Michaël Fernandez

List of Publications by Year
in descending order

88 papers	3,674 citations	126907 33 h-index	138484 58 g-index
91 all docs	91 docs citations	91 times ranked	3660 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.	16.0	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.	7.4	36
3	DeepCOP: deep learning-based approach to predict gene regulating effects of small molecules. Bioinformatics, 2020, 36, 813-818.	4.1	21
4	Editorial: Intelligent Systems for Genome Functional Annotations. Frontiers in Genetics, 2020, 11, 915.	2.3	0
5	The value of antimicrobial peptides in the age of resistance. Lancet Infectious Diseases, The, 2020, 20, e216-e230.	9.1	573
6	Quantitative Structure–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
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.	5.4	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.	5.5	15
9	Impact of distributions on the archetypes and prototypes in heterogeneous nanoparticle ensembles. Nanoscale, 2017, 9, 832-843.	5.6	10
10	Machine Learning for Silver Nanoparticle Electron Transfer Property Prediction. Journal of Chemical Information and Modeling, 2017, 57, 2413-2423.	5.4	60
11	Artificial neural network analysis of the catalytic efficiency of platinum nanoparticles. RSC Advances, 2017, 7, 48962-48971.	3.6	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.	2.6	19
14	Quantitative Structure–Property Relationship Models for Recognizing Metal Organic Frameworks (MOFs) with High CO_2 Working Capacity and CO_2/CH_4 Selectivity for Methane Purification. European Journal of Inorganic Chemistry, 2016, 2016, 4505-4511.	2.0	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.	8.2	14
16	QSAR Accelerated Discovery of Potent Ice Recrystallization Inhibitors. Scientific Reports, 2016, 6, 26403.	3.3	17
17	Geometrical Properties Can Predict CO_2 and N_2 Adsorption Performance of Metal–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

#	Article	IF	Citations
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.	10.3	35
21	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
22	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
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.	5.4	21
24	Identification of Nanoparticle Prototypes and Archetypes. ACS Nano, 2015, 9, 11980-11992.	14.6	31
25	Rapid and Accurate Machine Learning Recognition of High Performing Metal Organic Frameworks for CO_2 Capture. Journal of Physical Chemistry Letters, 2014, 5, 3056-3060.	4.6	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.	3.1	174
27	Molecular dynamics study of one dimensional nanoscale Si/SiO2 interfaces. European Physical Journal D, 2013, 67, 1.	1.3	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.	3.1	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.	14.5	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.	3.0	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.	3.9	81
33	Prediction of dinucleotide-specific RNA-binding sites in proteins. BMC Bioinformatics, 2011, 12, S5.	2.6	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.	3.2	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.	5.4	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.	1.5	2

#	ARTICLE	IF	CITATIONS
37	EVALUATION OF DNA INTRAMOLECULAR INTERACTIONS FOR NUCLEOSOME POSITIONING IN YEAST. , 2009, , .		0
38	Docking and quantitative structure–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
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.	3.1	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 pseudo–folding graph representation of protein sequences using support vector machines. Proteins: Structure, Function and Bioinformatics, 2008, 70, 167-175.	2.6	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.	2.4	4
43	Modeling of the Inhibition of the Intermediate–Conductance Ca^{2+}–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
44	2D Autocorrelation, CoMFA, and CoMSIA modeling of protein tyrosine kinases™ inhibition by substituted pyrido[2,3-d]pyrimidine derivatives. Bioorganic and Medicinal Chemistry, 2008, 16, 810-821.	3.0	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.	3.0	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.	3.0	32
47	Proteochemometric Modeling of the Inhibition Complexes of Matrix Metalloproteinases with *N*–Hydroxy–2–[(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
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.	2.0	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.	2.1	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.	2.0	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.	2.0	4
52	Analysis of protegrin structure–activity relationships: the structural characteristics important for antimicrobial activity using smoothed amino acid sequence descriptors. Molecular Simulation, 2007, 33, 689-702.	2.0	7
53	Quantitative Structure–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
54	QSAR analysis for heterocyclic antifungals. Bioorganic and Medicinal Chemistry, 2007, 15, 2680-2689.	3.0	42

#	Article	IF	Citations
55	QSAR modeling of matrix metalloproteinase inhibition by N-hydroxy-α-phenylsulfonylacetamide derivatives. Bioorganic and Medicinal Chemistry, 2007, 15, 6298-6310.	3.0	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.	2.4	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.	2.4	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.	1.4	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.	2.6	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.	3.2	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.	1.8	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.	5.2	23
63	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
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.	5.4	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.	3.2	22
66	QSAR for non-nucleoside inhibitors of HIV-1 reverse transcriptase. Bioorganic and Medicinal Chemistry, 2006, 14, 5876-5889.	3.0	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.	3.0	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.	3.0	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.	3.0	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.	3.0	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.	2.4	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.	1.8	73

#	Article	IF	Citations
73	Stabilization of Î±-chymotrypsin by chemical modification with monoamine cyclodextrin. Process Biochemistry, 2005, 40, 2091-2094.	3.7	17
74	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
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.	2.9	15
76	2D Autocorrelation modeling of the activity of trihalobenzocycloheptapyridine analogues as farnesyl protein transferase inhibitors. Molecular Simulation, 2005, 31, 575-584.	2.0	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.	5.4	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.	3.7	30
80	Effect of Î²-cyclodextrin-polysucrose polymer on the stability properties of soluble trypsin. Enzyme and Microbial Technology, 2004, 34, 78-82.	3.2	21
81	Thermal stabilization of trypsin by enzymic modification with Î²-cyclodextrin derivatives. Biotechnology and Applied Biochemistry, 2003, 38, 53.	3.1	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.	3.3	57
84	Effects of Î²-cyclodextrin-dextran polymer on stability properties of trypsin. Biotechnology and Bioengineering, 2003, 83, 743-747.	3.3	18
85	Functional Stabilization of Trypsin by Conjugation with Î²-Cyclodextrin-Modified Carboxymethylcellulose. Preparative Biochemistry and Biotechnology, 2003, 33, 53-66.	1.9	21
86	Chemical conjugation of trypsin with monoamine derivatives of cyclodextrins. Enzyme and Microbial Technology, 2002, 31, 543-548.	3.2	33
87	Stabilization of trypsin by chemical modification with Î²-cyclodextrin monoaldehyde. Biotechnology Letters, 2002, 24, 1455-1459.	2.2	27
88	Stabilization of Î±-chymotrypsin by modification with Î²-cyclodextrin derivatives. Biotechnology and Applied Biochemistry, 2002, 36, 235.	3.1	20