Alessandra Magistrato

List of Publications by Year
in descending order

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120 papers	3,587 citations	126907 33 h-index	182427 51 g-index
133 all docs	133 docs citations	133 times ranked	4236 citing authors

#	Article	IF	Citations
1	Is the Rigidity of SARS-CoV-2 Spike Receptor-Binding Motif the Hallmark for Its Enhanced Infectivity? Insights from All-Atom Simulations. Journal of Physical Chemistry Letters, 2020, 11, 4785-4790.	4.6	147
2	Role of protein frame and solvent for the redox properties of azurin from Pseudomonas aeruginosa. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 19641-19646.	7.1	135
3	Bioinorganic Chemistry of Parkinsonâ€™s Disease: Structural Determinants for the Copper-Mediated Amyloid Formation of Alpha-Synuclein. Inorganic Chemistry, 2010, 49, 10668-10679.	4.0	119
4	Fighting Cancer with Transition Metal Complexes: From Naked DNA to Protein and Chromatin Targeting Strategies. ChemMedChem, 2016, 11, 1199-1210.	3.2	104
5	Interfacing proteins with graphitic nanomaterials: from spontaneous attraction to tailored assemblies. Chemical Society Reviews, 2015, 44, 6916-6953.	38.1	91
6	Modeling anticancer drugâ€“DNA interactions via mixed QM/MM molecular dynamics simulations. Organic and Biomolecular Chemistry, 2006, 4, 2507-2517.	2.8	85
7	Who Activates the Nucleophile in Ribozyme Catalysis? An Answer from the Splicing Mechanism of Group II Introns. Journal of the American Chemical Society, 2016, 138, 10374-10377.	13.7	79
8	Copperâ^'1,10-Phenanthroline Complexes Binding to DNA: Structural Predictions from Molecular Simulations. Journal of Physical Chemistry B, 2009, 113, 10881-10890.	2.6	78
9	QM/MM Molecular Dynamics Studies of Metal Binding Proteins. Biomolecules, 2014, 4, 616-645.	4.0	74
10	Binding of Novel Azole-Bridged Dinuclear Platinum(II) Anticancer Drugs to DNA:Â Insights from Hybrid QM/MM Molecular Dynamics Simulationsâ€. Journal of Physical Chemistry B, 2006, 110, 3604-3613.	2.6	63
11	Influence of the Membrane Lipophilic Environment on the Structure and on the Substrate Access/Egress Routes of the Human Aromatase Enzyme. A Computational Study. Journal of Chemical Information and Modeling, 2012, 52, 1595-1606.	5.4	63
12	Hybrid QM/MM Car-Parrinello Simulations of Catalytic and Enzymatic Reactions. Chimia, 2002, 56, 13-19.	0.6	62
13	The Hydrolysis Mechanism of the Anticancer Ruthenium Drugs NAMI-A and ICR Investigated by DFTâ^'PCM Calculations. Journal of Physical Chemistry B, 2008, 112, 4401-4409.	2.6	60
14	Dissociation of minor groove binders from DNA: insights from metadynamics simulations. Nucleic Acids Research, 2008, 36, 5910-5921.	14.5	60
15	All-atom simulations disentangle the functional dynamics underlying gene maturation in the intron lariat spliceosome. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6584-6589.	7.1	59
16	Functionalized Feâ€Filled Multiwalled Carbon Nanotubes as Multifunctional Scaffolds for Magnetization of Cancer Cells. Advanced Functional Materials, 2013, 23, 3173-3184.	14.9	58
17	A Computational Assay of Estrogen Receptor Î± Antagonists Reveals the Key Common Structural Traits of Drugs Effectively Fighting Refractory Breast Cancers. Scientific Reports, 2018, 8, 649.	3.3	57
18	Common Mechanistic Features among Metallo-Î²-lactamases. Journal of Biological Chemistry, 2009, 284, 28164-28171.	3.4	54

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19	Nitrogen Fixation by a Molybdenum Catalyst Mimicking the Function of the Nitrogenase Enzyme:â€‰ A Critical Evaluation of DFT and Solvent Effects. Journal of Chemical Theory and Computation, 2007, 3, 1708-1720.	5.3	52
