Stefano Moro

List of Publications by Year in descending order

314 papers	13,040 citations	26567 56 h-index	38300 95 g-index
341 all docs	341 docs citations	341 times ranked	13934 citing authors

#	Article	IF	Citations
1	Medicinal Chemistry and the Molecular Operating Environment (MOE): Application of QSAR and Molecular Docking to Drug Discovery. Current Topics in Medicinal Chemistry, 2008, 8, 1555-1572.	1.0	831
2	FAM/USP9x, a Deubiquitinating Enzyme Essential for TGFÎ² Signaling, Controls Smad4 Monoubiquitination. Cell, 2009, 136, 123-135.	13.5	442
3	The mitochondrial calcium uniporter is a multimer that can include a dominant-negative pore-forming subunit. EMBO Journal, 2013, 32, 2362-2376.	3.5	408
4	Bridging Molecular Docking to Molecular Dynamics in Exploring Ligand-Protein Recognition Process: An Overview. Frontiers in Pharmacology, 2018, 9, 923.	1.6	401
5	Ciprofloxacin and levofloxacin attenuate microglia inflammatory response via TLR4/NF-kB pathway. Journal of Neuroinflammation, 2019, 16, 148.	3.1	275
6	Synthesis, CoMFA Analysis, and Receptor Docking of 3,5-Diacyl-2,4-Dialkylpyridine Derivatives as Selective A3Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 1999, 42, 706-721.	2.9	187
7	USP15 is a deubiquitylating enzyme for receptor-activated SMADs. Nature Cell Biology, 2011, 13, 1368-1375.	4.6	182
8	DNA Binding Site Selection of Dimeric and Tetrameric Stat5 Proteins Reveals a Large Repertoire of Divergent Tetrameric Stat5a Binding Sites. Molecular and Cellular Biology, 2000, 20, 389-401.	1.1	169
9	Progress in the pursuit of therapeutic adenosine receptor antagonists. Medicinal Research Reviews, 2006, 26, 131-159.	5.0	154
10	Human P2Y1Receptor:Â Molecular Modeling and Site-Directed Mutagenesis as Tools To Identify Agonist and Antagonist Recognition Sites. Journal of Medicinal Chemistry, 1998, 41, 1456-1466.	2.9	153
11	Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. Structure, 2014, 22, 1120-1139.	1.6	149
12	Quinalizarin as a potent, selective and cell-permeable inhibitor of protein kinase CK2. Biochemical Journal, 2009, 421, 387-395.	1.7	140
13	Toward the rational design of protein kinase casein kinase-2 inhibitors. , 2002, 93, 159-168.		139
14	Supervised Molecular Dynamics (SuMD) as a Helpful Tool To Depict GPCRâ€“Ligand Recognition Pathway in a Nanosecond Time Scale. Journal of Chemical Information and Modeling, 2014, 54, 372-376.	2.5	135
15	Identification of Ellagic Acid as Potent Inhibitor of Protein Kinase CK2:Â A Successful Example of a Virtual Screening Application. Journal of Medicinal Chemistry, 2006, 49, 2363-2366.	2.9	134
16	The Role of Amino Acids in Extracellular Loops of the Human P2Y1 Receptor in Surface Expression and Activation Processes. Journal of Biological Chemistry, 1999, 274, 14639-14647.	1.6	132
17	Synthesis, Biological Activity, and Molecular Modeling of Ribose-Modified Deoxyadenosine Bisphosphate Analogues as P2Y1Receptor Ligands. Journal of Medicinal Chemistry, 2000, 43, 829-842.	2.9	129
18	Structureâ^'Activity Relationships and Molecular Modeling of 3,5-Diacyl-2,4-dialkylpyridine Derivatives as Selective A3 Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 1998, 41, 3186-3201.	2.9	126

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19	Role of the Extracellular Loops of G Protein-Coupled Receptors in Ligand Recognition:Â A Molecular Modeling Study of the Human P2Y1Receptor. Biochemistry, 1999, 38, 3498-3507.	1.2	125
20	Coumarin as Attractive Casein Kinase 2 (CK2) Inhibitor Scaffold: An Integrate Approach To Elucidate the Putative Binding Motif and Explain Structureâ€“Activity Relationships. Journal of Medicinal Chemistry, 2008, 51, 752-759.	2.9	123
