

Andrea Mozzarelli

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

269 papers	6,855 citations	45 h-index	67 g-index
306 ext. papers	7,370 ext. citations	5.2 avg, IF	5.41 L-index

#	Paper	IF	Citations
269	From hemoglobin allostery to hemoglobin-based oxygen carriers. <i>Molecular Aspects of Medicine</i> , 2021 , 101050	16.7	2
268	Modulation of Oxygen Affinity in Hemoglobin-based Oxygen Carriers. <i>Regenerative Medicine, Artificial Cells and Nanomedicine</i> , 2021 , 375-403		1
267	A Competitive O-Acetylserine Sulfhydrylase Inhibitor Modulates the Formation of Cysteine Synthase Complex. <i>Catalysts</i> , 2021 , 11, 700	4	2
266	Human serine racemase is inhibited by glyceraldehyde 3-phosphate, but not by glyceraldehyde 3-phosphate dehydrogenase. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2021 , 1869, 140544	4	2
265	The allosteric interplay between S-nitrosylation and glycine binding controls the activity of human serine racemase. <i>FEBS Journal</i> , 2021 , 288, 3034-3054	5.7	4
264	Investigational Studies on a Hit Compound Cyclopropane-Carboxylic Acid Derivative Targeting -Acetylserine Sulfhydrylase as a Colistin Adjuvant. <i>ACS Infectious Diseases</i> , 2021 , 7, 281-292	5.5	3
263	Discovery of Substituted (2-Aminooxazol-4-yl)Isoxazole-3-carboxylic Acids as Inhibitors of Bacterial Serine Acetyltransferase in the Quest for Novel Potential Antibacterial Adjuvants. <i>Pharmaceuticals</i> , 2021 , 14,	5.2	3
262	Stability of Maleimide-PEG and Mono-Sulfone-PEG Conjugation to a Novel Engineered Cysteine in the Human Hemoglobin Alpha Subunit. <i>Frontiers in Chemistry</i> , 2021 , 9, 707797	5	2
261	A Key Silencing Histone Mark on Chromatin Is Lost When Colorectal Adenocarcinoma Cells Are Depleted of Methionine by Methionine Lyase. <i>Frontiers in Molecular Biosciences</i> , 2021 , 8, 735303	5.6	2
260	Engineering hemoglobin to enable homogenous PEGylation without modifying protein functionality. <i>Biomaterials Science</i> , 2020 , 8, 3896-3906	7.4	8
259	Inhibition of Nonessential Bacterial Targets: Discovery of a Novel Serine -Acetyltransferase Inhibitor. <i>ACS Medicinal Chemistry Letters</i> , 2020 , 11, 790-797	4.3	7
258	Model-based evaluation of the microhemodynamic effects of PEGylated HBOC molecules in the rat brain cortex: a laser speckle imaging study. <i>Biomedical Optics Express</i> , 2020 , 11, 4150-4175	3.5	
257	SP-B and SP-C analogues within CHF5633 synthetic surfactant probed by fluorescence labeling. <i>Journal of Molecular Liquids</i> , 2020 , 298, 111983	6	2
256	Rational Design of a User-Friendly Aptamer/Peptide-Based Device for the Detection of. <i>Sensors</i> , 2020 , 20,	3.8	3
255	Structural and Functional Characterization of the Globin-Coupled Sensors of and. <i>Antioxidants and Redox Signaling</i> , 2020 , 32, 378-395	8.4	4
254	Engineering tyrosine residues into hemoglobin enhances heme reduction, decreases oxidative stress and increases vascular retention of a hemoglobin based blood substitute. <i>Free Radical Biology and Medicine</i> , 2019 , 134, 106-118	7.8	14
253	ADIFAB fluorescence data used for the quantification of free fatty acids in media at different pH. <i>Data in Brief</i> , 2019 , 22, 158-163	1.2	1

252	Is the protein profile of pig Longissimus dorsi affected by gender and diet?. <i>Journal of Proteomics</i> , 2019 , 206, 103437	3.9	3
251	Combination of SAXS and Protein Painting Discloses the Three-Dimensional Organization of the Bacterial Cysteine Synthase Complex, a Potential Target for Enhancers of Antibiotic Action. <i>International Journal of Molecular Sciences</i> , 2019 , 20,	6.3	5