20	The Structural Role of Mg²⁺ Ions in a Class I RNA Polymerase Ribozyme: A Molecular Simulation Study. Journal of Physical Chemistry B, 2012, 116, 2259-2268.	2.6	51
21	Development of Site-Specific Mg²⁺â€“RNA Force Field Parameters: A Dream or Reality? Guidelines from Combined Molecular Dynamics and Quantum Mechanics Simulations. Journal of Chemical Theory and Computation, 2017, 13, 340-352.	5.3	51
22	Density Functional Theory Studies on Copper Phenanthroline Complexes. Inorganic Chemistry, 2007, 46, 5873-5881.	4.0	47
23	QM/MM MD Simulations on the Enzymatic Pathway of the Human Flap Endonuclease (hFEN1) Elucidating Common Cleavage Pathways to RNase H Enzymes. ACS Catalysis, 2015, 5, 3864-3875.	11.2	45
24	Characterization of the Dizinc Analogue of the Synthetic Diiron Protein DF1 Using ab Initio and Hybrid Quantum/Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2003, 107, 4182-4188.	2.6	43
25	Detecting DNA Mismatches with Metallo-Insertors: A Molecular Simulation Study. Inorganic Chemistry, 2012, 51, 2046-2057.	4.0	41
26	Computational Approaches Elucidate the Allosteric Mechanism of Human Aromatase Inhibition: A Novel Possible Route to Small-Molecule Regulation of CYP450s Activities?. Journal of Chemical Information and Modeling, 2014, 54, 2856-2868.	5.4	41
27	Single or Multiple Access Channels to the CYP450s Active Site? An Answer from Free Energy Simulations of the Human Aromatase Enzyme. Journal of Physical Chemistry Letters, 2017, 8, 2036-2042.	4.6	41
28	Dialkyl Effect on Enantioselectivity:Â Ï€-Stacking as a Structural Feature in P,N Complexes of Palladium(II). Organometallics, 2002, 21, 3033-3041.	2.3	40
29	Molecular basis for functional diversity among microbial Nep1-like proteins. PLoS Pathogens, 2019, 15, e1007951.	4.7	39
30	Copper trafficking in eukaryotic systems: current knowledge from experimental and computational efforts. Current Opinion in Structural Biology, 2019, 58, 26-33.	5.7	39
31	Direct observation of an equilibrium between two anion-cation orientations in olefin Pt(II) complex ion pairs by HOESY NMR spectroscopyElectronic supplementary information (ESI) available: details of the experimental measurements and calculations, along with the NMR intramolecular characterization of complexes 1â€“3. See http://www.rsc.org/suppdata/nj/b2/b212088g/. New Journal of Chemistry, 2003, 27, 455-458.	2.8	38
32	The Role of Ï€â‹¯Ï€ Stacking Interactions in Square Planar Palladium Complexes. Combined Quantum Mechanics/Molecular Mechanics QM/MM Studies. Organometallics, 2001, 20, 4178-4184.	2.3	37
33	Understanding the mechanistic basis of non-coding RNA through molecular dynamics simulations. Journal of Structural Biology, 2019, 206, 267-279.	2.8	37
34	A structural, functional, and computational analysis suggests pore flexibility as the base for the poor selectivity of CNG channels. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E3619-28.	7.1	35
35	Decrypting the Information Exchange Pathways across the Spliceosome Machinery. Journal of the American Chemical Society, 2020, 142, 8403-8411.	13.7	35
36	Enantioselective Palladium-Catalyzed Hydrosilylation of Styrene:Â Detailed Reaction Mechanism from First-Principles and Hybrid QM/MM Molecular Dynamics Simulations. Organometallics, 2004, 23, 3218-3227.	2.3	34

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37	Parameterization of azoleâ€bridged dinuclear platinum anticancer drugs via a QM/MM force matching procedure. Journal of Computational Chemistry, 2008, 29, 38-49.	3.3	34
