Stefano Moro

List of Publications by Year in Descending Order

304 papers	10,674 citations	55 h-index	86 g-index
339 ext. papers	11,846 ext. citations	5.4 avg, IF	6.19 L-index

#	Paper	IF	Citations
304	Re-Exploring the Ability of Common Docking Programs to Correctly Reproduce the Binding Modes of Non-Covalent Inhibitors of SARS-CoV-2 Protease M.. *Pharmaceuticals*, **2022**, 15,	5.2	4
303	Computationally driven discovery of SARS-CoV-2 M inhibitors: from design to experimental validation.. *Chemical Science*, **2022**, 13, 3674-3687	9.4	2
302	A new inactive conformation of SARS-CoV-2 main protease.. *Acta Crystallographica Section D: Structural Biology*, **2022**, 78, 363-378	5.5	5
301	Bat coronaviruses related to SARS-CoV-2: what about their 3CL proteases (MPro)?. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2022**, 37, 1077-1082	5.6	2
300	Developing novel classes of protein kinase CK1 inhibitors by fusing [1,2,4]triazole with different bicyclic heteroaromatic systems. *European Journal of Medicinal Chemistry*, **2021**, 216, 113331	6.8	3
299	Amphiphilic peptide-based MMP3 inhibitors for intra-articular treatment of knee OA. *Bioorganic and Medicinal Chemistry*, **2021**, 38, 116132	3.4	0
298	Inspecting the Mechanism of Fragment Hits Binding on SARS-CoV-2 M by Using Supervised Molecular Dynamics (SuMD) Simulations. *ChemMedChem*, **2021**, 16, 2075-2081	3.7	6
297	On the mechanism of tumor cell entry of aloe-emodin, a natural compound endowed with anticancer activity. *International Journal of Cancer*, **2021**, 149, 1129-1136	7.5	1
296	HT-SuMD: making molecular dynamics simulations suitable for fragment-based screening. A comparative study with NMR. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2021**, 36, 1-14	5.6	6
295	Potent and selective A adenosine receptor antagonists bearing aminoesters as heterobifunctional moieties. *RSC Medicinal Chemistry*, **2021**, 12, 254-262	3.5	
294	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, 1646-1650	5.6	22
293	Shedding Light on the Molecular Recognition of Sub-Kilodalton Macrocyclic Peptides on Thrombin by Supervised Molecular Dynamics. *Frontiers in Molecular Biosciences*, **2021**, 8, 707661	5.6	2
292	A Computational Workflow for the Identification of Novel Fragments Acting as Inhibitors of the Activity of Protein Kinase CK1 *International Journal of Molecular Sciences*, **2021**, 22,	6.3	5
291	Pyridazinones containing dithiocarbamoyl moieties as a new class of selective MAO-B inhibitors. *Bioorganic Chemistry*, **2021**, 115, 105203	5.1	1
290	Comparing Fragment Binding Poses Prediction Using HSP90 as a Key Study: When Bound Water Makes the Difference. *Molecules*, **2020**, 25,	4.8	2
289	New Insights into Key Determinants for Adenosine 1 Receptor Antagonists Selectivity Using Supervised Molecular Dynamics Simulations. *Biomolecules*, **2020**, 10,	5.9	3
288	A Deep-Learning Approach toward Rational Molecular Docking Protocol Selection. *Molecules*, **2020**, 25,	4.8	6

287	Exploring the RNA-Recognition Mechanism Using Supervised Molecular Dynamics (SuMD) Simulations: Toward a Rational Design for Ribonucleic-Targeting Molecules?. *Frontiers in Chemistry*, **2020**, 8, 107	5	6
286	A Supervised Molecular Dynamics Approach to Unbiased Ligand-Protein Unbinding. *Journal of Chemical Information and Modeling*, **2020**, 60, 1804-1817	6.1	14
285	The rise of molecular simulations in fragment-based drug design (FBDD): an overview. *Drug Discovery Today*, **2020**, 25, 1693-1701	8.8	10
284	A High-Throughput Screening Identifies MICU1 Targeting Compounds. *Cell Reports*, **2020**, 30, 2321-2331.e6	8.6	25