250	Covalent Inhibitors of Glyceraldehyde 3-Phosphate Dehydrogenase with Antimalarial Activity in Vitro. <i>ACS Medicinal Chemistry Letters</i> , 2019 , 10, 590-595	4.3	9
249	More than a Confinement: Soft and Hard Enzyme Entrapment Modulates Biological Catalyst Function. <i>Catalysts</i> , 2019 , 9, 1024	4	9
248	Refining the structure-activity relationships of 2-phenylcyclopropane carboxylic acids as inhibitors of O-acetylserine sulphydrylase isoforms. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2019 , 34, 31-43	5.6	11
247	The Energy Landscape of Human Serine Racemase. <i>Frontiers in Molecular Biosciences</i> , 2018 , 5, 112	5.6	17
246	Proteomics of Meat Products 2018 , 297-309		1
245	Human serine racemase is nitrosylated at multiple sites. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2018 , 1866, 813-821	4	5
244	Higher expression of miR-133b is associated with better efficacy of erlotinib as the second or third line in non-small cell lung cancer patients. <i>PLoS ONE</i> , 2018 , 13, e0196350	3.7	11
243	Soluble and Nanoporous Silica Gel-Entrapped Methionine -Lyase. <i>Journal of Nanoscience and Nanotechnology</i> , 2018 , 18, 2210-2219	1.3	4
242	Glutamine 89 is a key residue in the allosteric modulation of human serine racemase activity by ATP. <i>Scientific Reports</i> , 2018 , 8, 9016	4.9	8
241	Comparison of the oxidative reactivity of recombinant fetal and adult human hemoglobin: implications for the design of hemoglobin-based oxygen carriers. <i>Bioscience Reports</i> , 2018 , 38,	4.1	15
240	High- and low-affinity PEGylated hemoglobin-based oxygen carriers: Differential oxidative stress in a Guinea pig transfusion model. <i>Free Radical Biology and Medicine</i> , 2018 , 124, 299-310	7.8	10
239	Inhibition of O-acetylserine sulphydrylase by fluoroalanine derivatives. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2018 , 33, 1343-1351	5.6	11
238	Engineering methionine Lyase from <i>Citrobacter freundii</i> for anticancer activity. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2018 , 1866, 1260-1270	4	4
237	Phospholipid components of the synthetic pulmonary surfactant CHF5633 probed by fluorescence spectroscopy. <i>International Journal of Pharmaceutics</i> , 2018 , 553, 290-297	6.5	2
236	Insight into GFPmut2 pH Dependence by Single Crystal Microspectrophotometry and X-ray Crystallography. <i>Journal of Physical Chemistry B</i> , 2018 , 122, 11326-11337	3.4	2
235	Discovery of novel fragments inhibiting O-acetylserine sulphhydrylase by combining scaffold hopping and ligand-based drug design. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2018 , 33, 1444-1452	5.6	10

234	Protein carbonylation detection methods: A comparison. <i>Data in Brief</i> , 2018 , 19, 2215-2220	1.2	14
233	Magnesium and calcium ions differentially affect human serine racemase activity and modulate its quaternary equilibrium toward a tetrameric form. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2017 , 1865, 381-387	4	12
232	The Roles of Water in the Protein Matrix: A Largely Untapped Resource for Drug Discovery. <i>Journal of Medicinal Chemistry</i> , 2017 , 60, 6781-6827	8.3	77
231	Modulation of Escherichia coli serine acetyltransferase catalytic activity in the cysteine synthase complex. <i>FEBS Letters</i> , 2017 , 591, 1212-1224	3.8	10
