

# Giovanni Chillemi

## List of Publications by Year in descending order

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149  
papers

4,081  
citations

101543

36  
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168389

53  
g-index

158  
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158  
docs citations

158  
times ranked

5814  
citing authors

#	ARTICLE	IF	CITATIONS
1	Using of NMR Milk Metabolomics to Evaluate Mammary Gland Health Status in Dairy Cows. Lecture Notes in Civil Engineering, 2022, , 67-75.	0.4	0
2	Cow Milk Extracellular Vesicle Effects on an In Vitro Model of Intestinal Inflammation. Biomedicines, 2022, 10, 570.	3.2	19
3	Not just a Snapshot: An Italian Longitudinal Evaluation of Stability of Gut Microbiota Findings in Parkinson's Disease. Brain Sciences, 2022, 12, 739.	2.3	6
4	REDIportal: millions of novel A-to-I RNA editing events from thousands of RNAseq experiments. Nucleic Acids Research, 2021, 49, D1012-D1019.	14.5	86
5	Dissecting the Gene Expression Networks Associated with Variations in the Major Components of the Fatty Acid Semimembranosus Muscle Profile in Large White Heavy Pigs. Animals, 2021, 11, 628.	2.3	8
6	Co-occurring SYNJ1 and SHANK3 variants in a girl with intellectual disability, early-onset parkinsonism and catatonic episodes. Parkinsonism and Related Disorders, 2021, 84, 5-7.	2.2	1
7	Altered Local Interactions and Long-Range Communications in UK Variant (B.1.1.7) Spike Glycoprotein. International Journal of Molecular Sciences, 2021, 22, 5464.	4.1	9
8	Broadening the phenotypic spectrum of Beta3GalT6 associated phenotypes. American Journal of Medical Genetics, Part A, 2021, 185, 3153-3160.	1.2	3
9	MXAN: A new program for ab-initio structural quantitative analysis of XANES experiments. Computer Physics Communications, 2021, 265, 107992.	7.5	4
10	Epilepsy and BRAF Mutations: Phenotypes, Natural History and Genotype-Phenotype Correlations. Genes, 2021, 12, 1316.	2.4	13
11	The Quest for Genes Involved in Adaptation to Climate Change in Ruminant Livestock. Animals, 2021, 11, 2833.	2.3	18
12	Multiple Recombination Events and Strong Purifying Selection at the Origin of SARS-CoV-2 Spike Glycoprotein Increased Correlated Dynamic Movements. International Journal of Molecular Sciences, 2021, 22, 80.	4.1	21
13	SPRED2 loss-of-function causes a recessive Noonan syndrome-like phenotype. American Journal of Human Genetics, 2021, 108, 2112-2129.	6.2	23
14	Transcriptomic Characterization of Cow, Donkey and Goat Milk Extracellular Vesicles Reveals Their Anti-Inflammatory and Immunomodulatory Potential. International Journal of Molecular Sciences, 2021, 22, 12759.	4.1	27
15	Coding-Gene Coevolution Analysis of Rotavirus Proteins: A Bioinformatics and Statistical Approach. Genes, 2020, 11, 28.	2.4	1
16	Structural and dynamic analysis of G558R mutation in chicken <i>TSHR</i> gene shows altered signal transduction and corroborates its role as a domestication gene. Animal Genetics, 2020, 51, 51-57.	1.7	5
17	Anti-Inflammatory Potential of Cow, Donkey and Goat Milk Extracellular Vesicles as Revealed by Metabolomic Profile. Nutrients, 2020, 12, 2908.	4.1	19
18	New Insights into the Effect of Residue Mutations on the Rotavirus VP1 Function Using Molecular Dynamic Simulations. Journal of Chemical Information and Modeling, 2020, 60, 5011-5025.	5.4	4

