Antonella Ciancetta

List of Publications by Year
in descending order

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52 papers	1,500 citations	331259 21 h-index	329751 37 g-index
52 all docs	52 docs citations	52 times ranked	1987 citing authors

#	Article	IF	Citations
1	Enhancing Ligand and Protein Sampling Using Sequential Monte Carlo. Journal of Chemical Theory and Computation, 2022, , .	2.3	5
2	Sensitivity of Binding Free Energy Calculations to Initial Protein Crystal Structure. Journal of Chemical Theory and Computation, 2021, 17, 1806-1821.	2.3	13
3	Probe Confined Dynamic Mapping for G Protein-Coupled Receptor Allosteric Site Prediction. ACS Central Science, 2021, 7, 1847-1862.	5.3	15
4	A3 adenosine receptor activation mechanisms: molecular dynamics analysis of inactive, active, and fully active states. Journal of Computer-Aided Molecular Design, 2019, 33, 983-996.	1.3	10
5	Design and in Vivo Characterization of A₁ Adenosine Receptor Agonists in the Native Ribose and Conformationally Constrained (N)-Methanocarba Series. Journal of Medicinal Chemistry, 2019, 62, 1502-1522.	2.9	22
6	A₃ Adenosine Receptors as Modulators of Inflammation: From Medicinal Chemistry to Therapy. Medicinal Research Reviews, 2018, 38, 1031-1072.	5.0	111
7	Breakthrough in GPCR Crystallography and Its Impact on Computer-Aided Drug Design. Methods in Molecular Biology, 2018, 1705, 45-72.	0.4	16
8	Structure activity relationship of 2-arylalkynyl-adenine derivatives as human A₃ adenosine receptor antagonists. MedChemComm, 2018, 9, 1920-1932.	3.5	6
9	Repurposing of a Nucleoside Scaffold from Adenosine Receptor Agonists to Opioid Receptor Antagonists. ACS Omega, 2018, 3, 12658-12678.	1.6	13
10	Structure-Guided Modification of Heterocyclic Antagonists of the P2Y₁₄ Receptor. Journal of Medicinal Chemistry, 2018, 61, 4860-4882.	2.9	32
11	A2A Adenosine Receptor: Structures, Modeling, and Medicinal Chemistry. , 2018, , 91-136.		4
12	P2Y14 Receptor. , 2018, , 3713-3718.		2
13	Conjugates between minor groove binders and Zn(II)-tach complexes: Synthesis, characterization, and interaction with plasmid DNA. Tetrahedron, 2017, 73, 3014-3024.	1.0	5
14	Pyrimidine nucleotides containing a (S)-methanocarba ring as P2Y₆ receptor agonists. MedChemComm, 2017, 8, 1897-1908.	3.5	16
15	Polypharmacology of conformationally locked methanocarba nucleosides. Drug Discovery Today, 2017, 22, 1782-1791.	3.2	16
16	Demystifying P2Y₁ Receptor Ligand Recognition through Docking and Molecular Dynamics Analyses. Journal of Chemical Information and Modeling, 2017, 57, 3104-3123.	2.5	20
17	Bitopic fluorescent antagonists of the A_{2A} adenosine receptor based on pyrazolo[4,3-e][1,2,4]triazolo[1,5-c]pyrimidin-5-amine functionalized congeners. MedChemComm, 2017, 8, 1659-1667.	3.5	15
18	Structural Probing and Molecular Modeling of the A3 Adenosine Receptor: A Focus on Agonist Binding. Molecules, 2017, 22, 449.	1.7	30

