Laurent Emmanuel Dardenne

List of Publications by Year
in descending order

49 papers	1,620 citations	394421 19 h-index	377865 34 g-index
50 all docs	50 docs citations	50 times ranked	2173 citing authors

#	Article	IF	Citations
1	MHOLline 2.0: Workflow for automatic large-scale modeling and analysis of proteins. Revista Mundi Engenharia Tecnologia E GestÃ£o (ISSN 2525-4782), 2023, 5, .	0.0	4
2	Isobenzofuran-1(3H)-ones as new tyrosinase inhibitors: Biological activity and interaction studies by molecular docking and NMR. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2021, 1869, 140580.	2.3	6
3	New machine learning and physics-based scoring functions for drug discovery. Scientific Reports, 2021, 11, 3198.	3.3	91
4	Drug design and repurposing with DockThor-VS web server focusing on SARS-CoV-2 therapeutic targets and their non-synonym variants. Scientific Reports, 2021, 11, 5543.	3.3	63
5	Highly Flexible Ligand Docking: Benchmarking of the DockThor Program on the LEADS-PEP Proteinâ€“Peptide Data Set. Journal of Chemical Information and Modeling, 2020, 60, 667-683.	5.4	144
6	Cinnamoyl-N-Acylhydrazone-Donepezil Hybrids: Synthesis and Evaluation of Novel Multifunctional Ligands Against Neurodegenerative Diseases. Neurochemical Research, 2020, 45, 3003-3020.	3.3	7
7	Design, Synthesis and Biological Evaluation of Novel Triazole N-acylhydrazone Hybrids for Alzheimerâ€™s Disease. Molecules, 2020, 25, 3165.	3.8	14
8	Computational evaluation of natural compounds as potential inhibitors of human PEPCK-M: an alternative for lung cancer therapy . Advances and Applications in Bioinformatics and Chemistry, 2019, Volume 12, 15-32.	2.6	1
9	Synthesis of new lophineâ€“carbohydrate hybrids as cholinesterase inhibitors: cytotoxicity evaluation and molecular modeling. MedChemComm, 2019, 10, 2089-2101.	3.4	13
10	Design, synthesis and pharmacological evaluation of N -benzyl-piperidinyl-aryl-acylhydrazone derivatives as donepezil hybrids: Discovery of novel multi-target anti-alzheimer prototype drug candidates. European Journal of Medicinal Chemistry, 2018, 147, 48-65.	5.5	52
11	Discovery of naphthylâ€Nâ€acylhydrazone p38Î± MAPK inhibitors with in vivo antiâ€inflammatory and antiâ€TNFâ€Î± activity. Chemical Biology and Drug Design, 2018, 91, 391-397.	3.2	22
12	Inserting Co-Evolution Information from Contact Maps into a Multiobjective Genetic Algorithm for Protein Structure Prediction. , 2018, , .		3
13	Empirical Scoring Functions for Structure-Based Virtual Screening: Applications, Critical Aspects, and Challenges. Frontiers in Pharmacology, 2018, 9, 1089.	3.5	185
14	Design, synthesis, cholinesterase inhibition and molecular modelling study of novel tacrine hybrids with carbohydrate derivatives. Bioorganic and Medicinal Chemistry, 2018, 26, 5566-5577.	3.0	21
15	Estimating Protein Structure Prediction Models Quality Using Convolutional Neural Networks. , 2018, , .		3
16	Design, synthesis and evaluation of novel feruloyl-donepezil hybrids as potential multitarget drugs for the treatment of Alzheimer's disease. European Journal of Medicinal Chemistry, 2017, 130, 440-457.	5.5	67
17	In silico identification of inhibitors of ribose 5-phosphate isomerase from Trypanosoma cruzi using ligand and structure based approaches. Journal of Molecular Graphics and Modelling, 2017, 77, 168-180.	2.4	17
18	Improving de novo protein structure prediction using contact maps information. , 2017, , .		1

