MichaÃ«l Fernandez

List of Publications by Year
in descending order

88	3,674	126907	138484
papers	citations	33	58
		h-index	g-index

91	91	91	3660
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The value of antimicrobial peptides in the age of resistance. Lancet Infectious Diseases, The, 2020, 20, e216-e230.	9.1	573
2	Rapid and Accurate Machine Learning Recognition of High Performing Metal Organic Frameworks for CO₂ Capture. Journal of Physical Chemistry Letters, 2014, 5, 3056-3060.	4.6	234
3	Large-Scale Quantitative Structureâ€“Property Relationship (QSPR) Analysis of Methane Storage in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 7681-7689.	3.1	174
4	Atomic Property Weighted Radial Distribution Functions Descriptors of Metalâ€“Organic Frameworks for the Prediction of Gas Uptake Capacity. Journal of Physical Chemistry C, 2013, 117, 14095-14105.	3.1	113
5	Genome-wide enhancer prediction from epigenetic signatures using genetic algorithm-optimized support vector machines. Nucleic Acids Research, 2012, 40, e77-e77.	14.5	109
6	Toxic Colors: The Use of Deep Learning for Predicting Toxicity of Compounds Merely from Their Graphic Images. Journal of Chemical Information and Modeling, 2018, 58, 1533-1543.	5.4	101
7	Quantitative structureâ€“activity relationship to predict differential inhibition of aldose reductase by flavonoid compounds. Bioorganic and Medicinal Chemistry, 2005, 13, 3269-3277.	3.0	87
8	Genetic algorithm optimization in drug design QSAR: Bayesian-regularized genetic neural networks (BRGNN) and genetic algorithm-optimized support vectors machines (GA-SVM). Molecular Diversity, 2011, 15, 269-289.	3.9	81
9	QSAR for non-nucleoside inhibitors of HIV-1 reverse transcriptase. Bioorganic and Medicinal Chemistry, 2006, 14, 5876-5889.	3.0	80
10	Geometrical Properties Can Predict CO₂ and N₂ Adsorption Performance of Metalâ€“Organic Frameworks (MOFs) at Low Pressure. ACS Combinatorial Science, 2016, 18, 243-252.	3.8	77
11	Linear and nonlinear modeling of antifungal activity of some heterocyclic ring derivatives using multiple linear regression and Bayesian-regularized neural networks. Journal of Molecular Modeling, 2006, 12, 168-181.	1.8	73
12	The transformational role of GPU computing and deep learning in drug discovery. Nature Machine Intelligence, 2022, 4, 211-221.	16.0	73
13	Artificial Neural Networks from MATLAB® in Medicinal Chemistry. Bayesian-Regularized Genetic Neural Networks (BRGNN): Application to the Prediction of the Antagonistic Activity Against Human Platelet Thrombin Receptor (PAR-1). Current Topics in Medicinal Chemistry, 2008, 8, 1580-1605.	2.1	72
14	Quantitative Structureâ€“Property Relationship Models for Recognizing Metal Organic Frameworks (MOFs) with High CO₂ Working Capacity and CO₂/CH₄ Selectivity for Methane Purification. European Journal of Inorganic Chemistry, 2016, 2016, 4505-4511.	2.0	68
15	Linear and nonlinear QSAR study of N-hydroxy-2-[(phenylsulfonyl)amino]acetamide derivatives as matrix metalloproteinase inhibitors. Bioorganic and Medicinal Chemistry, 2006, 14, 4137-4150.	3.0	63
16	Modeling of farnesyltransferase inhibition by some thiol and non-thiol peptidomimetic inhibitors using genetic neural networks and RDF approaches. Bioorganic and Medicinal Chemistry, 2006, 14, 200-213.	3.0	62
17	Modeling of activity of cyclic urea HIV-1 protease inhibitors using regularized-artificial neural networks. Bioorganic and Medicinal Chemistry, 2006, 14, 280-294.	3.0	60
18	Machine Learning for Silver Nanoparticle Electron Transfer Property Prediction. Journal of Chemical Information and Modeling, 2017, 57, 2413-2423.	5.4	60

