Stefano Moro

List of Publications by Citations

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	Medicinal chemistry and the molecular operating environment (MOE): application of QSAR and molecular docking to drug discovery. *Current Topics in Medicinal Chemistry*, **2008**, 8, 1555-72	3	510
303	FAM/USP9x, a deubiquitinating enzyme essential for TGFbeta signaling, controls Smad4 monoubiquitination. *Cell*, **2009**, 136, 123-35	56.2	394
302	The mitochondrial calcium uniporter is a multimer that can include a dominant-negative pore-forming subunit. *EMBO Journal*, **2013**, 32, 2362-76	13	326
301	Bridging Molecular Docking to Molecular Dynamics in Exploring Ligand-Protein Recognition Process: An Overview. *Frontiers in Pharmacology*, **2018**, 9, 923	5.6	210
300	Synthesis, CoMFA analysis, and receptor docking of 3,5-diacyl-2, 4-dialkylpyridine derivatives as selective A3 adenosine receptor antagonists. *Journal of Medicinal Chemistry*, **1999**, 42, 706-21	8.3	171
299	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	4.8	158
298	USP15 is a deubiquitylating enzyme for receptor-activated SMADs. *Nature Cell Biology*, **2011**, 13, 1368-75	23.4	155
297	Progress in the pursuit of therapeutic adenosine receptor antagonists. *Medicinal Research Reviews*, **2006**, 26, 131-59	14.4	139
296	Human P2Y1 receptor: molecular modeling and site-directed mutagenesis as tools to identify agonist and antagonist recognition sites. *Journal of Medicinal Chemistry*, **1998**, 41, 1456-66	8.3	138
295	Advances in GPCR modeling evaluated by the GPCR Dock 2013 assessment: meeting new challenges. *Structure*, **2014**, 22, 1120-1139	5.2	136
294	Quinalizarin as a potent, selective and cell-permeable inhibitor of protein kinase CK2. *Biochemical Journal*, **2009**, 421, 387-95	3.8	127
293	Toward the rational design of protein kinase casein kinase-2 inhibitors **2002**, 93, 159-68		126
292	Identification of ellagic acid as potent inhibitor of protein kinase CK2: a successful example of a virtual screening application. *Journal of Medicinal Chemistry*, **2006**, 49, 2363-6	8.3	119
291	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, 14639-47	5.4	119
290	Ciprofloxacin and levofloxacin attenuate microglia inflammatory response via TLR4/NF-kB pathway. *Journal of Neuroinflammation*, **2019**, 16, 148	10.1	115
289	Structure-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, 3186-201	8.3	114
288	Synthesis, biological activity, and molecular modeling of ribose-modified deoxyadenosine bisphosphate analogues as P2Y(1) receptor ligands. *Journal of Medicinal Chemistry*, **2000**, 43, 829-42	8.3	113

287	Role of the extracellular loops of G protein-coupled receptors in ligand recognition: a molecular modeling study of the human P2Y1 receptor. *Biochemistry*, **1999**, 38, 3498-507	3.2	113
286	Coumarin as attractive casein kinase 2 (CK2) inhibitor scaffold: an integrate approach to elucidate the putative binding motif and explain structure-activity relationships. *Journal of Medicinal Chemistry*, **2008**, 51, 752-9	8.3	109
285	Tetrabromocinnamic acid (TBCA) and related compounds represent a new class of specific protein kinase CK2 inhibitors. *ChemBioChem*, **2007**, 8, 129-39	3.8	104
284	Hemolytic effects of water-soluble fullerene derivatives. *Journal of Medicinal Chemistry*, **2004**, 47, 6711-5	8.3	104
283	Toward efficient Zn(II)-based artificial nucleases. *Journal of the American Chemical Society*, **2004**, 126, 4543-9	16.4	101
282	Mimicking the vanadium bromoperoxidases reactions:Mild and selective bromination of arenes and alkenes in a two-phase system. *Tetrahedron Letters*, **1994**, 35, 7429-7432	2	101
281	Derivatives of the triazoloquinazoline adenosine antagonist (CGS 15943) having high potency at the human A2B and A3 receptor subtypes. *Journal of Medicinal Chemistry*, **1998**, 41, 2835-45	8.3	98
280	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
279	6-Aminoquinolones as new potential anti-HIV agents. *Journal of Medicinal Chemistry*, **2000**, 43, 3799-802	8.3	94
278	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
277	Synthesis, biological activity, and molecular modeling investigation of new pyrazolo[4,3-e]-1,2,4-triazolo[1,5-c]pyrimidine derivatives as human A(3) adenosine receptor antagonists. *Journal of Medicinal Chemistry*, **2002**, 45, 770-80	8.3	90
276	The ATP-binding site of protein kinase CK2 holds a positive electrostatic area and conserved water molecules. *ChemBioChem*, **2007**, 8, 1804-9	3.8	86
275	Kinase CK2 inhibition: an update. *Current Medicinal Chemistry*, **2013**, 20, 671-93	4.3	84
274	Quantitative correlation of solvent polarity with the alpha-/3(10)-helix equilibrium: a heptapeptide behaves as a solvent-driven molecular spring. *Angewandte Chemie - International Edition*, **2003**, 42, 3388-92	16.4	83
273	Inhibition of protein kinase CK2 by condensed polyphenolic derivatives. An in vitro and in vivo study. *Biochemistry*, **2004**, 43, 12931-6	3.2	82
272	Pyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidine derivatives as highly potent and selective human A(3) adenosine receptor antagonists: influence of the chain at the N(8) pyrazole nitrogen. *Journal of Medicinal Chemistry*, **2000**, 43, 4768-80	8.3	82
271	PEG-Ara-C conjugates for controlled release. *European Journal of Medicinal Chemistry*, **2004**, 39, 123-33	6.8	79
270	Fingerprint-based detection of acute aquatic toxicity. *Journal of Cheminformatics*, **2010**, 2,	8.6	78