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19	Genome-Wide DNA Methylation and Gene Expression Profiles in Cows Subjected to Different Stress Level as Assessed by Cortisol in Milk. <i>Genes</i> , 2020, 11, 850.	2.4	11
20	ELIXIR-IT HPC@CINECA: high performance computing resources for the bioinformatics community. <i>BMC Bioinformatics</i> , 2020, 21, 352.	2.6	25
21	HPC-REDIttools: a novel HPC-aware tool for improved large scale RNA-editing analysis. <i>BMC Bioinformatics</i> , 2020, 21, 353.	2.6	28
22	Muscle transcriptome analysis identifies genes involved in ciliogenesis and the molecular cascade associated with intramuscular fat content in Large White heavy pigs. <i>PLoS ONE</i> , 2020, 15, e0233372.	2.5	25
23	Evidence of distinct gene functional patterns in GC-poor and GC-rich isochores in <i>Bos taurus</i> . <i>Animal Genetics</i> , 2020, 51, 358-368.	1.7	6
24	Was the Cinta Senese Pig Already a Luxury Food in the Late Middle Ages? Ancient DNA and Archaeozoological Evidence from Central Italy. <i>Genes</i> , 2020, 11, 85.	2.4	1
25	Gallop Racing Shifts Mature mRNA towards Introns: Does Exercise-Induced Stress Enhance Genome Plasticity?. <i>Genes</i> , 2020, 11, 410.	2.4	7
26	A gene expression atlas for different kinds of stress in the mouse brain. <i>Scientific Data</i> , 2020, 7, 437.	5.3	34
27	DROPA: DRIP-seq optimized peak annotator. <i>BMC Bioinformatics</i> , 2019, 20, 414.	2.6	5
28	HECT-Type E3 Ubiquitin Ligases in Cancer. <i>Trends in Biochemical Sciences</i> , 2019, 44, 1057-1075.	7.5	59
29	Smyd2 conformational changes in response to p53 binding: role of the C-terminal domain. <i>Molecular Oncology</i> , 2019, 13, 1450-1461.	4.6	10
30	Clinical and functional characterization of a novel RASopathy-causing <i>SHOC2</i> mutation associated with prenatal-onset hypertrophic cardiomyopathy. <i>Human Mutation</i> , 2019, 40, 1046-1056.	2.5	18
31	MXAN and Molecular Dynamics: A New Way to Look to the XANES (X-ray Absorption Near Edge) Tj ETQq1 1 0.784314 rgBT /Overlock 0,2 1		
32	PeachVar-DB: A Curated Collection of Genetic Variations for the Interactive Analysis of Peach Genome Data. <i>Plant and Cell Physiology</i> , 2018, 59, e2-e2.	3.1	12
33	Molecular dynamics recipes for genome research. <i>Briefings in Bioinformatics</i> , 2018, 19, 853-862.	6.5	23
34	Missense mutations of NCPAG gene affect calving ease in Piedmontese cattle: preliminary evidences. <i>Italian Journal of Animal Science</i> , 2018, 17, 301-305.	1.9	0
35	Dynamic multiple-scattering treatment of X-ray absorption: Parameterization of a new molecular dynamics force field for myoglobin. <i>Structural Dynamics</i> , 2018, 5, 054101.	2.3	5
36	CoVaCS: a consensus variant calling system. <i>BMC Genomics</i> , 2018, 19, 120.	2.8	29

