1. An international database for pesticide risk assessments and management
2. The utility of QSARs in predicting acute fish toxicity of pesticide metabolites: A retrospective validation approach
3. Trend of Multi-Scale QSAR in Drug Design
4. The great descriptor melting pot: mixing descriptors for the common good of QSAR models
5. PaDEL-Descriptor: An Open Source Software to Calculate Molecular Descriptors and Fingerprints
6. Mordred: a molecular descriptor calculator
7. Dragon software: An easy approach to molecular descriptor calculations
8. A Java library for the calculation of molecular descriptors
9. Chemical Informatics functionality in R
10. PySpark and RDKit: Moving towards Big Data in Cheminformatics
11. QSRR: Quantitative Structure-(Chromatographic) retention relationships
12. A performance comparison of modem statistical techniques for molecular descriptor selection and retention prediction in chromatographic QSRR studies
13. Design, Synthesis, Antifungal Activity, and 3D-QASR of Novel Oxime Ether-Containing Coumarin Derivatives as Potential Fungicides
14. Risk mitigation strategy and mechanism analysis of neonicotinoid pesticides on earthworms.
15. Development of terpenoid repellents against Aedes albopictus: a combined study of biological activity evaluation and computational modelling
16. Unveiling first report on in silico modeling of aquatic toxicity of organic chemicals to Labeo rohita (Rohu) employing QSAR and q-RASAR.
17. Discovery of Novel Cinnamic Acid Derivatives as Fungicide Candidates
18. Rational Design of a Potential New Nematicide Targeting Chitin Deacetylase
19. Predictionof Environmental FateandToxicityofInsecticidesUsing Multi-Target QSAR Approach
20. QSAR Modeling of Pesticide Toxicity to Bees
21. A general QSAR model for predicting the acute toxicity of pesticides to Oncorhynchus mykiss
22. Ecotoxicological QSAR Modeling of Organophosphorus and Neonicotinoid Pesticides
23. Norm Index-Based QSAR Model for Acute Toxicity of Pesticides Toward Rainbow Trout
24. A Quantitative Structure Activity Relationship for acute oral toxicity of pesticides on rats: Validation, domain of application and prediction
25. Multi-scale QSAR Approach for Simultaneous Modeling of Ecotoxic Effects of Pesticides
26. Environmental Toxicity of Pesticides, and Its Modeling by QSAR Approaches
27. A general QSAR model for predicting the acute toxicity of pesticides to Lepomis macrochirus
28. Structure-toxicity modeling of pesticides to honey bees
29. Modeling pesticides toxicity to Sheepshead minnow using QSAR
30. QSAR Models for Identifying Pesticides Exhibiting High, Moderate, and Low Toxicity in Honey Bees
31. Use of EPI Suite™ fugacity model in assessing environmental fate
32. The future of the QSAR Toolbox: Moving to less uncertainty in predictive toxicology
33. Integrated in silico strategy for PBT assessment and prioritization under REACH
34. Comparison of two approaches to modeling ground water exposure with EPA's PRZM-GW model
35. 'China Pearl' peach
36. A comparative study of the predictive performance of different descriptor calculation tools: Molecular-based elution order modeling and interpretation of retention mechanism for isomeric compounds from METLIN database.