269	Models for the active site of vanadium-dependent haloperoxidases: insight into the solution structure of peroxo vanadium compounds. *Journal of Inorganic Biochemistry*, **2000**, 80, 41-9	4.2	78
268	Ligand-based homology modeling as attractive tool to inspect GPCR structural plasticity. *Current Pharmaceutical Design*, **2006**, 12, 2175-85	3.3	70
267	Titanium(IV)[R,R,R)-Tris(2-phenylethoxy)amine]Alkylperoxo Complex Mediated Oxidations: The Biphilic Nature of the Oxygen Transfer to Organic Sulfur Compounds. *Journal of the American Chemical Society*, **1997**, 119, 6935-6936	16.4	68
266	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	13.2	68
265	Synthesis, biological properties, and molecular modeling investigation of the first potent, selective, and water-soluble human A(3) adenosine receptor antagonist. *Journal of Medicinal Chemistry*, **2002**, 45, 3579-82	8.3	68
264	Enantioselective Ti(IV) Sulfoxidation Catalysts Bearing C3-Symmetric Trialkanolamine Ligands: Solution Speciation by 1H NMR and ESI-MS Analysis. *Journal of the American Chemical Society*, **1999**, 121, 6258-6268	16.4	67
263	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: pyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidine derivatives as a key study. *Journal of Medicinal Chemistry*, **2005**, 48, 152-62	8.3	66
262	Inhibition of protein kinase CK2 by anthraquinone-related compounds. A structural insight. *Journal of Biological Chemistry*, **2003**, 278, 1831-6	5.4	65
261	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
260	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	1.5	64
259	1,2,4-triazolo[4,3-a]quinoxalin-1-one moiety as an attractive scaffold to develop new potent and selective human A3 adenosine receptor antagonists: synthesis, pharmacological, and ligand-receptor modeling studies. *Journal of Medicinal Chemistry*, **2004**, 47, 3580-90	8.3	61
258	Novel camptothecin derivatives as topoisomerase I inhibitors. *Expert Opinion on Therapeutic Patents*, **2009**, 19, 555-74	6.8	58
257	MMsINC: a large-scale chemoinformatics database. *Nucleic Acids Research*, **2009**, 37, D284-90	20.1	58
256	51V-NMR investigation on the formation of peroxo vanadium complexes in aqueous solution: Some novel observations. *Journal of Molecular Catalysis*, **1994**, 94, 323-333		58
255	Protein kinase CK2 inhibitors: a patent review. *Expert Opinion on Therapeutic Patents*, **2012**, 22, 1081-97	6.8	56
254	Interactions of flavones and other phytochemicals with adenosine receptors. *Advances in Experimental Medicine and Biology*, **2002**, 505, 163-71	3.6	56
253	How druggable is protein kinase CK2?. *Medicinal Research Reviews*, **2010**, 30, 419-62	14.4	55
252	New 2-arylpyrazolo[3,4-c]quinoline derivatives as potent and selective human A3 adenosine receptor antagonists. Synthesis, pharmacological evaluation, and ligand-receptor modeling studies. *Journal of Medicinal Chemistry*, **2007**, 50, 4061-74	8.3	55

