Uko Maran

List of Publications by Year
in descending order

94 papers	3,196 citations	147726 31 h-index	168321 53 g-index
102 all docs	102 docs citations	102 times ranked	3114 citing authors

#	Article	IF	Citations
1	Machine Learning Quantitative Structureâ€“Property Relationships as a Function of Ionic Liquid Cations for the Gas-Ionic Liquid Partition Coefficient of Hydrocarbons. International Journal of Molecular Sciences, 2022, 23, 7534.	1.8	5
2	Binary and multi-class classification for androgen receptor agonists, antagonists and binders. Chemosphere, 2021, 262, 128313.	4.2	22
3	A role of flavonoids in cytochrome c-cardiolipin interactions. Bioorganic and Medicinal Chemistry, 2021, 33, 116043.	1.4	4
4	Combined NaÃ¯ve Bayesian, Chemical Fingerprints and Molecular Docking Classifiers to Model and Predict Androgen Receptor Binding Data for Environmentally- and Health-Sensitive Substances. International Journal of Molecular Sciences, 2021, 22, 6695.	1.8	4
5	The quantitative structure-property relationships for the gas-ionic liquid partition coefficient of a large variety of organic compounds in three ionic liquids. Journal of Molecular Liquids, 2021, 343, 117573.	2.3	8
6	Characterization and prediction of double-layer capacitance of nanoporous carbon materials using the Quantitative nano-Structure-Property Relationship approach based on experimentally determined porosity descriptors. Carbon, 2020, 158, 494-504.	5.4	12
7	Modelling of antiproliferative activity measured in HeLa cervical cancer cells in a series of xanthene derivatives. SAR and QSAR in Environmental Research, 2020, 31, 905-921.	1.0	5
8	CoMPARA: Collaborative Modeling Project for Androgen Receptor Activity. Environmental Health Perspectives, 2020, 128, 27002.	2.8	120
9	Logistic Classification Models for pHâ€“Permeability Profile: Predicting Permeability Classes for the Biopharmaceutical Classification System. Journal of Chemical Information and Modeling, 2019, 59, 2442-2455.	2.5	14
10	CHAPTER 6. Storing and Using Qualitative and Quantitative Structureâ€“Activity Relationships in the Era of Toxicological and Chemical Data Expansion. Issues in Toxicology, 2019, , 185-213.	0.2	8
11	Best Practices for QSAR Model Reporting: Physical and Chemical Properties, Ecotoxicity, Environmental Fate, Human Health, and Toxicokinetics Endpoints. Environmental Health Perspectives, 2018, 126, 126001.	2.8	51
12	Quantitative Nano-Structureâ€“Property Relationships for the Nanoporous Carbon: Predicting the Performance of Energy Storage Materials. ACS Applied Energy Materials, 2018, 1, 4016-4024.	2.5	14
13	pH-permeability profiles for drug substances: Experimental detection, comparison with human intestinal absorption and modelling. European Journal of Pharmaceutical Sciences, 2018, 123, 429-440.	1.9	26
14	QSAR modeling and chemical space analysis of antimalarial compounds. Journal of Computer-Aided Molecular Design, 2017, 31, 441-451.	1.3	13
15	Chemical structure and correlation analysis of HIV-1 NNRT and NRT inhibitors and database-curated, published inhibition constants with chemical structure in diverse datasets. Journal of Molecular Graphics and Modelling, 2017, 76, 205-223.	1.3	9
16	Public (Q)SAR Services, Integrated Modeling Environments, and Model Repositories on the Web: State of the Art and Perspectives for Future Development. Molecular Informatics, 2017, 36, 1600082.	1.4	32
17	In Silico Mining for Antimalarial Structure-Activity Knowledge and Discovery of Novel Antimalarial Curcuminoids. Molecules, 2016, 21, 853.	1.7	16
18	Design, discovery, modelling, synthesis, and biological evaluation of novel and small, low toxicity s-triazine derivatives as HIV-1 non-nucleoside reverse transcriptase inhibitors. Bioorganic and Medicinal Chemistry, 2016, 24, 2519-2529.	1.4	27