37. Structure Based Machine Learning Prediction of Retention Times for LC Method Development of Pharmaceuticals
38. Construction and application of a QSRR approach for identifying flavonoids
39. Modeling of small molecule's affinity to phospholipids using IAM-HPLC and QSRR approach enhanced by similarity-based machine algorithms
40. QSPR models for predicting the Kovats retention indices of synthetic ester derivatives based on pyrethrin essential oil
41. Support Vector Models-Based Quantitative Structure-Retention Relationship (QSRR) in the Development and Validation of RP-HPLC Method for Multi-component Analysis of Anti-diabetic Drugs
42. Liquid chromatographic retention time prediction models to secure and improve the feature annotation process in high-resolution mass spectrometry
43. A multi-target QSRR approach to model retention times of small molecules in RPLC
44. A practical strategy enabling more reliable identification of ginsenosides from Panax quinquefolius flower by dimension-enhanced liquid chromatography/mass spectrometry and quantitative structure-retention relationship-based retention behavior prediction
45. Quantitative structure-retention relationship by databases of illegal additives
46. Characterization and identification of alkaloids in Phellodendri Chinensis Cortex and Phellodendri Amurensis Cortex based on UHPLC-IM-Q-TOF-MS
47. QSRR and QSAR Studies of Antitumor Drugs in View of their Biological Activity Prediction
48. RPTLC study of QSRR and QSAR for some benzimidazole derivatives
49. The Application of Connected QSRR and QSAR Strategies to Predict the Physicochemical Interaction of Acridinone Derivatives with DNA
50. Prediction of Acridinones' Ability to Interstrand DNA Crosslinks Formation Using Connected QSRR and QSAR Analysis
51. Quantitative Structure-Retention Relationship Studies as an Analytical Tool in the Determination and Modeling of Pesticide Residues in Plant Organisms
52. Prediction of pesticide retention time in reversed-phase liquid chromatography using quantitative-structure retention relationship models: A comparative study of seven molecular descriptors datasets
53. Predicting reversed-phase liquid chromatographic retention times of pesticides by deep neural networks
54. Affinity of Antifungal Isoxazolo[3,4-b]pyridine-3(1H)-Ones to Phospholipids in Immobilized Artificial Membrane (IAM) Chromatography
55. Quantitative structure retention relationship modeling as potential tool in chromatographic determination of stability constants and thermodynamic parameters of β-cyclodextrin complexation process
56. Essential oils of coriander and sage: Investigation of chemical profile, thermal properties and QSRR analysis
57. Towards safer pesticide management: A quantitative structure-activity relationship based hazard prediction model
58. First report on pesticide sub-chronic and chronic toxicities against dogs using QSAR and chemical read-across
59. Artificial Intelligence and Machine Learning Methods to Evaluate Cardiotoxicity following the Adverse Outcome Pathway Frameworks
60. Applied aspects of neonicotinoid uses in crop protection
61. Overview of the Status and Global Strategy for Neonicotinoids
62. Urinary neonicotinoid concentrations and obesity: A cross-sectional study among Chinese adolescents
63. Non-acute exposure of neonicotinoids, health risk assessment, and evidence integration: a systematic review
64. Identification of key factors affecting neonicotinoid residues in crops and risk of dietary exposure
65. Toxicity and field control efficacy of bioinsecticides and neonicotinoid insecticides against<italic>Amrasca biguttula</italic>(Hemiptera: Cicadellidae) in north Hunan cotton area
66. Fitness effect and transcription profile reveal sublethal effect of nitenpyram on the predator Chrysopa pallens (Neuroptera: Chrysopidae)
67. Urinary neonicotinoids and metabolites are associated with obesity risk in Chinese school children
68. Maternal exposure to neonicotinoid insecticides and fetal growth restriction: A nested case-control study in the guangxi Zhuang birth cohort
69. Health risks of neonicotinoids chronic exposure and its association with glucose metabolism: A case-control study in rural China\*
70. Unintended consequences: Disrupting microbial communities of Nilaparvata lugens with non-target pesticides
71. Effect of Paclobutrazol Application on Enhancing the Efficacy of Nitenpyram against the Brown Planthopper, Nilaparvata lugens