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37	Role of the keratin 1 and keratin 10 tails in the pathogenesis of ichthyosis hystrix of Curth Macklin. PLoS ONE, 2018, 13, e0195792.	2.5	10
38	Massive NGS data analysis reveals hundreds of potential novel gene fusions in human cell lines. GigaScience, 2018, 7, .	6.4	6
39	Structural Evolution and Dynamics of the p53 Proteins. Cold Spring Harbor Perspectives in Medicine, 2017, 7, a028308.	6.2	41
40	Type I DNA Topoisomerases. Journal of Medicinal Chemistry, 2017, 60, 2169-2192.	6.4	98
41	Microcephaly, intractable seizures and developmental delay caused by biallelic variants in <i>TBCD</i> : further delineation of a new chaperone-mediated tubulinopathy. Clinical Genetics, 2017, 91, 725-738.	2.0	25
42	A molecular dynamics simulation study decodes the early stage of the disassembly process abolishing the human SAMHD1 function. Journal of Computer-Aided Molecular Design, 2017, 31, 497-505.	2.9	4
43	Whole-exome sequencing and targeted gene sequencing provide insights into the role of <i>PALB2</i> as a male breast cancer susceptibility gene. Cancer, 2017, 123, 210-218.	4.1	31
44	Genome assembly and transcriptome resource for river buffalo, <i>Bubalus bubalis</i> (2n = 50). GigaScience, 2017, 6, 1-6.	6.4	55
45	Structural and Dynamic Characterization of the C313Y Mutation in Myostatin Dimeric Protein, Responsible for the "Double Muscle" Phenotype in Piedmontese Cattle. Frontiers in Genetics, 2016, 7, 14.	2.3	6
46	Expanding the molecular diversity and phenotypic spectrum of glycerol 3-phosphate dehydrogenase 1 deficiency. Journal of Inherited Metabolic Disease, 2016, 39, 689-695.	3.6	24
47	Transcriptomic investigation of meat tenderness in two Italian cattle breeds. Animal Genetics, 2016, 47, 273-287.	1.7	37
48	Conformational Dynamics of Lysine Methyltransferase Smyd2. Insights into the Different Substrate Crevice Characteristics of Smyd2 and Smyd3. Journal of Chemical Information and Modeling, 2016, 56, 2467-2475.	5.4	10
49	Solvation structure of the halides from x-ray absorption spectroscopy. Journal of Chemical Physics, 2016, 145, 044318.	3.0	38
50	Skeletal muscle transcriptional profiles in two Italian beef breeds, Chianina and Maremmana, reveal breed specific variation. Molecular Biology Reports, 2016, 43, 253-268.	2.3	16
51	Equilibrium between 5- and 6-Fold Coordination in the First Hydration Shell of Cu(II). Journal of Physical Chemistry A, 2016, 120, 3958-3965.	2.5	17
52	Smyd3 open & closed lock mechanism for substrate recruitment: The hinge motion of C-terminal domain inferred from 1/4-second molecular dynamics simulations. Biochimica Et Biophysica Acta - General Subjects, 2016, 1860, 1466-1474.	2.4	12
53	Biallelic Mutations in TBCD , Encoding the Tubulin Folding Cofactor D, Perturb Microtubule Dynamics and Cause Early-Onset Encephalopathy. American Journal of Human Genetics, 2016, 99, 962-973.	6.2	66
54	SHOC2 subcellular shuttling requires the KEKE motif-rich region and N-terminal leucine-rich repeat domain and impacts on ERK signalling. Human Molecular Genetics, 2016, 25, 3824-3835.	2.9	17