230	Activation of an anti-bacterial toxin by the biosynthetic enzyme CysK: mechanism of binding, interaction specificity and competition with cysteine synthase. <i>Scientific Reports</i> , 2017 , 7, 8817	4.9	6
229	Proteomics of Parma Dry-Cured Ham: Analysis of Salting Exudates. <i>Journal of Agricultural and Food Chemistry</i> , 2017 , 65, 6307-6316	5.7	21
228	Gene cloning, characterization, and cytotoxic activity of methionine lyase from Clostridium novyi. <i>IUBMB Life</i> , 2017 , 69, 668-676	4.7	5
227	Insights on O-acetylserine sulphydrylase structure, function and biopharmaceutical applications. 2017 , 211-222		
226	Cyclopropane derivatives as potential human serine racemase inhibitors: unveiling novel insights into a difficult target. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2016 , 31, 645-52	5.6	11
225	Cyclopropane-1,2-dicarboxylic acids as new tools for the biophysical investigation of O-acetylserine sulphydrylases by fluorimetric methods and saturation transfer difference (STD) NMR. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2016 , 31, 78-87	5.6	19
224	Human serine racemase is allosterically modulated by NADH and reduced nicotinamide derivatives. <i>Biochemical Journal</i> , 2016 , 473, 3505-3516	3.8	9
223	Engineering tyrosine electron transfer pathways decreases oxidative toxicity in hemoglobin: implications for blood substitute design. <i>Biochemical Journal</i> , 2016 , 473, 3371-83	3.8	19
222	Rational Design, Synthesis, and Preliminary Structure-Activity Relationships of Substituted-2-Phenylcyclopropane Carboxylic Acids as Inhibitors of Salmonella typhimurium O-Acetylserine Sulphydrylase. <i>Journal of Medicinal Chemistry</i> , 2016 , 59, 2567-78	8.3	24
221	Insight of Saffron Proteome by Gel-Electrophoresis. <i>Molecules</i> , 2016 , 21, 167	4.8	8
220	Structural insight into the interaction of O-acetylserine sulphydrylase with competitive, peptidic inhibitors by saturation transfer difference-NMR. <i>FEBS Letters</i> , 2016 , 590, 943-53	3.8	9
219	Selectivity of 3-bromo-isoxazoline inhibitors between human and Plasmodium falciparum glyceraldehyde-3-phosphate dehydrogenases. <i>Bioorganic and Medicinal Chemistry</i> , 2016 , 24, 2654-9	3.4	13
218	Regulation of human serine racemase activity and dynamics by halides, ATP and malonate. <i>Amino Acids</i> , 2015 , 47, 163-73	3.5	18
217	Moonlighting O-acetylserine sulphydrylase: New functions for an old protein. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2015 , 1854, 1184-93	4	29

216	From protein structure to function via single crystal optical spectroscopy. <i>Frontiers in Molecular Biosciences</i> , 2015 , 2, 12	5.6	9
215	MediaChrom: Discovering a Class of Pyrimidoindolone-Based Polarity-Sensitive Dyes. <i>Journal of Organic Chemistry</i> , 2015 , 80, 10939-54	4.2	21
214	Expanding the chemical space of human serine racemase inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2015 , 25, 4297-303	2.9	19
213	Experiments on Hemoglobin in Single Crystals and Silica Gels Distinguish among Allosteric Models. <i>Biophysical Journal</i> , 2015 , 109, 1264-72	2.9	26
212	Understanding Water and Its Many Roles in Biological Structure: Ways to Exploit a Resource for Drug Discovery. <i>Methods in Pharmacology and Toxicology</i> , 2015 , 85-110	1.1	
211	Inhibitors of the sulfur assimilation pathway in bacterial pathogens as enhancers of antibiotic therapy. <i>Current Medicinal Chemistry</i> , 2015 , 22, 187-213	4.3	33