72. Monitoring of insecticide resistance for Apolygus lucorum populations in the apple orchard in China
73. Machine learning method for the management of acute kidney injury: more than just treating biomarkers individually
74. Preventing dataset shift from breaking machine-learning biomarkers
75. Identification of Tumor-Specific MRI Biomarkers Using Machine Learning (ML)
76. Machine Learning and Novel Biomarkers for the Diagnosis of Alzheimer's Disease
77. Can artificial intelligence accelerate preclinical drug discovery and precision medicine?
78. Proteomics and machine-learning models for alcohol-related liver disease biomarkers
79. Editorial: Identification of immune-related biomarkers for cancer diagnosis based on multi-omics data
80. A Significance Assessment of Diabetes Diagnostic Biomarkers Using Machine Learning
81. Artificial intelligence in dementia
82. Advances in auxiliary diagnosis of neuropsychiatric diseases based on machine learning
83. Human against Machine? Machine Learning Identifies MicroRNA Ratios as Biomarkers for Melanoma
84. Using Machine Learning Methods to Study Colorectal Cancer Tumor Micro-Environment and Its Biomarkers
85. Research progress of feature selection and machine learning methods for mass spectrometry-based protein biomarker discovery
86. Identifying Blood Biomarkers for Dementia Using Machine Learning Methods in the Framingham Heart Study
87. How to predict acute kidney injury
88. Machine-learning for osteoarthritis research
89. Predicting atopic asthma by using eNose breath profiles with machine learning
90. Machine Learning Algorithms Failed to Find Depression Biomarker
91. Machine Learning-Assisted Synchronous Fluorescence Sensing Approach for Rapid and Simultaneous Quantification of Thiabendazole and Fuberidazole in Red Wine
92. Detection of Pesticide Residue Level in Grape Using Hyperspectral Imaging with Machine Learning
93. Optimization of Pesticides Spray on Crops in Agriculture using Machine Learning
94. Predicting pesticide dissipation half-life intervals in plants with machine learning models
95. Performance of machine-learning algorithms to pattern recognition and classification of hearing impairment in Brazilian farmers exposed to pesticide and/or cigarette smoke
96. Nondestructive Detection of Pesticide Residue (Chlorpyrifos) on Bok Choi (Brassica rapa subsp. Chinensis) Using a Portable NIR Spectrometer Coupled with a Machine Learning Approach
97. Rapid detection of carbendazim residue in tea by machine learning assisted electrochemical sensor
98. Machine learning-assisted fluorescence sensor array for qualitative and quantitative analysis of pyrethroid pesticides
99. Identification of pesticide residues on black tea by fluorescence hyperspectral technology combined with machine learning
100. PesViT: a deep learning approach for detecting misuse of pesticides on farm
101. Non-Destructive Detection of Different Pesticide Residues on the Surface of Hami Melon Classification Based on tHBA-ELM Algorithm and SWIR Hyperspectral Imaging
102. Detection of Pesticide Residues in Cabbage Based on Fluorescence Spectroscopy Combined with Broad Learning
103. Surrogate biomarkers of pesticide toxicity among pesticide Handlers
104. Concentrations and temporal trends in pesticide biomarkers in urine of Swedish adolescents, 2000-2017
105. Occurrence of biomarkers of pesticide exposure in non-invasive human specimens
106. Investigating the relationship between non-occupational pesticide exposure and metabolomic biomarkers
107. Exposure to pesticides and oxidative stress in Brazilian agricultural communities
108. Validation of exposure indexes to pesticides through the analysis of exposure and effect biomarkers in ground pesticide applicators from Argentina
109. Assessment of pesticide toxicity on earthworms using multiple biomarkers: a review
110. Progress in researches on biological monitoring of chronic low dose pesticide exposure
111. Use of oxidative biomarkers in the evaluation of bioremediation efficiency
112. Effects of Pesticides and Electromagnetic Fields on Honeybees: A Field Study Using Biomarkers
113. Biomarkers of occupational exposure to pesticides: Systematic review of insecticides
114. Adverse Health Effects in Women Farmers Indirectly Exposed to Pesticides
115. New Toxicological Endpoints of Pesticides: Perspectives on Metabolomics
116. Application of metabolomics in pesticide environmental toxicology
117. Metabolomics-Based Mechanistic Insights into Revealing the Adverse Effects of Pesticides on Plants: An Interactive Review
118. Assessing Dietary Pesticide Intake and Potential Health Effects: The Application of Global Metabolomics Analysis
119. An Exploratory Study of the Metabolite Profiling from Pesticides Exposed Workers
120. Omics Approaches to Pesticide Biodegradation
121. Assessment of shade-unshade condition and subsequently pesticide treatment on first flush tea leaf metabolites through GC/MS based metabolomics approach
122. Stereoselective toxicity mechanism of neonicotinoid dinotefuran in honeybees: New perspective from a spatial metabolomics study
123. Soil metabolomics: A powerful tool for predicting and specifying pesticide sorption
124. Study on toxicity effects of environmental pollutants based on metabolomics: A review
125. Metabolomic analysis of the serum and urine of rats exposed to diazinon, dimethoate, and cypermethrin alone or in combination
126. Metabolomics, an Essential Tool in Exploring and Harnessing Microbial Chemical Ecology
127. Metabolomics and its application in environmental toxicology
128. Untargeted metabolomics reveals the preventive effect of quercetin on nephrotoxicity induced by four organophosphorus pesticide mixtures
129. Metabolomics analysis of cucumber fruit in response to foliar fertilizer and pesticides using UHPLC-Q-Orbitrap-HRMS
130. Impacts of dietary exposure to pesticides on faecal microbiome metabolism in adult twins
131. GC-MS based untargeted metabolomics reveals the metabolic response of earthworm (Eudrilus eugeniae) after chronic combinatorial exposure to three different pesticides
132. Current progress and prospects for future research on the rice pest metabolomes
133. Mechanism of Rotenone Toxicity against Plutella xylostella: New Perspective from a Spatial Metabolomics and Lipidomics Study
134. Effects of Different Pesticides on the Brewing of Wine Investigated by GC-MS-Based Metabolomics
135. Metabolomics and mass spectrometry imaging reveal the chronic toxicity of indoxacarb to adult zebrafish (Danio rerio) livers
136. Metabolomics study and meta-analysis on the association between maternal pesticide exposome and birth outcomes
137. PLS-regression: a basic tool of chemometrics
138. Orthogonal projections to latent structures (O-PLS)
139. Double-check: validation of diagnostic statistics for PLS-DA models in metabolomics studies
140. Analysis of the Human Adult Urinary Metabolome Variations with Age, Body Mass Index, and Gender by Implementing a Comprehensive Workflow for Univariate and OPLS Statistical Analyses