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55	RNA-Sequencing for profiling goat milk transcriptome in colostrum and mature milk. <i>BMC Veterinary Research</i> , 2016, 12, 264.	1.9	71
56	The p53 tetramer shows an induced-fit interaction of the C-terminal domain with the DNA-binding domain. <i>Oncogene</i> , 2016, 35, 3272-3281.	5.9	40
57	Molecular Signature of the Ebola Virus Associated with the Fishermen Community Outbreak in Aberdeen, Sierra Leone, in February 2015. <i>Genome Announcements</i> , 2015, 3, .	0.8	3
58	MD and Docking Studies Reveal That the Functional Switch of CYFIP1 is Mediated by a Butterfly-like Motion. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3401-3410.	5.3	24
59	Novel and known genetic variants for male breast cancer risk at 8q24.21, 9p21.3, 11q13.3 and 14q24.1: Results from a multicenter study in Italy. <i>European Journal of Cancer</i> , 2015, 51, 2289-2295.	2.8	25
60	Molecular Characterization of the First Ebola Virus Isolated in Italy, from a Health Care Worker Repatriated from Sierra Leone. <i>Genome Announcements</i> , 2015, 3, .	0.8	10
61	Modeling conformational transitions in kinases by molecular dynamics simulations: achievements, difficulties, and open challenges. <i>Frontiers in Genetics</i> , 2014, 5, 128.	2.3	12
62	Simulations of DNA topoisomerase 1B bound to supercoiled DNA reveal changes in the flexibility pattern of the enzyme and a secondary proteinâ€™DNA binding site. <i>Nucleic Acids Research</i> , 2014, 42, 9304-9312.	14.5	29
63	Signatures of selection in five Italian cattle breeds detected by a 54K SNP panel. <i>Molecular Biology Reports</i> , 2014, 41, 957-965.	2.3	26
64	Structural dynamics of V3 loop in a trimeric ambience, a molecular dynamics study on gp120â€™CD4 trimeric mimic. <i>Journal of Structural Biology</i> , 2014, 186, 132-140.	2.8	4
65	Performances of Bioinformatics Pipelines for the Identification of Pathogens in Clinical Samples with the De Novo Assembly Approaches: Focus on 2009 Pandemic Influenza A (H1N1). <i>Open Bioinformatics Journal</i> , 2014, 8, 1-5.	1.0	0
66	Massive screening of copy number population-scale variation in <i>Bos taurus</i> genome. <i>BMC Genomics</i> , 2013, 14, 124.	2.8	48
67	Microarray gene expression profiling of neural tissues in bovine spastic paresis. <i>BMC Veterinary Research</i> , 2013, 9, 122.	1.9	8
68	Association between single nucleotide polymorphisms (SNPs) and milk production traits in Italian Brown cattle. <i>Livestock Science</i> , 2013, 157, 93-99.	1.6	10
69	Structural dynamics of V3 loop with different electrostatics: implications on co-receptor recognition: a molecular dynamics study of HIV gp120. <i>Journal of Biomolecular Structure and Dynamics</i> , 2013, 31, 403-413.	3.5	14
70	The SNPs in the human genetic blueprint era. <i>New Biotechnology</i> , 2013, 30, 475-484.	4.4	10
71	Antisense transcripts enhanced by camptothecin at divergent CpG-island promoters associated with bursts of topoisomerase I-DNA cleavage complex and R-loop formation. <i>Nucleic Acids Research</i> , 2013, 41, 10110-10123.	14.5	57
72	Molecular dynamics of the full-length p53 monomer. <i>Cell Cycle</i> , 2013, 12, 3098-3108.	2.6	27