251	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, 5536-49	3.4	55
250	Flavonoid derivatives as adenosine receptor antagonists: a comparison of the hypothetical receptor binding site based on a comparative molecular field analysis model. *Journal of Medicinal Chemistry*, **1998**, 41, 46-52	8.3	55
249	Bridging molecular docking to membrane molecular dynamics to investigate GPCR-ligand recognition: the human A2A adenosine receptor as a key study. *Journal of Chemical Information and Modeling*, **2014**, 54, 169-83	6.1	54
248	Chiral resolution and stereospecificity of 6-phenyl-4-phenylethynyl- 1,4-dihydropyridines as selective A(3) adenosine receptor antagonists. *Journal of Medicinal Chemistry*, **1999**, 42, 3055-65	8.3	54
247	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	2.1	54
246	4-amido-2-aryl-1,2,4-triazolo[4,3-a]quinoxalin-1-ones as new potent and selective human A3 adenosine receptor antagonists. synthesis, pharmacological evaluation, and ligand-receptor modeling studies. *Journal of Medicinal Chemistry*, **2006**, 49, 3916-25	8.3	53
245	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 receptor-antagonist recognition. *Journal of Medicinal Chemistry*, **2009**, 52, 7640-52	8.3	51
244	Relationship between the structure and the DNA binding properties of diazoniapolycyclic duplex- and triplex-DNA binders: efficiency, selectivity, and binding mode. *Biochemistry*, **2007**, 46, 12721-36	3.2	51
243	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
242	Tuning the activity of Zn(II) complexes in DNA cleavage: clues for design of new efficient metallo-hydrolases. *Inorganic Chemistry*, **2008**, 47, 5473-84	5.1	50
241	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 A 3 and A 2B adenosine receptor subtypes: a molecular modeling investigation. *Journal of Medicinal Chemistry*, **2003**, 46, 4287-96	8.3	50
240	1,2,4-Triazolo[1,5-a]quinoxaline as a versatile tool for the design of selective human A3 adenosine receptor antagonists: synthesis, biological evaluation, and molecular modeling studies of 2-(hetero)aryl- and 2-carboxy-substituted derivatives. *Journal of Medicinal Chemistry*, **2005**, 48, 7932-45	8.3	48
239	Anthracyclines: recent developments in their separation and quantitation. *Biomedical Applications*, **2001**, 764, 161-71		48
238	Vanadium bromoperoxidases mimicking systems: Bromohydrins formation as evidence of the occurrence of a hypobromite-like vanadium complex. *Tetrahedron Letters*, **1995**, 36, 2675-2678	2	46
237	Mechanism of Arene Hydroxylation by Vanadium Picolinato Peroxo Complexes. *Journal of Organic Chemistry*, **1994**, 59, 6262-6267	4.2	45
236	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, 2588-605	6.1	44
235	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
234	Molecular modeling studies of human A3 adenosine antagonists: structural homology and receptor docking. *Journal of Chemical Information and Computer Sciences*, **1998**, 38, 1239-48		43

233	Novel point mutation in a leucine-rich repeat of the GPIbalpha 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, 1743-7	6.6	43
232	SAR and QSAR study on 2-aminothiazole derivatives, modulators of transcriptional repression in Huntington disease. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 5695-703	3.4	43
231	Prevalence, tumorigenic role, and biochemical implications of rare BRAF alterations. *Thyroid*, **2014**, 24, 809-19	6.2	42
230	Pharmaceutical perspectives of nonlinear QSAR strategies. *Journal of Chemical Information and Modeling*, **2010**, 50, 961-78	6.1	42
229	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		42
228	Exploring Protein-Peptide Recognition Pathways Using a Supervised Molecular Dynamics Approach. *Structure*, **2017**, 25, 655-662.e2	5.2	41
227	Discovery of novel A3 adenosine receptor ligands based on chromone scaffold. *Biochemical Pharmacology*, **2012**, 84, 21-9	6	41
226	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
225	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, 6015-26	8.3	41
224	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		41
223	Swimming into peptidomimetic chemical space using pepMMsMIMIC. *Nucleic Acids Research*, **2011**, 39, W261-9	20.1	38
222	Nature of the Radical Intermediates in the Decomposition of Peroxovanadium Species in Protic and Aprotic Media. *Inorganic Chemistry*, **1994**, 33, 1631-1637	5.1	37
221	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
220	Synthesis, ligand-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, 6086-102	3.4	36
219	DNA topoisomerase II structures and anthracycline activity: insights into ternary complex formation. *Current Pharmaceutical Design*, **2007**, 13, 2766-80	3.3	36
218	Demystifying the three dimensional structure of G protein-coupled receptors (GPCRs) with the aid of molecular modeling. *Chemical Communications*, **2003**, 2949-56	5.8	36
217	Fluorosulfonyl- and bis-(beta-chloroethyl)amino-phenylamino functionalized pyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidine derivatives: irreversible antagonists at the human A3 adenosine receptor and molecular modeling studies. *Journal of Medicinal Chemistry*, **2001**, 44, 2735-42	8.3	36
216	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