283	Halogen Bonds in Ligand-Protein Systems: Molecular Orbital Theory for Drug Design. *Journal of Chemical Information and Modeling*, **2020**, 60, 1317-1328	6.1	13
282	Scaffold Repurposing of in-House Chemical Library toward the Identification of New Casein Kinase 1 Inhibitors. *ACS Medicinal Chemistry Letters*, **2020**, 11, 1168-1174	4.3	2
281	A and A adenosine receptors: The extracellular loop 2 determines high (A) or low affinity (A) for adenosine. *Biochemical Pharmacology*, **2020**, 172, 113718	6	16
280	Conjugable A adenosine receptor antagonists for the development of functionalized ligands and their use in fluorescent probes. *European Journal of Medicinal Chemistry*, **2020**, 186, 111886	6.8	5
279	Targeting G Protein-Coupled Receptors with Magnetic Carbon Nanotubes: The Case of the A Adenosine Receptor. *ChemMedChem*, **2020**, 15, 1909-1920	3.7	2
278	Novel coumarin-pyridazine hybrids as selective MAO-B inhibitors for the Parkinson disease therapy. *Bioorganic Chemistry*, **2020**, 104, 104203	5.1	10
277	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	4.9	27
276	Evaluating the effects of fluorine on biological properties and metabolic stability of some antitubulin 3-substituted 7-phenyl-pyrroloquinolinones. *European Journal of Medicinal Chemistry*, **2019**, 178, 297-314	6.8	7
275	Peeking at G-protein-coupled receptors through the molecular dynamics keyhole. *Future Medicinal Chemistry*, **2019**, 11, 599-615	4.1	8
274	A Comparison in the Use of the Crystallographic Structure of the Human A1 or the A2A Adenosine Receptors as a Template for the Construction of a Homology Model of the A3 Subtype. *Applied Sciences (Switzerland)*, **2019**, 9, 821	2.6	4
273	Deciphering the Molecular Recognition Mechanism of Multidrug Resistance NorA Efflux Pump Using a Supervised Molecular Dynamics Approach. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	9
272	Ciprofloxacin and levofloxacin attenuate microglia inflammatory response via TLR4/NF-kB pathway. *Journal of Neuroinflammation*, **2019**, 16, 148	10.1	115
271	Can We Still Trust Docking Results? An Extension of the Applicability of DockBench on PDBbind Database. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	7
270	Revisiting the Allosteric Regulation of Sodium Cation on the Binding of Adenosine at the Human A Adenosine Receptor: Insights from Supervised Molecular Dynamics (SuMD) Simulations. *Molecules*, **2019**, 24,	4.8	6

269	Rethinking to riluzole mechanism of action: the molecular link among protein kinase CK1δ activity, TDP-43 phosphorylation, and amyotrophic lateral sclerosis pharmacological treatment. *Neural Regeneration Research*, **2019**, 14, 2083-2085	4.5	8
268	Pyrazolo[4,3-][1,2,4]triazolo[1,5-]pyrimidines to develop functionalized ligands to target adenosine receptors: fluorescent ligands as an example. *MedChemComm*, **2019**, 10, 1094-1108	5	4
267	Coupling Supervised Molecular Dynamics (SuMD) with Entropy Estimations To Shine Light on the Stability of Multiple Binding Sites. *ACS Medicinal Chemistry Letters*, **2019**, 10, 444-449	4.3	3
266	A Triazolotriazine-Based Dual GSK-3β/CK-1δ Ligand as a Potential Neuroprotective Agent Presenting Two Different Mechanisms of Enzymatic Inhibition. *ChemMedChem*, **2019**, 14, 310-314	3.7	16
265	Matrix metalloprotease 3 (MMP3) inhibition effect of a viscosupplement based on a hyaluronic acid amide derivative (HYADD4). *Osteoarthritis and Cartilage*, **2018**, 26, S286-S287	6.2	2