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73	Solvent Dependency of the UV-Vis Spectrum of Indenoisoquinolines: Role of Keto-Oxygens as Polarity Interaction Probes. <i>PLoS ONE</i> , 2013, 8, e73881.	2.5	4
74	Abstract 637: Antisense transcripts and R-loops caused by DNA topoisomerase I inhibition by camptothecin at human active CpG island promoters.. , 2013, , .		1
75	Carbon monoxide binding to the heme group at the dimeric interface modulates structure and copper accessibility in the Cu,Zn superoxide dismutase from <i>Haemophilus ducreyi</i> : in silico and in vitro evidences. <i>Journal of Biomolecular Structure and Dynamics</i> , 2012, 30, 269-279.	3.5	4
76	Role of Flexibility in Protein-DNA-Drug Recognition: The Case of Asp677Gly-Val703Ile Topoisomerase Mutant Hypersensitive to Camptothecin. <i>Journal of Amino Acids</i> , 2012, 2012, 1-8.	5.8	12
77	X-ray Absorption Study of the Solvation Structure of Cu <sup>2+</sup> in Methanol and Dimethyl Sulfoxide. <i>Inorganic Chemistry</i> , 2012, 51, 8827-8833.	4.0	23
78	Effects of the Pathological Q212P Mutation on Human Prion Protein Non-Octarepeat Copper-Binding Site. <i>Biochemistry</i> , 2012, 51, 6068-6079.	2.5	32
79	Binding of an Indenoisoquinoline to the Topoisomerase-DNA Complex Induces Reduction of Linker Mobility and Strengthening of Protein-DNA Interaction. <i>PLoS ONE</i> , 2012, 7, e51354.	2.5	14
80	Influence of the Second Coordination Shell on the XANES Spectra of the Zn <sup>2+</sup> Ion in Water and Methanol. <i>ChemPlusChem</i> , 2012, 77, 234-239.	2.8	40
81	Importance of V3 Loop Flexibility and Net Charge in the Context of Co-Receptor Recognition. A Molecular Dynamics Study on HIV gp120. <i>Journal of Biomolecular Structure and Dynamics</i> , 2012, 29, 879-891.	3.5	19
82	Identification of a Short Region on Chromosome 6 Affecting Direct Calving Ease in Piedmontese Cattle Breed. <i>PLoS ONE</i> , 2012, 7, e50137.	2.5	49
83	On the Solvation of the Zn <sup>2+</sup> Ion in Methanol: A Combined Quantum Mechanics, Molecular Dynamics, and EXAFS Approach. <i>Inorganic Chemistry</i> , 2011, 50, 8509-8515.	4.0	41
84	Simulative Analysis of a Truncated Octahedral DNA Nanocage Family Indicates the Single-Stranded Thymidine Linkers as the Major Player for the Conformational Variability. <i>Journal of Physical Chemistry C</i> , 2011, 115, 16819-16827.	3.1	14
85	Effect of the Zn <sup>2+</sup> and Hg <sup>2+</sup> Ions on the Structure of Liquid Water. <i>Journal of Physical Chemistry A</i> , 2011, 115, 4798-4803.	2.5	34
86	Revised Ionic Radii of Lanthanoid(III) Ions in Aqueous Solution. <i>Inorganic Chemistry</i> , 2011, 50, 4572-4579.	4.0	212
87	Analysis of co-receptor usage of circulating viral and proviral HIV genome quasispecies by ultra-deep pyrosequencing in patients who are candidates for CCR5 antagonist treatment. <i>Clinical Microbiology and Infection</i> , 2011, 17, 725-731.	6.0	32
88	Abstract 1180: Activation of antisense transcription by Top1cc in human colon cancer cells. , 2011, , .		0
89	Assembly and characterization of pandemic influenza A H1N1 genome in nasopharyngeal swabs using high-throughput pyrosequencing. <i>New Microbiologica</i> , 2011, 34, 391-7.	0.1	11
90	Erybraedin C, a natural compound from the plant <i>Bituminaria bituminosa</i> , inhibits both the cleavage and religation activities of human topoisomerase I. <i>Biochemical Journal</i> , 2010, 425, 531-539.	3.7	40