215	Autocorrelation of molecular electrostatic potential surface properties combined with partial least squares analysis as new strategy for the prediction of the activity of human A(3) adenosine receptor antagonists. *Journal of Medicinal Chemistry*, **2005**, 48, 5698-704	8.3	35
214	Vanadium-Bromoperoxidase-Mimicking Systems: Direct Evidence of a Hypobromite-Like Vanadium Intermediate. *European Journal of Inorganic Chemistry*, **2003**, 2003, 42-46	2.3	35
213	Synthesis of brominated compounds. A convenient molybdenum- catalyzed procedure inspired by the mode of action of haloperoxidases. *Tetrahedron Letters*, **1996**, 37, 8609-8612	2	35
212	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
211	Identification of novel protein kinase CK1 delta (CK1delta) inhibitors through structure-based virtual screening. *Bioorganic and Medicinal Chemistry Letters*, **2008**, 18, 5672-5	2.9	34
210	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
209	Investigation of Streptomyces antibioticus tyrosinase reactivity toward chlorophenols. *Archives of Biochemistry and Biophysics*, **2011**, 505, 67-74	4.1	33
208	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
207	A Adenosine Receptors: Protective vs. Damaging Effects Identified Using Novel Agonists and Antagonists. *Drug Development Research*, **1998**, 45, 113-124	5.1	33
206	Highlights on the development of A(2A) adenosine receptor agonists and antagonists. *ChemMedChem*, **2007**, 2, 260-81	3.7	33
205	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, 705-15	3.4	33
204	Design, synthesis, and structure-activity relationships of azolylmethylpyrroloquinolines as nonsteroidal aromatase inhibitors. *Journal of Medicinal Chemistry*, **2013**, 56, 7536-51	8.3	32
203	Interaction model for anthracycline activity against DNA topoisomerase II. *Biochemistry*, **2004**, 43, 7503-13	3.2	32
202	Advances in Computational Techniques to Study GPCR-Ligand Recognition. *Trends in Pharmacological Sciences*, **2015**, 36, 878-890	13.2	31
201	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		31
200	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
199	The dark side of protein kinase CK2 inhibition. *Current Medicinal Chemistry*, **2011**, 18, 2867-84	4.3	30
198	Use of electrospray ionization mass spectrometry to characterizechiral reactive intermediates in a titanium alkoxide mediatedsulfoxidation reaction. *Chemical Communications*, **1997**, 869-870	5.8	30

197	Novel strategies for the design of new potent and selective human A3 receptor antagonists: an update. *Current Medicinal Chemistry*, **2006**, 13, 639-45	4.3	30
196	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, 6596-606	8.3	30
195	A2B adenosine receptor antagonists: recent developments. *Mini-Reviews in Medicinal Chemistry*, **2005**, 5, 1053-60	3.2	30
194	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
193	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
192	In silico binding free energy predictability by using the linear interaction energy (LIE) method: bromobenzimidazole CK2 inhibitors as a case study. *Journal of Chemical Information and Modeling*, **2007**, 47, 572-82	6.1	29
191	Histidine-Containing Bisperoxovanadium(V) Compounds: Insight Into the Solution Structure by an ESI-MS and 51V-NMR Comparative Study. *European Journal of Inorganic Chemistry*, **1999**, 1999, 1489-1495	2.3	29
190	A theoretical and experimental investigation of the electrophilic oxidation of thioethers and sulfoxides by peroxides. *Tetrahedron*, **1995**, 51, 12363-12372	2.4	29
189	Hydroxylation of aromatics with hydrogen peroxide catalyzed by vanadium (V) peroxocomplexes. *Journal of Molecular Catalysis*, **1993**, 83, 107-116		29
188	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
187	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
186	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	2.7	28
185	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	2.5	28
184	Fluorescent ligands for adenosine receptors. *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 26-36	2.9	27
183	Adenosiland: walking through adenosine receptors landscape. *European Journal of Medicinal Chemistry*, **2012**, 58, 248-57	6.8	27
182	Direct Evidence of Solvent-Peroxovanadium Clusters by Electrospray Ionization Mass Spectrometry. *European Journal of Inorganic Chemistry*, **1998**, 1998, 1193-1197	2.3	27
181	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 A2A receptor. *Journal of Chemical Information and Modeling*, **2008**, 48, 350-63	6.1	27
180	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, 354-61	3.4	27