21	Mimicking the vanadium bromoperoxidases reactions:Mild and selective bromination of arenes and alkenes in a two-phase system. Tetrahedron Letters, 1994, 35, 7429-7432.	0.7	121
22	Hemolytic Effects of Water-Soluble Fullerene Derivatives. Journal of Medicinal Chemistry, 2004, 47, 6711-6715.	2.9	114
23	Toward Efficient Zn(II)-Based Artificial Nucleases. Journal of the American Chemical Society, 2004, 126, 4543-4549.	6.6	112
24	MG-2477, a new tubulin inhibitor, induces autophagy through inhibition of the Akt/mTOR pathway and delayed apoptosis in A549 cells. Biochemical Pharmacology, 2012, 83, 16-26.	2.0	111
25	Tetrabromocinnamic Acid (TBCA) and Related Compounds Represent a New Class of Specific Protein Kinase CK2 Inhibitors. ChemBioChem, 2007, 8, 129-139.	1.3	109
26	Derivatives of the Triazoloquinazoline Adenosine Antagonist (CGS 15943) Having High Potency at the Human A2Band A3Receptor Subtypes. Journal of Medicinal Chemistry, 1998, 41, 2835-2845.	2.9	106
27	6-Aminoquinolones as New Potential Anti-HIV Agents. Journal of Medicinal Chemistry, 2000, 43, 3799-3802.	2.9	105
28	Synthesis, Biological Activity, and Molecular Modeling Investigation of New Pyrazolo[4,3-e]-1,2,4-triazolo[1,5-c]pyrimidine Derivatives as Human A3 Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 2002, 45, 770-780.	2.9	99
29	The ATPâ€Binding Site of Protein Kinase CK2 Holds a Positive Electrostatic Area and Conserved Water Molecules. ChemBioChem, 2007, 8, 1804-1809.	1.3	98
30	Kinase CK2 Inhibition: An Update. Current Medicinal Chemistry, 2013, 20, 671-693.	1.2	94
31	Quantitative Correlation of Solvent Polarity with the Î±-/310-Helix Equilibrium: A Heptapeptide Behaves as a Solvent-Driven Molecular Spring. Angewandte Chemie - International Edition, 2003, 42, 3388-3392.	7.2	91
32	Pyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidine Derivatives as Highly Potent and Selective Human A3Adenosine Receptor Antagonists:Â Influence of the Chain at the N8Pyrazole Nitrogen. Journal of Medicinal Chemistry, 2000, 43, 4768-4780.	2.9	89
33	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
34	Models for the active site of vanadium-dependent haloperoxidases: insight into the solution structure of peroxo vanadium compounds. Journal of Inorganic Biochemistry, 2000, 80, 41-49.	1.5	87
35	Inhibition of Protein Kinase CK2 by Condensed Polyphenolic Derivatives. An in Vitro and in Vivo Study. Biochemistry, 2004, 43, 12931-12936.	1.2	87
36	PEGâ€“Ara-C conjugates for controlled release. European Journal of Medicinal Chemistry, 2004, 39, 123-133.	2.6	85

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37	Enantioselective Ti(IV) Sulfoxidation Catalysts BearingC3-Symmetric Trialkanolamine Ligands:Â Solution Speciation by1H NMR and ESI-MS Analysis. Journal of the American Chemical Society, 1999, 121, 6258-6268.	6.6	83
38	Titanium(IV)â^'(R,R,R)-Tris(2-phenylethoxy)amineâ^' Alkylperoxo Complex Mediated Oxidations:Â The Biphilic Nature of the Oxygen Transfer to Organic Sulfur Compounds. Journal of the American Chemical Society, 1997, 119, 6935-6936.	6.6	81
39	Ligand-Based Homology Modeling as Attractive Tool to Inspect GPCR Structural Plasticity. Current Pharmaceutical Design, 2006, 12, 2175-2185.	0.9	80
40	Inhibition of Protein Kinase CK2 by Anthraquinone-related Compounds. Journal of Biological Chemistry, 2003, 278, 1831-1836.	1.6	75
41	Synthesis, Biological Properties, and Molecular Modeling Investigation of the First Potent, Selective, and Water-Soluble Human A3 Adenosine Receptor Antagonist. Journal of Medicinal Chemistry, 2002, 45, 3579-3582.	2.9	74
