Giorgio Colombo

List of Publications by Year in Descending Order

221 papers	6,447 citations	44 h-index	68 g-index
237 ext. papers	7,273 ext. citations	6 avg, IF	5.93 L-index

#	Paper	IF	Citations
221	Protein allostery and ligand design: Computational design meets experiments to discover novel chemical probes.. *Journal of Molecular Biology*, **2022**, 167468	6.5	2
220	Transcription factor protein interactomes reveal genetic determinants in heart disease.. *Cell*, **2022**,	56.2	3
219	Machine Learning of Allosteric Effects: The Analysis of Ligand-Induced Dynamics to Predict Functional Effects in TRAP1. *Journal of Physical Chemistry B*, **2021**, 125, 101-114	3.4	14
218	Bow to the enemy: How flexibility of host protein receptors can favor SARS-CoV-2. *Biophysical Journal*, **2021**, 120, 977-979	2.9	0
217	Honokiol Bis-Dichloroacetate Is a Selective Allosteric Inhibitor of the Mitochondrial Chaperone TRAP1. *Antioxidants and Redox Signaling*, **2021**, 34, 505-516	8.4	11
216	Machine Learning Prediction of Allosteric Drug Activity from Molecular Dynamics. *Journal of Physical Chemistry Letters*, **2021**, 12, 3724-3732	6.4	14
215	HIF1α-dependent induction of the mitochondrial chaperone TRAP1 regulates bioenergetic adaptations to hypoxia. *Cell Death and Disease*, **2021**, 12, 434	9.8	5
214	Atomistic Simulations of the Mechanisms of the Poorly Catalytic Mitochondrial Chaperone Trap1: Insights into the Effects of Structural Asymmetry on Reactivity. *ACS Catalysis*, **2021**, 11, 8605-8620	13.1	2
213	The molecular chaperone TRAP1 in cancer: From the basics of biology to pharmacological targeting. *Seminars in Cancer Biology*, **2021**, 76, 45-53	12.7	5
212	On the binding of naphthalene diimides to a human telomeric G-quadruplex multimer model. *International Journal of Biological Macromolecules*, **2021**, 166, 1320-1334	7.9	14
211	Visualizing the Dynamics of a Protein Folding Machinery: The Mechanism of Asymmetric ATP Processing in Hsp90 and its Implications for Client Remodelling. *Journal of Molecular Biology*, **2021**, 433, 166728	6.5	3
210	Disruption of protein phosphatase 1 complexes with the use of bioportides as a novel approach to target sperm motility. *Fertility and Sterility*, **2021**, 115, 348-362	4.8	3
209	Biocompatible graft copolymers from bacterial poly(γ-glutamic acid) and poly(lactic acid). *Polymer Chemistry*, **2021**, 12, 3784-3793	4.9	6
208	New perspectives in cancer drug development: computational advances with an eye to design. *RSC Medicinal Chemistry*, **2021**, 12, 1491-1502	3.5	4
207	Exploiting Folding and Degradation Machineries To Target Undruggable Proteins: What Can a Computational Approach Tell Us?. *ChemMedChem*, **2021**, 16, 1593-1599	3.7	1
206	The Binding Pocket at the Interface of Multimeric Telomere G-quadruplexes: Myth or Reality?. *Chemistry - A European Journal*, **2021**, 27, 11707-11720	4.8	1
205	Targeting the mitochondrial chaperone TRAP1: strategies and therapeutic perspectives. *Trends in Pharmacological Sciences*, **2021**, 42, 566-576	13.2	9