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19	Using an aggregation tree to arrange energy function terms for protein structure prediction. , 2017, , .		1
20	Critical Features of Fragment Libraries for Protein Structure Prediction. PLoS ONE, 2017, 12, e0170131.	2.5	20
21	LASSBioâ€1829 Hydrochloride: Development of a New Orally Active Nâ€Acylhydrazone IKK2 Inhibitor with Antiâ€inflammatory Properties. ChemMedChem, 2016, 11, 234-244.	3.2	7
22	Using Crowding-Distance in a Multiobjective Genetic Algorithm for Protein Structure Prediction. , 2016, , .		4
23	Novel series of tacrine-tianeptine hybrids: Synthesis, cholinesterase inhibitory activity, S100B secretion and a molecular modeling approach. European Journal of Medicinal Chemistry, 2016, 121, 758-772.	5.5	39
24	A unique SaeS allele overrides cell-density dependent expression of saeR and lukSF-PV in the ST30-SCCmecIV lineage of CA-MRSA. International Journal of Medical Microbiology, 2016, 306, 367-380.	3.6	10
25	Comparison of differential evolution variants for the molecular ligand-receptor docking problem. , 2015, , .		2
26	Genetic operators based on backbone constraint angles for protein structure prediction. , 2015, , .		3
27	A multiobjective approach for protein structure prediction using a steady-state genetic algorithm with phenotypic crowding. , 2015, , .		6
28	Structural modeling and docking studies of ribose 5-phosphate isomerase from Leishmania major and Homo sapiens: A comparative analysis for Leishmaniasis treatment. Journal of Molecular Graphics and Modelling, 2015, 55, 134-147.	2.4	23
29	Receptorâ€“ligand molecular docking. Biophysical Reviews, 2014, 6, 75-87.	3.2	324
30	A dynamic niching genetic algorithm strategy for docking highly flexible ligands. Information Sciences, 2014, 289, 206-224.	6.9	116
31	A multiple minima genetic algorithm for protein structure prediction. Applied Soft Computing Journal, 2014, 15, 88-99.	7.2	59
32	Structural modelling and comparative analysis of homologous, analogous and specific proteins from Trypanosoma cruzi versus Homo sapiens: putative drug targets for chagas' disease treatment. BMC Genomics, 2010, 11, 610.	2.8	45
33	Understanding the HIV-1 protease nelfinavir resistance mutation D30N in subtypes B and C through molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2010, 29, 137-147.	2.4	24
34	Analysis of Î±4 Î²1integrin specific antagonists binding modes: structural insights by molecular docking, molecular dynamics and linear interaction energy method for free energy calculations. Journal of the Brazilian Chemical Society, 2010, 21, 546-555.	0.6	7
35	Full-atom ab initio protein structure prediction with a Genetic Algorithm using a similarity-based surrogate model. , 2010, , .		10
36	A new approach for potential drug target discovery through in silico metabolic pathway analysis using Trypanosoma cruzi genome information. Memorias Do Instituto Oswaldo Cruz, 2009, 104, 1100-1110.	1.6	27

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37	General Methodology to Optimize Damping Functions to Account for Charge Penetration Effects in Electrostatic Calculations Using Multicentered Multipolar Expansions. Journal of Physical Chemistry A, 2008, 112, 268-280.	2.5	11
38	Molecular Dynamics Simulations of Cruzipains 1 and 2 at Different Temperatures. , 2007, , 158-162.		1
39	Genetic Algorithm for Finding Multiple Low Energy Conformations of Poly Alanine Sequences Under an Atomistic Protein Model. , 2007, , 163-166.		1
40	Molecular docking study and development of an empirical binding free energy model for phosphodiesterase 4 inhibitors. Bioorganic and Medicinal Chemistry, 2006, 14, 6001-6011.	3.0	15
41	Investigation of the three-dimensional lattice HP protein folding model using a genetic algorithm. Genetics and Molecular Biology, 2004, 27, 611-615.	1.3	33
42	A genetic algorithm for the ligand-protein docking problem. Genetics and Molecular Biology, 2004, 27, 605-610.	1.3	40
43	Selection-Insertion Schemes in Genetic Algorithms for the Flexible Ligand Docking Problem. Lecture Notes in Computer Science, 2004, , 368-379.	1.3	19
44	Performance and parameterization of the algorithm Simplified Generalized Simulated Annealing. Genetics and Molecular Biology, 2004, 27, 616-622.	1.3	17
45	Electrostatic properties in the catalytic site of papain: A possible regulatory mechanism for the reactivity of the ion pair. Proteins: Structure, Function and Bioinformatics, 2003, 52, 236-253.	2.6	33
46	Chiral Bistacrine Analogues: Synthesis, Cholinesterase Inhibitory Activity and a Molecular Modeling Approach. Journal of the Brazilian Chemical Society, 0, , .	0.6	5
47	Expedient Microwave-Assisted Synthesis of Bis(n)-lophine Analogues as Selective Butyrylcholinesterase Inhibitors: Cytotoxicity Evaluation and Molecular Modelling. Journal of the Brazilian Chemical Society, 0, , .	0.6	1
48	An Expedient Synthesis of Tacrine-Squaric Hybrids as Potent, Selective and Dualâ€'Binding Cholinesterase Inhibitors. Journal of the Brazilian Chemical Society, 0, , .	0.6	0
49	Design, synthesis, and biological evaluation of new thalidomideâ€"donepezil hybrids as neuroprotective agents targeting cholinesterases and neuroinflammation. RSC Medicinal Chemistry, 0, , .	3.9	1