210	Immobilization of Proteins in Silica Gel: Biochemical and Biophysical Properties. <i>Current Organic Chemistry</i> , 2015 , 19, 1653-1668	1.7	17
209	Ormosil gels doped with engineered catechol 1,2 dioxygenases for chlorocatechol bioremediation. <i>Biotechnology and Applied Biochemistry</i> , 2014 , 61, 297-303	2.8	1
208	Experimental basis for a new allosteric model for multisubunit proteins. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2014 , 111, 12758-63	11.5	37
207	Discovery of covalent inhibitors of glyceraldehyde-3-phosphate dehydrogenase, a target for the treatment of malaria. <i>Journal of Medicinal Chemistry</i> , 2014 , 57, 7465-71	8.3	34
206	Molecular insights into dimerization inhibition of c-Maf transcription factor. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2014 , 1844, 2108-15	4	12
205	Identification of a small molecule that increases hemoglobin oxygen affinity and reduces SS erythrocyte sickling. <i>ACS Chemical Biology</i> , 2014 , 9, 2318-25	4.9	32
204	Targeting cystalysin, a virulence factor of treponema denticola-supported periodontitis. <i>ChemMedChem</i> , 2014 , 9, 1501-11	3.7	21
203	ATP binding to human serine racemase is cooperative and modulated by glycine. <i>FEBS Journal</i> , 2013 , 280, 5853-63	5.7	27
202	Unintended consequences? Water molecules at biological and crystallographic protein-protein interfaces. <i>Computational Biology and Chemistry</i> , 2013 , 47, 126-41	3.6	11
201	Fine tuning of the active site modulates specificity in the interaction of O-acetylserine sulphydrylase isozymes with serine acetyltransferase. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2013 , 1834, 169-81	4	30
200	Role of tertiary structures on the Root effect in fish hemoglobins. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2013 , 1834, 1885-93	4	7
199	Muscle and meat: new horizons and applications for proteomics on a farm to fork perspective. <i>Journal of Proteomics</i> , 2013 , 88, 58-82	3.9	45

198	Tertiary and quaternary allostery in tetrameric hemoglobin from <i>Scapharca inaequalis</i> . <i>Biochemistry</i> , 2013 , 52, 2108-17	3.2	6
197	Chemogenomics of pyridoxal 5'-phosphate dependent enzymes. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2013 , 28, 183-94	5.6	11
196	Asymmetry of the active site loop conformation between subunits of glutamate-1-semialdehyde aminomutase in solution. <i>BioMed Research International</i> , 2013 , 2013, 353270	3	12
195	Development of a novel, hemolysis-resistant reagent for assessment of α -amylase in biological fluids. <i>Clinical Chemistry and Laboratory Medicine</i> , 2013 , 51, 1409-15	5.9	1
194	Serine racemase: a key player in neuron activity and in neuropathologies. <i>Frontiers in Bioscience - Landmark</i> , 2013 , 18, 1112-28	2.8	31
193	CO rebinding kinetics and molecular dynamics simulations highlight dynamic regulation of internal cavities in human cytoglobin. <i>PLoS ONE</i> , 2013 , 8, e49770	3.7	24
192	Isozyme-specific ligands for O-acetylserine sulfhydrylase, a novel antibiotic target. <i>PLoS ONE</i> , 2013 , 8, e77558	3.7	39
191	Biochemistry of Hemoglobin 2013 , 55-73		1
190	International Consortium for Development of Hemoglobin-Based Oxygen Carriers, Oxygen Therapeutics and Multifunctional Resuscitation Fluids: A White Paper 2013 , 737-746		1
189	"Muscle to meat" molecular events and technological transformations: the proteomics insight. <i>Journal of Proteomics</i> , 2012 , 75, 4275-89	3.9	85