38	Discovery of a natural cyan blue: A unique food-sourced anthocyanin could replace synthetic brilliant blue. Science Advances, 2021, 7, .	10.3	34
39	Protonation state and substrate binding to B2 metalloâ€Î²â€lactamase CphA from Aeromonas hydrofila. Proteins: Structure, Function and Bioinformatics, 2007, 69, 595-605.	2.6	33
40	Rational design of allosteric modulators of the aromatase enzyme: AnÂunprecedented therapeutic strategy to fight breast cancer. European Journal of Medicinal Chemistry, 2019, 168, 253-262.	5.5	33
41	Allosteric Cross-Talk among Spikeâ€™s Receptor-Binding Domain Mutations of the SARS-CoV-2 South African Variant Triggers an Effective Hijacking of Human Cell Receptor. Journal of Physical Chemistry Letters, 2021, 12, 5987-5993.	4.6	33
42	Computational Study of the DNA-Binding Protein Helicobacter pylori NikR: The Role of Ni2+ 2 Francesco Musiani and Branimir BertoÅ¡a contributed equally to the simulations presented here.. Journal of Chemical Theory and Computation, 2010, 6, 3503-3515.	5.3	32
43	A Dehydrogenase Dual Hydrogen Abstraction Mechanism Promotes Estrogen Biosynthesis: Can We Expand the Functional Annotation of the Aromatase Enzyme?. Chemistry - A European Journal, 2018, 24, 10840-10849.	3.3	31
44	Unusual Arâ^'H/Rhâ^'HJHHNMR Coupling in Complexes of Rhodium(III):Â Experimental Evidence and Theoretical Support for an Î·1â^'Arene Structure. Journal of the American Chemical Society, 2004, 126, 12492-12502.	13.7	29
45	Azole-Bridged Diplatinum Anticancer Compounds. Modulating DNA Flexibility to Escape Repair Mechanism and Avoid Cross Resistance. Journal of Physical Chemistry B, 2007, 111, 11873-11876.	2.6	29
46	Molecular Basis for Endocrine Disruption by Pesticides Targeting Aromatase and Estrogen Receptor. International Journal of Environmental Research and Public Health, 2020, 17, 5664.	2.6	29
47	Frontiers of metal-coordinating drug design. Expert Opinion on Drug Discovery, 2021, 16, 497-511.	5.0	28
48	Synthesis, photophysical, electrochemical, and electrochemiluminescent properties of 5,15-bis(9-anthracenyl)porphyrin derivatives. Organic and Biomolecular Chemistry, 2009, 7, 2402.	2.8	27
49	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. Inorganic Chemistry, 2014, 53, 7999-8008.	4.0	27
50	A Candidate Ion-Retaining State in the Inward-Facing Conformation of Sodium/Galactose Symporter: Clues from Atomistic Simulations. Journal of Chemical Theory and Computation, 2013, 9, 1240-1246.	5.3	26
51	All-Atom Simulations Decrypt the Molecular Terms of RNA Catalysis in the Exon-Ligation Step of the Spliceosome. ACS Catalysis, 2020, 10, 5328-5334.	11.2	26
52	Enantioselective Palladium-Catalyzed Hydrosilylation of Styrene:Â Influence of Electronic and Steric Effects on Enantioselectivity and Catalyst Design via Hybrid QM/MM Molecular Dynamics Simulations. Organometallics, 2006, 25, 1151-1157.	2.3	25
53	Sliding of Alkylating Anticancer Drugs along the Minor Groove of DNA: New Insights on Sequence Selectivity. Biophysical Journal, 2008, 94, 550-561.	0.5	25
54	Atomisticâ€Level Portrayal of Drugâ€“DNA Interplay: A History of Courtships and Meetings Revealed by Molecular Simulations. ChemMedChem, 2014, 9, 1966-1981.	3.2	25

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55	Role of Water in the Puzzling Mechanism of the Final Aromatization Step Promoted by the Human Aromatase Enzyme. Insights from QM/MM MD Simulations. Journal of Chemical Information and Modeling, 2015, 55, 2218-2226.	5.4	25
56	A Synthetic Derivative of Antimicrobial Peptide Holothuroidin 2 from Mediterranean Sea Cucumber (Holothuria tubulosa) in the Control of Listeria monocytogenes. Marine Drugs, 2019, 17, 159.	4.6	25