264	Discovery of 2-aminoimidazole and 2-amino imidazolyl-thiazoles as non-xanthine human adenosine A receptor antagonists: SAR and molecular modeling studies. *MedChemComm*, **2018**, 9, 676-684	5	2
263	Combining self- and cross-docking as benchmark tools: the performance of DockBench in the D3R Grand Challenge 2. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 251-264	4.2	17
262	Supervised Molecular Dynamics (SuMD) Approaches in Drug Design. *Methods in Molecular Biology*, **2018**, 1824, 287-298	1.4	9
261	[1,2,4]Triazolo[1,5-c]pyrimidines as adenosine receptor antagonists: Modifications at the 8 position to reach selectivity towards A adenosine receptor subtype. *European Journal of Medicinal Chemistry* , **2018**, 157, 837-851	6.8	8
260	AquaMMapS: An Alternative Tool to Monitor the Role of Water Molecules During Protein-Ligand Association. *ChemMedChem*, **2018**, 13, 522-531	3.7	17
259	Targeting tubulin polymerization by novel 7-aryl-pyrroloquinolinones: Synthesis, biological activity and SARs. *European Journal of Medicinal Chemistry*, **2018**, 143, 244-258	6.8	7
258	Molecular Dynamics Applications to GPCR Ligand Design. *Methods and Principles in Medicinal Chemistry*, **2018**, 225-246	0.4	
257	Bridging Molecular Docking to Molecular Dynamics in Exploring Ligand-Protein Recognition Process: An Overview. *Frontiers in Pharmacology*, **2018**, 9, 923	5.6	210
256	Targeting Protein Kinase CK1δ with Riluzole: Could It Be One of the Possible Missing Bricks to Interpret Its Effect in the Treatment of ALS from a Molecular Point of View?. *ChemMedChem*, **2018**, 13, 2601-2605	3.7	10
255	Could the presence of sodium ion influence the accuracy and precision of the ligand-posing in the human A adenosine receptor orthosteric binding site using a molecular docking approach? Insights from Dockbench. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 1337-1346	4.2	6
254	Could Adenosine Recognize its Receptors with a Stoichiometry Other than 1 : 1?. *Molecular Informatics*, **2018**, 37, e1800009	3.8	5
253	The role of 5-arylalkylamino- and 5-piperazino- moieties on the 7-aminopyrazolo[4,3-d]pyrimidine core in affecting adenosine A and A receptor affinity and selectivity profiles. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2017**, 32, 248-263	5.6	14
252	Phenolic 1,3-diketones attenuate lipopolysaccharide-induced inflammatory response by an alternative magnesium-mediated mechanism. *British Journal of Pharmacology*, **2017**, 174, 1090-1103	8.6	18

251	Conjugates between minor groove binders and Zn(II)-tach complexes: Synthesis, characterization, and interaction with plasmid DNA. *Tetrahedron*, **2017**, 73, 3014-3024	2.4	5
250	Comparison of the Human A Adenosine Receptor Recognition by Adenosine and Inosine: New Insight from Supervised Molecular Dynamics Simulations. *ChemMedChem*, **2017**, 12, 1319-1326	3.7	22
249	Estimation of kinetic and thermodynamic ligand-binding parameters using computational strategies. *Future Medicinal Chemistry*, **2017**, 9, 507-523	4.1	21
248	Exploring Protein-Peptide Recognition Pathways Using a Supervised Molecular Dynamics Approach. *Structure*, **2017**, 25, 655-662.e2	5.2	41
247	Sulfonamido-derivatives of unsubstituted carbazoles as BACE1 inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2017**, 27, 4812-4816	2.9	7
246	Synthesis, structure-activity relationships and biological evaluation of 7-phenyl-pyrroloquinolinone 3-amide derivatives as potent antimitotic agents. *European Journal of Medicinal Chemistry*, **2017**, 127, 643-660	6.8	12
