# Uko Maran

List of Publications by Year
in descending order



| 94 | 3,196 | 147566 | 168136 |
|---|---|---|---|
| papers | citations | 31 h-index | 53 g-index |

| 102 | 102 | 102 | 3114 |
|---|---|---|---|
| all docs | docs citations | times ranked | 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 |

| # | Article | IF | Citations |
|---|---|---|---|
| 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 |