1065-1076.	5.0	14
28	Unraveling the Impact of Cysteine-to-Serine Mutations on the Structural and Functional Properties of Cu(I)-Binding Proteins. <i>International Journal of Molecular Sciences</i> , 2019, 20, 3462.	4.1	16
29	Unraveling the Molecular Mechanism of Pre-mRNA Splicing From Multi-Scale Simulations. <i>Frontiers in Molecular Biosciences</i> , 2019, 6, 62.	3.5	7
30	Disclosing the Impact of Carcinogenic SF3b Mutations on Pre-mRNA Recognition Via All-Atom Simulations. <i>Biomolecules</i> , 2019, 9, 633.	4.0	23
31	Molecular basis for functional diversity among microbial Nep1-like proteins. <i>PLoS Pathogens</i> , 2019, 15, e1007951.	4.7	39
32	Structural, Thermodynamic, and Kinetic Traits of Antiestrogen-Compounds Selectively Targeting the Y537S Mutant Estrogen Receptor ± Transcriptional Activity in Breast Cancer Cell Lines. <i>Frontiers in Chemistry</i> , 2019, 7, 602.	3.6	6
33	The pivotal role of MBD4-ATP7B in the human Cu excretion path as revealed by EPR experiments and all-atom simulations. <i>Metallomics</i> , 2019, 11, 1288-1297.	2.4	15
34	Copper trafficking in eukaryotic systems: current knowledge from experimental and computational efforts. <i>Current Opinion in Structural Biology</i> , 2019, 58, 26-33.	5.7	39
35	Post-Translational Regulation of CYP450s Metabolism As Revealed by All-Atoms Simulations of the Aromatase Enzyme. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 2930-2940.	5.4	22
36	Unraveling the molecular mechanisms of color expression in anthocyanins. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 8757-8766.	2.8	20

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37	Pre-mRNA Splicing: The Gene Maturation Symphony of the Intron Lariat Spliceosome Revealed by Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2019, 116, 299a.	0.5	0
38	Understanding the mechanistic basis of non-coding RNA through molecular dynamics simulations. <i>Journal of Structural Biology</i> , 2019, 206, 267-279.	2.8	37
39	A Synthetic Derivative of Antimicrobial Peptide Holothuroidin 2 from Mediterranean Sea Cucumber (<i>Holothuria tubulosa</i>) in the Control of <i>Listeria monocytogenes</i> . <i>Marine Drugs</i> , 2019, 17, 159.	4.6	25
40	Can multiscale simulations unravel the function of metallo-enzymes to improve knowledge-based drug discovery?. <i>Future Medicinal Chemistry</i> , 2019, 11, 771-791.	2.3	9
41	Rational design of allosteric modulators of the aromatase enzyme: An unprecedented therapeutic strategy to fight breast cancer. <i>European Journal of Medicinal Chemistry</i> , 2019, 168, 253-262.	5.5	33
42	How Can Interleukin-1 Receptor Antagonist Modulate Distinct Cell Death Pathways?. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 351-359.	5.4	21
43	The Catalytic Mechanism of Steroidogenic Cytochromes P450 from All-Atom Simulations: Entwinement with Membrane Environment, Redox Partners, and Post-Transcriptional Regulation. <i>Catalysts</i> , 2019, 9, 81.	3.5	23
44	A Computational Assay of Estrogen Receptor ± Antagonists Reveals the Key Common Structural Traits of Drugs Effectively Fighting Refractory Breast Cancers. <i>Scientific Reports</i> , 2018, 8, 649.	3.3	57
45	A Dehydrogenase Dual Hydrogen Abstraction Mechanism Promotes Estrogen Biosynthesis: Can We Expand the Functional Annotation of the Aromatase Enzyme?. <i>Chemistry - A European Journal</i> , 2018, 24, 10840-10849.	3.3	31
46	All-atom simulations disentangle the functional dynamics underlying gene maturation in the intron lariat spliceosome. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 6584-6589.	7.1	59