204	The tumor suppressor folliculin inhibits lactate dehydrogenase A and regulates the Warburg effect. *Nature Structural and Molecular Biology*, **2021**, 28, 662-670	17.6	4
203	Chemical Chaperones Modulate the Formation of Metabolite Assemblies. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	1
202	SARS-CoV-2 Spike Protein Mutations and Escape from Antibodies: A Computational Model of Epitope Loss in Variants of Concern. *Journal of Chemical Information and Modeling*, **2021**, 61, 4687-4700	6.1	10
201	Revealing Escherichia coli type II L-asparaginase active site flexible loop in its open, ligand-free conformation. *Scientific Reports*, **2021**, 11, 18885	4.9	1
200	Analysis of Hsp90 allosteric modulators interactome reveals a potential dual action mode involving mitochondrial MDH2. *Bioorganic Chemistry*, **2021**, 115, 105258	5.1	
199	Chemical Perturbation of Oncogenic Protein Folding: from the Prediction of Locally Unstable Structures to the Design of Disruptors of Hsp90-Client Interactions. *Chemistry - A European Journal*, **2020**, 26, 9459-9465	4.8	28
198	Mechanistic Model for the Hsp90-Driven Opening of Human Argonaute. *Journal of Chemical Information and Modeling*, **2020**, 60, 1469-1480	6.1	2
197	Dual Binding to Orthosteric and Allosteric Sites Enhances the Anticancer Activity of a TRAP1-Targeting Drug. *Journal of Medicinal Chemistry*, **2020**, 63, 2930-2940	8.3	10
196	Tryptophan scanning mutagenesis as a way to mimic the compound-bound state and probe the selectivity of allosteric inhibitors in cells. *Chemical Science*, **2020**, 11, 1892-1904	9.4	6
195	Design of Disruptors of the Hsp90-Cdc37 Interface. *Molecules*, **2020**, 25,	4.8	8
194	Frontispiece: Designing Molecular Spanners to Throw in the Protein Networks. *Chemistry - A European Journal*, **2020**, 26,	4.8	2
193	Molecular Dynamics Performance Evaluation with Modern Computer Architecture. *Lecture Notes in Computer Science*, **2020**, 322-329	0.9	
192	Designing Molecular Spanners to Throw in the Protein Networks. *Chemistry - A European Journal*, **2020**, 26, 4656-4670	4.8	22
191	Setup and Validation of a Reliable Docking Protocol for the Development of Neuroprotective Agents by Targeting the Sigma-1 Receptor (S1R). *International Journal of Molecular Sciences*, **2020**, 21,	6.3	2
190	Simple Model of Protein Energetics To Identify Ab Initio Folding Transitions from All-Atom MD Simulations of Proteins. *Journal of Chemical Theory and Computation*, **2020**, 16, 5960-5971	6.4	6
189	Dynamically Shaping Chaperones. Allosteric Modulators of HSP90 Family as Regulatory Tools of Cell Metabolism in Neoplastic Progression. *Frontiers in Oncology*, **2020**, 10, 1177	5.3	11
188	The Answer Lies in the Energy: How Simple Atomistic Molecular Dynamics Simulations May Hold the Key to Epitope Prediction on the Fully Glycosylated SARS-CoV-2 Spike Protein. *Journal of Physical Chemistry Letters*, **2020**, 11, 8084-8093	6.4	24
187	Rational Design of Allosteric and Selective Inhibitors of the Molecular Chaperone TRAP1. *Cell Reports*, **2020**, 31, 107531	10.6	32

186	Ligand Binding, Unbinding, and Allosteric Effects: Deciphering Small-Molecule Modulation of HSP90. *Journal of Chemical Theory and Computation*, **2019**, 15, 6368-6381	6.4	26
185	Computational Analysis of Dengue Virus Envelope Protein (E) Reveals an Epitope with Flavivirus Immunodiagnostic Potential in Peptide Microarrays. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	21
184	The Subtle Trade-Off between Evolutionary and Energetic Constraints in Protein-Protein Interactions. *Journal of Physical Chemistry Letters*, **2019**, 10, 1489-1497	6.4	16
183	Peptides for Infectious Diseases: From Probe Design to Diagnostic Microarrays. *Antibodies*, **2019**, 8,	7	12
182	Mechanisms of Metabolite Amyloid Formation: Computational Studies for Drug Design against Metabolic Disorders. *ACS Medicinal Chemistry Letters*, **2019**, 10, 666-670	4.3	4
181	Rational design of allosteric modulators of the aromatase enzyme: An unprecedented therapeutic strategy to fight breast cancer. *European Journal of Medicinal Chemistry*, **2019**, 168, 253-262	6.8	24
180	Allosteric Modulators of HSP90 and HSP70: Dynamics Meets Function through Structure-Based Drug Design. *Journal of Medicinal Chemistry*, **2019**, 62, 60-87	8.3	59
179	Impact of Mutations on NPAC Structural Dynamics: Mechanistic Insights from MD Simulations. *Journal of Chemical Information and Modeling*, **2019**, 59, 3927-3937	6.1	22
178	ADAMDEC1 Maintains a Growth Factor Signaling Loop in Cancer Stem Cells. *Cancer Discovery*, **2019**, 9, 1574-1589	24.4	28
177	The Importance of Detail: How Differences in Ligand Structures Determine Distinct Functional Responses in Integrin *Chemistry - A European Journal*, **2019**, 25, 5959-5970	4.8	6
176	The calcium-binding type III repeats domain of thrombospondin-2 binds to fibroblast growth factor 2 (FGF2). *Angiogenesis*, **2019**, 22, 133-144	10.6	24
175	The Structural Asymmetry of Mitochondrial Hsp90 (Trap1) Determines Fine Tuning of Functional Dynamics. *Journal of Chemical Theory and Computation*, **2018**, 14, 1033-1044	6.4	31
174	A Computational Assay of Estrogen Receptor Antagonists Reveals the Key Common Structural Traits of Drugs Effectively Fighting Refractory Breast Cancers. *Scientific Reports*, **2018**, 8, 649	4.9	44
173	The Interplay between Structural Stability and Plasticity Determines Mutation Profiles and Chaperone Dependence in Protein Kinases. *Journal of Chemical Theory and Computation*, **2018**, 14, 1059-1070	6.4	13
172	Chemo-enzymatic synthesis of (E)-2,3-diaryl-5-styryl-trans-2,3-dihydrobenzofuran-based scaffolds and their in vitro and in silico evaluation as a novel sub-family of potential allosteric modulators of the 90 kDa heat shock protein (Hsp90). *Organic and Biomolecular Chemistry*, **2018**, 16, 3741-3753	3.9	13
171	Enhancing Antibody Serodiagnosis Using a Controlled Peptide Coimmobilization Strategy. *ACS Infectious Diseases*, **2018**, 4, 998-1006	5.5	20
170	Are Amyloid Fibrils RNA-Traps? A Molecular Dynamics Perspective. *Frontiers in Molecular Biosciences*, **2018**, 5, 53	5.6	3
169	BPSL1626: Reverse and Structural Vaccinology Reveal a Novel Candidate for Vaccine Design against. *Antibodies*, **2018**, 7,	7	5