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19	Transglutaminase-catalyzed synthesis of trypsin-cyclodextrin conjugates: Kinetics and stability properties. Biotechnology and Bioengineering, 2003, 81, 732-737.	3.3	57
20	Amino Acid Sequence Autocorrelation Vectors and Ensembles of Bayesian-Regularized Genetic Neural Networks for Prediction of Conformational Stability of Human Lysozyme Mutants. Journal of Chemical Information and Modeling, 2006, 46, 1255-1268.	5.4	57
21	Modeling of Cyclin-Dependent Kinase Inhibition by 1H-Pyrazolo[3,4-d]Pyrimidine Derivatives Using Artificial Neural Network Ensembles. Journal of Chemical Information and Modeling, 2005, 45, 1884-1895.	5.4	54
22	Proteometric study of ghrelin receptor function variations upon mutations using amino acid sequence autocorrelation vectors and genetic algorithm-based least square support vector machines. Journal of Molecular Graphics and Modelling, 2007, 26, 166-178.	2.4	53
23	Amino acid sequence autocorrelation vectors and bayesian-regularized genetic neural networks for modeling protein conformational stability: Gene V protein mutants. Proteins: Structure, Function and Bioinformatics, 2007, 67, 834-852.	2.6	46
24	Identification of a potent and selective Ïƒ1 receptor agonist potentiating NGF-induced neurite outgrowth in PC12 cells. Bioorganic and Medicinal Chemistry, 2011, 19, 6210-6224.	3.0	45
25	Thermal stabilization of trypsin by enzymic modification with Î²-cyclodextrin derivatives. Biotechnology and Applied Biochemistry, 2003, 38, 53.	3.1	42
26	QSAR analysis for heterocyclic antifungals. Bioorganic and Medicinal Chemistry, 2007, 15, 2680-2689.	3.0	42
27	QSAR modeling of matrix metalloproteinase inhibition by N-hydroxy-Î±-phenylsulfonylacetamide derivatives. Bioorganic and Medicinal Chemistry, 2007, 15, 6298-6310.	3.0	40
28	Prediction of dinucleotide-specific RNA-binding sites in proteins. BMC Bioinformatics, 2011, 12, S5.	2.6	38
29	Quantitative Structureâ€“Activity Relationship of Rubiscolin Analogues as Î´ Opioid Peptides Using Comparative Molecular Field Analysis (CoMFA) and Comparative Molecular Similarity Indices Analysis (CoMSIA). Journal of Agricultural and Food Chemistry, 2007, 55, 8101-8104.	5.2	36
30	Automated discovery of noncovalent inhibitors of SARS-CoV-2 main protease by consensus Deep Docking of 40 billion small molecules. Chemical Science, 2021, 12, 15960-15974.	7.4	36
31	Bayesian-regularized genetic neural networks applied to the modeling of non-peptide antagonists for the human luteinizing hormone-releasing hormone receptor. Journal of Molecular Graphics and Modelling, 2006, 25, 410-422.	2.4	35
32	Geometrical features can predict electronic properties of graphene nanoflakes. Carbon, 2016, 103, 142-150.	10.3	35
33	Improved functional properties of trypsin modified by monosubstituted amino-Î²-cyclodextrins. Journal of Molecular Catalysis B: Enzymatic, 2003, 21, 133-141.	1.8	34
34	Statistics, damned statistics and nanoscience â€“ using data science to meet the challenge of nanomaterial complexity. Nanoscale Horizons, 2016, 1, 89-95.	8.0	34
35	Chemical conjugation of trypsin with monoamine derivatives of cyclodextrins. Enzyme and Microbial Technology, 2002, 31, 543-548.	3.2	33
36	Modeling of the Inhibition Constant (Ki) of Some Cruzain Ketone-Based Inhibitors Using 2D Spatial Autocorrelation Vectors and Data-Diverse Ensembles of Bayesian-Regularized Genetic Neural Networks. QSAR and Combinatorial Science, 2007, 26, 27-40.	1.4	33