188	Design and synthesis of trans-2-substituted-cyclopropane-1-carboxylic acids as the first non-natural small molecule inhibitors of O-acetylserine sulfhydrylase. <i>MedChemComm</i> , 2012 , 3, 1111	5	34
187	Histidine E7 dynamics modulates ligand exchange between distal pocket and solvent in AHb1 from <i>Arabidopsis thaliana</i> . <i>Journal of Physical Chemistry B</i> , 2011 , 115, 4138-46	3.4	15
186	Proteomic analysis of pork meat in the production of cooked ham. <i>Molecular BioSystems</i> , 2011 , 7, 2252-60		29
185	Modulation of expression and polymerization of hemoglobin Polytaur, a potential blood substitute. <i>Archives of Biochemistry and Biophysics</i> , 2011 , 505, 42-7	4.1	12
184	Exploring O-acetylserine sulfhydrylase-B isoenzyme from <i>Salmonella typhimurium</i> by fluorescence spectroscopy. <i>Archives of Biochemistry and Biophysics</i> , 2011 , 505, 178-85	4.1	8
183	The multifaceted pyridoxal 5'-phosphate-dependent O-acetylserine sulfhydrylase. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011 , 1814, 1497-510	4	35
182	Drug discovery targeting amino acid racemases. <i>Chemical Reviews</i> , 2011 , 111, 6919-46	68.1	83
181	Oxygen Delivery by Natural and Artificial Oxygen Carriers 2011 , 317-325		

180	Human kynurenine aminotransferase II--reactivity with substrates and inhibitors. <i>FEBS Journal</i> , 2011 , 278, 1882-900	5.7	22
179	Low affinity PEGylated hemoglobin from <i>Trematomus bernacchii</i> , a model for hemoglobin-based blood substitutes. <i>BMC Biochemistry</i> , 2011 , 12, 66	4.8	8
178	Oxygen binding to <i>Arabidopsis thaliana</i> AHb2 nonsymbiotic hemoglobin: evidence for a role in oxygen transport. <i>IUBMB Life</i> , 2011 , 63, 355-62	4.7	17
177	Oxygen and nitric oxide rebinding kinetics in nonsymbiotic hemoglobin AHb1 from <i>Arabidopsis thaliana</i> . <i>IUBMB Life</i> , 2011 , 63, 1094-100	4.7	13
176	Electrophoretic analysis of PEGylated hemoglobin-based blood substitutes. <i>Analytical Biochemistry</i> , 2011 , 408, 118-23	3.1	8
175	Exploring methionine lyase structure-function relationship via microspectrophotometry and X-ray crystallography. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011 , 1814, 834-42	4	16
174	Ligand migration and hexacoordination in type 1 non-symbiotic rice hemoglobin. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011 , 1814, 1042-53	4	13
173	Exploring and exploiting allostery: Models, evolution, and drug targeting. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011 , 1814, 922-33	4	46
172	Protein crystal microspectrophotometry. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011 , 1814, 734-41	4	9
171	X-ray crystallography marries spectroscopy to unveil structure and function of biological macromolecules. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2011 , 1814, 731-3	4	10
170	Bound water at protein-protein interfaces: partners, roles and hydrophobic bubbles as a conserved motif. <i>PLoS ONE</i> , 2011 , 6, e24712	3.7	48
169	2011 ,		7
168	Oxygen Delivery via Allosteric Effectors of Hemoglobin and Blood Substitutes 2010 , 609-660		1
167	A two-step process controls the formation of the bienzyme cysteine synthase complex. <i>Journal of Biological Chemistry</i> , 2010 , 285, 12813-22	5.4	30
166	Pyridoxal 5'-Phosphate-Dependent Enzymes: Catalysis, Conformation, and Genomics 2010 , 273-350		8
165	Identification of the structural determinants for the stability of substrate and aminoacrylate external Schiff bases in O-acetylserine sulfhydrylase-A. <i>Biochemistry</i> , 2010 , 49, 6093-103	3.2	25