47	Single or Multiple Access Channels to the CYP450s Active Site? An Answer from Free Energy Simulations of the Human Aromatase Enzyme. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 2036-2042.	4.6	41
48	An omics perspective to the molecular mechanisms of anticancer metallo-drugs in the computational microscope era. <i>Expert Opinion on Drug Discovery</i> , 2017, 12, 1-13.	5.0	14
49	Development of Site-Specific Mg ²⁺ RNA Force Field Parameters: A Dream or Reality? Guidelines from Combined Molecular Dynamics and Quantum Mechanics Simulations. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 340-352.	5.3	51
50	Direct in silico visualization of ligands channelling through proteins: The next-generation frontier of computational biology. <i>Physics of Life Reviews</i> , 2017, 22-23, 82-84.	2.8	2
51	Fighting Cancer with Transition Metal Complexes: From Naked DNA to Protein and Chromatin Targeting Strategies. <i>ChemMedChem</i> , 2016, 11, 1199-1210.	3.2	104
52	Who Activates the Nucleophile in Ribozyme Catalysis? An Answer from the Splicing Mechanism of Group II Introns. <i>Journal of the American Chemical Society</i> , 2016, 138, 10374-10377.	13.7	79
53	Structural, dynamical and catalytic interplay between Mg ²⁺ ions and RNA. Vices and virtues of atomistic simulations. <i>Inorganica Chimica Acta</i> , 2016, 452, 73-81.	2.4	16
54	The molecular mechanism of secondary sodium symporters elucidated through the lens of the computational microscope. <i>RSC Advances</i> , 2016, 6, 9522-9540.	3.6	13

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55	Enzymatic and Inhibition Mechanism of Human Aromatase (CYP19A1) Enzyme. A Computational Perspective from QM/MM and Classical Molecular Dynamics Simulations. <i>Mini-Reviews in Medicinal Chemistry</i> , 2016, 16, 1112-1124.	2.4	20
56	Role of Water in the Puzzling Mechanism of the Final Aromatization Step Promoted by the Human Aromatase Enzyme. Insights from QM/MM MD Simulations. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 2218-2226.	5.4	25
57	QM/MM MD Simulations on the Enzymatic Pathway of the Human Flap Endonuclease (hFEN1) Elucidating Common Cleavage Pathways to RNase H Enzymes. <i>ACS Catalysis</i> , 2015, 5, 3864-3875.	11.2	45
58	Interfacing proteins with graphitic nanomaterials: from spontaneous attraction to tailored assemblies. <i>Chemical Society Reviews</i> , 2015, 44, 6916-6953.	38.1	91
59	A structural, functional, and computational analysis suggests pore flexibility as the base for the poor selectivity of CNG channels. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, E3619-28.	7.1	35
60	Metadynamics Simulations Reveal a Na ⁺ Independent Exiting Path of Galactose for the Inward-Facing Conformation of vSGLT. <i>PLoS Computational Biology</i> , 2014, 10, e1004017.	3.2	20
61	QM/MM Molecular Dynamics Studies of Metal Binding Proteins. <i>Biomolecules</i> , 2014, 4, 616-645.	4.0	74
62	Atomistic-Level Portrayal of Drug-DNA Interplay: A History of Courtships and Meetings Revealed by Molecular Simulations. <i>ChemMedChem</i> , 2014, 9, 1966-1981.	3.2	25
63	Computational Approaches Elucidate the Allosteric Mechanism of Human Aromatase Inhibition: A Novel Possible Route to Small-Molecule Regulation of CYP450s Activities?. <i>Journal of Chemical Information and Modeling</i> , 2014, 54, 2856-2868.	5.4	41
64	Ru[(bpy) ₂ (dppz)] ²⁺ and Rh[(bpy) ₂ (chrysi)] ³⁺ Targeting Double Strand DNA: The Shape of the Intercalating Ligand Tunes the Free Energy Landscape of Deintercalation. <i>Inorganic Chemistry</i> , 2014, 53, 7999-8008.	4.0	27
