Giorgio Colombo

List of Publications by Citations

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	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
220	Rational design of shepherdin, a novel anticancer agent. *Cancer Cell*, **2005**, 7, 457-68	24.3	275
219	Combinatorial drug design targeting multiple cancer signaling networks controlled by mitochondrial Hsp90. *Journal of Clinical Investigation*, **2009**, 119, 454-64	15.9	168
218	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
217	Swe1Wee1-dependent tyrosine phosphorylation of Hsp90 regulates distinct facets of chaperone function. *Molecular Cell*, **2010**, 37, 333-43	17.6	143
216	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
215	Peptide self-assembly at the nanoscale: a challenging target for computational and experimental biotechnology. *Trends in Biotechnology*, **2007**, 25, 211-8	15.1	117
214	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
213	Sequence dependence of amyloid fibril formation: insights from molecular dynamics simulations. *Journal of Molecular Biology*, **2005**, 349, 583-96	6.5	83
212	Corresponding functional dynamics across the Hsp90 Chaperone family: insights from a multiscale analysis of MD simulations. *PLoS Computational Biology*, **2012**, 8, e1002433	5	82
211	Enantioselective mukaiyama-michael reactions of 2-carbomethoxy cyclopentenone catalyzed by chiral bis(Oxazoline)-Cu(II) complexes. *Tetrahedron Letters*, **1996**, 37, 8921-8924	2	81
210	Long-Pentraxin 3 Derivative as a Small-Molecule FGF Trap for Cancer Therapy. *Cancer Cell*, **2015**, 28, 225-39	24.3	80
209	Antileukemic activity of shepherdin and molecular diversity of hsp90 inhibitors. *Journal of the National Cancer Institute*, **2006**, 98, 1068-77	9.7	80
208	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
207	Human and chicken antibodies to CCR5-ECL1 block mucosal and systemic HIV infection. *Retrovirology*, **2006**, 3, 1	3.6	78
206	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
205	The Chaperone TRAP1 As a Modulator of the Mitochondrial Adaptations in Cancer Cells. *Frontiers in Oncology*, **2017**, 7, 58	5.3	77

204	Pharmacological enhancement of □glucosidase by the allosteric chaperone N-acetylcysteine. *Molecular Therapy*, **2012**, 20, 2201-11	11.7	72
203	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
202	Understanding the determinants of stability and folding of small globular proteins from their energetics. *Protein Science*, **2004**, 13, 113-24	6.3	70
201	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
200	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
199	Simulation of MscL gating in a bilayer under stress. *Biophysical Journal*, **2003**, 84, 2331-7	2.9	67
198	Effect of hexafluoroisopropanol alcohol on the structure of melittin: a molecular dynamics simulation study. *Protein Science*, **2005**, 14, 2582-9	6.3	65
197	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
196	Predicting interaction sites from the energetics of isolated proteins: a new approach to epitope mapping. *Biophysical Journal*, **2010**, 98, 1966-75	2.9	62
195	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
194	Molecular Dynamics Simulations Reveal the Mechanisms of Allosteric Activation of Hsp90 by Designed Ligands. *Scientific Reports*, **2016**, 6, 23830	4.9	60
193	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
192	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
191	Activation of Hsp90 Enzymatic Activity and Conformational Dynamics through Rationally Designed Allosteric Ligands. *Chemistry - A European Journal*, **2015**, 21, 13598-608	4.8	54
190	Targeting tumor angiogenesis with TSP-1-based compounds: rational design of antiangiogenic mimetics of endogenous inhibitors. *Oncotarget*, **2010**, 1, 662-673	3.3	53
189	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
188	Dynamic diagnosis of familial prion diseases supports the □-□ loop as a universal interference target. *PLoS ONE*, **2011**, 6, e19093	3.7	51
187	Fast three dimensional pharmacophore virtual screening of new potent non-steroid aromatase inhibitors. *Journal of Medicinal Chemistry*, **2009**, 52, 143-50	8.3	49

186	Methionine sulfoxides on prion protein Helix-3 switch on the alpha-fold destabilization required for conversion. *PLoS ONE*, **2009**, 4, e4296	3.7	49
185	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
184	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
183	Immunogenic and structural properties of the Asn-Gly-Arg (NGR) tumor neovasculature-homing motif. *Molecular Immunology*, **2006**, 43, 1509-18	4.3	46
182	Allosteric Regulation Points Control the Conformational Dynamics of the Molecular Chaperone Hsp90. *Journal of Molecular Biology*, **2016**, 428, 4559-4571	6.5	45
181	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
180	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
179	Misfolding of the amyloid beta-protein: a molecular dynamics study. *Proteins: Structure, Function and Bioinformatics*, **2006**, 62, 183-92	4.2	45
178	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
177	Investigating the mechanism of peptide aggregation: insights from mixed monte carlo-molecular dynamics simulations. *Biophysical Journal*, **2008**, 94, 4414-26	2.9	44
176	Molecular mechanism of allosteric communication in Hsp70 revealed by molecular dynamics simulations. *PLoS Computational Biology*, **2012**, 8, e1002844	5	43
175	Anharmonicity and self-similarity of the free energy landscape of protein G. *Physical Review Letters*, **2007**, 98, 048102	7.4	43
174	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
173	Chaperones rescue the energetic landscape of mutant CFTR at single molecule and in cell. *Nature Communications*, **2017**, 8, 398	17.4	42
172	Rationalization of the Enantioselectivity of Subtilisin in DMF. *Journal of the American Chemical Society*, **1999**, 121, 3486-3493	16.4	42
171	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
170	Peptides for immunological purposes: design, strategies and applications. *Amino Acids*, **2013**, 45, 257-68	3.5	41
169	Exploiting antigenic diversity for vaccine design: the chlamydia ArtJ paradigm. *Journal of Biological Chemistry*, **2010**, 285, 30126-38	5.4	39