168	Expedient Access to 2-Benzazepines by Palladium-Catalyzed C-H Activation: Identification of a Unique Hsp90 Inhibitor Scaffold. *Chemistry - A European Journal*, **2018**, 24, 16516-16520	4.8	8
167	Understanding Allostery to Design New Drugs. *Methods and Principles in Medicinal Chemistry*, **2018**, 281-300		
166	How the Ligand-Induced Reorganization of Protein Internal Energies Is Coupled to Conformational Events. *Journal of Chemical Theory and Computation*, **2018**, 14, 5992-6001	6.4	7
165	A Local Allosteric Network in Heat Shock Protein 70 (Hsp70) Links Inhibitor Binding to Enzyme Activity and Distal Protein-Protein Interactions. *ACS Chemical Biology*, **2018**, 13, 3142-3152	4.9	10
164	Targeting Difficult Protein-Protein Interactions with Plain and General Computational Approaches. *Molecules*, **2018**, 23,	4.8	4
163	Understanding Complex Mechanisms of Enzyme Reactivity: The Case of Limonene-1,2-Epoxide Hydrolases. *ACS Catalysis*, **2018**, 8, 5698-5707	13.1	17
162	Design of Allosteric Stimulators of the Hsp90 ATPase as New Anticancer Leads. *Chemistry - A European Journal*, **2017**, 23, 5188-5192	4.8	27
161	Protein design: from computer models to artificial intelligence. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2017**, 7, e1318	7.9	15
160	Unraveling Energy and Dynamics Determinants to Interpret Protein Functional Plasticity: The Limonene-1,2-epoxide-hydrolase Case Study. *Journal of Chemical Information and Modeling*, **2017**, 57, 717-725	6.1	2
159	SAGE: A Fast Computational Tool for Linear Epitope Grafting onto a Foreign Protein Scaffold. *Journal of Chemical Information and Modeling*, **2017**, 57, 6-10	6.1	6
158	Crystal Structure of the DFNKF Segment of Human Calcitonin Unveils Aromatic Interactions between Phenylalanines. *Chemistry - A European Journal*, **2017**, 23, 1985-1985	4.8	1
157	Role of Terahertz (THz) Fluctuations in the Allosteric Properties of the PDZ Domains. *Journal of Physical Chemistry B*, **2017**, 121, 10200-10208	3.4	3
156	Chaperones rescue the energetic landscape of mutant CFTR at single molecule and in cell. *Nature Communications*, **2017**, 8, 398	17.4	42
155	Structure and Computation in Immunoreagent Design: From Diagnostics to Vaccines. *Trends in Biotechnology*, **2017**, 35, 1208-1220	15.1	14
154	Designing Probes for Immunodiagnostics: Structural Insights into an Epitope Targeting Burkholderia Infections. *ACS Infectious Diseases*, **2017**, 3, 736-743	5.5	4
153	Structural Vaccinology for Melioidosis Vaccine Design and Immunodiagnostics. *Current Tropical Medicine Reports*, **2017**, 4, 103-110	5	1
152	A protease-resistant Escherichia coli asparaginase with outstanding stability and enhanced anti-leukaemic activity in vitro. *Scientific Reports*, **2017**, 7, 14479	4.9	22
151	Crystal Structure of the DFNKF Segment of Human Calcitonin Unveils Aromatic Interactions between Phenylalanines. *Chemistry - A European Journal*, **2017**, 23, 2051-2058	4.8	22