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19	Effects of temperature and concentration on particle size in a lactose solution using dynamic light scattering analysis. International Dairy Journal, 2016, 61, 205-210.	1.5	6
20	Quantitative structureâ€“permeability relationships at various pH values for neutral and amphoteric drugs and drug-like compounds. SAR and QSAR in Environmental Research, 2016, 27, 813-832.	1.0	16
21	Natural Variation in Arabidopsis Cvi-0 Accession Reveals an Important Role of MPK12 in Guard Cell CO2 Signaling. PLoS Biology, 2016, 14, e2000322.	2.6	69
22	The Permeability of an Artificial Membrane for Wide Range of pH in Human Gastrointestinal Tract: Experimental Measurements and Quantitative Structureï£¿Activity Relationship. Molecular Informatics, 2015, 34, 493-506.	1.4	21
23	Quantitative structureâ€“permeability relationships at various pH values for acidic and basic drugs and drug-like compounds. SAR and QSAR in Environmental Research, 2015, 26, 701-719.	1.0	19
24	QSAR DataBank repository: open and linked qualitative and quantitative structureâ€“activity relationship models. Journal of Cheminformatics, 2015, 7, 32.	2.8	58
25	Classifying bio-concentration factor with random forest algorithm, influence of the bio-accumulative vs. non-bio-accumulative compound ratio to modelling result, and applicability domain for random forest model. SAR and QSAR in Environmental Research, 2014, 25, 967-981.	1.0	13
26	Measurement of baseline toxicity and QSAR analysis of 50 non-polar and 58 polar narcotic chemicals for the alga Pseudokirchneriella subcapitata. Chemosphere, 2014, 96, 23-32.	4.2	59
27	Improving the Use of Ranking in Virtual Screening against HIV-1 Integrase with Triangular Numbers and Including Ligand Profiling with Antitargets. Journal of Chemical Information and Modeling, 2014, 54, 3172-3185.	2.5	18
28	QSAR DataBank - an approach for the digital organization and archiving of QSAR model information. Journal of Cheminformatics, 2014, 6, 25.	2.8	39
29	From data point timelines to a well curated data set, data mining of experimental data and chemical structure data from scientific articles, problems and possible solutions. Journal of Computer-Aided Molecular Design, 2013, 27, 583-603.	1.3	21
30	Quantitative relationship between rate constants and molecular structure descriptors for the gas phase hydrogen abstraction reactions. SAR and QSAR in Environmental Research, 2013, 24, 501-518.	1.0	0
31	Comparative analysis of local and consensus quantitative structure-activity relationship approaches for the prediction of bioconcentration factor. SAR and QSAR in Environmental Research, 2013, 24, 175-199.	1.0	8
32	Drugs, non-drugs, and disease category specificity: organ effects by ligand pharmacology1. SAR and QSAR in Environmental Research, 2013, 24, 319-331.	1.0	9
33	QSAR2012 Workshop - Preface. SAR and QSAR in Environmental Research, 2013, 24, 253-254.	1.0	0
34	Molecular Property Filters Describing Pharmacokinetics and Drug Binding. Current Medicinal Chemistry, 2012, 19, 1646-1662.	1.2	36
35	DrugLogit: Logistic Discrimination between Drugs and Nondrugs Including Disease-Specificity by Assigning Probabilities Based on Molecular Properties. Journal of Chemical Information and Modeling, 2012, 52, 2165-2180.	2.5	38
36	Diseaseâ€Specific Differentiation Between Drugs and Nonâ€Drugs Using Principal Component Analysis of Their Molecular Descriptor Space. Molecular Informatics, 2012, 31, 369-383.	1.4	11