57	Second step of hydrolytic dehalogenation in haloalkane dehalogenase investigated by QM/MM methods. Proteins: Structure, Function and Bioinformatics, 2008, 70, 707-717.	2.6	24
58	Theoretical Studies of Homogeneous Catalysts Mimicking Nitrogenase. Molecules, 2011, 16, 442-465.	3.8	24
59	Structural and Dynamic Properties of Monoclonal Antibodies Immobilized on CNTs: A Computational Study. Chemistry - A European Journal, 2013, 19, 12281-12293.	3.3	24
60	Exploiting Cryo-EM Structural Information and All-Atom Simulations To Decrypt the Molecular Mechanism of Splicing Modulators. Journal of Chemical Information and Modeling, 2020, 60, 2510-2521.	5.4	24
61	Peptide Inhibitors of Bacterial Protein Synthesis with Broad Spectrum and SbmA-Independent Bactericidal Activity against Clinical Pathogens. Journal of Medicinal Chemistry, 2020, 63, 9590-9602.	6.4	24
62	First-Principles Modeling of Biological Systems and Structure-Based Drug-Design. Current Computer-Aided Drug Design, 2013, 9, 15-34.	1.2	24
63	Anthramycinâ^'DNA Binding Explored by Molecular Simulations. Journal of Physical Chemistry B, 2006, 110, 24687-24695.	2.6	23
64	Disclosing the Impact of Carcinogenic SF3b Mutations on Pre-mRNA Recognition Via All-Atom Simulations. Biomolecules, 2019, 9, 633.	4.0	23
65	The Catalytic Mechanism of Steroidogenic Cytochromes P450 from All-Atom Simulations: Entwinement with Membrane Environment, Redox Partners, and Post-Transcriptional Regulation. Catalysts, 2019, 9, 81.	3.5	23
66	All-atom simulations to studying metallodrugs/target interactions. Current Opinion in Chemical Biology, 2021, 61, 1-8.	6.1	23
67	Atomic-Level Mechanism of Pre-mRNA Splicing in Health and Disease. Accounts of Chemical Research, 2021, 54, 144-154.	15.6	23
68	Post-Translational Regulation of CYP450s Metabolism As Revealed by All-Atoms Simulations of the Aromatase Enzyme. Journal of Chemical Information and Modeling, 2019, 59, 2930-2940.	5.4	22
69	First-Principles Simulations of Câ^'S Bond Cleavage in Rhenium Thioether Complexes. Journal of Physical Chemistry A, 2004, 108, 2008-2013.	2.5	21
70	How Can Interleukin-1 Receptor Antagonist Modulate Distinct Cell Death Pathways?. Journal of Chemical Information and Modeling, 2019, 59, 351-359.	5.4	21
71	Electronically and Sterically Induced Structural Distortions in Square-Planar d8 Complexes. Organometallics, 2000, 19, 3591-3596.	2.3	20
72	Interaction between the DNA Model Base 9-Ethylguanine and a Group of Ruthenium Polypyridyl Complexes:Â Kinetics and Conformational Temperature Dependence. Inorganic Chemistry, 2007, 46, 6715-6722.	4.0	20

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73	Metadynamics Simulations Reveal a Na+ Independent Exiting Path of Galactose for the Inward-Facing Conformation of vSGLT. PLoS Computational Biology, 2014, 10, e1004017.	3.2	20
74	Unraveling the molecular mechanisms of color expression in anthocyanins. Physical Chemistry Chemical Physics, 2019, 21, 8757-8766.	2.8	20
75	Enzymatic and Inhibition Mechanism of Human Aromatase (CYP19A1) Enzyme. A Computational Perspective from QM/MM and Classical Molecular Dynamics Simulations. Mini-Reviews in Medicinal Chemistry, 2016, 16, 1112-1124.	2.4	20
76	Structural Properties of Polyglutamine Aggregates Investigated via Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2008, 112, 16843-16850.	2.6	19
77	Theoretical Studies of the Reductive Câ^'S Bond Cleavage in Complexes of the Form [M(9S3)2]2+ (M = Re,) Tj ETQq1 1 0.784314 rgB	2.5	18
78	Targeting Orthosteric and Allosteric Pockets of Aromatase via Dual-Mode Novel Azole Inhibitors. ACS Medicinal Chemistry Letters, 2020, 11, 732-739.	2.8	18
