Paolo Tosco

List of Publications by Year in descending order

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Ρλοιο Τοςςο

#	Article	IF	CITATIONS
1	Open3DQSAR: a new open-source software aimed at high-throughput chemometric analysis of molecular interaction fields. Journal of Molecular Modeling, 2011, 17, 201-208.	0.8	135
2	Bringing the MMFF force field to the RDKit: implementation and validation. Journal of Cheminformatics, 2014, 6, .	2.8	121
3	Open3DALIGN: an open-source software aimed at unsupervised ligand alignment. Journal of Computer-Aided Molecular Design, 2011, 25, 777-783.	1.3	99
4	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, 1449-1457.	2.9	58
5	Physicochemical Profiling of Sartans: A Detailed Study of Ionization Constants and Distribution Coefficients. Helvetica Chimica Acta, 2008, 91, 468-482.	1.0	51
6	COSMO <i>sar3D</i> : Molecular Field Analysis Based on Local COSMO σ-Profiles. Journal of Chemical Information and Modeling, 2012, 52, 2157-2164.	2.5	36
7	Mechanistic Insights into Cyclooxygenase Irreversible Inactivation by Aspirin. ChemMedChem, 2009, 4, 939-945.	1.6	35
8	Edaravone Derivatives Containing NO-Donor Functions. Journal of Medicinal Chemistry, 2009, 52, 574-578.	2.9	35
9	Novel small molecule protein arginine deiminase 4 (PAD4) inhibitors. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 715-719.	1.0	32
10	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, 102-109.	2.6	29
11	1,2,5-Oxadiazole analogues of leflunomide and related compounds. European Journal of Medicinal Chemistry, 2011, 46, 383-392.	2.6	28
12	A 3D-QSAR-Driven Approach to Binding Mode and Affinity Prediction. Journal of Chemical Information and Modeling, 2012, 52, 302-307.	2.5	27
13	[3-(1 H -Imidazol-4-yl)propyl]guanidines containing furoxan moieties. Bioorganic and Medicinal Chemistry, 2003, 11, 1197-1205.	1.4	22
14	Synthesis and preliminary pharmacological characterisation of a new class of nitrogen-containing bisphosphonates (N-BPs). Bioorganic and Medicinal Chemistry, 2010, 18, 2428-2438.	1.4	22
15	Multitarget drugs: Focus on the NO-donor hybrid drugs. Pure and Applied Chemistry, 2008, 80, 1693-1701.	0.9	19
16	The role of fluorine in stabilizing the bioactive conformation of dihydroorotate dehydrogenase inhibitors. Journal of Molecular Modeling, 2013, 19, 1099-1107.	0.8	19
17	A Mechanistic Hypothesis for the Aspirin-Induced Switch in Lipid Mediator Production by Cyclooxygenase-2. Journal of the American Chemical Society, 2013, 135, 10404-10410.	6.6	18
18	Design and Synthesis of a γ ¹ β ⁸ yclodextrin Oligomer: A New Platform with Potential Application as a Dendrimeric Multicarrier. Chemistry - A European Journal, 2013, 19, 12086-12092.	1.7	17

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19	6-Cyclohexylmethoxy-5-(cyano-NNO-azoxy)pyrimidine-4-amine: AÂnew scaffold endowed with potent CDK2 inhibitory activity. European Journal of Medicinal Chemistry, 2013, 68, 333-338.	2.6	16
20	Hydroxy-1,2,5-oxadiazolyl moiety as bioisoster of the carboxy function. A computational study on γ-aminobutyric acid (GABA) related compounds. Journal of Molecular Modeling, 2008, 14, 279-291.	0.8	15
21	Furoxan analogues of the histamine H3-receptor antagonist imoproxifan and related furazan derivatives. Bioorganic and Medicinal Chemistry, 2005, 13, 4750-4759.	1.4	14
22	Complementary Three-Dimensional Quantitative Structureâ^'Activity Relationship Modeling of Binding Affinity and Functional Potency: A Study on α ₄ β ₂ Nicotinic Ligands. Journal of Medicinal Chemistry, 2009, 52, 2311-2316.	2.9	14
23	NO-donor melatonin derivatives: synthesis and in vitro pharmacological characterization. Journal of Pineal Research, 2007, 42, 371-385.	3.4	13
24	A new class of NO-donor H3-antagonists. Il Farmaco, 2004, 59, 359-371.	0.9	12
25	SDF2XYZ2SDF: how to exploit TINKER power in cheminformatics projects. Journal of Molecular Modeling, 2011, 17, 3021-3023.	0.8	11
26	Thymopentin down-regulates both activity and expression of iNOS in blood cells of Sézary syndrome patients. Nitric Oxide - Biology and Chemistry, 2012, 27, 143-149.	1.2	8
27	Nitrooxyacyl Derivatives of Salicylic Acid: Aspirinâ€Like Molecules that Covalently Inactivate Cyclooxygenaseâ€L. ChemMedChem, 2011, 6, 523-530.	1.6	7
28	Structure-Antioxidant Activity Relationships in a Series of NO-Donor Phenols. ChemMedChem, 2008, 3, 1443-1448.	1.6	6
29	The integration of Open3DTOOLS into the RDKit and KNIME. Journal of Cheminformatics, 2014, 6, .	2.8	6
30	Non-imidazole histamine NO-donor H3-antagonists. Il Farmaco, 2005, 60, 507-512.	0.9	5
31	A New Class of NO-Donor H3-Antagonists ChemInform, 2004, 35, no.	0.1	0
32	3D-QSAR reloaded: Open3DALIGN meets COSMOsar3D. Journal of Cheminformatics, 2013, 5, .	2.8	0