245	Impact of protein-ligand solvation and desolvation on transition state thermodynamic properties of adenosine A ligand binding kinetics. *In Silico Pharmacology*, **2017**, 5, 16	4.3	15
244	Supporting the Identification of Novel Fragment-Based Positive Allosteric Modulators Using a Supervised Molecular Dynamics Approach: A Retrospective Analysis Considering the Human A2A Adenosine Receptor as a Key Example. *Molecules*, **2017**, 22,	4.8	15
243	Synthesis and preliminary structure-activity relationship study of 2-aryl-2H-pyrazolo[4,3-c]quinolin-3-ones as potential checkpoint kinase 1 (Chk1) inhibitors. *Journal of Enzyme Inhibition and Medicinal Chemistry*, **2017**, 33, 171-183	5.6	5
242	In Silico 3D Modeling of Binding Activities. *Methods in Molecular Biology*, **2016**, 1425, 23-35	1.4	3
241	New Trends in Inspecting GPCR-ligand Recognition Process: the Contribution of the Molecular Modeling Section (MMS) at the University of Padova. *Molecular Informatics*, **2016**, 35, 440-8	3.8	3
240	DockBench as docking selector tool: the lesson learned from D3R Grand Challenge 2015. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 773-789	4.2	10
239	Deciphering the Complexity of Ligand-Protein Recognition Pathways Using Supervised Molecular Dynamics (SuMD) Simulations. *Journal of Chemical Information and Modeling*, **2016**, 56, 687-705	6.1	64
238	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	6.8	16
237	Structural refinement of pyrazolo[4,3-d]pyrimidine derivatives to obtain highly potent and selective antagonists for the human A3 adenosine receptor. *European Journal of Medicinal Chemistry*, **2016**, 108, 117-133	6.8	16
236	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	3	10
235	Synthesis, biological evaluation and molecular modeling studies of phthalazin-1(2H)-one derivatives as novel cholinesterase inhibitors. *RSC Advances*, **2016**, 6, 46170-46185	3.7	15
234	Modeling ligand recognition at the P2Y12 receptor in light of X-ray structural information. *Journal of Computer-Aided Molecular Design*, **2015**, 29, 737-56	4.2	34

233	Exploring the recognition pathway at the human A2A adenosine receptor of the endogenous agonist adenosine using supervised molecular dynamics simulations. *MedChemComm*, **2015**, 6, 1081-1085	5	29
232	Advances in Computational Techniques to Study GPCR-Ligand Recognition. *Trends in Pharmacological Sciences*, **2015**, 36, 878-890	13.2	31
231	Novel 3-Substituted 7-Phenylpyrrolo[3,2-f]quinolin-9(6H)-ones as Single Entities with Multitarget Antiproliferative Activity. *Journal of Medicinal Chemistry*, **2015**, 58, 7991-8010	8.3	20
230	The xylanase inhibitor TAXI-III counteracts the necrotic activity of a Fusarium graminearum xylanase in vitro and in durum wheat transgenic plants. *Molecular Plant Pathology*, **2015**, 16, 583-92	5.7	13
229	Novel insights on the DNA interaction of calicheamicin (I). *Biopolymers*, **2015**, 103, 449-59	2.2	3
228	NMR-Assisted Molecular Docking Methodologies. *Molecular Informatics*, **2015**, 34, 513-25	3.8	11
227	DockBench: An Integrated Informatic Platform Bridging the Gap between the Robust Validation of Docking Protocols and Virtual Screening Simulations. *Molecules*, **2015**, 20, 9977-93	4.8	33
226	ALK kinase domain mutations in primary anaplastic large cell lymphoma: consequences on NPM-ALK activity and sensitivity to tyrosine kinase inhibitors. *PLoS ONE*, **2015**, 10, e0121378	3.7	6
225	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, 4065-71	3.4	43
224	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	3.7	5