42	Techniques: Recent developments in computer-aided engineering of GPCR ligands using the human adenosine A3 receptor as an example. Trends in Pharmacological Sciences, 2005, 26, 44-51.	4.0	72
43	Novel camptothecin derivatives as topoisomerase I inhibitors. Expert Opinion on Therapeutic Patents, 2009, 19, 555-574.	2.4	72
44	Autocorrelation of Molecular Electrostatic Potential Surface Properties Combined with Partial Least Squares Analysis as Alternative Attractive Tool to Generate Ligand-Based 3D-QSARs. Current Drug Discovery Technologies, 2005, 2, 13-21.	0.6	71
45	MMsINC: a large-scale chemoinformatics database. Nucleic Acids Research, 2009, 37, D284-D290.	6.5	71
46	Combined Target-Based and Ligand-Based Drug Design Approach as a Tool To Define a Novel 3D-Pharmacophore Model of Human A3 Adenosine Receptor Antagonists:â€‰ Pyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidine Derivatives as a Key Study. Journal of Medicinal Chemistry, 2005, 48, 152-162.	2.9	69
47	Interactions of Flavones and Other Phytochemicals with Adenosine Receptors. Advances in Experimental Medicine and Biology, 2002, 505, 163-171.	0.8	69
48	1,2,4-Triazolo[4,3-a]quinoxalin-1-one Moiety as an Attractive Scaffold To Develop New Potent and Selective Human A3Adenosine Receptor Antagonists:Â Synthesis, Pharmacological, and Ligandâ^'Receptor Modeling Studies. Journal of Medicinal Chemistry, 2004, 47, 3580-3590.	2.9	67
49	Protein kinase CK2 inhibitors: a patent review. Expert Opinion on Therapeutic Patents, 2012, 22, 1081-1097.	2.4	67
50	Exploring Protein-Peptide Recognition Pathways Using a Supervised Molecular Dynamics Approach. Structure, 2017, 25, 655-662.e2.	1.6	67
51	51V-NMR investigation on the formation of peroxo vanadium complexes in aqueous solution: Some novel observations. Journal of Molecular Catalysis, 1994, 94, 323-333.	1.2	66
52	1-Substituted pyrazolo[1,5-c]quinazolines as novel Gly/NMDA receptor antagonists: Synthesis, biological evaluation, and molecular modeling study. Bioorganic and Medicinal Chemistry, 2005, 13, 5536-5549.	1.4	64
53	The versatile chemistry of peroxo complexes of vanadium, molybdenum and tungsten as oxidants of organic compounds. Journal of Physical Organic Chemistry, 1996, 9, 329-336.	0.9	60
54	How druggable is protein kinase CK2?. Medicinal Research Reviews, 2010, 30, 419-462.	5.0	60

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55	Supervised Molecular Dynamics (SuMD) Insights into the mechanism of action of SARS-CoV-2 main protease inhibitor PF-07321332. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 1645-1649.	2.5	60
56	Flavonoid Derivatives as Adenosine Receptor Antagonists:Â A Comparison of the Hypothetical Receptor Binding Site Based on a Comparative Molecular Field Analysis Model. Journal of Medicinal Chemistry, 1998, 41, 46-52.	2.9	59
57	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
58	New 2-Arylpyrazolo[3,4-c]quinoline Derivatives as Potent and Selective Human A₃Adenosine Receptor Antagonists. Synthesis, Pharmacological Evaluation, and Ligandâ^'Receptor Modeling Studies. Journal of Medicinal Chemistry, 2007, 50, 4061-4074.	2.9	58
59	The Identification of the 2-Phenylphthalazin-1(2H)-one Scaffold as a New Decorable Core Skeleton for the Design of Potent and Selective Human A₃ Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 2011, 54, 2102-2113.	2.9	57
60	Chiral Resolution and Stereospecificity of 6-Phenyl-4-phenylethynyl- 1,4-dihydropyridines as Selective A3 Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 1999, 42, 3055-3065.	2.9	56