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91	An amber compatible molecular mechanics force field for the anticancer drug topotecan. <i>Theoretical Chemistry Accounts</i> , 2010, 127, 293-302.	1.4	11
92	Hif1 $\beta$ down-regulation is associated with transposition of great arteries in mice treated with a retinoic acid antagonist. <i>BMC Genomics</i> , 2010, 11, 497.	2.8	20
93	Structural and Dynamical Effects Induced by the Anticancer Drug Topotecan on the Human Topoisomerase I $\alpha$ DNA Complex. <i>PLoS ONE</i> , 2010, 5, e10934.	2.5	32
94	All-Atom Molecular Dynamics Simulations of the K <sup>+</sup> Channel Chimera Kv1.2/Kv2.1. <i>Biophysical Journal</i> , 2010, 98, 519a.	0.5	0
95	ADP/ATP mitochondrial carrier MD simulations to shed light on the structural $\alpha$ dynamical events that, after an additional mutation, restore the function in a pathological single mutant. <i>Journal of Structural Biology</i> , 2010, 172, 225-232.	2.8	10
96	Dynamic Investigation of Protein Metal Active Sites: Interplay of XANES and Molecular Dynamics Simulations. <i>Journal of the American Chemical Society</i> , 2010, 132, 14901-14909.	13.7	18
97	Assignment of UV $\alpha$ Vis Spectrum of (3,3 $\alpha$ )-Diindolylmethane, a <i>Leishmania donovani</i> Topoisomerase IB Inhibitor and a Candidate DNA Minor Groove Binder. <i>Journal of Physical Chemistry A</i> , 2010, 114, 7121-7126.	2.5	7
98	Solvent Effects on the Valence UV $\alpha$ Vis Absorption Spectra of Topotecan Anticancer Drug in Aqueous Solution at Room Temperature: A Nanoseconds Time-Scale TD-DFT/MD Computational Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 6770-6778.	2.6	13
99	A Tool for Sheep Product Quality: Custom Microarrays from Public Databases. <i>Nutrients</i> , 2009, 1, 235-250.	4.1	6
100	Structural-Dynamical Properties of the <i>Deinococcus Radiodurans</i> Topoisomerase IB in Absence of DNA: Correlation with the Human Enzyme. <i>Journal of Biomolecular Structure and Dynamics</i> , 2009, 27, 307-317.	3.5	30
101	Evidence of the crucial role of the linker domain on the catalytic activity of human topoisomerase I by experimental and simulative characterization of the Lys681Ala mutant. <i>Nucleic Acids Research</i> , 2009, 37, 6849-6858.	14.5	29
102	Archived HIV-1 minority variants detected by ultra-deep pyrosequencing in provirus may be fully replication competent. <i>Aids</i> , 2009, 23, 2541-2543.	2.2	17
103	A specific transcriptional response of yeast cells to camptothecin dependent on the Swi4 and Mbp1 factors. <i>European Journal of Pharmacology</i> , 2009, 603, 29-36.	3.5	8
104	Microarrays and high-throughput transcriptomic analysis in species with incomplete availability of genomic sequences. <i>New Biotechnology</i> , 2009, 25, 272-279.	4.4	30
105	Structural Investigation of Lanthanoid Coordination: a Combined XANES and Molecular Dynamics Study. <i>Inorganic Chemistry</i> , 2009, 48, 10239-10248.	4.0	51
106	Deciphering the Structural Properties That Confer Stability to a DNA Nanocage. <i>ACS Nano</i> , 2009, 3, 1813-1822.	14.6	25
107	Massively parallel pyrosequencing highlights minority variants in the HIV-1 env quasispecies deriving from lymphomonocyte sub-populations. <i>Retrovirology</i> , 2009, 6, 15.	2.0	89
108	Molecular Modelling Of BCRP (ABCG2) Multidrug Resistance Protein And Docking Of New Camptothecin Analogues. <i>Biophysical Journal</i> , 2009, 96, 599a.	0.5	0