223	Bridging molecular docking to membrane molecular dynamics to investigate GPCR-ligand recognition: the human A□A adenosine receptor as a key study. *Journal of Chemical Information and Modeling*, **2014**, 54, 169-83	6.1	54
222	Prevalence, tumorigenic role, and biochemical implications of rare BRAF alterations. *Thyroid*, **2014**, 24, 809-19	6.2	42
221	7-Amino-2-phenylpyrazolo[4,3-d]pyrimidine derivatives: structural investigations at the 5-position to target human A□and A(2A) adenosine receptors. Molecular modeling and pharmacological studies. *European Journal of Medicinal Chemistry*, **2014**, 84, 614-27	6.8	22
220	Advances in GPCR modeling evaluated by the GPCR Dock 2013 assessment: meeting new challenges. *Structure*, **2014**, 22, 1120-1139	5.2	136
219	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 structure-activity relationship study. *Journal of Medicinal Chemistry*, **2014**, 57, 6210-25	8.3	10
218	Perturbation of fluid dynamics properties of water molecules during G protein-coupled receptor-ligand recognition: the human A2A adenosine receptor as a key study. *Journal of Chemical Information and Modeling*, **2014**, 54, 2846-55	6.1	23
217	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, 2243-54	6.1	22
216	Supervised molecular dynamics (SuMD) as a helpful tool to depict GPCR-ligand recognition pathway in a nanosecond time scale. *Journal of Chemical Information and Modeling*, **2014**, 54, 372-6	6.1	97

215	Carboxylation-dependent conformational changes of human osteocalcin. *Frontiers in Bioscience - Landmark*, **2014**, 19, 1105-16	2.8	10
214	Evaluation of the steric impact of flavin adenine dinucleotide in Drosophila melanogaster cryptochrome function. *Biochemical and Biophysical Research Communications*, **2014**, 450, 1606-11	3.4	3
213	Leukaemic cells from chronic lymphocytic leukaemia patients undergo apoptosis following microtubule depolymerization and Lyn inhibition by nocodazole. *British Journal of Haematology*, **2014**, 165, 659-72	4.5	17
212	The A3 adenosine receptor as multifaceted therapeutic target: pharmacology, medicinal chemistry, and in silico approaches. *Medicinal Research Reviews*, **2013**, 33, 235-335	14.4	35
211	In silico investigation of PHD-3 specific HIF1-α proline 567 hydroxylation: a new player in the VHL/HIF-1α interaction pathway?. *FEBS Letters*, **2013**, 587, 2996-3001	3.8	10
210	The mitochondrial calcium uniporter is a multimer that can include a dominant-negative pore-forming subunit. *EMBO Journal*, **2013**, 32, 2362-76	13	326
209	MMsDusty: an Alternative InChI-Based Tool to Minimize Chemical Redundancy. *Molecular Informatics*, **2013**, 32, 681-4	3.8	2
208	Implementing the "Best Template Searching" tool into Adenosiland platform. *In Silico Pharmacology*, **2013**, 1, 25	4.3	10
207	Design, synthesis, and structure-activity relationships of azolylmethylpyrroloquinolines as nonsteroidal aromatase inhibitors. *Journal of Medicinal Chemistry*, **2013**, 56, 7536-51	8.3	32
206	Molecular docking methodologies. *Methods in Molecular Biology*, **2013**, 924, 339-60	1.4	11
205	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, 2256-69	8.3	24
204	Fluorescent ligands for adenosine receptors. *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 26-36	2.9	27
203	Revisiting a receptor-based pharmacophore hypothesis for human A(2A) adenosine receptor antagonists. *Journal of Chemical Information and Modeling*, **2013**, 53, 1620-37	6.1	12
202	New insight into adenosine receptors selectivity derived from a novel series of [5-substituted-4-phenyl-1,3-thiazol-2-yl] benzamides and furamides. *European Journal of Medicinal Chemistry*, **2013**, 63, 924-34	6.8	25