61	4-Amido-2-aryl-1,2,4-triazolo[4,3-a]quinoxalin-1-ones as New Potent and Selective Human A3Adenosine Receptor Antagonists. Synthesis, Pharmacological Evaluation, and Ligandâ^'Receptor Modeling Studies. Journal of Medicinal Chemistry, 2006, 49, 3916-3925.	2.9	56
62	Pyrazolo[4,3-e]-1,2,4-triazolo[1,5-c]pyrimidine Derivatives as Adenosine Receptor Antagonists. Influence of the N5 Substituent on the Affinity at the Human A3and A2BAdenosine Receptor Subtypes:Â A Molecular Modeling Investigation. Journal of Medicinal Chemistry, 2003, 46, 4287-4296.	2.9	55
63	Relationship between the Structure and the DNA Binding Properties of Diazoniapolycyclic Duplex- and Triplex-DNA Binders:â€‰ Efficiency, Selectivity, and Binding Mode. Biochemistry, 2007, 46, 12721-12736.	1.2	55
64	A High-Throughput Screening Identifies MICU1 Targeting Compounds. Cell Reports, 2020, 30, 2321-2331.e6.	2.9	54
65	Vanadium bromoperoxidases mimicking systems: Bromohydrins formation as evidence of the occurrence of a hypobromite-like vanadium complex. Tetrahedron Letters, 1995, 36, 2675-2678.	0.7	53
66	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
67	1,2,4-Triazolo[1,5-a]quinoxaline as a Versatile Tool for the Design of Selective Human A3 Adenosine Receptor Antagonists:â€‰ Synthesis, Biological Evaluation, and Molecular Modeling Studies of 2-(Hetero)aryl- and 2-Carboxy-Substitued Derivatives. Journal of Medicinal Chemistry, 2005, 48, 7932-7945.	2.9	52
68	Tuning the Activity of Zn(II) Complexes in DNA Cleavage: Clues for Design of New Efficient Metallo-Hydrolases. Inorganic Chemistry, 2008, 47, 5473-5484.	1.9	52
69	Molecular Modeling Studies of Human A3Adenosine Antagonists:â€‰ Structural Homology and Receptor Docking. Journal of Chemical Information and Computer Sciences, 1998, 38, 1239-1248.	2.8	51
70	Anthracyclines: recent developments in their separation and quantitation. Biomedical Applications, 2001, 764, 161-171.	1.7	51
71	2-Phenylpyrazolo[4,3-d]pyrimidin-7-one as a New Scaffold To Obtain Potent and Selective Human A₃ Adenosine Receptor Antagonists: New Insights into the Receptorâ^'Antagonist Recognition. Journal of Medicinal Chemistry, 2009, 52, 7640-7652.	2.9	51
72	Prevalence, Tumorigenic Role, and Biochemical Implications of Rare BRAF Alterations. Thyroid, 2014, 24, 809-819.	2.4	51

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73	Novel point mutation in a leucine-rich repeat of the GPIbÂ chain of the platelet von Willebrand factor receptor, GPIb/IX/V, resulting in an inherited dominant form of Bernard-Soulier syndrome affecting two unrelated families: the N41H variant. Haematologica, 2008, 93, 1743-1747.	1.7	50
74	Comparison of Multilabel and Single-Label Classification Applied to the Prediction of the Isoform Specificity of Cytochrome P450 Substrates. Journal of Chemical Information and Modeling, 2009, 49, 2588-2605.	2.5	50
75	Mechanism of Arene Hydroxylation by Vanadium Picolinato Peroxo Complexes. Journal of Organic Chemistry, 1994, 59, 6262-6267.	1.7	49
76	SAR and QSAR study on 2-aminothiazole derivatives, modulators of transcriptional repression in Huntingtonâ€™s disease. Bioorganic and Medicinal Chemistry, 2008, 16, 5695-5703.	1.4	49
77	Swimming into peptidomimetic chemical space using pepMMsMIMIC. Nucleic Acids Research, 2011, 39, W261-W269.	6.5	49
78	Studies directed toward the prediction of the oxidative reactivity of vanadium peroxo complexes in water. Correlations between the nature of the ligands and 51V-NMR chemical shifts. Journal of Molecular Catalysis A, 1995, 104, 159-169.	4.8	48
79	A mechanistic investigation of bromoperoxidases mimicking systems. Evidence of a hypobromite-like vanadium intermediate from experimental data and ab initio calculations. Journal of Molecular Catalysis A, 1996, 113, 175-184.	4.8	48