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37	Structural requirements of pyrido[2,3-d]pyrimidin-7-one as CDK4/D inhibitors: 2D autocorrelation, CoMFA and CoMSIA analyses. Bioorganic and Medicinal Chemistry, 2008, 16, 6103-6115.	3.0	32
38	Identification of Nanoparticle Prototypes and Archetypes. ACS Nano, 2015, 9, 11980-11992.	14.6	31
39	Î±-Chymotrypsin stabilization by chemical conjugation with O-carboxymethyl-poly-Î²-cyclodextrin. Process Biochemistry, 2004, 39, 535-539.	3.7	30
40	Proteochemometric Recognition of Stable Kinase Inhibition Complexes Using Topological Autocorrelation and Support Vector Machines. Journal of Chemical Information and Modeling, 2010, 50, 1179-1188.	5.4	30
41	2D Autocorrelation modeling of the activity of trihalobenzocycloheptapyridine analogues as farnesyl protein transferase inhibitors. Molecular Simulation, 2005, 31, 575-584.	2.0	29
42	2D Autocorrelation modeling of the negative inotropic activity of calcium entry blockers using Bayesian-regularized genetic neural networks. Bioorganic and Medicinal Chemistry, 2006, 14, 3330-3340.	3.0	29
43	2D Autocorrelation, CoMFA, and CoMSIA modeling of protein tyrosine kinasesâ€™ inhibition by substituted pyrido[2,3-d]pyrimidine derivatives. Bioorganic and Medicinal Chemistry, 2008, 16, 810-821.	3.0	29
44	2D Autocorrelation Modelling of the Inhibitory Activity of Cytokinin-Derived Cyclin-Dependent Kinase Inhibitors. Bulletin of Mathematical Biology, 2006, 68, 735-751.	1.9	28
45	Stabilization of trypsin by chemical modification with Î²-cyclodextrin monoaldehyde. Biotechnology Letters, 2002, 24, 1455-1459.	2.2	27
46	Machine Learning Prediction of the Energy Gap of Graphene Nanoflakes Using Topological Autocorrelation Vectors. ACS Combinatorial Science, 2016, 18, 661-664.	3.8	26
47	Artificial neural network analysis of the catalytic efficiency of platinum nanoparticles. RSC Advances, 2017, 7, 48962-48971.	3.6	24
48	Modeling of acetylcholinesterase inhibition by tacrine analogues using Bayesian-regularized Genetic Neural Networks and ensemble averaging. Journal of Enzyme Inhibition and Medicinal Chemistry, 2006, 21, 647-661.	5.2	23
49	Functional properties and application in peptide synthesis of trypsin modified with cyclodextrin-containing dicarboxylic acids. Journal of Molecular Catalysis B: Enzymatic, 2004, 31, 47-52.	1.8	22
50	Ensembles of Bayesian-regularized Genetic Neural Networks for Modeling of Acetylcholinesterase Inhibition by Huprines. Chemical Biology and Drug Design, 2006, 68, 201-212.	3.2	22
51	Functional Stabilization of Trypsin by Conjugation with Î²-Cyclodextrin-Modified Carboxymethylcellulose. Preparative Biochemistry and Biotechnology, 2003, 33, 53-66.	1.9	21
52	Effect of Î²-cyclodextrin-polysucrose polymer on the stability properties of soluble trypsin. Enzyme and Microbial Technology, 2004, 34, 78-82.	3.2	21
53	Quantitative Structureâ€“Property Relationship Modeling of Electronic Properties of Graphene Using Atomic Radial Distribution Function Scores. Journal of Chemical Information and Modeling, 2015, 55, 2500-2506.	5.4	21
54	DeepCOP: deep learning-based approach to predict gene regulating effects of small molecules. Bioinformatics, 2020, 36, 813-818.	4.1	21

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55	Stabilization of Î±-chymotrypsin by modification with Î²-cyclodextrin derivatives. Biotechnology and Applied Biochemistry, 2002, 36, 235.	3.1	20
56	Classification of conformational stability of protein mutants from 3D pseudoâ€folding graph representation of protein sequences using support vector machines. Proteins: Structure, Function and Bioinformatics, 2008, 70, 167-175.	2.6	20
57	Protein radial distribution function (P-RDF) and Bayesian-Regularized Genetic Neural Networks for modeling protein conformational stability: Chymotrypsin inhibitor 2 mutants. Journal of Molecular Graphics and Modelling, 2007, 26, 748-759.	2.4	19
58	Docking and quantitative structureâ€“activity relationship studies for sulfonyl hydrazides as inhibitors of cytosolic human branched-chain amino acid aminotransferase. Molecular Diversity, 2009, 13, 493-500.	3.9	19
59	Machine learning and genetic algorithm prediction of energy differences between electronic calculations of graphene nanoflakes. Nanotechnology, 2017, 28, 38LT03.	2.6	19
60	Effects of Î²-cyclodextrin-dextran polymer on stability properties of trypsin. Biotechnology and Bioengineering, 2003, 83, 743-747.	3.3	18
61	Stabilization of Î±-chymotrypsin by chemical modification with monoamine cyclodextrin. Process Biochemistry, 2005, 40, 2091-2094.	3.7	17
62	QSAR models for predicting the activity of non-peptide luteinizing hormone-releasing hormone (LHRH) antagonists derived from erythromycin A using quantum chemical properties. Journal of Molecular Modeling, 2007, 13, 465-476.	1.8	17
63	QSAR Accelerated Discovery of Potent Ice Recrystallization Inhibitors. Scientific Reports, 2016, 6, 26403.	3.3	17
64	Genetic neural network modeling of the selective inhibition of the intermediate-conductance Ca2+-activated K+ channel by some triarylmethanes using topological charge indexes descriptors. Journal of Computer-Aided Molecular Design, 2005, 19, 771-789.	2.9	15
65	Small molecule-induced degradation of the full length and V7 truncated variant forms of human androgen receptor. European Journal of Medicinal Chemistry, 2018, 157, 1164-1173.	5.5	15
66	Modeling corrosion inhibition efficacy of small organic molecules as non-toxic chromate alternatives using comparative molecular surface analysis (CoMSA). Chemosphere, 2016, 160, 80-88.	8.2	14
67	Impact of distributions on the archetypes and prototypes in heterogeneous nanoparticle ensembles. Nanoscale, 2017, 9, 832-843.	5.6	10
68	Bias-Free Chemically Diverse Test Sets from Machine Learning. ACS Combinatorial Science, 2017, 19, 544-554.	3.8	10
69	Analysis of protegrin structureâ€“activity relationships: the structural characteristics important for antimicrobial activity using smoothed amino acid sequence descriptors. Molecular Simulation, 2007, 33, 689-702.	2.0	7
70	Quantitative Structure?Activity Relationship Modeling of Growth Hormone Secretagogues Agonist Activity of some Tetrahydroisoquinoline 1-Carboxamides. Chemical Biology and Drug Design, 2007, 69, 48-55.	3.2	7
71	Quantitative Structureâ€“Activity Relationship of Organosulphur Compounds as Soybean 15â€Lipoxygenase Inhibitors Using CoMFA and CoMSIA. Chemical Biology and Drug Design, 2010, 76, 511-517.	3.2	7
72	A CoMSIA study on the adenosine kinase inhibition of pyrrolo[2,3-d]pyrimidine nucleoside analogues. Bioorganic and Medicinal Chemistry, 2008, 16, 5103-5108.	3.0	5