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109	UV-Vis Spectra of the Anticancer Camptothecin Family Drugs in Aqueous Solution: Specific Spectroscopic Signatures Unraveled by a Combined Computational and Experimental Study. <i>Journal of Physical Chemistry B</i> , 2009, 113, 5369-5375.	2.6	42
110	Ion hydration in high-density water. <i>Journal of Physics: Conference Series</i> , 2009, 190, 012057.	0.4	9
111	Transcriptomic analysis of two sheep breeds during lactation, using a new custom microarray platform. <i>Italian Journal of Animal Science</i> , 2009, 8, 33-35.	1.9	2
112	Global Transcription Regulation by DNA Topoisomerase I in Exponentially Growing <i>Saccharomyces cerevisiae</i> Cells: Activation of Telomere-Proximal Genes by TOP1 Deletion. <i>Journal of Molecular Biology</i> , 2008, 377, 311-322.	4.2	34
113	A Coupled Molecular Dynamics and XANES Data Analysis Investigation of Aqueous Cadmium(II). <i>Journal of Physical Chemistry A</i> , 2008, 112, 11833-11841.	2.5	50
114	Structural and Dynamical Properties of the Hg <sup>2+</sup> Aqua Ion: A Molecular Dynamics Study. <i>Journal of Physical Chemistry B</i> , 2008, 112, 4694-4702.	2.6	48
115	Thr729 in human topoisomerase I modulates anti-cancer drug resistance by altering protein domain communications as suggested by molecular dynamics simulations. <i>Nucleic Acids Research</i> , 2008, 36, 5645-5651.	14.5	49
116	A single mutation in the 729 residue modulates human DNA topoisomerase I DNA binding and drug resistance. <i>Nucleic Acids Research</i> , 2008, 36, 5635-5644.	14.5	24
117	Integrated experimental and theoretical approach for the structural characterization of Hg <sup>2+</sup> aqueous solutions. <i>Journal of Chemical Physics</i> , 2008, 128, 084502.	3.0	50
118	Valproic Acid Induces Neuroendocrine Differentiation and UGT2B7 Up-Regulation in Human Prostate Carcinoma Cell Line. <i>Drug Metabolism and Disposition</i> , 2007, 35, 968-972.	3.3	40
119	The open state of human topoisomerase I as probed by molecular dynamics simulation. <i>Nucleic Acids Research</i> , 2007, 35, 3032-3038.	14.5	21
120	Evidence for Sevenfold Coordination in the First Solvation Shell of Hg(II) Aqua Ion. <i>Journal of the American Chemical Society</i> , 2007, 129, 5430-5436.	13.7	78
121	Dynamic changes in gene expression profiles of 22q11 and related orthologous genes during mouse development. <i>Gene</i> , 2007, 391, 91-102.	2.2	12
122	Effects of dutasteride on the expression of genes related to androgen metabolism and related pathway in human prostate cancer cell lines. <i>Investigational New Drugs</i> , 2007, 25, 491-497.	2.6	41
123	Role of flexibility and long range communication on the function of human topoisomerase I. <i>Italian Journal of Biochemistry</i> , 2007, 56, 110-4.	0.3	2
124	A Coupled Car-Parrinello Molecular Dynamics and EXAFS Data Analysis Investigation of Aqueous Co <sup>2+</sup> . <i>Journal of Physical Chemistry A</i> , 2006, 110, 13081-13088.	2.5	46
125	Theoretical modeling of the valence UV spectra of 1,2,3-triazine and uracil in solution. <i>Physical Chemistry Chemical Physics</i> , 2006, 8, 1385.	2.8	39
126	Detection of Second Hydration Shells in Ionic Solutions by XANES: Computed Spectra for Ni <sup>2+</sup> in Water Based on Molecular Dynamics. <i>Journal of the American Chemical Society</i> , 2006, 128, 1853-1858.	13.7	59

