Alessandro Pedretti

List of Publications by Year
in descending order

38 papers	2,373 citations	394421 19 h-index	302126 39 g-index
39 all docs	39 docs citations	39 times ranked	3728 citing authors

#	Article	IF	Citations
1	VEGA â€“ An open platform to develop chemo-bio-informatics applications, using plug-in architecture and script programming. Journal of Computer-Aided Molecular Design, 2004, 18, 167-173.	2.9	635
2	VEGA: a versatile program to convert, handle and visualize molecular structure on Windows-based PCs. Journal of Molecular Graphics and Modelling, 2002, 21, 47-49.	2.4	404
3	Assessing drug-likeness â€“ what are we missing?. Drug Discovery Today, 2008, 13, 285-294.	6.4	235
4	Type 2 Diabetes Mellitus: A Review of Multi-Target Drugs. Molecules, 2020, 25, 1987.	3.8	208
5	Reactions and enzymes in the metabolism of drugs and other xenobiotics. Drug Discovery Today, 2012, 17, 549-560.	6.4	183
6	The VEGA suite of programs: an versatile platform for cheminformatics and drug design projects. Bioinformatics, 2021, 37, 1174-1175.	4.1	90
7	FAME 3: Predicting the Sites of Metabolism in Synthetic Compounds and Natural Products for Phase 1 and Phase 2 Metabolic Enzymes. Journal of Chemical Information and Modeling, 2019, 59, 3400-3412.	5.4	60
8	Design, Synthesis, and Evaluation of Carnosine Derivatives as Selective and Efficient Sequestering Agents of Cytotoxic Reactive Carbonyl Species. ChemMedChem, 2009, 4, 967-975.	3.2	55
9	Comparative modeling of the quaternary structure for the human TRPM8 channel and analysis of its binding features. Biochimica Et Biophysica Acta - Biomembranes, 2009, 1788, 973-982.	2.6	45
10	In silico prediction of human carboxylesterase-1 (hCES1) metabolism combining docking analyses and MD simulations. Bioorganic and Medicinal Chemistry, 2010, 18, 320-329.	3.0	42
11	Homology modeling and metabolism prediction of human carboxylesterase-2 using docking analyses by GriDock: a parallelized tool based on AutoDock 4.0. Journal of Computer-Aided Molecular Design, 2010, 24, 771-787.	2.9	40
12	Modeling of Binding Modes and Inhibition Mechanism of Some Natural Ligands of Farnesyl Transferase Using Molecular Docking. Journal of Medicinal Chemistry, 2002, 45, 1460-1465.	6.4	37
13	A Comprehensive Mapping of the Druggable Cavities within the SARS-CoV-2 Therapeutically Relevant Proteins by Combining Pocket and Docking Searches as Implemented in Pockets 2.0. International Journal of Molecular Sciences, 2020, 21, 5152.	4.1	34
14	Binding Space Concept: A New Approach To Enhance the Reliability of Docking Scores and Its Application to Predicting Butyrylcholinesterase Hydrolytic Activity. Journal of Chemical Information and Modeling, 2017, 57, 1691-1702.	5.4	31
15	Biological and computational evaluation of an oxadiazole derivative (MD77) as a new lead for direct STAT3 inhibitors. MedChemComm, 2012, 3, 592.	3.4	26
16	Homology Modeling of Leishmanolysin (gp63) from Leishmania panamensis and Molecular Docking of Flavonoids. ACS Omega, 2020, 5, 14741-14749.	3.5	26
17	Novel selective, potent naphthyl TRPM8 antagonists identified through a combined ligand- and structure-based virtual screening approach. Scientific Reports, 2017, 7, 10999.	3.3	23
18	Computational approaches in the rational design of improved carbonyl quenchers: focus on histidine containing dipeptides. Future Medicinal Chemistry, 2016, 8, 1721-1737.	2.3	21