80	Structural Investigation of the 7-Chloro-3-hydroxy-1H-quinazoline-2,4-dione Scaffold to Obtain AMPA and Kainate Receptor Selective Antagonists. Synthesis, Pharmacological, and Molecular Modeling Studies. Journal of Medicinal Chemistry, 2006, 49, 6015-6026.	2.9	48
81	Urolithin as a Converging Scaffold Linking Ellagic acid and Coumarin Analogues: Design of Potent Protein Kinase CK2 Inhibitors. ChemMedChem, 2011, 6, 2273-2286.	1.6	47
82	Ligand-Based Drug Design Methodologies in Drug Discovery Process: An Overview. Current Drug Discovery Technologies, 2006, 3, 155-165.	0.6	46
83	Pharmaceutical Perspectives of Nonlinear QSAR Strategies. Journal of Chemical Information and Modeling, 2010, 50, 961-978.	2.5	46
84	Discovery of novel A3 adenosine receptor ligands based on chromone scaffold. Biochemical Pharmacology, 2012, 84, 21-29.	2.0	46
85	Targeting the coronavirus SARS-CoV-2: computational insights into the mechanism of action of the protease inhibitors lopinavir, ritonavir and nelfinavir. Scientific Reports, 2020, 10, 20927.	1.6	44
86	Nature of the Radical Intermediates in the Decomposition of Peroxovanadium Species in Protic and Aprotic Media. Inorganic Chemistry, 1994, 33, 1631-1637.	1.9	43
87	Synthesis of brominated compounds. A convenient molybdenum- catalyzed procedure inspired by the mode of action of haloperoxidases. Tetrahedron Letters, 1996, 37, 8609-8612.	0.7	42
88	Modeling ligand recognition at the P2Y12 receptor in light of X-ray structural information. Journal of Computer-Aided Molecular Design, 2015, 29, 737-756.	1.3	42
89	DNA Topoisomerase II Structures and Anthracycline Activity: Insights into Ternary Complex Formation. Current Pharmaceutical Design, 2007, 13, 2766-2780.	0.9	41
90	The Significance of 2-Furyl Ring Substitution with a 2-(para-substituted) Aryl Group in a New Series of Pyrazolo-triazolo-pyrimidines as Potent and Highly Selective hA₃ Adenosine Receptors Antagonists: New Insights into Structureâ^'Affinity Relationship and Receptorâ^'Antagonist Recognition. Journal of Medicinal Chemistry, 2010, 53, 3361-3375.	2.9	40

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91	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
92	Advances in Computational Techniques to Study GPCRâ€“Ligand Recognition. Trends in Pharmacological Sciences, 2015, 36, 878-890.	4.0	40
93	Interaction Model for Anthracycline Activity against DNA Topoisomerase IIâ€. Biochemistry, 2004, 43, 7503-7513.	1.2	39
94	Identification of novel protein kinase CK1 delta (CK1Î´) inhibitors through structure-based virtual screening. Bioorganic and Medicinal Chemistry Letters, 2008, 18, 5672-5675.	1.0	39
95	Demystifying the three dimensional structure of G protein-coupled receptors (GPCRs) with the aid of molecular modeling. Chemical Communications, 2003, , 2949.	2.2	38
96	Autocorrelation of Molecular Electrostatic Potential Surface Properties Combined with Partial Least Squares Analysis as New Strategy for the Prediction of the Activity of Human A3Adenosine Receptor Antagonists. Journal of Medicinal Chemistry, 2005, 48, 5698-5704.	2.9	38
97	Highlights on the Development of A2A Adenosine Receptor Agonists and Antagonists. ChemMedChem, 2007, 2, 260-281.	1.6	38
98	Synthesis, ligandâ€“receptor modeling studies and pharmacological evaluation of novel 4-modified-2-aryl-1,2,4-triazolo[4,3-a]quinoxalin-1-one derivatives as potent and selective human A3 adenosine receptor antagonists. Bioorganic and Medicinal Chemistry, 2008, 16, 6086-6102.	1.4	38