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127	Structural dynamics of the mitochondrial ADP/ATP carrier revealed by molecular dynamics simulation studies. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 65, 681-691.	2.6	29
128	Gene expression profile study in CFTR mutated bronchial cell lines. <i>Clinical and Experimental Medicine</i> , 2006, 6, 157-165.	3.6	8
129	The different cleavage DNA sequence specificity explains the camptothecin resistance of the human topoisomerase I Glu418Lys mutant. <i>Nucleic Acids Research</i> , 2006, 34, 5093-5100.	14.5	21
130	Quantitative analysis of XANES spectra of disordered systems based on molecular dynamics. <i>Journal of Synchrotron Radiation</i> , 2005, 12, 75-79.	2.4	16
131	Effect on DNA relaxation of the single Thr718Ala mutation in human topoisomerase I: a functional and molecular dynamics study. <i>Nucleic Acids Research</i> , 2005, 33, 3339-3350.	14.5	47
132	Computational Evidence for a Variable First Shell Coordination of the Cadmium(II) Ion in Aqueous Solution. <i>Journal of Physical Chemistry B</i> , 2005, 109, 9186-9193.	2.6	49
133	New Hints on the pH-Driven Tautomeric Equilibria of the Topotecan Anticancer Drug in Aqueous Solutions from an Integrated Spectroscopic and Quantum-Mechanical Approach. <i>Journal of the American Chemical Society</i> , 2005, 127, 15429-15436.	13.7	43
134	Experimental Evidence for a Variable First Coordination Shell of the Cadmium(II) Ion in Aqueous, Dimethyl Sulfoxide, and N,N-Dimethylpropyleneurea Solution. <i>Journal of Physical Chemistry B</i> , 2005, 109, 9178-9185.	2.6	53
135	Role of the Linker Domain and the 203-214 N-Terminal Residues in the Human Topoisomerase I DNA Complex Dynamics. <i>Biophysical Journal</i> , 2004, 87, 4087-4097.	0.5	25
136	Protein concerted motions in the DNA-human topoisomerase I complex. <i>Nucleic Acids Research</i> , 2003, 31, 1525-1535.	14.5	44
137	Single Mutation in the Linker Domain Confers Protein Flexibility and Camptothecin Resistance to Human Topoisomerase I. <i>Journal of Biological Chemistry</i> , 2003, 278, 43268-43275.	3.4	81
138	Hydrogen and Higher Shell Contributions in Zn <sup>2+</sup> , Ni <sup>2+</sup> , and Co <sup>2+</sup> Aqueous Solutions: An X-ray Absorption Fine Structure and Molecular Dynamics Study. <i>Journal of the American Chemical Society</i> , 2002, 124, 1958-1967.	13.7	175
139	Development and Validation of an Integrated Computational Approach for the Study of Ionic Species in Solution by Means of Effective Two-Body Potentials. The Case of Zn <sup>2+</sup> , Ni <sup>2+</sup> , and Co <sup>2+</sup> in Aqueous Solutions. <i>Journal of the American Chemical Society</i> , 2002, 124, 1968-1976.	13.7	92
140	Molecular Dynamics Simulation of the RNA Complex of a Double-Stranded RNA-Binding Domain Reveals Dynamic Features of the Intermolecular Interface and Its Hydration. <i>Biophysical Journal</i> , 2002, 83, 3542-3552.	0.5	27
141	Structure and Hydration of the DNA-Human Topoisomerase I Covalent Complex. <i>Biophysical Journal</i> , 2001, 81, 490-500.	0.5	26
142	On the Use of the Quasi-Gaussian Entropy Theory in Systems of Polyatomic Flexible Molecules. <i>Journal of Physical Chemistry B</i> , 2001, 105, 1834-1844.	2.6	8
143	The role of computer technology in applied computational chemical-physics. <i>Computer Physics Communications</i> , 2001, 139, 1-19.	7.5	5
144	Molecular dynamics simulations with constrained roto-translational motions: Theoretical basis and statistical mechanical consistency. <i>Journal of Chemical Physics</i> , 2000, 112, 9-23.	3.0	103

#	ARTICLE	IF	CITATIONS
145	Structure and Hydration of BamHI DNA Recognition Site: A Molecular Dynamics Investigation. <i>Biophysical Journal</i> , 2000, 79, 1263-1272.	0.5	23
146	Derivation of a general fluid equation of state based on the quasi-Gaussian entropy theory: application to the Lennard-Jones fluid. <i>Molecular Physics</i> , 1999, 96, 1469-1490.	1.7	16
147	Development of a parallel molecular dynamics code on SIMD computers: Algorithm for use of pair list criterion. <i>Journal of Computational Chemistry</i> , 1998, 19, 685-694.	3.3	4
148	The essential dynamics of Cu, Zn superoxide dismutase: suggestion of intersubunit communication. <i>Biophysical Journal</i> , 1997, 73, 1007-1018.	0.5	48
149	Elite Food Between the Late Middle Ages and Renaissance: Some Case Studies from Latium. <i>Environmental Archaeology</i> , 0, , 1-15.	1.2	2