179	Ligand-based drug design methodologies in drug discovery process: an overview. *Current Drug Discovery Technologies*, **2006**, 3, 155-65	1.5	27
178	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
177	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
176	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
175	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, 5733-42	3.4	26
174	Anchimeric assistance effect on regioselective hydrolysis of branched PEGs: a mechanistic investigation. *Bioorganic and Medicinal Chemistry*, **2004**, 12, 5031-7	3.4	26
173	Application of QSAR analysis to organic anion transporting polypeptide 1a5 (Oatp1a5) substrates. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 463-71	3.4	26
172	Mapping drug interactions at the covalent topoisomerase II-DNA complex by bisantrene/amsacrine congeners. *Journal of Biological Chemistry*, **1998**, 273, 12732-9	5.4	26
171	A High-Throughput Screening Identifies MICU1 Targeting Compounds. *Cell Reports*, **2020**, 30, 2321-2331.e6	8.6	25
170	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
169	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
168	Synthesis and biological studies of a new series of 5-heteroarylcarbamoylaminopyrazolo[4,3-e]1,2,4-triazolo[1,5-c]pyrimidines as human A3 adenosine receptor antagonists. Influence of the heteroaryl substituent on binding affinity and molecular modeling investigations. *Journal of Medicinal Chemistry*, **2006**, 49, 1720-3	8.3	24
167	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, 4923-32	3.4	24
166	Evidence for the Recognition of Non-Nucleotide Antagonists Within the Transmembrane Domains of the Human P2Y(1) Receptor. *Drug Development Research*, **2002**, 57, 173-181	5.1	24
165	The topoisomerase II poison clerocidin alkylates non-paired guanines of DNA: implications for irreversible stimulation of DNA cleavage. *Nucleic Acids Research*, **2001**, 29, 4224-30	20.1	24
164	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
163	Elucidation of the ribonuclease A aggregation process mediated by 3D domain swapping: a computational approach reveals possible new multimeric structures. *Biopolymers*, **2008**, 89, 26-39	2.2	23
162	Indolo[2,3-b]-quinolizinium bromide: an efficient intercalator with DNA-photodamaging properties. *ChemBioChem*, **2002**, 3, 550-8	3.8	23

161	Sequence-specific interactions of drugs interfering with the topoisomerase-DNA cleavage complex. *Biochimica Et Biophysica Acta - Molecular Basis of Disease*, **2002**, 1587, 145-54	6.9	23
160	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
159	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
158	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
157	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
156	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
155	Quantitation of camptothecin and related compounds. *Biomedical Applications*, **2001**, 764, 121-40		22
154	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
153	Estimation of kinetic and thermodynamic ligand-binding parameters using computational strategies. *Future Medicinal Chemistry*, **2017**, 9, 507-523	4.1	21
152	2 -Glycoprotein binds to thrombin and selectively inhibits the enzyme procoagulant functions. *Journal of Thrombosis and Haemostasis*, **2013**, 11, 1093-102	15.4	21
151	Peroxovanadium complexes as radical oxidants in organic solvents and in aqueous solutions. *Journal of Molecular Catalysis A*, **1997**, 117, 139-149		21
150	alpha-Naphthylaminopropan-2-ol Derivatives as BACE1 Inhibitors. *ChemMedChem*, **2008**, 3, 1530-4	3.7	21
149	Characterization and Reactivity of Triperoxo Vanadium Complexes In Protic Solvents. *European Journal of Inorganic Chemistry*, **2001**, 2001, 2913	2.3	21
148	Correlation between one-electron reduction and oxygen-oxygen bond strength in d0 transition metal peroxo complexes. *Inorganic Chemistry*, **1993**, 32, 5797-5799	5.1	21
147	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
146	Molecular modeling as a tool to investigate molecular recognition in P2Y receptors. *Current Pharmaceutical Design*, **2002**, 8, 2401-13	3.3	20
145	Mimicking Peptides In Silico. *Molecular Informatics*, **2012**, 31, 12-20	3.8	19
144	Ab Initio Calculations on Water Peroxovanadium Clusters, VO(O2)(H2O)n+ (n = 1). Implications for the Structure in Aqueous Solution. *Journal of Physical Chemistry A*, **1997**, 101, 4637-4640	2.8	19

143	Synthesis and Molecular Modeling Studies of Fullerene–5,6,7-Trimethoxyindole–Oligonucleotide Conjugates as Possible Probes for Study of Photochemical Reactions in DNA Triple Helices. *European Journal of Organic Chemistry*, **2002**, 2002, 405-413	3.2	19
142	New 1,4-anthracene-9,10-dione derivatives as potential anticancer agents. *Il Farmaco*, **2000**, 55, 1-5		19
141	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
140	Semisynthesis, biological activity, and molecular modeling studies of C-ring-modified camptothecins. *Journal of Medicinal Chemistry*, **2009**, 52, 1029-39	8.3	18
139	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
138	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
137	Carbazole-containing arylcarboxamides as BACE1 inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2011**, 21, 6657-61	2.9	17
136	Pyrazolo-triazolo-pyrimidines as adenosine receptor antagonists: A complete structure-activity profile. *Purinergic Signalling*, **2007**, 3, 183-93	3.8	17
135	On the Mechanism of the Oxygen Transfer to Sulfoxides by (Peroxo)[tris(hydroxyalkyl)amine]TiIV Complexes – Evidence for a Metal-Template-Assisted Process. *European Journal of Organic Chemistry*, **2003**, 2003, 507-511	3.2	17
134	Molecular recognition in P2 receptors: ligand development aided by molecular modeling and mutagenesis. *Progress in Brain Research*, **1999**, 120, 119-32	2.9	17
133	AquaMMapS: An Alternative Tool to Monitor the Role of Water Molecules During Protein-Ligand Association. *ChemMedChem*, **2018**, 13, 522-531	3.7	17
132	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
131	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
130	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
129	Tandem 3D-QSARs approach as a valuable tool to predict binding affinity data: design of new Gly/NMDA receptor antagonists as a key study. *Journal of Chemical Information and Modeling*, **2007**, 47, 1913-22	6.1	16
128	G protein-coupled receptors as challenging druggable targets: insights from in silico studies. *New Journal of Chemistry*, **2006**, 30, 301	3.6	16
127	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
126	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