79	All-Atom Simulations Disclose How Cytochrome Reductase Reshapes the Substrate Access/Egress Routes of Its Partner CYP450s. Journal of Physical Chemistry Letters, 2020, 11, 1189-1193.	4.6	18
80	Hydrogen Bonding Cooperativity in polyQ Î²-Sheets from First Principle Calculations. Journal of Chemical Theory and Computation, 2010, 6, 1777-1782.	5.3	17
81	Structural, dynamical and catalytic interplay between Mg2+ ions and RNA. Vices and virtues of atomistic simulations. Inorganica Chimica Acta, 2016, 452, 73-81.	2.4	16
82	Unraveling the Impact of Cysteine-to-Serine Mutations on the Structural and Functional Properties of Cu(I)-Binding Proteins. International Journal of Molecular Sciences, 2019, 20, 3462.	4.1	16
83	The pivotal role of MBD4â€"ATP7B in the human Cu(<scp>i</scp>) excretion path as revealed by EPR experiments and all-atom simulations. Metallomics, 2019, 11, 1288-1297.	2.4	15
84	An omics perspective to the molecular mechanisms of anticancer metallo-drugs in the computational microscope era. Expert Opinion on Drug Discovery, 2017, 12, 1-13.	5.0	14
85	Recent advances in computational design of potent aromatase inhibitors: open-eye on endocrine-resistant breast cancers. Expert Opinion on Drug Discovery, 2019, 14, 1065-1076.	5.0	14
86	Anthrax Lethal Factor Investigated by Molecular Simulations. Journal of Chemical Theory and Computation, 2008, 4, 1745-1756.	5.3	13
87	The molecular mechanism of secondary sodium symporters elucidated through the lens of the computational microscope. RSC Advances, 2016, 6, 9522-9540.	3.6	13
88	Three- and Four-Center Trans Effects in Triply Bonded Ditungsten Complexes:Â An ab Initio Molecular Dynamics Study of Compounds with Stoichiometry W2Cl4(NHEt)2(PMe3)2. Inorganic Chemistry, 2000, 39, 5553-5560.	4.0	12
89	Computing Metalâ€Binding Proteins for Therapeutic Benefit. ChemMedChem, 2021, 16, 2034-2049.	3.2	12
90	Spontaneous Production of Ultrastable Reactive Oxygen Species on Titanium Oxide Surfaces Modified with Organic Ligands. Advanced Materials Interfaces, 2021, 8, 2100629.	3.7	11

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91	Balanced dual acting compounds targeting aromatase and estrogen receptor Î± as an emerging therapeutic opportunity to counteract estrogen responsive breast cancer. European Journal of Medicinal Chemistry, 2021, 224, 113733.	5.5	11
92	An oomycete NLP cytolysin forms transient small pores in lipid membranes. Science Advances, 2022, 8, eabj9406.	10.3	11
93	Cu(I) Controls Conformational States in Human Atox1 Metallochaperone: An EPR and Multiscale Simulation Study. Journal of Physical Chemistry B, 2020, 124, 4399-4411.	2.6	10
94	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. Journal of the American Society for Mass Spectrometry, 2009, 20, 1327-1333.	2.8	9
95	Can multiscale simulations unravel the function of metallo-enzymes to improve knowledge-based drug discovery?. Future Medicinal Chemistry, 2019, 11, 771-791.	2.3	9
96	Nep1-like proteins as a target for plant pathogen control. PLoS Pathogens, 2021, 17, e1009477.	4.7	9
97	All-Atom Simulations Uncover the Molecular Terms of the NKCC1 Transport Mechanism. Journal of Chemical Information and Modeling, 2021, 61, 3649-3658.	5.4	9
98	Investigating the Molecular Mechanism of H3B-8800: A Splicing Modulator Inducing Preferential Lethality in Spliceosome-Mutant Cancers. International Journal of Molecular Sciences, 2021, 22, 11222.	4.1	9
99	Cisâ^'TransIsomerization in Triply-Bonded Ditungsten Complexes:Â A Multitude of Possible Pathways. Inorganic Chemistry, 2001, 40, 5780-5786.	4.0	8