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73	Proteochemometric Modeling of the Inhibition Complexes of Matrix Metalloproteinases with Nâ€Hydroxyâ€2â€[(Phenylsulfonyl)Amino]Acetamide Derivatives Using Topological Autocorrelation Interaction Matrix and Model Ensemble Averaging. Chemical Biology and Drug Design, 2008, 72, 65-78.	3.2	5
74	Quantitative Structureâ€“Price Relationship (QS$R) Modeling and the Development of Economically Feasible Drug Discovery Projects. Journal of Chemical Information and Modeling, 2019, 59, 1306-1313.	5.4	5
75	Classification of conformational stability of protein mutants from 2D graph representation of protein sequences using support vector machines. Molecular Simulation, 2007, 33, 889-896.	2.0	4
76	Comparative modeling of the conformational stability of chymotrypsin inhibitor 2 protein mutants using amino acid sequence autocorrelation (AASA) and amino acid 3D autocorrelation (AA3DA) vectors and ensembles of Bayesian-regularized genetic neural networks. Molecular Simulation, 2007, 33, 1045-1056.	2.0	4
77	Classification of voltage-gated K+ ion channels from 3D pseudo-folding graph representation of protein sequences using genetic algorithm-optimized support vector machines. Journal of Molecular Graphics and Modelling, 2008, 26, 1306-1314.	2.4	4
78	Modeling of the Inhibition of the Intermediateâ€Conductance Ca²⁺â€Activated K⁺ Channel (IKCa1) by Some Triarylmethanes Using Quantum Chemical Properties Derived From Ab Initio Calculations. QSAR and Combinatorial Science, 2008, 27, 866-875.	1.4	4
79	Modeling of lattice parameters of the and phases of the superalloys with base nickel by using a multiple linear regression analysis. Superlattices and Microstructures, 2009, 45, 117-124.	3.1	4
80	Proteometric modelling of protein conformational stability using amino acid sequence autocorrelation vectors and genetic algorithm-optimised support vector machines. Molecular Simulation, 2008, 34, 857-872.	2.0	3
81	Large-scale recognition of high-affinity proteaseâ€“inhibitor complexes using topological autocorrelation and support vector machines. Molecular Simulation, 2016, 42, 420-433.	2.0	2
82	Graphical Representations of Protein Sequences for Alignment-Free Comparative and Predictive Studies. Recognition of Protease Inhibition Pattern from H-Depleted Molecular Graph Representation of Protease Sequences. Current Bioinformatics, 2010, 5, 241-252.	1.5	2
83	Recognition of drug-target interaction patterns using genetic algorithm-optimized Bayesian-regularized neural networks and support vector machines. , 2009, , .		1
84	Molecular dynamics study of one dimensional nanoscale Si/SiO2 interfaces. European Physical Journal D, 2013, 67, 1.	1.3	1
85	Genetic Algorithm Optimization of Bayesian-Regularized Artificial Neural Networks in Drug Design. , 2016, , 83-102.		1
86	EVALUATION OF DNA INTRAMOLECULAR INTERACTIONS FOR NUCLEOSOME POSITIONING IN YEAST. , 2009, , .		0
87	MOFIA: a chemoinformatic webserver for the prediction of CO2 adsorption in metal organic frameworks (MOF). Materials Research Society Symposia Proceedings, 2013, 1523, 801.	0.1	0
88	Editorial: Intelligent Systems for Genome Functional Annotations. Frontiers in Genetics, 2020, 11, 915.	2.3	0