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19	Synthesis, modeling, and crystallographic study of 3,4-disubstituted-1,2,5-oxadiazoles and evaluation of their ability to decrease STAT3 activity. MedChemComm, 2010, 1, 156.	3.4	20
20	Structural Effects of Some Relevant Missense Mutations on the MECP2â€Ð NA Binding: A MD Study Analyzed by Rescore+, a Versatile Rescoring Tool of the VEGA ZZ Program. Molecular Informatics, 2016, 35, 424-433.	2.5	18
21	MetaQSAR: An Integrated Database Engine to Manage and Analyze Metabolic Data. Journal of Medicinal Chemistry, 2018, 61, 1019-1030.	6.4	18
22	Rescoring and Linearly Combining: A Highly Effective Consensus Strategy for Virtual Screening Campaigns. International Journal of Molecular Sciences, 2019, 20, 2060.	4.1	17
23	Synthesis, structureâ€“activity relationships and stereochemical investigations of new tricyclic pyridazinone derivatives as potential STAT3 inhibitors. MedChemComm, 2013, 4, 1181.	3.4	16
24	Combining Molecular Dynamics and Docking Simulations to Develop Targeted Protocols for Performing Optimized Virtual Screening Campaigns on the hTRPM8 Channel. International Journal of Molecular Sciences, 2020, 21, 2265.	4.1	15
25	Combining Different Docking Engines and Consensus Strategies to Design and Validate Optimized Virtual Screening Protocols for the SARS-CoV-2 3CL Protease. Molecules, 2021, 26, 797.	3.8	14
26	Prediction of UGT-mediated Metabolism Using the Manually Curated MetaQSAR Database. ACS Medicinal Chemistry Letters, 2019, 10, 633-638.	2.8	10
27	Prediction of the Formation of Reactive Metabolites by A Novel Classifier Approach Based on Enrichment Factor Optimization (EFO) as Implemented in the VEGA Program. Molecules, 2018, 23, 2955.	3.8	9
28	Repositioning Dequalinium as Potent Muscarinic Allosteric Ligand by Combining Virtual Screening Campaigns and Experimental Binding Assays. International Journal of Molecular Sciences, 2020, 21, 5961.	4.1	9
29	A multiscale approach to predict the binding mode of metallo betaâ€lactamase inhibitors. Proteins: Structure, Function and Bioinformatics, 2022, 90, 372-384.	2.6	8
30	In-Depth AGE and ALE Profiling of Human Albumin in Heart Failure: Ex Vivo Studies. Antioxidants, 2021, 10, 358.	5.1	4
31	MetaClass, a Comprehensive Classification System for Predicting the Occurrence of Metabolic Reactions Based on the MetaQSAR Database. Molecules, 2021, 26, 5857.	3.8	4
32	Key factors regulating protein carbonylation by Î±,Î² unsaturated carbonyls: A structural study based on a retrospective meta-analysis. Biophysical Chemistry, 2017, 230, 20-26.	2.8	3
33	WarpEngine, a Flexible Platform for Distributed Computing Implemented in the VEGA Program and Specially Targeted for Virtual Screening Studies. Journal of Chemical Information and Modeling, 2018, 58, 1154-1160.	5.4	3
34	Tree2C: A Flexible Tool for Enabling Model Deployment with Special Focus on Cheminformatics Applications. Applied Sciences (Switzerland), 2020, 10, 7704.	2.5	3
35	Enhancing the Reliability of GPCR Models by Accounting for Flexibility of Their Proâ€Containing Helices: the Case of the Human mAChR1 Receptor. Molecular Informatics, 2015, 34, 216-227.	2.5	2
36	MetaTREE, a Novel Database Focused on Metabolic Trees, Predicts an Important Detoxification Mechanism: The Glutathione Conjugation. Molecules, 2021, 26, 2098.	3.8	2

#	Article	IF	Citations
37	Towards the Inhibition of Proteinâ€“Protein Interactions (PPIs) in STAT3: Insights into a New Class of Benzothiadiazole Derivatives. Molecules, 2020, 25, 3509.	3.8	1
38	Extensive Sampling of Molecular Dynamics Simulations to Identify Reliable Protein Structures for Optimized Virtual Screening Studies: The Case of the hTRPM8 Channel. International Journal of Molecular Sciences, 2022, 23, 7558.	4.1	1