65	Sodium-Galactose Transporter: The First Steps of the Transport Mechanism Investigated by Molecular Dynamics. <i>Biophysical Journal</i> , 2014, 106, 365a-366a.	0.5	0
66	Structural and Dynamical Properties of Monoclonal Antibodies Immobilized on CNTs: A Computational Study. <i>Biophysical Journal</i> , 2014, 106, 620a.	0.5	0
67	Structural and Dynamic Properties of Monoclonal Antibodies Immobilized on CNTs: A Computational Study. <i>Chemistry - A European Journal</i> , 2013, 19, 12281-12293.	3.3	24
68	A Candidate Ion-Retaining State in the Inward-Facing Conformation of Sodium/Galactose Symporter: Clues from Atomistic Simulations. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 1240-1246.	5.3	26
69	Functionalized Fe-Filled Multiwalled Carbon Nanotubes as Multifunctional Scaffolds for Magnetization of Cancer Cells. <i>Advanced Functional Materials</i> , 2013, 23, 3173-3184.	14.9	58
70	Structural Role of Uracil DNA Glycosylase for the Recognition of Uracil in DNA Duplexes. Clues from Atomistic Simulations. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1371-1387.	5.4	4
71	First-Principles Modeling of Biological Systems and Structure-Based Drug-Design. <i>Current Computer-Aided Drug Design</i> , 2013, 9, 15-34.	1.2	3
72	Magnetic Carbon Nanotubes: Functionalized Fe-Filled Multiwalled Carbon Nanotubes as Multifunctional Scaffolds for Magnetization of Cancer Cells (<i>Adv. Funct. Mater.</i> 25/2013). <i>Advanced Functional Materials</i> , 2013, 23, 3172-3172.	14.9	1

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73	First-Principles Modeling of Biological Systems and Structure-Based Drug-Design. <i>Current Computer-Aided Drug Design</i> , 2013, 9, 15-34.	1.2	24
74	First-principles modeling of biological systems and structure-based drug-design. <i>Current Computer-Aided Drug Design</i> , 2013, 9, 15-34.	1.2	8
75	Detecting DNA Mismatches with Metallo-Insertors: A Molecular Simulation Study. <i>Inorganic Chemistry</i> , 2012, 51, 2046-2057.	4.0	41
76	Influence of the Membrane Lipophilic Environment on the Structure and on the Substrate Access/Egress Routes of the Human Aromatase Enzyme. A Computational Study. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1595-1606.	5.4	63
77	The Structural Role of Mg ²⁺ Ions in a Class I RNA Polymerase Ribozyme: A Molecular Simulation Study. <i>Journal of Physical Chemistry B</i> , 2012, 116, 2259-2268.	2.6	51
78	On the active site of mononuclear B1 metallo- β -lactamases: a computational study. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 425-435.	2.9	7
79	Theoretical Studies of Homogeneous Catalysts Mimicking Nitrogenase. <i>Molecules</i> , 2011, 16, 442-465.	3.8	24
80	Bioinorganic Chemistry of Parkinson's Disease: Structural Determinants for the Copper-Mediated Amyloid Formation of Alpha-Synuclein. <i>Inorganic Chemistry</i> , 2010, 49, 10668-10679.	4.0	119
81	Hydrogen Bonding Cooperativity in polyQ β -Sheets from First Principle Calculations. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 1777-1782.	5.3	17
82	Computational Study of the DNA-Binding Protein Helicobacter pylori NikR: The Role of Ni ²⁺ 2 Francesco Musiani and Branimir Bertović contributed equally to the simulations presented here.. <i>Journal of Chemical Theory and Computation</i> , 2010, 6, 3503-3515.	5.3	32
83	Huntingtin: Stability and Interaction with Molecular Partner from Computational Biophysics Studies. <i>Biophysical Journal</i> , 2010, 98, 637a.	0.5	0
