

Paolo Tosco

List of Publications by Citations

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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	Open3DQSAR: a new open-source software aimed at high-throughput chemometric analysis of molecular interaction fields. <i>Journal of Molecular Modeling</i> , 2011 , 17, 201-8	2	109
30	3D-QSAR reloaded: Open3DALIGN meets COSMOsar3D. <i>Journal of Cheminformatics</i> , 2013 , 5,	8.6	78
29	Open3DALIGN: an open-source software aimed at unsupervised ligand alignment. <i>Journal of Computer-Aided Molecular Design</i> , 2011 , 25, 777-83	4.2	74
28	Bringing the MMFF force field to the RDKit: implementation and validation. <i>Journal of Cheminformatics</i> , 2014 , 6,	8.6	70
27	NO-donor COX-2 inhibitors. New nitrooxy-substituted 1,5-diarylimidazoles endowed with COX-2 inhibitory and vasodilator properties. <i>Journal of Medicinal Chemistry</i> , 2007 , 50, 1449-57	8.3	52
26	Physicochemical Profiling of Sartans: A Detailed Study of Ionization Constants and Distribution Coefficients. <i>Helvetica Chimica Acta</i> , 2008 , 91, 468-482	2	43
25	Edaravone derivatives containing NO-donor functions. <i>Journal of Medicinal Chemistry</i> , 2009 , 52, 574-8	8.3	31
24	Mechanistic insights into cyclooxygenase irreversible inactivation by aspirin. <i>ChemMedChem</i> , 2009 , 4, 939-45	3.7	30
23	Novel small molecule protein arginine deiminase 4 (PAD4) inhibitors. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013 , 23, 715-9	2.9	28
22	COSMOsar3D: molecular field analysis based on local COSMO ϵ profiles. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 2157-64	6.1	26
21	New inhibitors of dihydroorotate dehydrogenase (DHODH) based on the 4-hydroxy-1,2,5-oxadiazol-3-yl (hydroxyfurazanyl) scaffold. <i>European Journal of Medicinal Chemistry</i> , 2012 , 49, 102-9	6.8	25
20	1,2,5-Oxadiazole analogues of leflunomide and related compounds. <i>European Journal of Medicinal Chemistry</i> , 2011 , 46, 383-92	6.8	23
19	A 3D-QSAR-driven approach to binding mode and affinity prediction. <i>Journal of Chemical Information and Modeling</i> , 2012 , 52, 302-7	6.1	22
18	Synthesis and preliminary pharmacological characterisation of a new class of nitrogen-containing bisphosphonates (N-BPs). <i>Bioorganic and Medicinal Chemistry</i> , 2010 , 18, 2428-38	3.4	21
17	[3-(1H-imidazol-4-yl)propyl]guanidines containing furoxan moieties: a new class of H3-antagonists endowed with NO-donor properties. <i>Bioorganic and Medicinal Chemistry</i> , 2003 , 11, 1197-205	3.4	21
16	The role of fluorine in stabilizing the bioactive conformation of dihydroorotate dehydrogenase inhibitors. <i>Journal of Molecular Modeling</i> , 2013 , 19, 1099-107	2	18
15	Multitarget drugs: Focus on the NO-donor hybrid drugs. <i>Pure and Applied Chemistry</i> , 2008 , 80, 1693-1701	2.1	17

14	Design and Synthesis of a (1)(B)-Cyclodextrin Oligomer: A New Platform with Potential Application as a Dendrimeric Multicarrier. <i>Chemistry - A European Journal</i> , 2013 , 19, 12086-92	4.8	16
13	A mechanistic hypothesis for the aspirin-induced switch in lipid mediator production by cyclooxygenase-2. <i>Journal of the American Chemical Society</i> , 2013 , 135, 10404-10	16.4	16
12	6-Cyclohexylmethoxy-5-(cyano-NNO-azoxy)pyrimidine-4-amine: a new scaffold endowed with potent CDK2 inhibitory activity. <i>European Journal of Medicinal Chemistry</i> , 2013 , 68, 333-8	6.8	14
11	Complementary three-dimensional quantitative structure-activity relationship modeling of binding affinity and functional potency: a study on alpha4beta2 nicotinic ligands. <i>Journal of Medicinal Chemistry</i> , 2009 , 52, 2311-6	8.3	13
10	Hydroxy-1,2,5-oxadiazolyl moiety as bioisoster of the carboxy function. A computational study on gamma-aminobutyric acid (GABA) related compounds. <i>Journal of Molecular Modeling</i> , 2008 , 14, 279-91	2	13
9	Furoxan analogues of the histamine H3-receptor antagonist imoproxifan and related furazan derivatives. <i>Bioorganic and Medicinal Chemistry</i> , 2005 , 13, 4750-9	3.4	13
8	NO-donor melatonin derivatives: synthesis and in vitro pharmacological characterization. <i>Journal of Pineal Research</i> , 2007 , 42, 371-85	10.4	12
7	A new class of NO-donor H3-antagonists. <i>Il Farmaco</i> , 2004 , 59, 359-71		11
6	SDF2XYZ2SDF: how to exploit TINKER power in cheminformatics projects. <i>Journal of Molecular Modeling</i> , 2011 , 17, 3021-3	2	9
5	Thymopentin down-regulates both activity and expression of iNOS in blood cells of Sjögren syndrome patients. <i>Nitric Oxide - Biology and Chemistry</i> , 2012 , 27, 143-9	5	8
4	Nitrooxyacyl derivatives of salicylic acid: aspirin-like molecules that covalently inactivate cyclooxygenase-1. <i>ChemMedChem</i> , 2011 , 6, 523-30	3.7	7
3	Non-imidazole histamine NO-donor H3-antagonists. <i>Il Farmaco</i> , 2005 , 60, 507-12		5
2	Structure-antioxidant activity relationships in a series of NO-donor phenols. <i>ChemMedChem</i> , 2008 , 3, 1443-8	3.7	4
1	The integration of Open3DTOOLS into the RDKit and KNIME. <i>Journal of Cheminformatics</i> , 2014 , 6,	8.6	3