150	The Chaperone TRAP1 As a Modulator of the Mitochondrial Adaptations in Cancer Cells. *Frontiers in Oncology*, **2017**, 7, 58	5.3	77
149	High Affinity vs. Native Fibronectin in the Modulation of 4β1 Integrin Conformational Dynamics: Insights from Computational Analyses and Implications for Molecular Design. *PLoS Computational Biology*, **2017**, 13, e1005334	5	10
148	Novel PARP-1 Inhibitor Scaffolds Disclosed by a Dynamic Structure-Based Pharmacophore Approach. *PLoS ONE*, **2017**, 12, e0170846	3.7	10
147	Molecular Dynamics Simulations Reveal the Mechanisms of Allosteric Activation of Hsp90 by Designed Ligands. *Scientific Reports*, **2016**, 6, 23830	4.9	60
146	Allosteric Regulation Points Control the Conformational Dynamics of the Molecular Chaperone Hsp90. *Journal of Molecular Biology*, **2016**, 428, 4559-4571	6.5	45
145	An atomistic view of Hsp70 allosteric crosstalk: from the nucleotide to the substrate binding domain and back. *Scientific Reports*, **2016**, 6, 23474	4.9	24
144	Evolving serodiagnostics by rationally designed peptide arrays: the Burkholderia paradigm in Cystic Fibrosis. *Scientific Reports*, **2016**, 6, 32873	4.9	19
143	Integrating computational and chemical biology tools in the discovery of antiangiogenic small molecule ligands of FGF2 derived from endogenous inhibitors. *Scientific Reports*, **2016**, 6, 23432	4.9	18
142	Balancing Accuracy and Cost of Confinement Simulations by Interpolation and Extrapolation of Confinement Energies. *Journal of Chemical Theory and Computation*, **2016**, 12, 2779-89	6.4	5
141	Assessment of Mutational Effects on Peptide Stability through Confinement Simulations. *Journal of Physical Chemistry Letters*, **2016**, 7, 126-30	6.4	9
140	Flexible vs Rigid Epitope Conformations for Diagnostic- and Vaccine-Oriented Applications: Novel Insights from the Burkholderia pseudomallei BPSL2765 Pal3 Epitope. *ACS Infectious Diseases*, **2016**, 2, 221-30	5.5	19
139	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, 1112-24	3.2	16
138	DNA Polymerase Conformational Dynamics and the Role of Fidelity-Conferring Residues: Insights from Computational Simulations. *Frontiers in Molecular Biosciences*, **2016**, 3, 20	5.6	8
137	Synthesis of Functionalized 2-(4-Hydroxyphenyl)-3-methylbenzofuran Allosteric Modulators of Hsp90 Activity. *European Journal of Organic Chemistry*, **2016**, 2016, 3349-3364	3.2	15
136	Surface energetics and protein-protein interactions: analysis and mechanistic implications. *Scientific Reports*, **2016**, 6, 24035	4.9	10
135	Structure-based approach for identification of novel phenylboronic acids as serine-β-lactamase inhibitors. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 851-861	4.2	8
134	Screening Complex Biological Samples with Peptide Microarrays: The Favorable Impact of Probe Orientation via Chemoselective Immobilization Strategies on Clickable Polymeric Coatings. *Bioconjugate Chemistry*, **2016**, 27, 2669-2677	6.3	31
133	Structural Stability and Flexibility Direct the Selection of Activating Mutations in Epidermal Growth Factor Receptor Kinase. *Journal of Chemical Information and Modeling*, **2015**, 55, 1377-87	6.1	20

132	From crystal structure to in silico epitope discovery in the Burkholderia pseudomallei flagellar hook-associated protein FlgK. *FEBS Journal*, **2015**, 282, 1319-33	5.7	30
131	Long-Pentraxin 3 Derivative as a Small-Molecule FGF Trap for Cancer Therapy. *Cancer Cell*, **2015**, 28, 225-38	24.3	80
130	Structure-based design of a B cell antigen from B. pseudomallei. *ACS Chemical Biology*, **2015**, 10, 803-12	4.9	11
129	Design, synthesis and biological evaluation of biphenylamide derivatives as Hsp90 C-terminal inhibitors. *European Journal of Medicinal Chemistry*, **2015**, 89, 442-66	6.8	37
128	Activation of Hsp90 Enzymatic Activity and Conformational Dynamics through Rationally Designed Allosteric Ligands. *Chemistry - A European Journal*, **2015**, 21, 13598-608	4.8	54
127	Long range Trp-Trp interaction initiates the folding pathway of a pro-angiogenic hairpin peptide. *Scientific Reports*, **2015**, 5, 16651	4.9	6
126	Sequence- and Structure-Based Immunoreactive Epitope Discovery for Burkholderia pseudomallei Flagellin. *PLoS Neglected Tropical Diseases*, **2015**, 9, e0003917	4.8	27
125	Covalent docking of selected boron-based serine beta-lactamase inhibitors. *Journal of Computer-Aided Molecular Design*, **2015**, 29, 441-50	4.2	18
124	The Dynamics of Drug Discovery. *Current Topics in Medicinal Chemistry*, **2015**, 15, 2043-2055	3	20
123	Prediction of Antigenic B and T Cell Epitopes via Energy Decomposition Analysis: Description of the Web-Based Prediction Tool BEPPE. *Methods in Molecular Biology*, **2015**, 1348, 13-22	1.4	5
122	The Dynamics of Drug Discovery. *Current Topics in Medicinal Chemistry*, **2015**, 15, 2043-55	3	7
121	Mechanisms of Differential Allosteric Modulation in Homologous Proteins: Insights from the Analysis of Internal Dynamics and Energetics of PDZ Domains. *Journal of Chemical Theory and Computation*, **2014**, 10, 5677-89	6.4	31
120	Inactivation of TEM-1 by avibactam (NXL-104): insights from quantum mechanics/molecular mechanics metadynamics simulations. *Biochemistry*, **2014**, 53, 5174-85	3.2	26
119	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, 2856-68	6.1	33
118	Identification of a new scaffold for hsp90 C-terminal inhibition. *ACS Medicinal Chemistry Letters*, **2014**, 5, 84-8	4.3	28
117	Exploiting conformational dynamics in drug discovery: design of C-terminal inhibitors of Hsp90 with improved activities. *Journal of Chemical Information and Modeling*, **2014**, 54, 195-208	6.1	46
116	Investigating the dynamic aspects of drug-protein recognition through a combination of MD and NMR analyses: implications for the development of protein-protein interaction inhibitors. *PLoS ONE* , **2014**, 9, e97153	3.7	10
115	The five-to-six-coordination transition of ferric human serum heme-albumin is allosterically-modulated by ibuprofen and warfarin: a combined XAS and MD study. *PLoS ONE*, **2014** , 9, e104231	3.7	24