99	The A₃ adenosine receptor as multifaceted therapeutic target: pharmacology, medicinal chemistry, and in silico approaches. Medicinal Research Reviews, 2013, 33, 235-335.	5.0	38
100	Fluorosulfonyl- and Bis-(Î²-chloroethyl)amino-phenylamino Functionalized Pyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidine Derivatives:â€‰ Irreversible Antagonists at the Human A3 Adenosine Receptor and Molecular Modeling Studies. Journal of Medicinal Chemistry, 2001, 44, 2735-2742.	2.9	37
101	Vanadium-Bromoperoxidase-Mimicking Systems: Direct Evidence of a Hypobromite-Like Vanadium Intermediate. European Journal of Inorganic Chemistry, 2003, 2003, 42-46.	1.0	37
102	Investigation of Streptomyces antibioticus tyrosinase reactivity toward chlorophenols. Archives of Biochemistry and Biophysics, 2011, 505, 67-74.	1.4	37
103	The Dark Side of Protein Kinase CK2 Inhibition. Current Medicinal Chemistry, 2011, 18, 2867-2884.	1.2	37
104	Design, Synthesis, and Structureâ€“Activity Relationships of Azolylmethylpyrroloquinolines as Nonsteroidal Aromatase Inhibitors. Journal of Medicinal Chemistry, 2013, 56, 7536-7551.	2.9	37
105	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
106	Pyrido[2,3-e]-1,2,4-triazolo[4,3-a]pyrazin-1-one as a New Scaffold To Develop Potent and Selective Human A3 Adenosine Receptor Antagonists. Synthesis, Pharmacological Evaluation, and Ligandâ^'Receptor Modeling Studies. Journal of Medicinal Chemistry, 2009, 52, 2407-2419.	2.9	35
107	Hydroxylation of aromatics with hydrogen peroxide catalyzed by vanadium (V) peroxocomplexes. Journal of Molecular Catalysis, 1993, 83, 107-116.	1.2	34
108	The chemistry of peroxovanadium species in aqueous solutions. Structure and reactivity of a neutral diperoxovanadium complex as provided by 51V-NMR data, ab initio calculations and kinetic results. Journal of Molecular Catalysis A, 1997, 120, 93-99.	4.8	34

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109	A3 adenosine receptors: Protective vs. damaging effects identified using novel agonists and antagonists. , 1998, 45, 113-124.		34
110	GTP-dependent packing of a three-helix bundle is required for atlastin-mediated fusion. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 16283-16288.	3.3	34
111	A theoretical and experimental investigation of the electrophilic oxidation of thioethers and sulfoxides by peroxides. Tetrahedron, 1995, 51, 12363-12372.	1.0	33
112	Use of electrospray ionization mass spectrometry to characterize chiral reactive intermediates in a titanium alkoxide mediated sulfoxidation reaction. Chemical Communications, 1997, , 869-870.	2.2	33
113	Solvation, preferential solvation and complexation by the solvent of peroxovanadium complexes studied by 51V NMR spectroscopy. Correlations with the oxidative reactivity. Inorganica Chimica Acta, 1998, 272, 62-67.	1.2	33
114	2-Aryl-8-chloro-1,2,4-triazolo[1,5-a]quinoxalin-4-amines as highly potent A1 and A3 adenosine receptor antagonists. Bioorganic and Medicinal Chemistry, 2005, 13, 705-715.	1.4	33
115	Flavonoids Diosmetin and Hesperetin are Potent Inhibitors of Cytochrome P450 2C9-mediated Drug Metabolism in vitro. Drug Metabolism and Pharmacokinetics, 2010, 25, 466-476.	1.1	33
116	Novel fluorescent antagonist as a molecular probe in A3 adenosine receptor binding assays using flow cytometry. Biochemical Pharmacology, 2012, 83, 1552-1561.	2.0	33
117	Histidine-Containing Bisperoxovanadium(V) Compounds: Insight Into the Solution Structure by an ESI-MS and51V-NMR Comparative Study. European Journal of Inorganic Chemistry, 1999, 1999, 1489-1495.	1.0	32
118	The Furoxan System: Design of Selective Nitric Oxide (NO) Donor Inhibitors of COX-2 Endowed with Anti-Aggregatory and Vasodilating Activities. Chemistry and Biodiversity, 2005, 2, 886-900.	1.0	32