141. SIMCA-P, version 7.0.
142. PlantMetSuite: A User-Friendly Web-Based Tool for Metabolomics Analysis and Visualisation
143. MSCAT: A Machine Learning Assisted Catalog of Metabolomics Software Tools
144. Downloading and Analysis of Metabolomic and Lipidomic Data from Metabolomics Workbench Using MetaboAnalyst 5.0.
145. MetaboAnalyst 2.0-a comprehensive server for metabolomic data analysis
146. Using MetaboAnalyst 3.0 for Comprehensive Metabolomics Data Analysis.
147. MetaboAnalyst 4.0: towards more transparent and integrative metabolomics analysis
148. Unified and Standardized Mass Spectrometry Data Processing in Python Using spectrum\_utils
149. The mwtab Python Library for RESTful Access and Enhanced Quality Control, Deposition, and Curation of the Metabolomics Workbench Data Repository
150. A Python library for FAIRer access and deposition to the Metabolomics Workbench Data Repository
151. The metabolomics workbench file status website: a metadata repository promoting FAIR principles of metabolomics data
152. MESSES: Software for Transforming Messy Research Datasets into Clean Submissions to Metabolomics Workbench for Public Sharing
153. A Python-Based Pipeline for Preprocessing LC-MS Data for Untargeted Metabolomics Workflows
154. Xconnector: Retrieving and visualizing metabolites and pathways information from various database resources
155. DBDIpy: a Python library for processing of untargeted datasets from real-time plasma ionization mass spectrometry
156. Phenonaut: multiomics data integration for phenotypic space exploration
157. UmetaFlow: an untargeted metabolomics workflow for high-throughput data processing and analysis
158. MetaboDiff: an R package for differential metabolomic analysis
159. MobilityTransformR: an R package for effective mobility transformation of CE-MS data
160. maplet: an extensible R toolbox for modular and reproducible metabolomics pipelines
161. MetaboAnalystR: an R package for flexible and reproducible analysis of metabolomics data
162. Lilikoi V2.0: a deep learning-enabled, personalized pathway-based R package for diagnosis and prognosis predictions using metabolomics data
163. imputomics: web server and R package for missing values imputation in metabolomics data
164. Lilikoi: an R package for personalized pathway-based classification modeling using metabolomics data
165. A Modular and Expandable Ecosystem for Metabolomics Data Annotation in R
166. Pesticide effect on earthworm lethality via interpretable machine learning
167. DFT study on substituted aromatic compounds' caused acute toxicities to on Daphnia Magna Straus
168. Acute Toxicity of Substituted Phenols to Daphnia Magna Strausat Different pH Values by Kier's Shape IndeX
169. DFT study on the structure of aromatic derivatives and its toxicity to fathead minnows
170. Evaluation of the lipophilicity of chalcones by RP-TLC and computational methods
171. Toxicology of arsenic in fish and aquatic systems
172. Determination of the use of Ligula intestinalis as a bioindicator in malathion residues
173. Mechanisms of Cyanide and Azide Binding to Cobalt Complexes Relevant to Their Antidotal Action
174. Oxidized liposomal artificial red blood cells rescue azide-poisoned mice from lethal toxidrome by recovering cytochrome c oxidase activity
175. A Cobalt Schiff-Base Complex as a Putative Therapeutic for Azide Poisoning
176. Retention time prediction in hydrophilic interaction liquid chromatography with graph neural network and transfer learning