MichaÃ«l Fernandez

List of Publications by Year
in descending order

88	3,674	145106 33	156644 58
papers	citations	h-index	g-index

91	91	91	4153
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The transformational role of GPU computing and deep learning in drug discovery. Nature Machine Intelligence, 2022, 4, 211-221.	8.3	73
2	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.	3.7	36
3	DeepCOP: deep learning-based approach to predict gene regulating effects of small molecules. Bioinformatics, 2020, 36, 813-818.	1.8	21
4	Editorial: Intelligent Systems for Genome Functional Annotations. Frontiers in Genetics, 2020, 11, 915.	1.1	0
5	The value of antimicrobial peptides in the age of resistance. Lancet Infectious Diseases, The, 2020, 20, e216-e230.	4.6	573
6	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.	2.5	5
7	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.	2.5	101
8	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.	2.6	15
9	Impact of distributions on the archetypes and prototypes in heterogeneous nanoparticle ensembles. Nanoscale, 2017, 9, 832-843.	2.8	10
10	Machine Learning for Silver Nanoparticle Electron Transfer Property Prediction. Journal of Chemical Information and Modeling, 2017, 57, 2413-2423.	2.5	60
11	Artificial neural network analysis of the catalytic efficiency of platinum nanoparticles. RSC Advances, 2017, 7, 48962-48971.	1.7	24
12	Bias-Free Chemically Diverse Test Sets from Machine Learning. ACS Combinatorial Science, 2017, 19, 544-554.	3.8	10
13	Machine learning and genetic algorithm prediction of energy differences between electronic calculations of graphene nanoflakes. Nanotechnology, 2017, 28, 38LT03.	1.3	19
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.	1.0	68
15	Modeling corrosion inhibition efficacy of small organic molecules as non-toxic chromate alternatives using comparative molecular surface analysis (CoMSA). Chemosphere, 2016, 160, 80-88.	4.2	14
16	QSAR Accelerated Discovery of Potent Ice Recrystallization Inhibitors. Scientific Reports, 2016, 6, 26403.	1.6	17
17	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
18	Machine Learning Prediction of the Energy Gap of Graphene Nanoflakes Using Topological Autocorrelation Vectors. ACS Combinatorial Science, 2016, 18, 661-664.	3.8	26

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19	Genetic Algorithm Optimization of Bayesian-Regularized Artificial Neural Networks in Drug Design. , 2016, , 83-102.		1
20	Geometrical features can predict electronic properties of graphene nanoflakes. Carbon, 2016, 103, 142-150.	5.4	35
21	Statistics, damned statistics and nanoscience â€“ using data science to meet the challenge of nanomaterial complexity. Nanoscale Horizons, 2016, 1, 89-95.	4.1	34
22	Large-scale recognition of high-affinity proteaseâ€“inhibitor complexes using topological autocorrelation and support vector machines. Molecular Simulation, 2016, 42, 420-433.	0.9	2
23	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.	2.5	21
24	Identification of Nanoparticle Prototypes and Archetypes. ACS Nano, 2015, 9, 11980-11992.	7.3	31
25	Rapid and Accurate Machine Learning Recognition of High Performing Metal Organic Frameworks for CO₂ Capture. Journal of Physical Chemistry Letters, 2014, 5, 3056-3060.	2.1	234
26	Large-Scale Quantitative Structureâ€“Property Relationship (QSPR) Analysis of Methane Storage in Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2013, 117, 7681-7689.	1.5	174
27	Molecular dynamics study of one dimensional nanoscale Si/SiO2 interfaces. European Physical Journal D, 2013, 67, 1.	0.6	1
28	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.	1.5	113
29	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
30	Genome-wide enhancer prediction from epigenetic signatures using genetic algorithm-optimized support vector machines. Nucleic Acids Research, 2012, 40, e77-e77.	6.5	109
31	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.	1.4	45
32	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.	2.1	81
33	Prediction of dinucleotide-specific RNA-binding sites in proteins. BMC Bioinformatics, 2011, 12, S5.	1.2	38
34	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.	1.5	7
35	Proteochemometric Recognition of Stable Kinase Inhibition Complexes Using Topological Autocorrelation and Support Vector Machines. Journal of Chemical Information and Modeling, 2010, 50, 1179-1188.	2.5	30
36	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.	0.7	2