125	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
124	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
123	Exploring potency and selectivity receptor antagonist profiles using a multilabel classification approach: the human adenosine receptors as a key study. *Journal of Chemical Information and Modeling*, **2009**, 49, 2820-36	6.1	15
122	Comparative studies on the DNA-binding properties of linear and angular dibenzoquinolizinium ions. *Journal of Organic Chemistry*, **2006**, 71, 8401-11	4.2	15
121	Antitumor AZA-anthrapyrazoles: biophysical and biochemical studies on 8- and 9-aza regioisomers. *Biochemical Pharmacology*, **2004**, 67, 631-42	6	15
120	New water soluble pyrroloquinoline derivatives as new potential anticancer agents. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 4733-9	3.4	15
119	DNA-interactive anticancer aza-anthrapyrazoles: biophysical and biochemical studies relevant to the mechanism of action. *Molecular Pharmacology*, **2001**, 59, 96-103	4.3	15
118	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
117	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
116	A Supervised Molecular Dynamics Approach to Unbiased Ligand-Protein Unbinding. *Journal of Chemical Information and Modeling*, **2020**, 60, 1804-1817	6.1	14
115	Inhibition of cytochrome P450 2C8-mediated drug metabolism by the flavonoid diosmetin. *Drug Metabolism and Pharmacokinetics*, **2011**, 26, 559-68	2.2	14
114	Diazoniapolycyclic ions inhibit the activity of topoisomerase I and the growth of certain tumor cell lines. *ChemMedChem*, **2008**, 3, 1671-6	3.7	14
113	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
112	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
111	Rational design, synthesis, and DNA binding properties of novel sequence-selective peptidyl congeners of ametantrone. *ChemMedChem*, **2010**, 5, 1080-91	3.7	13
110	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
109	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
108	Acute in vitro effects of dronedarone, an iodine-free derivative, and amiodarone, on the rabbit sinoatrial node automaticity: a comparative study. *Journal of Cardiovascular Pharmacology and Therapeutics*, **2007**, 12, 248-57	2.6	12

107	Combining ligand-based and structure-based drug design in the virtual screening arena. *Expert Opinion on Drug Discovery*, **2007**, 2, 37-49	6.2	12
106	DNA-binding preferences of bisantrene analogues: relevance to the sequence specificity of drug-mediated topoisomerase II poisoning. *Molecular Pharmacology*, **1998**, 54, 1036-45	4.3	12
105	Molecular docking methodologies. *Methods in Molecular Biology*, **2013**, 924, 339-60	1.4	11
104	NMR-Assisted Molecular Docking Methodologies. *Molecular Informatics*, **2015**, 34, 513-25	3.8	11
103	Metabolism of 2-hydroxy-3-deoxyestradiol by rat liver microsomes. *Biochemical Pharmacology*, **1977**, 26, 769-73	6	11
102	The rise of molecular simulations in fragment-based drug design (FBDD): an overview. *Drug Discovery Today*, **2020**, 25, 1693-1701	8.8	10
101	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
100	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
99	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
98	Implementing the "Best Template Searching" tool into Adenosiland platform. *In Silico Pharmacology*, **2013**, 1, 25	4.3	10
97	Carboxylation-dependent conformational changes of human osteocalcin. *Frontiers in Bioscience - Landmark*, **2014**, 19, 1105-16	2.8	10
96	Does the combination of optimal substitutions at the C2-, N6- and N9-positions of the pyrazolo-triazolo-pyrimidine scaffold guarantee selective modulation of the human A2A adenosine receptors?. *Bioorganic and Medicinal Chemistry*, **2011**, 19, 6120-34	3.4	10
95	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
94	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, 3224-3237	3	10
93	Novel coumarin-pyridazine hybrids as selective MAO-B inhibitors for the Parkinson's disease therapy. *Bioorganic Chemistry*, **2020**, 104, 104203	5.1	10
92	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
91	Supervised Molecular Dynamics (SuMD) Approaches in Drug Design. *Methods in Molecular Biology*, **2018**, 1824, 287-298	1.4	9
90	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