201	Kinase CK2 inhibition: an update. *Current Medicinal Chemistry*, **2013**, 20, 671-93	4.3	84
200	Functional significance of the novel H-RAS gene mutation M72I in a patient with medullary thyroid cancer. *Experimental and Clinical Endocrinology and Diabetes*, **2013**, 121, 546-50	2.3	6
199	β2 -Glycoprotein I binds to thrombin and selectively inhibits the enzyme procoagulant functions. *Journal of Thrombosis and Haemostasis*, **2013**, 11, 1093-102	15.4	21
198	Conformational Changes of Congenital FVII Variants with Defective Binding to Tissue Factor ARG304GLN (FVII Padua), ARG 304TRP (FVII Nagoya) and ARG79GLN (FVII Shinjo or Tondabayashi). *International Journal of Biomedical Science*, **2013**, 9, 185-93		1

197	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	6	93
196	Novel fluorescent antagonist as a molecular probe in A(3) adenosine receptor binding assays using flow cytometry. *Biochemical Pharmacology*, **2012**, 83, 1552-61	6	28
195	Discovery of novel A3 adenosine receptor ligands based on chromone scaffold. *Biochemical Pharmacology*, **2012**, 84, 21-9	6	41
194	A cluster of factor XI-deficient patients due to a new mutation (Ile 436 Lys) in northeastern Italy. *European Journal of Haematology*, **2012**, 88, 229-36	3.8	4
193	Mimicking Peptides In Silico. *Molecular Informatics*, **2012**, 31, 12-20	3.8	19
192	Adenosiland: walking through adenosine receptors landscape. *European Journal of Medicinal Chemistry*, **2012**, 58, 248-57	6.8	27
191	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 a(3) adenosine receptor antagonists. *Journal of Medicinal Chemistry*, **2012**, 55, 9654-68	8.3	16
190	Protein kinase CK2 inhibitors: a patent review. *Expert Opinion on Therapeutic Patents*, **2012**, 22, 1081-97	6.8	56
189	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, 470-82	6.8	28
188	Ellagic acid and polyhydroxylated urolithins are potent catalytic inhibitors of human topoisomerase II: an in vitro study. *Journal of Agricultural and Food Chemistry*, **2012**, 60, 9162-70	5.7	22
187	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, 2102-13	8.3	50
186	USP15 is a deubiquitylating enzyme for receptor-activated SMADs. *Nature Cell Biology*, **2011**, 13, 1368-75	23.4	155
185	Investigation of Streptomyces antibioticus tyrosinase reactivity toward chlorophenols. *Archives of Biochemistry and Biophysics*, **2011**, 505, 67-74	4.1	33
184	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, 877-89	8.3	30
183	Does the combination of optimal substitutions at the C, N and N positions of the pyrazolo-triazolo-pyrimidine scaffold guarantee selective modulation of the human A adenosine receptors?. *Bioorganic and Medicinal Chemistry*, **2011**, 19, 6120-34	3.4	10
182	Carbazole-containing arylcarboxamides as BACE1 inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2011**, 21, 6657-61	2.9	17
181	A Novel Generalized 3D-QSAR Model of Camptothecin Analogs. *Molecular Informatics*, **2011**, 30, 927-38	3.8	2
180	The role of the N-terminal domain in the regulation of the "constitutively active" conformation of protein kinase CK2 insight from a molecular dynamics investigation. *ChemMedChem*, **2011**, 6, 1207-16	3.7	5

179	Urolithin as a converging scaffold linking ellagic acid and coumarin analogues: design of potent protein kinase CK2 inhibitors. *ChemMedChem*, **2011**, 6, 2273-86	3.7	41
178	ClickMD: an intuitive web-oriented molecular dynamics platform. *Future Medicinal Chemistry*, **2011**, 3, 923-31	4.1	4
177	The dark side of protein kinase CK2 inhibition. *Current Medicinal Chemistry*, **2011**, 18, 2867-84	4.3	30