168	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
167	A structure-based strategy for epitope discovery in Burkholderia pseudomallei OppA antigen. *Structure*, **2013**, 21, 167-175	5.2	37
166	An efficient steroid pharmacophore-based strategy to identify new aromatase inhibitors. *European Journal of Medicinal Chemistry*, **2009**, 44, 4121-7	6.8	36
165	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
164	Identification of domains in protein structures from the analysis of intramolecular interactions. *Journal of Physical Chemistry B*, **2012**, 116, 3331-43	3.4	34
163	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
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161	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
160	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
159	Targeting tumor angiogenesis with TSP-1-based compounds: rational design of antiangiogenic mimetics of endogenous inhibitors. *Oncotarget*, **2010**, 1, 662-73	3.3	33
158	Rational Design of Allosteric and Selective Inhibitors of the Molecular Chaperone TRAP1. *Cell Reports*, **2020**, 31, 107531	10.6	32
157	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
156	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
155	Molecular recognition and drug-lead identification: what can molecular simulations tell us?. *Current Medicinal Chemistry*, **2010**, 17, 25-41	4.3	31
154	Interplay between hydrophobic cluster and loop propensity in beta-hairpin formation: a mechanistic study. *Protein Science*, **2003**, 12, 538-50	6.3	31
153	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
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151	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

150	Rational epitope design for protein targeting. *ACS Chemical Biology*, **2013**, 8, 397-404	4.9	30
149	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
148	ADAMDEC1 Maintains a Growth Factor Signaling Loop in Cancer Stem Cells. *Cancer Discovery*, **2019**, 9, 1574-1589	24.4	28
147	Identification of a new scaffold for hsp90 C-terminal inhibition. *ACS Medicinal Chemistry Letters*, **2014**, 5, 84-8	4.3	28
146	Combining computational and biochemical studies for a rationale on the anti-aromatase activity of natural polyphenols. *ChemMedChem*, **2007**, 2, 1750-62	3.7	28
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144	Sequence- and Structure-Based Immunoreactive Epitope Discovery for Burkholderia pseudomallei Flagellin. *PLoS Neglected Tropical Diseases*, **2015**, 9, e0003917	4.8	27
143	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
142	Inactivation of TEM-1 by avibactam (NXL-104): insights from quantum mechanics/molecular mechanics metadynamics simulations. *Biochemistry*, **2014**, 53, 5174-85	3.2	26
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140	Application of structure-based thermodynamic calculations to the rationalization of the enantioselectivity of subtilisin in organic solvents. *Tetrahedron: Asymmetry*, **1998**, 9, 1205-1214		25
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137	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
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135	Molecular dynamics simulations of proteins and peptides: from folding to drug design. *Current Protein and Peptide Science*, **2008**, 9, 181-96	2.8	24
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130	Probing the hirudin-thrombin interaction by incorporation of noncoded amino acids and molecular dynamics simulation. *Biochemistry*, **2002**, 41, 13556-69	3.2	23
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128	A protease-resistant Escherichia coli asparaginase with outstanding stability and enhanced anti-leukaemic activity in vitro. *Scientific Reports*, **2017**, 7, 14479	4.9	22
127	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
126	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
125	Designing Molecular Spanners to Throw in the Protein Networks. *Chemistry - A European Journal*, **2020**, 26, 4656-4670	4.8	22
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120	Enhancing Antibody Serodiagnosis Using a Controlled Peptide Coimmobilization Strategy. *ACS Infectious Diseases*, **2018**, 4, 998-1006	5.5	20
119	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
118	The Dynamics of Drug Discovery. *Current Topics in Medicinal Chemistry*, **2015**, 15, 2043-2055	3	20
117	Evolving serodiagnostics by rationally designed peptide arrays: the Burkholderia paradigm in Cystic Fibrosis. *Scientific Reports*, **2016**, 6, 32873	4.9	19
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112	Covalent docking of selected boron-based serine beta-lactamase inhibitors. *Journal of Computer-Aided Molecular Design*, **2015**, 29, 441-50	4.2	18
111	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
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101	Protein Folding Simulations: Combining Coarse-grained Models and All-atom Molecular Dynamics. *Theoretical Chemistry Accounts*, **2006**, 116, 75-86	1.9	16
100	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
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97	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

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79	Honokiol Bis-Dichloroacetate Is a Selective Allosteric Inhibitor of the Mitochondrial Chaperone TRAP1. *Antioxidants and Redox Signaling*, **2021**, 34, 505-516	8.4	11

78	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
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