84	A density functional theory (DFT) study on gas-phase proton transfer reactions of derivatized and underivatized peptide ions generated by matrix-assisted laser desorption ionization. <i>Journal of the American Society for Mass Spectrometry</i> , 2009, 20, 1327-1333.	2.8	9
85	Molecular Recognition Routes Of DNA By Anticancer Ligands: Mechanisms and Free Energies Explored Via Molecular Dynamics Simulations. <i>Biophysical Journal</i> , 2009, 96, 84a.	0.5	0
86	Copper ^{1,10} -Phenanthroline Complexes Binding to DNA: Structural Predictions from Molecular Simulations. <i>Journal of Physical Chemistry B</i> , 2009, 113, 10881-10890.	2.6	78
87	Synthesis, photophysical, electrochemical, and electrochemiluminescent properties of 5,15-bis(9-anthracenyl)porphyrin derivatives. <i>Organic and Biomolecular Chemistry</i> , 2009, 7, 2402.	2.8	27
88	Common Mechanistic Features among Metallo- β -lactamases. <i>Journal of Biological Chemistry</i> , 2009, 284, 28164-28171.	3.4	54
89	Simulations of Copper-1,10-Phenanthroline Complexes Binding the DNA. <i>Biophysical Journal</i> , 2009, 96, 577a.	0.5	0
90	Second step of hydrolytic dehalogenation in haloalkane dehalogenase investigated by QM/MM methods. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 70, 707-717.	2.6	24

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91	Parameterization of azole-bridged dinuclear platinum anticancer drugs via a QM/MM force matching procedure. <i>Journal of Computational Chemistry</i> , 2008, 29, 38-49.	3.3	34
92	Sliding of Alkylating Anticancer Drugs along the Minor Groove of DNA: New Insights on Sequence Selectivity. <i>Biophysical Journal</i> , 2008, 94, 550-561.	0.5	25
93	The Hydrolysis Mechanism of the Anticancer Ruthenium Drugs NAMI-A and ICR Investigated by DFT-PCM Calculations. <i>Journal of Physical Chemistry B</i> , 2008, 112, 4401-4409.	2.6	60
94	Structural Properties of Polyglutamine Aggregates Investigated via Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2008, 112, 16843-16850.	2.6	19
95	Anthrax Lethal Factor Investigated by Molecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1745-1756.	5.3	13
96	Dissociation of minor groove binders from DNA: insights from metadynamics simulations. <i>Nucleic Acids Research</i> , 2008, 36, 5910-5921.	14.5	60
97	Azole-Bridged Diplatinum Anticancer Compounds. Modulating DNA Flexibility to Escape Repair Mechanism and Avoid Cross Resistance. <i>Journal of Physical Chemistry B</i> , 2007, 111, 11873-11876.	2.6	29
98	Density Functional Theory Studies on Copper Phenanthroline Complexes. <i>Inorganic Chemistry</i> , 2007, 46, 5873-5881.	4.0	47
99	Interaction between the DNA Model Base 9-Ethylguanine and a Group of Ruthenium Polypyridyl Complexes: Kinetics and Conformational Temperature Dependence. <i>Inorganic Chemistry</i> , 2007, 46, 6715-6722.	4.0	20
100	Nitrogen Fixation by a Molybdenum Catalyst Mimicking the Function of the Nitrogenase Enzyme: A Critical Evaluation of DFT and Solvent Effects. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1708-1720.	5.3	52
101	Protonation state and substrate binding to B2 metallo- β -lactamase CphA from <i>Aeromonas hydrophila</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 69, 595-605.	2.6	33
102	Modeling anticancer drug-DNA interactions via mixed QM/MM molecular dynamics simulations. <i>Organic and Biomolecular Chemistry</i> , 2006, 4, 2507-2517.	2.8	85
103	Anthramycin-DNA Binding Explored by Molecular Simulations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 24687-24695.	2.6	23