164	Design of O-acetylserine sulfhydrylase inhibitors by mimicking nature. <i>Journal of Medicinal Chemistry</i> , 2010 , 53, 345-56	8.3	67
163	Polymerized and polyethylene glycol-conjugated hemoglobins: a globin-based calibration curve for dynamic light scattering analysis. <i>Analytical Biochemistry</i> , 2010 , 401, 266-70	3.1	4

162	Haemoglobin-based oxygen carriers: research and reality towards an alternative to blood transfusions. <i>Blood Transfusion</i> , 2010 , 8 Suppl 3, s59-68	3.6	21
161	Ligand migration through the internal hydrophobic cavities in human neuroglobin. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2009 , 106, 18984-9	11.5	42
160	Tryptophan synthase: a mine for enzymologists. <i>Cellular and Molecular Life Sciences</i> , 2009 , 66, 2391-403	10.3	62
159	Hemoglobin, an "evergreen" red protein. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2009 , 1794, 1317-24	4	14
158	PEGylation promotes hemoglobin tetramer dissociation. <i>Bioconjugate Chemistry</i> , 2009 , 20, 1356-66	6.3	42
157	Identification of xenoestrogens in food additives by an integrated in silico and in vitro approach. <i>Chemical Research in Toxicology</i> , 2009 , 22, 52-63	4	64
156	Cofactor chemogenomics. <i>Methods in Molecular Biology</i> , 2009 , 575, 93-122	1.4	4
155	Structural plasticity and functional implications of internal cavities in distal mutants of type 1 non-symbiotic hemoglobin AHB1 from <i>Arabidopsis thaliana</i> . <i>Journal of Physical Chemistry B</i> , 2009 , 113, 16028-38	3.4	17
154	Chemogenomic strategies to expand the bioactive chemical space. <i>Current Medicinal Chemistry</i> , 2009 , 16, 4374-81	4.3	23
153	Ligand-induced tertiary relaxations during the T-to-R quaternary transition in hemoglobin. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 12790-4	3.4	9
152	Characterization of ligand migration mechanisms inside hemoglobins from the analysis of geminate rebinding kinetics. <i>Methods in Enzymology</i> , 2008 , 437, 329-45	1.7	4
151	Robust classification of "relevant" water molecules in putative protein binding sites. <i>Journal of Medicinal Chemistry</i> , 2008 , 51, 1063-7	8.3	81
150	Trapping of the thioacylglyceraldehyde-3-phosphate dehydrogenase intermediate from <i>Bacillus stearothermophilus</i> . Direct evidence for a flip-flop mechanism. <i>Journal of Biological Chemistry</i> , 2008 , 283, 21693-702	5.4	31
149	Oxygen binding to heme proteins in solution, encapsulated in silica gels, and in the crystalline state. <i>Methods in Enzymology</i> , 2008 , 437, 311-28	1.7	28
148	Energy-based prediction of amino acid-nucleotide base recognition. <i>Journal of Computational Chemistry</i> , 2008 , 29, 1955-69	3.5	39
147	Towards a novel haemoglobin-based oxygen carrier: Euro-PEG-Hb, physico-chemical properties, vasoactivity and renal filtration. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2008 , 1784, 1402-9	4.9	38
146	Structure, mechanism, and conformational dynamics of O-acetylserine sulfhydrylase from <i>Salmonella typhimurium</i> : comparison of A and B isozymes. <i>Biochemistry</i> , 2007 , 46, 8315-30	3.2	53
145	Ligand migration in nonsymbiotic hemoglobin AHB1 from <i>Arabidopsis thaliana</i> . <i>Journal of Physical Chemistry B</i> , 2007 , 111, 12582-90	3.4	25

144	Control of ionizable residues in the catalytic mechanism of tryptophan synthase from <i>Salmonella typhimurium</i> . <i>Biochemistry</i> , 2007 , 46, 13223-34	3.2	12
143	Evidence of discrete substates and unfolding pathways in green fluorescent protein. <i>Biophysical Journal</i> , 2007 , 92, 1724-31	2.9	15