176	Swimming into peptidomimetic chemical space using pepMMsMIMIC. *Nucleic Acids Research*, **2011**, 39, W261-9	20.1	38
175	Inhibitory effects of glycosaminoglycans on basal and stimulated transforming growth factor-1 expression in mesangial cells: biochemical and structural considerations. *Glycobiology*, **2011**, 21, 1029-37	5.8	4
174	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, 16283-8	11.5	26
173	Inhibition of cytochrome P450 2C8-mediated drug metabolism by the flavonoid diosmetin. *Drug Metabolism and Pharmacokinetics*, **2011**, 26, 559-68	2.2	14
172	Receptor-driven identification of novel human A adenosine receptor antagonists as potential therapeutic agents. *Methods in Enzymology*, **2010**, 485, 225-44	1.7	7
171	Pharmaceutical perspectives of nonlinear QSAR strategies. *Journal of Chemical Information and Modeling*, **2010**, 50, 961-78	6.1	42
170	Flavonoids diosmetin and hesperetin are potent inhibitors of cytochrome P450 2C9-mediated drug metabolism in vitro. *Drug Metabolism and Pharmacokinetics*, **2010**, 25, 466-76	2.2	26
169	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 hA(3) adenosine receptors antagonists: new insights into structure-affinity relationship and receptor-antagonist recognition. *Journal of Medicinal Chemistry*, **2010**, 53, 3361-75	8.3	36
168	Rational design, synthesis, and DNA binding properties of novel sequence-selective peptidyl congeners of ametantrone. *ChemMedChem*, **2010**, 5, 1080-91	3.7	13
167	Structure-activity relationship study of 16 a-thiocamptothecins: an integrated in vitro and in silico approach. *ChemMedChem*, **2010**, 5, 2006-15	3.7	5
166	How druggable is protein kinase CK2?. *Medicinal Research Reviews*, **2010**, 30, 419-62	14.4	55
165	Support Vector Machine (SVM) as Alternative Tool to Assign Acute Aquatic Toxicity Warning Labels to Chemicals. *Molecular Informatics*, **2010**, 29, 51-64	3.8	10
164	A novel glucosyltransferase from Catharanthus roseus cell suspensions. *Process Biochemistry*, **2010**, 45, 655-659	4.8	7
163	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 ligand-receptor recognition process. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 2524-36	3.4	29
162	BACE1 inhibitory activities of enantiomerically pure, variously substituted N-(3-(4-benzhydrylpiperazin-1-yl)-2-hydroxypropyl) arylsulfonamides. *Bioorganic and Medicinal Chemistry*, **2010**, 18, 7991-6	3.4	5

161	Fingerprint-based detection of acute aquatic toxicity. *Journal of Cheminformatics*, **2010**, 2,	8.6	78
160	Molecular Modeling and Reengineering of A3 Adenosine Receptors **2010**, 149-161		
159	Novel camptothecin derivatives as topoisomerase I inhibitors. *Expert Opinion on Therapeutic Patents*, **2009**, 19, 555-74	6.8	58
158	MMsINC: a large-scale chemoinformatics database. *Nucleic Acids Research*, **2009**, 37, D284-90	20.1	58
157	Combining selectivity and affinity predictions using an integrated Support Vector Machine (SVM) approach: An alternative tool to discriminate between the human adenosine A(2A) and A(3) receptor pyrazolo-triazolo-pyrimidine antagonists binding sites. *Bioorganic and Medicinal Chemistry*, **2009**, 17, 5259-74	3.4	22
156	A novel splicing variant encoding putative catalytic alpha subunit of maize protein kinase CK2. *Physiologia Plantarum*, **2009**, 136, 251-63	4.6	4
155	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 ligand-receptor modeling studies. *Journal of Medicinal Chemistry*, **2009**, 52, 2407-19	8.3	33
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