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37	Quantitative structureâ€“activity relationship analysis of acute toxicity of diverse chemicals to Daphnia magna with whole molecule descriptors. SAR and QSAR in Environmental Research, 2011, 22, 757-774.	1.0	27
38	Combined Approach Using Ligand Efficiency, Cross-Docking, and Antitarget Hits for Wild-Type and Drug-Resistant Y181C HIV-1 Reverse Transcriptase. Journal of Chemical Information and Modeling, 2011, 51, 2595-2611.	2.5	27
39	Drug efficiency indices for improvement of molecular docking scoring functions. Journal of Computational Chemistry, 2010, 31, 174-184.	1.5	53
40	A General Treatment of Solubility 4. Description and Analysis of a PCA Model for Ostwald Solubility Coefficients. Journal of Chemical Information and Modeling, 2010, 50, 1275-1283.	2.5	15
41	QSAR model for the prediction of bio-concentration factor using aqueous solubility and descriptors considering various electronic effects. SAR and QSAR in Environmental Research, 2010, 21, 711-729.	1.0	18
42	Chapter 6. Molecular Descriptors from Two-Dimensional Chemical Structure. Issues in Toxicology, 2010, , 148-192.	0.2	7
43	Docking and Virtual Screening Using Distributed Grid Technology. QSAR and Combinatorial Science, 2009, 28, 815-821.	1.5	21
44	Relationship Between Structure and Permeability in Artificial Membranes: Theoretical Whole Molecule Descriptors in Development of QSAR Models. QSAR and Combinatorial Science, 2009, 28, 811-814.	1.5	7
45	The QSAR Modeling of Cytotoxicity on Anthraquinones. QSAR and Combinatorial Science, 2009, 28, 829-833.	1.5	3
46	UNICORE. , 2009, , 615-643.		4
47	The autoimmune regulator PHD finger binds to nonâ€methylated histone H3K4 to activate gene expression. EMBO Reports, 2008, 9, 370-376.	2.0	210
48	The proposal of architecture for chemical splitting to optimize QSAR models for aquatic toxicity. Chemosphere, 2008, 72, 772-780.	4.2	31
49	QSPR Modeling of the Polarizability of Polyaromatic Hydrocarbons and Fullerenes. Journal of Physical Chemistry C, 2008, 112, 4785-4790.	1.5	18
50	Design of Multi-Binding-Site Inhibitors, Ligand Efficiency, and Consensus Screening of Avian Influenza H5N1 Wild-Type Neuraminidase and of the Oseltamivir-Resistant H274Y Variant. Journal of Chemical Information and Modeling, 2008, 48, 2074-2080.	2.5	47
51	Chemomentum - UNICORE 6 Based Infrastructure for Complex Applications in Science and Technology. Lecture Notes in Computer Science, 2008, , 82-93.	1.0	26
52	The autoimmune regulator PHD finger binds to non-methylated histone H3K4 to activate gene expression. EMBO Reports, 2008, 9, 370-376.	2.0	131
53	Structure-based calculation of drug efficiency indices. Bioinformatics, 2007, 23, 2678-2685.	1.8	26
54	Modeling the Toxicity of Chemicals to Tetrahymena pyriformis Using Heuristic Multilinear Regression and Heuristic Back-Propagation Neural Networks. Journal of Chemical Information and Modeling, 2007, 47, 2271-2279.	2.5	37

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55	QSPR Modeling of Solubility of Polyaromatic Hydrocarbons and Fullerene in 1-Octanol and n-Heptane. Journal of Physical Chemistry B, 2007, 111, 9853-9857.	1.2	33
56	Comparative Quantitative Structureâ€“Activityâ€“Activity Relationships for Toxicity to Tetrahymena pyriformis and Pimephales promelas. ATLA Alternatives To Laboratory Animals, 2007, 35, 15-24.	0.7	30
57	Mining of the chemical information in GRID environment. Future Generation Computer Systems, 2007, 23, 76-83.	4.9	14
58	Grid Computing for the Estimation of Toxicity: Acute Toxicity on Fathead Minnow (Pimephales) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 62	14	
59	Open Computing Grid for Molecular Science and Engineering. Journal of Chemical Information and Modeling, 2006, 46, 953-959.	2.5	32
60	Combination of a Modified Scoring Function with Two-Dimensional Descriptors for Calculation of Binding Affinities of Bulky, Flexible Ligands to Proteins. Journal of the American Chemical Society, 2006, 128, 1233-1239.	6.6	31
61	QSPR Treatment of the Soil Sorption Coefficients of Organic Pollutants.. ChemInform, 2005, 36, no.	0.1	0
62	Description of the Electronic Structure of Organic Chemicals Using Semiempirical and ab initio Methods for Development of Toxicological QSARs.. ChemInform, 2005, 36, no.	0.1	0
63	OpenMolGRID: Using Automated Workflows in GRID Computing Environment. Lecture Notes in Computer Science, 2005, , 464-473.	1.0	14
64	A General Treatment of Solubility. 3. Principal Component Analysis (PCA) of the Solubilities of Diverse Solutes in Diverse Solvents. Journal of Chemical Information and Modeling, 2005, 45, 913-923.	2.5	36
65	Description of the Electronic Structure of Organic Chemicals Using Semiempirical and Ab Initio Methods for Development of Toxicological QSARs. Journal of Chemical Information and Modeling, 2005, 45, 106-114.	2.5	51
66	QSPR Treatment of the Soil Sorption Coefficients of Organic Pollutants. Journal of Chemical Information and Modeling, 2005, 45, 94-105.	2.5	41
67	QSAR Modeling of Genotoxicity on Non-congeneric Sets of Organic Compounds. Artificial Intelligence Review, 2003, 20, 13-38.	9.7	15
68	A General Treatment of Solubility. 2. QSPR Prediction of Free Energies of Solvation of Specified Solutes in Ranges of Solvents. Journal of Chemical Information and Computer Sciences, 2003, 43, 1806-1814.	2.8	44
69	The Present Utility and Future Potential for Medicinal Chemistry of QSAR/QSPR with Whole Molecule Descriptors. ChemInform, 2003, 34, no.	0.1	0
70	A Comprehensive Docking Study on the Selectivity of Binding of Aromatic Compounds to Proteins.. ChemInform, 2003, 34, no.	0.1	0
71	A Comprehensive Docking Study on the Selectivity of Binding of Aromatic Compounds to Proteins. Journal of Chemical Information and Computer Sciences, 2003, 43, 1576-1583.	2.8	13
72	A General Treatment of Solubility. 1. The QSPR Correlation of Solvation Free Energies of Single Solutes in Series of Solvents. Journal of Chemical Information and Computer Sciences, 2003, 43, 1794-1805.	2.8	97