114	Dimerization capacities of FGF2 purified with or without heparin-affinity chromatography. *PLoS ONE*, **2014**, 9, e110055	3.7	8
113	Investigating allostery in molecular recognition: insights from a computational study of multiple antibody-antigen complexes. *Journal of Physical Chemistry B*, **2013**, 117, 535-52	3.4	15
112	Exploiting the Burkholderia pseudomallei acute phase antigen BPSL2765 for structure-based epitope discovery/design in structural vaccinology. *Chemistry and Biology*, **2013**, 20, 1147-56		41
111	Energetic and dynamic aspects of the affinity maturation process: characterizing improved variants from the bevacizumab antibody with molecular simulations. *Journal of Chemical Information and Modeling*, **2013**, 53, 2937-50	6.1	17
110	Rational epitope design for protein targeting. *ACS Chemical Biology*, **2013**, 8, 397-404	4.9	30
109	A structure-based strategy for epitope discovery in Burkholderia pseudomallei OppA antigen. *Structure*, **2013**, 21, 167-175	5.2	37
108	Inhibiting Peptide and Protein Self-Aggregation: What Can Simulations Tell Us?. *Modecular Medicine and Medicinal*, **2013**, 401-437		
107	Peptides for immunological purposes: design, strategies and applications. *Amino Acids*, **2013**, 45, 257-68	3.5	41
106	A Hamiltonian replica exchange molecular dynamics (MD) method for the study of folding, based on the analysis of the stabilization determinants of proteins. *International Journal of Molecular Sciences*, **2013**, 14, 12157-69	6.3	17
105	3D-QSAR Assisted Design, Synthesis and Evaluation of Novobiocin Analogues. *ACS Medicinal Chemistry Letters*, **2012**, 4, 57-62	4.3	21
104	Ligand selection from the analysis of protein conformational substates: new leads targeting the N-terminal domain of Hsp90. *RSC Advances*, **2012**, 2, 4268	3.7	7
103	Identification of domains in protein structures from the analysis of intramolecular interactions. *Journal of Physical Chemistry B*, **2012**, 116, 3331-43	3.4	34
102	Corresponding functional dynamics across the Hsp90 Chaperone family: insights from a multiscale analysis of MD simulations. *PLoS Computational Biology*, **2012**, 8, e1002433	5	82
101	Molecular mechanism of allosteric communication in Hsp70 revealed by molecular dynamics simulations. *PLoS Computational Biology*, **2012**, 8, e1002844	5	43
100	Pharmacological enhancement of □glucosidase by the allosteric chaperone N-acetylcysteine. *Molecular Therapy*, **2012**, 20, 2201-11	11.7	72
99	Molecular dynamics simulations of hsp90 with an eye to inhibitor design. *Pharmaceuticals*, **2012**, 5, 944-62	3.2	1
98	Direct and allosteric inhibition of the FGF2/HSPGs/FGFR1 ternary complex formation by an antiangiogenic, thrombospondin-1-mimic small molecule. *PLoS ONE*, **2012**, 7, e36990	3.7	33
97	Dynamic diagnosis of familial prion diseases supports the □-□ loop as a universal interference target. *PLoS ONE*, **2011**, 6, e19093	3.7	51

96	HMGB1-carbenoxolone interactions: dynamics insights from combined nuclear magnetic resonance and molecular dynamics. *Chemistry - an Asian Journal*, **2011**, 6, 1171-80	4.5	6
95	A multiscale approach to characterize the early aggregation steps of the amyloid-forming peptide GNNQQNY from the yeast prion sup-35. *PLoS Computational Biology*, **2011**, 7, e1002051	5	68
94	Combined in silico and experimental approach for drug design: the binding mode of peptidic and non-peptidic inhibitors to hsp90 N-terminal domain. *Chemical Biology and Drug Design*, **2010**, 76, 382-91	2.9	10
93	Non-peptidic thrombospondin-1 mimics as fibroblast growth factor-2 inhibitors: an integrated strategy for the development of new antiangiogenic compounds. *Journal of Biological Chemistry*, **2010**, 285, 8733-42	5.4	61
92	Exploiting antigenic diversity for vaccine design: the chlamydia ArtJ paradigm. *Journal of Biological Chemistry*, **2010**, 285, 30126-38	5.4	39
91	Molecular recognition and drug-lead identification: what can molecular simulations tell us?. *Current Medicinal Chemistry*, **2010**, 17, 25-41	4.3	31
90	Computational study of the resistance shown by the subtype B/HIV-1 protease to currently known inhibitors. *Biochemistry*, **2010**, 49, 4283-95	3.2	18
89	Predicting interaction sites from the energetics of isolated proteins: a new approach to epitope mapping. *Biophysical Journal*, **2010**, 98, 1966-75	2.9	62
88	Dynamics-Based Discovery of Allosteric Inhibitors: Selection of New Ligands for the C-terminal Domain of Hsp90. *Journal of Chemical Theory and Computation*, **2010**, 6, 2978-89	6.4	70
87	Protein Dynamics and Drug Design: The Role of Molecular Simulations **2010**, 340-385		
86	Swe1Wee1-dependent tyrosine phosphorylation of Hsp90 regulates distinct facets of chaperone function. *Molecular Cell*, **2010**, 37, 333-43	17.6	143
85	The structural intolerance of the PrP alpha-fold for polar substitution of the helix-3 methionines. *Cellular and Molecular Life Sciences*, **2010**, 67, 2825-38	10.3	14
84	Structural analysis of a helical peptide unfolding pathway. *Chemistry - A European Journal*, **2010**, 16, 5400-7	4.8	23
83	Selecting sequences that fold into a defined 3D structure: A new approach for protein design based on molecular dynamics and energetics. *Biophysical Chemistry*, **2010**, 146, 76-84	3.5	14
82	Investigating dynamic and energetic determinants of protein nucleic acid recognition: analysis of the zinc finger zif268-DNA complexes. *BMC Structural Biology*, **2010**, 10, 42	2.7	13
81	Targeting tumor angiogenesis with TSP-1-based compounds: rational design of antiangiogenic mimetics of endogenous inhibitors. *Oncotarget*, **2010**, 1, 662-673	3.3	53
80	Targeting tumor angiogenesis with TSP-1-based compounds: rational design of antiangiogenic mimetics of endogenous inhibitors. *Oncotarget*, **2010**, 1, 662-73	3.3	33
79	Structure and sequence determinants of aggregation investigated with molecular dynamics. *Frontiers in Bioscience - Landmark*, **2009**, 14, 523-39	2.8	5