100	Deciphering the Molecular Terms of Arp2/3 Allosteric Regulation from All-Atom Simulations and Dynamical Network Theory. Journal of Physical Chemistry Letters, 2021, 12, 5384-5389.	4.6	8
101	First-principles modeling of biological systems and structure-based drug-design. Current Computer-Aided Drug Design, 2013, 9, 15-34.	1.2	8
102	On the active site of mononuclear B1 metallo Î²-lactamases: a computational study. Journal of Computer-Aided Molecular Design, 2012, 26, 425-435.	2.9	7
103	Unraveling the Molecular Mechanism of Pre-mRNA Splicing From Multi-Scale Simulations. Frontiers in Molecular Biosciences, 2019, 6, 62.	3.5	7
104	Molecular Mechanisms of the Blockage of Glioblastoma Motility. Journal of Chemical Information and Modeling, 2021, 61, 2967-2980.	5.4	7
105	Molecular Basis of SARS-CoV-2 Nsp1-Induced Immune Translational Shutdown as Revealed by All-Atom Simulations. Journal of Physical Chemistry Letters, 2021, 12, 11745-11750.	4.6	7
106	Structural, Thermodynamic, and Kinetic Traits of Antiestrogen-Compounds Selectively Targeting the Y537S Mutant Estrogen Receptor Î± Transcriptional Activity in Breast Cancer Cell Lines. Frontiers in Chemistry, 2019, 7, 602.	3.6	6
107	An Expanded Two-Zn²⁺-Ion Motif Orchestrates Pre-mRNA Maturation in the 3â€²-End Processing Endonuclease Machinery. ACS Catalysis, 2021, 11, 4319-4326.	11.2	6
108	Dynamical interplay between the human high-affinity copper transporter hCtr1 and its cognate metal ion. Biophysical Journal, 2022, 121, 1194-1204.	0.5	6

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109	Structural Role of Uracil DNA Glycosylase for the Recognition of Uracil in DNA Duplexes. Clues from Atomistic Simulations. Journal of Chemical Information and Modeling, 2013, 53, 1371-1387.	5.4	4
110	First-Principles Modeling of Biological Systems and Structure-Based Drug-Design. Current Computer-Aided Drug Design, 2013, 9, 15-34.	1.2	3
111	Isolation of a Highly Persistent Diphosphanyl Radical: The Phosphorus Analogue of a Hydrazyl This work was supported by the ETH ZÃ¼rich and Swiss National Science Foundation.. Angewandte Chemie - International Edition, 2001, 40, 723-726.	13.8	3
112	Direct in silico visualization of ligands channelling through proteins: The next-generation frontier of computational biology. Physics of Life Reviews, 2017, 22-23, 82-84.	2.8	2
113	Magnetic Carbon Nanotubes: Functionalized Fe-Filled Multiwalled Carbon Nanotubes as Multifunctional Scaffolds for Magnetization of Cancer Cells (Adv. Funct. Mater. 25/2013). Advanced Functional Materials, 2013, 23, 3172-3172.	14.9	1
114	Molecular Mechanism of Huntingtonâ€™s Disease â€" A Computational Perspective. , 0, , .		1
115	Molecular Recognition Routes Of DNA By Anticancer Ligands: Mechanisms and Free Energies Explored Via Molecular Dynamics Simulations. Biophysical Journal, 2009, 96, 84a.	0.5	0
116	Simulations of Copper-1,10-Phenanthroline Complexes Binding the DNA. Biophysical Journal, 2009, 96, 577a.	0.5	0
117	Huntingtin: Stability and Interaction with Molecular Partner from Computational Biophysics Studies. Biophysical Journal, 2010, 98, 637a.	0.5	0
118	Sodium-Galactose Transporter: The First Steps of the Transport Mechanism Investigated by Molecular Dynamics. Biophysical Journal, 2014, 106, 365a-366a.	0.5	0
119	Structural and Dynamical Properties of Monoclonal Antibodies Immobilized on CNTs: A Computational Study. Biophysical Journal, 2014, 106, 620a.	0.5	0
120	Pre-mRNA Splicing: The Gene Maturation Symphony of the Intron Lariat Spliceosome Revealed by Molecular Dynamics Simulations. Biophysical Journal, 2019, 116, 299a.	0.5	0