119	A2B Adenosine Receptor Antagonists: Recent Developments. Mini-Reviews in Medicinal Chemistry, 2005, 5, 1053-1060.	1.1	32
120	Novel Strategies for the Design of New Potent and Selective Human A3 Receptor Antagonists: An Update. Current Medicinal Chemistry, 2006, 13, 639-645.	1.2	32
121	Amide bond direction modulates G-quadruplex recognition and telomerase inhibition by 2,6 and 2,7 bis-substituted anthracenedione derivatives. Bioorganic and Medicinal Chemistry, 2008, 16, 354-361.	1.4	31
122	Prediction of the aqueous solvation free energy of organic compounds by using autocorrelation of molecular electrostatic potential surface properties combined with response surface analysis. Bioorganic and Medicinal Chemistry, 2008, 16, 5733-5742.	1.4	31
123	3-Hydroxy-1H-quinazoline-2,4-dione derivatives as new antagonists at ionotropic glutamate receptors: Molecular modeling and pharmacological studies. European Journal of Medicinal Chemistry, 2012, 54, 470-482.	2.6	31
124	Scouting Human A3 Adenosine Receptor Antagonist Binding Mode Using a Molecular Simplification Approach: From Triazoloquinoxaline to a Pyrimidine Skeleton as a Key Study. Journal of Medicinal Chemistry, 2007, 50, 6596-6606.	2.9	30
125	Linear and Nonlinear 3D-QSAR Approaches in Tandem with Ligand-Based Homology Modeling as a Computational Strategy To Depict the Pyrazolo-Triazolo-Pyrimidine Antagonists Binding Site of the Human Adenosine A_{2A} Receptor. Journal of Chemical Information and Modeling, 2008, 48, 350-363.	2.5	30
126	Synthesis and Biological Evaluation of a New Series of 1,2,4-Triazolo[1,5-a]-1,3,5-triazines as Human A_{2A} Adenosine Receptor Antagonists with Improved Water Solubility. Journal of Medicinal Chemistry, 2011, 54, 877-889.	2.9	30

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128	Estimation of kinetic and thermodynamic ligand-binding parameters using computational strategies. Future Medicinal Chemistry, 2017, 9, 507-523.	1.1	30
129	The application of a 3D-QSAR (autoMEP/PLS) approach as an efficient pharmacodynamic-driven filtering method for small-sized virtual library: Application to a lead optimization of a human A3 adenosine receptor antagonist. Bioorganic and Medicinal Chemistry, 2006, 14, 4923-4932.	1.4	29
130	In Silico Binding Free Energy Predictability by Using the Linear Interaction Energy (LIE) Method:â€‰Bromobenzimidazole CK2 Inhibitors as a Case Study. Journal of Chemical Information and Modeling, 2007, 47, 572-582.	2.5	29
131	Synthesis and pharmacological characterization of a new series of 5,7-disubstituted-[1,2,4]triazolo[1,5-a][1,3,5]triazine derivatives as adenosine receptor antagonists: A preliminary inspection of ligandâ€“receptor recognition process. Bioorganic and Medicinal Chemistry, 2010, 18, 2524-2536.	1.4	29
132	Adenosiland: Walking through adenosine receptors landscape. European Journal of Medicinal Chemistry, 2012, 58, 248-257.	2.6	29
133	AquaMMapS: An Alternative Tool to Monitor the Role of Water Molecules During Proteinâ€“Ligand Association. ChemMedChem, 2018, 13, 522-531.	1.6	29
134	The rise of molecular simulations in fragment-based drug design (FBDD): an overview. Drug Discovery Today, 2020, 25, 1693-1701.	3.2	29
135	Correlation between one-electron reduction and oxygen-oxygen bond strength in d0 transition metal peroxo complexes. Inorganic Chemistry, 1993, 32, 5797-5799.	1.9	28
136	Direct Evidence of Solvent-Peroxovanadium Clusters by Electrospray Ionization Mass Spectrometry. European Journal of Inorganic Chemistry, 1998, 1998, 1193-1197.	1.0	28
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