78	Why is a protective antigen protective?. *Hum Vaccin*, **2009**, 5, 872-5		4
77	Structural and computational biology of the molecular chaperone Hsp90: from understanding molecular mechanisms to computer-based inhibitor design. *Current Topics in Medicinal Chemistry*, **2009**, 9, 1369-85	3	22
76	Modeling signal propagation mechanisms and ligand-based conformational dynamics of the Hsp90 molecular chaperone full-length dimer. *PLoS Computational Biology*, **2009**, 5, e1000323	5	125
75	2?-O-Alkyl Derivatives and 5?-Analogues of 5-Aminoimidazole-4-carboxamide-1-□D-ribofuranoside (AICAR) as Potential Hsp90 Inhibitors. *European Journal of Organic Chemistry*, **2009**, 2009, 5913-5919	3.2	11
74	An efficient steroid pharmacophore-based strategy to identify new aromatase inhibitors. *European Journal of Medicinal Chemistry*, **2009**, 44, 4121-7	6.8	36
73	Fast three dimensional pharmacophore virtual screening of new potent non-steroid aromatase inhibitors. *Journal of Medicinal Chemistry*, **2009**, 52, 143-50	8.3	49
72	Combinatorial drug design targeting multiple cancer signaling networks controlled by mitochondrial Hsp90. *Journal of Clinical Investigation*, **2009**, 119, 454-64	15.9	168
71	Methionine sulfoxides on prion protein Helix-3 switch on the alpha-fold destabilization required for conversion. *PLoS ONE*, **2009**, 4, e4296	3.7	49
70	Molecular simulations of peptides: a useful tool for the development of new drugs and for the study of molecular recognition. *Methods in Molecular Biology*, **2009**, 570, 77-153	1.4	6
69	Investigating the mechanism of peptide aggregation: insights from mixed monte carlo-molecular dynamics simulations. *Biophysical Journal*, **2008**, 94, 4414-26	2.9	44
68	Biochemical and computational insights into the anti-aromatase activity of natural catechol estrogens. *Journal of Steroid Biochemistry and Molecular Biology*, **2008**, 110, 10-7	5.1	8
67	A molecular dynamics study of the interaction of D-peptide amyloid inhibitors with their target sequence reveals a potential inhibitory pharmacophore conformation. *Journal of Molecular Biology*, **2008**, 383, 266-80	6.5	14
66	Understanding ligand-based modulation of the Hsp90 molecular chaperone dynamics at atomic resolution. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 7976-81	11.5	60
65	Two amino acid substitutions within the first external loop of CCR5 induce human immunodeficiency virus-blocking antibodies in mice and chickens. *Journal of Virology*, **2008**, 82, 4125-34	6.6	19
64	Molecular dynamics simulations of proteins and peptides: from folding to drug design. *Current Protein and Peptide Science*, **2008**, 9, 181-96	2.8	24
63	Computational studies of the structure, dynamics and native content of amyloid-like fibrils of ribonuclease A. *Proteins: Structure, Function and Bioinformatics*, **2008**, 70, 863-72	4.2	18
62	Relationship between energy distribution and fold stability: Insights from molecular dynamics simulations of native and mutant proteins. *Proteins: Structure, Function and Bioinformatics*, **2008**, 72, 660-72	4.2	45
61	Structural determinants of the unusual helix stability of a de novo engineered vascular endothelial growth factor (VEGF) mimicking peptide. *Chemistry - A European Journal*, **2008**, 14, 4164-6	4.8	34