142	Complexity in modeling and understanding protonation states: computational titration of HIV-1-protease-inhibitor complexes. <i>Chemistry and Biodiversity</i> , 2007 , 4, 2564-77	2.5	9
141	The consequences of scoring docked ligand conformations using free energy correlations. <i>European Journal of Medicinal Chemistry</i> , 2007 , 42, 921-33	6.8	52
140	Energetics of the protein-DNA-water interaction. <i>BMC Structural Biology</i> , 2007 , 7, 4	2.7	48
139	Evolution of allosteric models for hemoglobin. <i>IUBMB Life</i> , 2007 , 59, 586-99	4.7	93
138	Environment effects on the oscillatory unfolding kinetics of GFP. <i>European Biophysics Journal</i> , 2007 , 36, 795-803	1.9	5
137	Trapping hemoglobin in rigid matrices: fine tuning of oxygen binding properties by modulation of encapsulation protocols. <i>Artificial Cells, Blood Substitutes, and Biotechnology</i> , 2007 , 35, 69-79		9
136	Pyridoxal 5'-phosphate enzymes as targets for therapeutic agents. <i>Current Medicinal Chemistry</i> , 2007 , 14, 1291-324	4.3	153
135	Hemocyanin from <i>E. californicum</i> encapsulated in silica gels: oxygen binding and conformational states. <i>Gene</i> , 2007 , 398, 202-7	3.8	7
134	Different roles of protein dynamics and ligand migration in non-symbiotic hemoglobins AHb1 and AHb2 from <i>Arabidopsis thaliana</i> . <i>Gene</i> , 2007 , 398, 224-33	3.8	27
133	The reactivity with CO of AHb1 and AHb2 from <i>Arabidopsis thaliana</i> is controlled by the distal HisE7 and internal hydrophobic cavities. <i>Journal of the American Chemical Society</i> , 2007 , 129, 2880-9	16.4	49
132	Monitoring the T-R transition of human hemoglobin encapsulated in silica gels. <i>FASEB Journal</i> , 2007 , 21, A637	0.9	
131	Is cooperative oxygen binding by hemoglobin really understood?. <i>Rendiconti Lincei</i> , 2006 , 17, 147-162	1.7	4
130	Sulfur mobilization in cyanobacteria: the catalytic mechanism of L-cystine C-S lyase (C-DES) from <i>synechocystis</i> . <i>Journal of Biological Chemistry</i> , 2006 , 281, 38769-80	5.4	15
129	Time-resolved methods in Biophysics. 2. Monitoring haem proteins at work with nanosecond laser flash photolysis. <i>Photochemical and Photobiological Sciences</i> , 2006 , 5, 1109-20	4.2	47
128	Mapping the energetics of water-protein and water-ligand interactions with the "natural" HINT forcefield: predictive tools for characterizing the roles of water in biomolecules. <i>Journal of Molecular Biology</i> , 2006 , 358, 289-309	6.5	75
127	Water: How to evaluate its contribution in protein-ligand interactions. <i>International Journal of Quantum Chemistry</i> , 2006 , 106, 647-651	2.1	11

126	Exploring the pyridoxal 5'-phosphate-dependent enzymes. <i>Chemical Record</i> , 2006 , 6, 275-87	6.6	38
125	Allosteric communication between alpha and beta subunits of tryptophan synthase: modelling the open-closed transition of the alpha subunit. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2006 , 1764, 1102-9	4	19
124	Tools for building a comprehensive modeling system for virtual screening under real biological conditions: The Computational Titration algorithm. <i>Journal of Molecular Graphics and Modelling</i> , 2006 , 24, 434-9	2.8	16
123	Circular dichroism spectroscopy of tertiary and quaternary conformations of human hemoglobin entrapped in wet silica gels. <i>Protein Science</i> , 2006 , 15, 1961-7	6.3	26