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73	The Present Utility and Future Potential for Medicinal Chemistry of QSAR / QSPR with Whole Molecule Descriptors. Current Topics in Medicinal Chemistry, 2002, 2, 1333-1356.	1.0	70
74	General and Class Specific Models for Prediction of Soil Sorption Using Various Physicochemical Descriptors. Journal of Chemical Information and Computer Sciences, 2002, 42, 1450-1459.	2.8	12
75	Interpretation of Quantitative Structureâ^'Property and â^'Activity Relationships. Journal of Chemical Information and Computer Sciences, 2001, 41, 679-685.	2.8	110
76	Perspective on the Relationship between Melting Points and Chemical Structure. Crystal Growth and Design, 2001, 1, 261-265.	1.4	167
77	Correlation of the Solubilities of Gases and Vapors in Methanol and Ethanol with Their Molecular Structures. Journal of Chemical Information and Computer Sciences, 2001, 41, 358-363.	2.8	28
78	Theoretical Descriptors for the Correlation of Aquatic Toxicity of Environmental Pollutants by Quantitative Structure-Toxicity Relationships. Journal of Chemical Information and Computer Sciences, 2001, 41, 1162-1176.	2.8	80
79	Non-Linear QSAR Treatment of Genotoxicity. Molecular Simulation, 2000, 24, 229-242.	0.9	31
80	QSPR Correlation and Predictions of GC Retention Indexes for Methyl-Branched Hydrocarbons Produced by Insects. Analytical Chemistry, 2000, 72, 101-109.	3.2	101
81	Structurally Diverse Quantitative Structureâ^'Property Relationship Correlations of Technologically Relevant Physical Properties. Journal of Chemical Information and Computer Sciences, 2000, 40, 1-18.	2.8	238
82	QSPR and QSAR Models Derived Using Large Molecular Descriptor Spaces. A Review of CODESSA Applications. Collection of Czechoslovak Chemical Communications, 1999, 64, 1551-1571.	1.0	70
83	A Comprehensive QSAR Treatment of the Genotoxicity of Heteroaromatic and Aromatic Amines. QSAR and Combinatorial Science, 1999, 18, 03-10.	1.4	65
84	Theoretical study of aminoalkylation in the Mannich reaction of furan with methyleneimminium salt. International Journal of Quantum Chemistry, 1998, 67, 359-366.	1.0	2
85	Fourier transform ion cyclotron resonance mass spectrometry and theoretical studies of gas phase SN2 nucleophilic substitution reactions at sp3-carbon atoms. Journal of the Chemical Society Perkin Transactions II, 1998, , 825-834.	0.9	3
86	New podands with terminal chromogenic moieties derived from formazans. Journal of the Chemical Society Perkin Transactions II, 1998, , 611-616.	0.9	16
87	Prediction of Melting Points for the Substituted Benzenes:â€‰ A QSPR Approach. Journal of Chemical Information and Computer Sciences, 1997, 37, 913-919.	2.8	70
88	A gas phase ab initio study of the Menshutkin reaction. Computational and Theoretical Chemistry, 1997, 397, 263-272.	1.5	12
89	Theoretical study of the keto-enol tautomerism in aqueous solutions. Tetrahedron, 1996, 52, 11325-11328.	1.0	18
90	A comparative AM1 and ab initio study of the intramolecular proton transfer in tautomeric organic compounds. International Journal of Quantum Chemistry, 1996, 60, 1765-1773.	1.0	6

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91	Semiempirical study of the solvent effect on the Menshutkin reaction. Journal of the Chemical Society Perkin Transactions II, 1994, , 2445.	0.9	23
92	About the mutagenicity of chlorine-substituted furanones and halopropenals. A QSAR study using molecular orbital indices. Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis, 1991, 247, 97-102.	0.4	63
93	ELIXIR and Toxicology: a community in development. F1000Research, 0, 10, 1129.	0.8	3
94	Synthesis of 6â€²-galactosyllactose, a deviant human milk oligosaccharide, with the aid of Candida antarctica lipase-B. Organic and Biomolecular Chemistry, 0, , .	1.5	0