60	Molecular simulation of multistate peptide dynamics: a comparison between microsecond timescale sampling and multiple shorter trajectories. *Journal of Computational Chemistry*, **2008**, 29, 1740-52	3.5	47
59	Combining computational and biochemical studies for a rationale on the anti-aromatase activity of natural polyphenols. *ChemMedChem*, **2007**, 2, 1750-62	3.7	28
58	Peptide self-assembly at the nanoscale: a challenging target for computational and experimental biotechnology. *Trends in Biotechnology*, **2007**, 25, 211-8	15.1	117
57	The molecular dynamics of assembly of the ubiquitous aortic medial amyloidal medin fragment. *Journal of Molecular Graphics and Modelling*, **2007**, 25, 903-11	2.8	5
56	Anharmonicity and self-similarity of the free energy landscape of protein G. *Physical Review Letters*, **2007**, 98, 048102	7.4	43
55	Protein Folding Simulations: Combining Coarse-grained Models and All-atom Molecular Dynamics. *Theoretical Chemistry Accounts*, **2006**, 116, 75-86	1.9	16
54	Assessing the influence of electrostatic schemes on molecular dynamics simulations of secondary structure forming peptides. *Journal of Physics Condensed Matter*, **2006**, 18, S329-S345	1.8	18
53	Antileukemic activity of shepherdin and molecular diversity of hsp90 inhibitors. *Journal of the National Cancer Institute*, **2006**, 98, 1068-77	9.7	80
52	Human and chicken antibodies to CCR5-ECL1 block mucosal and systemic HIV infection. *Retrovirology*, **2006**, 3, 1	3.6	78
51	Small-molecule targeting of heat shock protein 90 chaperone function: rational identification of a new anticancer lead. *Journal of Medicinal Chemistry*, **2006**, 49, 7721-30	8.3	79
50	Immunogenic and structural properties of the Asn-Gly-Arg (NGR) tumor neovasculature-homing motif. *Molecular Immunology*, **2006**, 43, 1509-18	4.3	46
49	Similar folds with different stabilization mechanisms: the cases of Prion and Doppel proteins. *BMC Structural Biology*, **2006**, 6, 17	2.7	17
48	Modeling enzymatic processes: A molecular simulation analysis of the origins of regioselectivity. *Chemical Physics Letters*, **2006**, 418, 373-376	2.5	9
47	Misfolding of the amyloid beta-protein: a molecular dynamics study. *Proteins: Structure, Function and Bioinformatics*, **2006**, 62, 183-92	4.2	45
46	The determinants of stability in the human prion protein: insights into folding and misfolding from the analysis of the change in the stabilization energy distribution in different conditions. *Proteins: Structure, Function and Bioinformatics*, **2006**, 62, 698-707	4.2	31
45	Sequence dependence of amyloid fibril formation: insights from molecular dynamics simulations. *Journal of Molecular Biology*, **2005**, 349, 583-96	6.5	83
44	Mechanism of helix nucleation and propagation: microscopic view from microsecond time scale MD simulations. *Journal of Physical Chemistry B*, **2005**, 109, 20064-7	3.4	33
43	Study of the Villin headpiece folding dynamics by combining coarse-grained Monte Carlo evolution and all-atom molecular dynamics. *Proteins: Structure, Function and Bioinformatics*, **2005**, 58, 459-71	4.2	52

42	A dynamic perspective on the molecular recognition of chitooligosaccharide ligands by hevein domains. *Carbohydrate Research*, **2005**, 340, 1039-49	2.9	11
41	Effect of hexafluoroisopropanol alcohol on the structure of melittin: a molecular dynamics simulation study. *Protein Science*, **2005**, 14, 2582-9	6.3	65
40	Rational design of shepherdin, a novel anticancer agent. *Cancer Cell*, **2005**, 7, 457-68	24.3	275
39	A decoy set for the thermostable subdomain from chicken villin headpiece, comparison of different free energy estimators. *BMC Bioinformatics*, **2005**, 6, 301	3.6	14
38	Structure elucidation and 3D solution conformation of the antibiotic enduracidin determined by NMR spectroscopy and molecular dynamics. *Magnetic Resonance in Chemistry*, **2005**, 43, 603-10	2.1	19
37	Molecular dynamics simulation of the aggregation of the core-recognition motif of the islet amyloid polypeptide in explicit water. *Proteins: Structure, Function and Bioinformatics*, **2005**, 59, 519-27	4.2	43
36	Determinants of protein stability and folding: comparative analysis of beta-lactoglobulins and liver basic fatty acid binding protein. *Proteins: Structure, Function and Bioinformatics*, **2005**, 61, 366-76	4.2	20
35	Folding and mis-folding of peptides and proteins: insights from molecular simulations. *Mini-Reviews in Medicinal Chemistry*, **2005**, 5, 353-9	3.2	7
34	Antileukemic Activity of Shepherdin, a Novel Targeted Inhibitor of the Survivin-Hsp90 Complex.. *Blood*, **2005**, 106, 242-242	2.2	1
33	Thermodynamics of beta-amyloid fibril formation. *Journal of Chemical Physics*, **2004**, 120, 8307-17	3.9	26
32	Understanding the determinants of stability and folding of small globular proteins from their energetics. *Protein Science*, **2004**, 13, 113-24	6.3	70
31	The influence of simulation conditions in molecular dynamics investigations of model β-sheet peptides. *Theoretical Chemistry Accounts*, **2004**, 112, 145	1.9	18
30	Beta-hairpin conformation of fibrillogenic peptides: structure and alpha-beta transition mechanism revealed by molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 198-204	4.2	78
29	Characterization of the conformational space of a triple-stranded beta-sheet forming peptide with molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2004**, 57, 734-46	4.2	6
28	Remote control of enzyme selectivity: the case of stevioside and steviolbioside. *Tetrahedron*, **2004**, 60, 741-746	2.4	11
27	Modeling the alpha-helix to beta-hairpin transition mechanism and the formation of oligomeric aggregates of the fibrillogenic peptide Abeta(12-28): insights from all-atom molecular dynamics simulations. *Journal of Molecular Graphics and Modelling*, **2004**, 23, 263-73	2.8	25
26	Toward the understanding of the structure and dynamics of protein-carbohydrate interactions: molecular dynamics studies of the complexes between hevein and oligosaccharidic ligands. *Carbohydrate Research*, **2004**, 339, 985-94	2.9	23
25	All-Atom Folding Simulations of the Villin Headpiece from Stochastically Selected Coarse-Grained Structures. *Journal of Physical Chemistry B*, **2004**, 108, 12267-12270	3.4	36