122	Kinetics of acid-induced spectral changes in the GFPmut2 chromophore. <i>Journal of the American Chemical Society</i> , 2005 , 127, 626-35	16.4	52
121	Determination of microscopic rate constants for CO binding and migration in myoglobin encapsulated in silica gels. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 19523-8	3.4	27
120	Geminate rebinding in R-state hemoglobin: kinetic and computational evidence for multiple hydrophobic pockets. <i>Journal of the American Chemical Society</i> , 2005 , 127, 17427-32	16.4	28
119	Confinement and crowding effects on tryptophan synthase alpha2beta2 complex. <i>FEBS Letters</i> , 2005 , 579, 2197-202	3.8	20
118	Unfolding of Green Fluorescent Protein mut2 in wet nanoporous silica gels. <i>Protein Science</i> , 2005 , 14, 1125-33	6.3	54
117	Tracking unfolding and refolding of single GFPmut2 molecules. <i>Biophysical Journal</i> , 2005 , 89, 2033-45	2.9	29
116	Interaction of serine acetyltransferase with O-acetylserine sulfhydrylase active site: evidence from fluorescence spectroscopy. <i>Protein Science</i> , 2005 , 14, 2115-24	6.3	72
115	Identification of the geometric requirements for allosteric communication between the alpha- and beta-subunits of tryptophan synthase. <i>Journal of Biological Chemistry</i> , 2005 , 280, 13450-6	5.4	24
114	Evidence for two geminate rebinding states following laser photolysis of R state hemoglobin encapsulated in wet silica gels. <i>Journal of Physical Chemistry B</i> , 2005 , 109, 11411-3	3.4	28
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28	Water induced TSDC in hemoglobin and myoglobin		2
27	Red Blood Cells from Stem Cells257-271		
26	Red-Cell Transfusion in Clinical Practice213-220		
25	Biochemistry of Storage of Red Blood Cells231-241		1
24	Conscientious Objection in Patient Blood Management205-211		
23	Diagnosis and Treatment of Haemorrhages in Nonsurgical Patients107-119		
22	The Major Physiological Control Mechanisms of Blood Flow and Oxygen Delivery23-45		
21	Hb Octamers by Introduction of Surface Cysteines371-380		
20	Animal Models and Oxidative Biomarkers to Evaluate Preclinical Safety of Extracellular Hemoglobins391-411		
19	Oxygenation in the Preterm Neonate131-143		

18	Transfusion: Political, Administrative and Logistic Issues	193-204	
17	AcademiaIndustry Collaboration in Blood Substitute Development: Issues, Case Histories and a Proposal	413-428	
16	Transfusion Therapy in β -Thalassemia and Sickle Cell Disease	179-191	
15	Causes and Consequences of Red Cell Incompatibility	221-230	
14	The Universal Red Blood Cell	273-284	
13	Hemoglobin Vesicles as a Cellular-Type Hemoglobin-Based Oxygen Carrier	381-390	
12	Hemoglobin Reactivity and Regulation	9-22	1
11	Normobaric and Hyperbaric Oxygen Therapy for Ischemic Stroke and Other Neurological Conditions	159-177	
10	Engineering the Molecular Shape of PEG-Hemoglobin Adducts for Supraperfusion	345-369	1
9	Ischemia	145-158	1
8	Proteomic Investigations of Stored Red Blood Cells	243-256	1
7	Allosteric Effectors of Hemoglobin: Past, Present and Future	285-300	7
6	Hemoglobin-Based Oxygen Carriers: History, Limits, Brief Summary of the State of the Art, Including Clinical Trials	301-316	15
5	Crosslinked and Polymerized Hemoglobins as Potential Blood Substitutes	327-344	1
4	The Main Players: Hemoglobin and Myoglobin; Nitric Oxide and Oxygen	47-62	1
3	The Role of Reactive Oxygen and Nitrogen Species in Ischemia/Reperfusion Injury	63-77	1
2	Acute Traumatic Hemorrhage and Anemia	79-106	2
1	Management of Perioperative Bleeding	121-130	0