89	Human A3 adenosine receptor as versatile G protein-coupled receptor example to validate the receptor homology modeling technology. *Current Pharmaceutical Design*, **2009**, 15, 4069-84	3.3	9
88	Pyrazolo-triazolo-pyrimidines as adenosine receptor antagonists: Effect of the N-5 bond type on the affinity and selectivity at the four adenosine receptor subtypes. *Purinergic Signalling*, **2008**, 4, 39-46	3.8	9
87	Design, synthesis and biological properties of fulleropyrrolidine derivatives as potential DNA photo-probes. *Journal of Supramolecular Chemistry*, **2002**, 2, 327-334		9
86	Interactions between DNA and benzo- and tetrahydrobenzofurocoumarins: thermodynamic and molecular modeling studies. *Il Farmaco*, **2000**, 55, 276-86		9
85	Photophysical properties of the lowest excited singlet and triplet states of thio- and seleno-psoralens. *Photochemistry and Photobiology*, **2000**, 71, 506-13	3.6	9
84	Discovery of HIV-1 integrase inhibitors through a novel combination of ligand and structure-based drug design. *Medicinal Chemistry*, **2005**, 1, 263-75	1.8	9
83	ATP non-competitive Ser/Thr kinase inhibitors as potential anticancer agents. *Anti-Cancer Agents in Medicinal Chemistry*, **2009**, 9, 778-86	2.2	9
82	Peeking at G-protein-coupled receptors through the molecular dynamics keyhole. *Future Medicinal Chemistry*, **2019**, 11, 599-615	4.1	8
81	[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
80	Reactivity of clerocidin towards adenine: implications for base-modulated DNA damage. *Organic and Biomolecular Chemistry*, **2009**, 7, 976-85	3.9	8
79	Protein kinase CK2 inhibitors: emerging anticancer therapeutic agents?. *Anti-Cancer Agents in Medicinal Chemistry*, **2008**, 8, 798-806	2.2	8
78	2-Hydroxy-3-carboxy-dihydrocinnamic acid: Complexation properties towards aluminium(III) and iron(III). *Polyhedron*, **2007**, 26, 3419-3427	2.7	8
77	Pyrazoloquinazoline Tricyclic System as Novel Scaffold to Design New Kinase CK2 Inhibitors. *Letters in Drug Design and Discovery*, **2006**, 3, 281-284	0.8	8
76	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
75	Sulfonamido-derivatives of unsubstituted carbazoles as BACE1 inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2017**, 27, 4812-4816	2.9	7
74	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
73	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
72	Receptor-driven identification of novel human A2B adenosine receptor antagonists as potential therapeutic agents. *Methods in Enzymology*, **2010**, 485, 225-44	1.7	7

71	A novel glucosyltransferase from Catharanthus roseus cell suspensions. *Process Biochemistry*, **2010**, 45, 655-659	4.8	7
70	A versatile synthesis of the 1,4-dihydroxynaphthoquinone nucleus. *Tetrahedron Letters*, **2000**, 41, 6631-6634		7
69	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
68	A Deep-Learning Approach toward Rational Molecular Docking Protocol Selection. *Molecules*, **2020**, 25,	4.8	6
67	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
66	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
65	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
64	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
63	Response Surface Analysis as Alternative 3D-QSAR Tool: Human A3 Adenosine Receptor Antagonists as a Key Study. *Letters in Drug Design and Discovery*, **2007**, 4, 122-127	0.8	6
62	Ribose modified nucleosides and nucleotides as ligands for purine receptors. *Nucleosides, Nucleotides and Nucleic Acids*, **2001**, 20, 333-41	1.4	6
61	Isolation and characterization of a Golgi-rich fraction from the Harding-Passey mouse melanoma. *Tohoku Journal of Experimental Medicine*, **1978**, 126, 63-70	2.4	6
60	Scouting Novel Protein Kinase A (PKA) Inhibitors by Using a Consensus Docking-Based Virtual Screening Approach. *Letters in Drug Design and Discovery*, **2009**, 6, 327-336	0.8	6
59	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
58	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
57	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
56	1-Thiopsoralen, a new photobiologically active heteropsoralen. Photophysical, photochemical and computer aided studies. *Il Farmaco*, **1997**, 52, 645-52		6
55	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
54	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