104	Binding of Novel Azole-Bridged Dinuclear Platinum(II) Anticancer Drugs to DNA: Insights from Hybrid QM/MM Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2006, 110, 3604-3613.	2.6	63
105	Enantioselective Palladium-Catalyzed Hydrosilylation of Styrene: Influence of Electronic and Steric Effects on Enantioselectivity and Catalyst Design via Hybrid QM/MM Molecular Dynamics Simulations. <i>Organometallics</i> , 2006, 25, 1151-1157.	2.3	25
106	Role of protein frame and solvent for the redox properties of azurin from <i>Pseudomonas aeruginosa</i> . <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2006, 103, 19641-19646.	7.1	135
107	Enantioselective Palladium-Catalyzed Hydrosilylation of Styrene: Detailed Reaction Mechanism from First-Principles and Hybrid QM/MM Molecular Dynamics Simulations. <i>Organometallics</i> , 2004, 23, 3218-3227.	2.3	34
108	Unusual Ar-H/Rh-H NMR Coupling in Complexes of Rhodium(III): Experimental Evidence and Theoretical Support for an η^1 -Arene Structure. <i>Journal of the American Chemical Society</i> , 2004, 126, 12492-12502.	13.7	29

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109	Theoretical Studies of the Reductive C-S Bond Cleavage in Complexes of the Form $[M(9S3)2]^{2+}$ (M = Re,) Tj ETQq1.1 0.784314 rgB	2.5	18
110	First-Principles Simulations of C-S Bond Cleavage in Rhenium Thioether Complexes. <i>Journal of Physical Chemistry A</i> , 2004, 108, 2008-2013.	2.5	21
111	Characterization of the Dizinc Analogue of the Synthetic Diiron Protein DF1 Using ab Initio and Hybrid Quantum/Classical Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2003, 107, 4182-4188.	2.6	43
112	Direct observation of an equilibrium between two anion-cation orientations in olefin Pt(II) complex ion pairs by HOESY NMR spectroscopy Electronic supplementary information (ESI) available: details of the experimental measurements and calculations, along with the NMR intramolecular characterization of complexes 1-3. See http://www.rsc.org/suppdata/nj/b2/b212088g/ . <i>New Journal of Chemistry</i> , 2003, 27, 455-458.	2.8	38
113	Hybrid QM/MM Car-Parrinello Simulations of Catalytic and Enzymatic Reactions. <i>Chimia</i> , 2002, 56, 13-19.	0.6	62
114	Dialkyl Effect on Enantioselectivity: π -Stacking as a Structural Feature in P,N Complexes of Palladium(II). <i>Organometallics</i> , 2002, 21, 3033-3041.	2.3	40
115	The Role of π - π Stacking Interactions in Square Planar Palladium Complexes. Combined Quantum Mechanics/Molecular Mechanics QM/MM Studies. <i>Organometallics</i> , 2001, 20, 4178-4184.	2.3	37
116	Cis-Trans Isomerization in Triply-Bonded Ditungsten Complexes: A Multitude of Possible Pathways. <i>Inorganic Chemistry</i> , 2001, 40, 5780-5786.	4.0	8
117	Isolation of a Highly Persistent Diphosphanyl Radical: The Phosphorus Analogue of a Hydrazyl This work was supported by the ETH Zürich and Swiss National Science Foundation.. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 723-726.	13.8	3
118	Three- and Four-Center Trans Effects in Triply Bonded Ditungsten Complexes: An ab Initio Molecular Dynamics Study of Compounds with Stoichiometry $W_2Cl_4(NHEt)_2(PMe_3)_2$. <i>Inorganic Chemistry</i> , 2000, 39, 5553-5560.	4.0	12
119	Electronically and Sterically Induced Structural Distortions in Square-Planar d8 Complexes. <i>Organometallics</i> , 2000, 19, 3591-3596.	2.3	20
120	Molecular Mechanism of Huntington's Disease - A Computational Perspective. , 0, , .		1