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37	EVALUATION OF DNA INTRAMOLECULAR INTERACTIONS FOR NUCLEOSOME POSITIONING IN YEAST. , 2009, , .		0
38	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.	2.1	19
39	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.	1.4	4
40	Recognition of drug-target interaction patterns using genetic algorithm-optimized Bayesian-regularized neural networks and support vector machines. , 2009, , .		1
41	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.	1.5	20
42	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.	1.3	4
43	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.	1.5	4
44	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.	1.4	29
45	A CoMSIA study on the adenosine kinase inhibition of pyrrolo[2,3-d]pyrimidine nucleoside analogues. Bioorganic and Medicinal Chemistry, 2008, 16, 5103-5108.	1.4	5
46	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.	1.4	32
47	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.	1.5	5
48	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.	0.9	3
49	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.	1.0	72
50	Classification of conformational stability of protein mutants from 2D graph representation of protein sequences using support vector machines. Molecular Simulation, 2007, 33, 889-896.	0.9	4
51	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.	0.9	4
52	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.	0.9	7
53	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.	2.4	36
54	QSAR analysis for heterocyclic antifungals. Bioorganic and Medicinal Chemistry, 2007, 15, 2680-2689.	1.4	42

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55	QSAR modeling of matrix metalloproteinase inhibition by N-hydroxy-Î±-phenylsulfonylacetamide derivatives. Bioorganic and Medicinal Chemistry, 2007, 15, 6298-6310.	1.4	40
56	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.	1.3	53
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.	1.3	19
58	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.	1.5	33
59	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.	1.5	46
60	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.	1.5	7
61	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.	0.8	17
62	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.	2.5	23
63	2D Autocorrelation Modelling of the Inhibitory Activity of Cytokinin-Derived Cyclin-Dependent Kinase Inhibitors. Bulletin of Mathematical Biology, 2006, 68, 735-751.	0.9	28
64	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.	2.5	57
65	Ensembles of Bayesian-regularized Genetic Neural Networks for Modeling of Acetylcholinesterase Inhibition by Huprines. Chemical Biology and Drug Design, 2006, 68, 201-212.	1.5	22
66	QSAR for non-nucleoside inhibitors of HIV-1 reverse transcriptase. Bioorganic and Medicinal Chemistry, 2006, 14, 5876-5889.	1.4	80
67	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.	1.4	62
68	Modeling of activity of cyclic urea HIV-1 protease inhibitors using regularized-artificial neural networks. Bioorganic and Medicinal Chemistry, 2006, 14, 280-294.	1.4	60
69	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.	1.4	29
70	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.	1.4	63
71	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.	1.3	35
72	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.	0.8	73

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73	Stabilization of Î±-chymotrypsin by chemical modification with monoamine cyclodextrin. Process Biochemistry, 2005, 40, 2091-2094.	1.8	17
74	Quantitative structureâ€“activity relationship to predict differential inhibition of aldose reductase by flavonoid compounds. Bioorganic and Medicinal Chemistry, 2005, 13, 3269-3277.	1.4	87
75	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.	1.3	15
76	2D Autocorrelation modeling of the activity of trihalobenzocycloheptapyridine analogues as farnesyl protein transferase inhibitors. Molecular Simulation, 2005, 31, 575-584.	0.9	29
77	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.	2.5	54
78	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
79	Î±-Chymotrypsin stabilization by chemical conjugation with O-carboxymethyl-poly-Î²-cyclodextrin. Process Biochemistry, 2004, 39, 535-539.	1.8	30
80	Effect of Î²-cyclodextrin-polysucrose polymer on the stability properties of soluble trypsin. Enzyme and Microbial Technology, 2004, 34, 78-82.	1.6	21
81	Thermal stabilization of trypsin by enzymic modification with Î²-cyclodextrin derivatives. Biotechnology and Applied Biochemistry, 2003, 38, 53.	1.4	42
82	Improved functional properties of trypsin modified by monosubstituted amino-Î²-cyclodextrins. Journal of Molecular Catalysis B: Enzymatic, 2003, 21, 133-141.	1.8	34
83	Transglutaminase-catalyzed synthesis of trypsin-cyclodextrin conjugates: Kinetics and stability properties. Biotechnology and Bioengineering, 2003, 81, 732-737.	1.7	57
84	Effects of Î²-cyclodextrin-dextran polymer on stability properties of trypsin. Biotechnology and Bioengineering, 2003, 83, 743-747.	1.7	18
85	Functional Stabilization of Trypsin by Conjugation with Î²-Cyclodextrin-Modified Carboxymethylcellulose. Preparative Biochemistry and Biotechnology, 2003, 33, 53-66.	1.0	21
86	Chemical conjugation of trypsin with monoamine derivatives of cyclodextrins. Enzyme and Microbial Technology, 2002, 31, 543-548.	1.6	33
87	Stabilization of trypsin by chemical modification with Î²-cyclodextrin monoaldehyde. Biotechnology Letters, 2002, 24, 1455-1459.	1.1	27
88	Stabilization of Î±-chymotrypsin by modification with Î²-cyclodextrin derivatives. Biotechnology and Applied Biochemistry, 2002, 36, 235.	1.4	20