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19	Structure-Based Scaffold Repurposing for G Protein-Coupled Receptors: Transformation of Adenosine Derivatives into 5HT_{2B}/5HT_{2C} Serotonin Receptor Antagonists. Journal of Medicinal Chemistry, 2016, 59, 11006-11026.	2.9	18
20	In Silico 3D Modeling of Binding Activities. Methods in Molecular Biology, 2016, 1425, 23-35.	0.4	4
21	New Trends in Inspecting GPCRâ€ligand Recognition Process: the Contribution of the Molecular Modeling Section (MMS) at the University of Padova. Molecular Informatics, 2016, 35, 440-448.	1.4	3
22	South (S)- and North (N)-Methanocarba-7-Deazaadenosine Analogues as Inhibitors of Human Adenosine Kinase. Journal of Medicinal Chemistry, 2016, 59, 6860-6877.	2.9	41
23	Structure-Based Design of 3-(4-Aryl-1H-1,2,3-triazol-1-yl)-Biphenyl Derivatives as P2Y₁₄ Receptor Antagonists. Journal of Medicinal Chemistry, 2016, 59, 6149-6168.	2.9	38
24	Deciphering the Complexity of Ligandâ€"Protein Recognition Pathways Using Supervised Molecular Dynamics (SuMD) Simulations. Journal of Chemical Information and Modeling, 2016, 56, 687-705.	2.5	88
25	Purine (N)-Methanocarba Nucleoside Derivatives Lacking an Exocyclic Amine as Selective A3 Adenosine Receptor Agonists. Journal of Medicinal Chemistry, 2016, 59, 3249-3263.	2.9	14
26	5,7-Disubstituted-[1,2,4]triazolo[1,5- a][1,3,5]triazines as pharmacological tools to explore the antagonist selectivity profiles toward adenosine receptors. European Journal of Medicinal Chemistry, 2016, 108, 529-541.	2.6	18
27	Structural refinement of pyrazolo[4,3- d]pyrimidine derivatives to obtain highly potent and selective antagonists for the human A 3 adenosine receptor. European Journal of Medicinal Chemistry, 2016, 108, 117-133.	2.6	18
28	Pyrazolo[4,3-e][1,2,4]triazolo[1,5-c]pyrimidines and Structurally Simplified Analogs. Chemistry and SAR Profile as Adenosine Receptor Antagonists. Current Topics in Medicinal Chemistry, 2016, 16, 3224-3257.	1.0	13
29	P2Y14 Receptor. , 2016, , 1-5.		0
30	DockBench: An Integrated Informatic Platform Bridging the Gap between the Robust Validation of Docking Protocols and Virtual Screening Simulations. Molecules, 2015, 20, 9977-9993.	1.7	40
31	Understanding allosteric interactions in G protein-coupled receptors using Supervised Molecular Dynamics: A prototype study analysing the human A3 adenosine receptor positive allosteric modulator LUF6000. Bioorganic and Medicinal Chemistry, 2015, 23, 4065-4071.	1.4	53
32	Influence of key amino acid mutation on the active site structure and on folding in acetyl-CoA synthase: a theoretical perspective. Chemical Communications, 2015, 51, 8551-8554.	2.2	4
33	Exploring the recognition pathway at the human A_{2A} adenosine receptor of the endogenous agonist adenosine using supervised molecular dynamics simulations. MedChemComm, 2015, 6, 1081-1085.	3.5	36
34	Advances in Computational Techniques to Study GPCRâ€"Ligand Recognition. Trends in Pharmacological Sciences, 2015, 36, 878-890.	4.0	40
35	The Influence of the 1-(3-Trifluoromethyl-Benzyl)-1H-Pyrazole-4-yl Moiety on the Adenosine Receptors Affinity Profile of Pyrazolo[4,3-e][1,2,4]Triazolo[1,5-c]Pyrimidine Derivatives. PLoS ONE, 2015, 10, e0143504.	1.1	6
36	Bridging Molecular Docking to Membrane Molecular Dynamics To Investigate GPCRâ€"Ligand Recognition: The Human A_{2A} Adenosine Receptor as a Key Study. Journal of Chemical Information and Modeling, 2014, 54, 169-183.	2.5	59

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37	7-Amino-2-phenylpyrazolo[4,3-d]pyrimidine derivatives: Structural investigations at the 5-position to target human A1 and A2A adenosine receptors. Molecular modeling and pharmacological studies. European Journal of Medicinal Chemistry, 2014, 84, 614-627.	2.6	22
38	Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. Structure, 2014, 22, 1120-1139.	1.6	149
39	Scaffold Decoration at Positions 5 and 8 of 1,2,4-Triazolo[1,5-c]Pyrimidines to Explore the Antagonist Profiling on Adenosine Receptors: A Preliminary Structureâ€“Activity Relationship Study. Journal of Medicinal Chemistry, 2014, 57, 6210-6225.	2.9	13
40	Perturbation of Fluid Dynamics Properties of Water Molecules during G Protein-Coupled Receptorâ€“Ligand Recognition: The Human A_{2A} Adenosine Receptor as a Key Study. Journal of Chemical Information and Modeling, 2014, 54, 2846-2855.	2.5	24
41	Alternative Quality Assessment Strategy to Compare Performances of GPCR-Ligand Docking Protocols: The Human Adenosine A_{2A} Receptor as a Case Study. Journal of Chemical Information and Modeling, 2014, 54, 2243-2254.	2.5	26
42	Aquaporin Inhibition by Gold(III) Compounds: New Insights. ChemMedChem, 2013, 8, 1086-1092.	1.6	77
43	Implementing the â€œBest Template Searchingâ€•tool into Adenosiland platform. In Silico Pharmacology, 2013, 1, 25.	1.8	10
44	2-Arylpyrazolo[4,3-d]pyrimidin-7-amino Derivatives As New Potent and Selective Human A₃ Adenosine Receptor Antagonists. Molecular Modeling Studies and Pharmacological Evaluation. Journal of Medicinal Chemistry, 2013, 56, 2256-2269.	2.9	24
45	Revisiting a Receptor-Based Pharmacophore Hypothesis for Human A_{2A} Adenosine Receptor Antagonists. Journal of Chemical Information and Modeling, 2013, 53, 1620-1637.	2.5	16
46	Exploring the Directionality of 5-Substitutions in a New Series of 5-Alkylaminopyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidine as a Strategy To Design Novel Human A₃ Adenosine Receptor Antagonists.. Journal of Medicinal Chemistry, 2012, 55, 9654-9668.	2.9	17
47	Activation of carboplatin by carbonate: a theoretical investigation. Dalton Transactions, 2012, 41, 12960.	1.6	27
48	Synthesis and Spectroscopic Characterisation of a Heterodinuclear Iron(III)â€Copper(II) Complex Based on an Asymmetric Dinucleating Ligand System. European Journal of Inorganic Chemistry, 2012, 2012, 4565-4569.	1.0	8
49	Targeting Aquaporin Function: Potent Inhibition of Aquaglyceroporin-3 by a Gold-Based Compound. PLoS ONE, 2012, 7, e37435.	1.1	108
50	A QM/MM study of the binding of RAPTA ligands to cathepsin B. Journal of Computer-Aided Molecular Design, 2011, 25, 729-742.	1.3	36
51	Activation of carboplatin by chloride ions: a theoretical investigation. Theoretical Chemistry Accounts, 2011, 129, 757-769.	0.5	20
52	Rationalization of the inhibition activity of structurally related organometallic compounds against the drug target cathepsin B by DFT. Dalton Transactions, 2010, 39, 5556.	1.6	79