24	Synthesis, structure and conformation of partially-modified retro- and retro-inverso psi[NHCH(CF3)]Gly peptides. *Chemistry - A European Journal*, **2003**, 9, 4510-22	4.8	70
23	Interplay between hydrophobic cluster and loop propensity in beta-hairpin formation: a mechanistic study. *Protein Science*, **2003**, 12, 538-50	6.3	31
22	Structure determination and dynamics of peptides overlapping the catalytic hairpin of the Ras-specific GEF Cdc25(Mm). *Biochemistry*, **2003**, 42, 12154-62	3.2	6
21	Simulation of MscL gating in a bilayer under stress. *Biophysical Journal*, **2003**, 84, 2331-7	2.9	67
20	Folding and stability of the three-stranded beta-sheet peptide Betanova: insights from molecular dynamics simulations. *Proteins: Structure, Function and Bioinformatics*, **2002**, 46, 380-92	4.2	45
19	Structure-activity relationships of linear and cyclic peptides containing the NGR tumor-homing motif. *Journal of Biological Chemistry*, **2002**, 277, 47891-7	5.4	144
18	Mechanism by which 2,2,2-trifluoroethanol/water mixtures stabilize secondary-structure formation in peptides: a molecular dynamics study. *Proceedings of the National Academy of Sciences of the United States of America*, **2002**, 99, 12179-84	11.5	406
17	Probing the hirudin-thrombin interaction by incorporation of noncoded amino acids and molecular dynamics simulation. *Biochemistry*, **2002**, 41, 13556-69	3.2	23
16	Modeling enzyme reactivity in organic solvents and water through computer simulations. *Journal of Biotechnology*, **2002**, 96, 23-33	3.7	21
15	□ -Adrenergic receptor ligands: insight into structure□ctivity relationships using Monte-Carlo conformational analysis in water. *Tetrahedron*, **2001**, 57, 1849-1855	2.4	4
14	Simulation of carbohydrate-protein interactions: computer-aided design of a second generation GM1 mimic. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 117-28	4.2	8
13	Optimization of Enzymatic Enantiomeric Resolutions Through Solvent Selection **2001**, 319-324		
12	Coupling high enzyme activity and stability: a challenging target. *Trends in Biotechnology*, **2000**, 18, 401	15.1	6
11	Modelling of Enzyme Properties in Organic Solvents. *Monatshefte F□ Chemie*, **2000**, 131, 527-547	1.4	18
10	Modelling the enantioselectivity of subtilisin in water and organic solvents: insights from molecular dynamics and quantum mechanical/molecular mechanical studies. *Chemical Communications*, **2000**, 559-560	5.8	6
9	Modelling of Enzyme Properties in Organic Solvents **2000**, 1-21		1
8	Rationalization of the Enantioselectivity of Subtilisin in DMF. *Journal of the American Chemical Society*, **1999**, 121, 3486-3493	16.4	42
7	Stability and Activity of Mesophilic Subtilisin E and Its Thermophilic Homolog: Insights from Molecular Dynamics Simulations. *Journal of the American Chemical Society*, **1999**, 121, 6895-6903	16.4	63

6	Solvent Dynamics and Mechanism of Proton Transfer in Human Carbonic Anhydrase II. *Journal of the American Chemical Society*, **1999**, 121, 2290-2302	16.4	107
5	Application of structure-based thermodynamic calculations to the rationalization of the enantioselectivity of subtilisin in organic solvents. *Tetrahedron: Asymmetry*, **1998**, 9, 1205-1214		25
4	Enantioselective mukaiyama-michael reactions of 2-carbomethoxy cyclopentenone catalyzed by chiral bis(Oxazoline)-Cu(II) complexes. *Tetrahedron Letters*, **1996**, 37, 8921-8924	2	81
3	The answer lies in the energy: how simple atomistic molecular dynamics simulations may hold the key to epitope prediction on the fully glycosylated SARS-CoV-2 spike protein		1
2	Differential Antibody Recognition by Novel SARS-CoV-2 and SARS-CoV Spike Protein Receptor Binding Domains: Mechanistic Insights and Implications for the Design of Diagnostics and Therapeutics		2
1	ADAMDEC1 maintains a novel growth factor signaling loop in cancer stem cells		3