53	Structure-activity relationship study of 16 a-thiocamptothecins: an integrated in vitro and in silico approach. *ChemMedChem*, **2010**, 5, 2006-15	3.7	5
52	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
51	1-Thioangelicin: crystal structure, computer-aided studies and photobiological activity. *Il Farmaco*, **2004**, 59, 125-32		5
50	Synthesis, biological studies and molecular modeling investigation of 1,3-dimethyl-2,4-dioxo-6-methyl-8-(substituted) 1,2,3,4-tetrahydro [1,2,4]-triazolo [3,4-f]-purines as potential adenosine receptor antagonists. *Il Farmaco*, **2005**, 60, 299-306		5
49	Synthesis, biological and modeling studies of 1,3-di-n-propyl-2,4-dioxo-6-methyl-8-(substituted) 1,2,3,4-tetrahydro [1,2,4]-triazolo [3,4-f]-purines as adenosine receptor antagonists. *Il Farmaco*, **2005**, 60, 643-51		5
48	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
47	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
46	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
45	Could Adenosine Recognize its Receptors with a Stoichiometry Other than 1 : 1?. *Molecular Informatics*, **2018**, 37, e1800009	3.8	5
44	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
43	A new inactive conformation of SARS-CoV-2 main protease.. *Acta Crystallographica Section D: Structural Biology*, **2022**, 78, 363-378	5.5	5
42	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
41	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
40	A novel splicing variant encoding putative catalytic alpha subunit of maize protein kinase CK2. *Physiologia Plantarum*, **2009**, 136, 251-63	4.6	4
39	ClickMD: an intuitive web-oriented molecular dynamics platform. *Future Medicinal Chemistry*, **2011**, 3, 923-31	4.1	4
38	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
37	Designing a ligand for pharmaceutical purposes. *Expert Opinion on Drug Discovery*, **2008**, 3, 579-90	6.2	4
36	Structurally related nucleotides as selective agonists and antagonists at P2Y1 receptors. *Il Farmaco*, **2001**, 56, 71-5		4

35	New benzoquinolizin-5-one derivatives as furocoumarin analogs: DNA-interactions and molecular modeling studies. *Il Farmaco*, **1999**, 54, 551-61		4
34	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
33	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
32	New Insights into Key Determinants for Adenosine 1 Receptor Antagonists Selectivity Using Supervised Molecular Dynamics Simulations. *Biomolecules*, **2020**, 10,	5.9	3
31	In Silico 3D Modeling of Binding Activities. *Methods in Molecular Biology*, **2016**, 1425, 23-35	1.4	3
30	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
29	Novel insights on the DNA interaction of calicheamicin (). *Biopolymers*, **2015**, 103, 449-59	2.2	3
28	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
27	Dissecting reactivity of clerocidin toward common buffer systems by means of selected drug analogues. *Chemical Research in Toxicology*, **2005**, 18, 35-40	4	3
26	A novel conformational state for SARS-CoV-2 main protease		3
25	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
24	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
23	Comparing Fragment Binding Poses Prediction Using HSP90 as a Key Study: When Bound Water Makes the Difference. *Molecules*, **2020**, 25,	4.8	2
22	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
21	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
20	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
19	MMsDusty: an Alternative InChI-Based Tool to Minimize Chemical Redundancy. *Molecular Informatics*, **2013**, 32, 681-4	3.8	2
18	A Novel Generalized 3D-QSAR Model of Camptothecin Analogs. *Molecular Informatics*, **2011**, 30, 927-38	3.8	2

17	Computationally driven discovery of SARS-CoV-2 M inhibitors: from design to experimental validation.. *Chemical Science*, **2022**, 13, 3674-3687	9.4	2
16	Targeting G Protein-Coupled Receptors with Magnetic Carbon Nanotubes: The Case of the A Adenosine Receptor. *ChemMedChem*, **2020**, 15, 1909-1920	3.7	2
15	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
14	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
13	MMsINC : A New Public Large-Scale Chemoinformatics Database System **2008**,		1
12	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
11	PCA-Based Representations of Graphs for Prediction in QSAR Studies. *Lecture Notes in Computer Science*, **2009**, 105-114	0.9	1
10	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
9	Pyridazinones containing dithiocarbamoyl moieties as a new class of selective MAO-B inhibitors. *Bioorganic Chemistry*, **2021**, 115, 105203	5.1	1
8	Amphiphilic peptide-based MMP3 inhibitors for intra-articular treatment of knee OA. *Bioorganic and Medicinal Chemistry*, **2021**, 38, 116132	3.4	0
7	Editorial [Hot Topic: Computational Applications in Medicinal Chemistry Executive (Editor: Stefano Moro)]. *Current Pharmaceutical Design*, **2006**, 12, 2065-2066	3.3	
6	Potent and Selective A2A Adenosine Receptor Antagonists: Recent Improvements. *Frontiers in Drug Design and Discovery*, **2005**, 2, 49-62		
5	Tetralogy of Fallot in a blastocystic implantation. *American Journal of Cardiology*, **1987**, 60, 1206	3	
4	Electrophoretic profile of tyrosinase treated with neuraminidase in various subcellular fractions from mouse melanoma. *Journal of Dermatology*, **1979**, 6, 125-7	1.6	
3	Molecular Modeling and Reengineering of A3 Adenosine Receptors **2010**, 149-161		
2	Potent and selective A adenosine receptor antagonists bearing aminoesters as heterobifunctional moieties. *RSC Medicinal Chemistry*, **2021**, 12, 254-262	3.5	
1	Molecular Dynamics Applications to GPCR Ligand Design. *Methods and Principles in Medicinal Chemistry*, **2018**, 225-246	0.4	