Paolo Tosco

List of Publications by Year in Descending Order

31 papers	832 citations	17 h-index	28 g-index
33 ext. papers	938 ext. citations	5.3 avg, IF	4.15 L-index

#	Paper	IF	Citations
31	Bringing the MMFF force field to the RDKit: implementation and validation. *Journal of Cheminformatics*, **2014**, 6,	8.6	70
30	The integration of Open3DTOOLS into the RDKit and KNIME. *Journal of Cheminformatics*, **2014**, 6,	8.6	3
29	3D-QSAR reloaded: Open3DALIGN meets COSMOsar3D. *Journal of Cheminformatics*, **2013**, 5,	8.6	78
28	Design and Synthesis of a (1)(3)-Cyclodextrin Oligomer: A New Platform with Potential Application as a Dendrimeric Multicarrier. *Chemistry - A European Journal*, **2013**, 19, 12086-92	4.8	16
27	The role of fluorine in stabilizing the bioactive conformation of dihydroorotate dehydrogenase inhibitors. *Journal of Molecular Modeling*, **2013**, 19, 1099-107	2	18
26	6-Cyclohexylmethoxy-5-(cyano-NNO-azoxy)pyrimidine-4-amine: a new scaffold endowed with potent CDK2 inhibitory activity. *European Journal of Medicinal Chemistry*, **2013**, 68, 333-8	6.8	14
25	Novel small molecule protein arginine deiminase 4 (PAD4) inhibitors. *Bioorganic and Medicinal Chemistry Letters*, **2013**, 23, 715-9	2.9	28
24	A mechanistic hypothesis for the aspirin-induced switch in lipid mediator production by cyclooxygenase-2. *Journal of the American Chemical Society*, **2013**, 135, 10404-10	16.4	16
23	New inhibitors of dihydroorotate dehydrogenase (DHODH) based on the 4-hydroxy-1,2,5-oxadiazol-3-yl (hydroxyfurazanyl) scaffold. *European Journal of Medicinal Chemistry*, **2012**, 49, 102-9	6.8	25
22	Thymopentin down-regulates both activity and expression of iNOS in blood cells of S□ary syndrome patients. *Nitric Oxide - Biology and Chemistry*, **2012**, 27, 143-9	5	8
21	COSMOsar3D: molecular field analysis based on local COSMO □profiles. *Journal of Chemical Information and Modeling*, **2012**, 52, 2157-64	6.1	26
20	A 3D-QSAR-driven approach to binding mode and affinity prediction. *Journal of Chemical Information and Modeling*, **2012**, 52, 302-7	6.1	22
19	Open3DALIGN: an open-source software aimed at unsupervised ligand alignment. *Journal of Computer-Aided Molecular Design*, **2011**, 25, 777-83	4.2	74
18	Open3DQSAR: a new open-source software aimed at high-throughput chemometric analysis of molecular interaction fields. *Journal of Molecular Modeling*, **2011**, 17, 201-8	2	109
17	SDF2XYZ2SDF: how to exploit TINKER power in cheminformatics projects. *Journal of Molecular Modeling*, **2011**, 17, 3021-3	2	9
16	1,2,5-Oxadiazole analogues of leflunomide and related compounds. *European Journal of Medicinal Chemistry*, **2011**, 46, 383-92	6.8	23
15	Nitrooxyacyl derivatives of salicylic acid: aspirin-like molecules that covalently inactivate cyclooxygenase-1. *ChemMedChem*, **2011**, 6, 523-30	3.7	7

14	Synthesis and preliminary pharmacological characterisation of a new class of nitrogen-containing bisphosphonates (N-BPs). *Bioorganic and Medicinal Chemistry*, **2010**, 18, 2428-38	3.4	21
13	Mechanistic insights into cyclooxygenase irreversible inactivation by aspirin. *ChemMedChem*, **2009**, 4, 939-45	3.7	30
12	Complementary three-dimensional quantitative structure-activity relationship modeling of binding affinity and functional potency: a study on alpha4beta2 nicotinic ligands. *Journal of Medicinal Chemistry*, **2009**, 52, 2311-6	8.3	13
11	Edaravone derivatives containing NO-donor functions. *Journal of Medicinal Chemistry*, **2009**, 52, 574-8	8.3	31
10	Multitarget drugs: Focus on the NO-donor hybrid drugs. *Pure and Applied Chemistry*, **2008**, 80, 1693-1701	2.1	17
9	Hydroxy-1,2,5-oxadiazolyl moiety as bioisoster of the carboxy function. A computational study on gamma-aminobutyric acid (GABA) related compounds. *Journal of Molecular Modeling*, **2008**, 14, 279-91	2	13
8	Structure-antioxidant activity relationships in a series of NO-donor phenols. *ChemMedChem*, **2008**, 3, 1443-8	3.7	4
7	Physicochemical Profiling of Sartans: A Detailed Study of Ionization Constants and Distribution Coefficients. *Helvetica Chimica Acta*, **2008**, 91, 468-482	2	43
6	NO-donor COX-2 inhibitors. New nitrooxy-substituted 1,5-diarylimidazoles endowed with COX-2 inhibitory and vasodilator properties. *Journal of Medicinal Chemistry*, **2007**, 50, 1449-57	8.3	52
5	NO-donor melatonin derivatives: synthesis and in vitro pharmacological characterization. *Journal of Pineal Research*, **2007**, 42, 371-85	10.4	12
4	Furoxan analogues of the histamine H3-receptor antagonist imoproxifan and related furazan derivatives. *Bioorganic and Medicinal Chemistry*, **2005**, 13, 4750-9	3.4	13
3	Non-imidazole histamine NO-donor H3-antagonists. *Il Farmaco*, **2005**, 60, 507-12		5
2	A new class of NO-donor H3-antagonists. *Il Farmaco*, **2004**, 59, 359-71		11
1	[3-(1H-imidazol-4-yl)propyl]guanidines containing furoxan moieties: a new class of H3-antagonists endowed with NO-donor properties. *Bioorganic and Medicinal Chemistry*, **2003**, 11, 1197-205	3.4	21