# Yu Zong Chen

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5016405/publications.pdf

Version: 2024-02-01

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|---|---|---|---|
| 149 papers | 8,897 citations | 44069 48 h-index | 45317 90 g-index |
| 150 all docs | 150 docs citations | 150 times ranked | 10452 citing authors |

| # | Article | IF | Citations |
|---|---|---|---|
| 1 | Mechanisms of drug combinations: interaction and network perspectives. Nature Reviews Drug Discovery, 2009, 8, 111-128. | 46.4 | 779 |
| 2 | Therapeutic target database 2020: enriched resource for facilitating research and early development of targeted therapeutics. Nucleic Acids Research, 2020, 48, D1031-D1041. | 14.5 | 488 |
| 3 | Therapeutic target database update 2018: enriched resource for facilitating bench-to-clinic research of targeted therapeutics. Nucleic Acids Research, 2018, 46, D1121-D1127. | 14.5 | 462 |
| 4 | Therapeutic target database update 2012: a resource for facilitating target-oriented drug discovery. Nucleic Acids Research, 2012, 40, D1128-D1136. | 14.5 | 459 |
| 5 | Therapeutic target database update 2022: facilitating drug discovery with enriched comparative data of targeted agents. Nucleic Acids Research, 2022, 50, D1398-D1407. | 14.5 | 310 |
| 6 | NOREVA: normalization and evaluation of MS-based metabolomics data. Nucleic Acids Research, 2017, 45, W162-W170. | 14.5 | 305 |
| 7 | Therapeutic target database update 2016: enriched resource for bench to clinical drug target and targeted pathway information. Nucleic Acids Research, 2016, 44, D1069-D1074. | 14.5 | 278 |
| 8 | Update of TTD: Therapeutic Target Database. Nucleic Acids Research, 2010, 38, D787-D791. | 14.5 | 243 |
| 9 | What Contributes to Serotoninâ€“Norepinephrine Reuptake Inhibitorsâ€™ Dual-Targeting Mechanism? The Key Role of Transmembrane Domain 6 in Human Serotonin and Norepinephrine Transporters Revealed by Molecular Dynamics Simulation. ACS Chemical Neuroscience, 2018, 9, 1128-1140. | 3.5 | 225 |
| 10 | Clustered patterns of species origins of nature-derived drugs and clues for future bioprospecting. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 12943-12948. | 7.1 | 223 |
| 11 | NPASS: natural product activity and species source database for natural product research, discovery and tool development. Nucleic Acids Research, 2018, 46, D1217-D1222. | 14.5 | 177 |
| 12 | Consistent gene signature of schizophrenia identified by a novel feature selection strategy from comprehensive sets of transcriptomic data. Briefings in Bioinformatics, 2020, 21, 1058-1068. | 6.5 | 177 |
| 13 | ANPELA: analysis and performance assessment of the label-free quantification workflow for metaproteomic studies. Briefings in Bioinformatics, 2020, 21, 621-636. | 6.5 | 151 |
| 14 | Effect of Selection of Molecular Descriptors on the Prediction of Bloodâ^'Brain Barrier Penetrating and Nonpenetrating Agents by Statistical Learning Methods. Journal of Chemical Information and Modeling, 2005, 45, 1376-1384. | 5.4 | 145 |
| 15 | Clinical trials, progression-speed differentiating features and swiftness rule of the innovative targets of first-in-class drugs. Briefings in Bioinformatics, 2020, 21, 649-662. | 6.5 | 139 |
| 16 | In-Silico Approaches to Multi-target Drug Discovery. Pharmaceutical Research, 2010, 27, 739-749. | 3.5 | 135 |
| 17 | Computational identification of the binding mechanism of a triple reuptake inhibitor amitifadine for the treatment of major depressive disorder. Physical Chemistry Chemical Physics, 2018, 20, 6606-6616. | 2.8 | 125 |
| 18 | Therapeutic target database update 2014: a resource for targeted therapeutics. Nucleic Acids Research, 2014, 42, D1118-D1123. | 14.5 | 116 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | Simultaneous Improvement in the Precision, Accuracy, and Robustness of Label-free Proteome Quantification by Optimizing Data Manipulation Chains*. Molecular and Cellular Proteomics, 2019, 18, 1683-1699. | 3.8 | 113 |
| 20 | Prediction of RNA-binding proteins from primary sequence by a support vector machine approach. Rna, 2004, 10, 355-368. | 3.5 | 109 |
| 21 | Exploring the Binding Mechanism of Metabotropic Glutamate Receptor 5 Negative Allosteric Modulators in Clinical Trials by Molecular Dynamics Simulations. ACS Chemical Neuroscience, 2018, 9, 1492-1502. | 3.5 | 108 |
| 22 | SVM-Prot 2016: A Web-Server for Machine Learning Prediction of Protein Functional Families from Sequence Irrespective of Similarity. PLoS ONE, 2016, 11, e0155290. | 2.5 | 98 |
| 23 | Discovery of benzimidazole derivatives as novel multi-target EGFR, VEGFR-2 and PDGFR kinase inhibitors. Bioorganic and Medicinal Chemistry, 2011, 19, 4529-4535. | 3.0 | 97 |
| 24 | Clinical Success of Drug Targets Prospectively Predicted by In Silico Study. Trends in Pharmacological Sciences, 2018, 39, 229-231. | 8.7 | 97 |
| 25 | Inhibition of epidermal growth factor receptor tyrosine kinase by chalcone derivatives. BBA - Proteins and Proteomics, 2001, 1550, 144-152. | 2.1 | 86 |
| 26 | Are herb-pairs of traditional Chinese medicine distinguishable from others? Pattern analysis and artificial intelligence classification study of traditionally defined herbal properties. Journal of Ethnopharmacology, 2007, 111, 371-377. | 4.1 | 82 |
| 27 | Fluorescence Array-Based Sensing of Metal Ions Using Conjugated Polyelectrolytes. ACS Applied Materials & Interfaces, 2015, 7, 6882-6888. | 8.0 | 82 |
| 28 | Effect of training datasets on support vector machine prediction of protein-protein interactions. Proteomics, 2005, 5, 876-884. | 2.2 | 73 |
| 29 | Phthalimide conjugations for the degradation of oncogenic PI3K. European Journal of Medicinal Chemistry, 2018, 151, 237-247. | 5.5 | 73 |
| 30 | Recent progresses in the application of machine learning approach for predicting protein functional class independent of sequence similarity. Proteomics, 2006, 6, 4023-4037. | 2.2 | 72 |
| 31 | Can an in silico drug-target search method be used to probe potential mechanisms of medicinal plant ingredients?. Natural Product Reports, 2003, 20, 432. | 10.3 | 70 |
| 32 | Computer prediction of allergen proteins from sequence-derived protein structural and physicochemical properties. Molecular Immunology, 2007, 44, 514-520. | 2.2 | 69 |
| 33 | Support vector machines approach for predicting druggable proteins: recent progress in its exploration and investigation of its usefulness. Drug Discovery Today, 2007, 12, 304-313. | 6.4 | 69 |
| 34 | Discovery of the Consistently Well-Performed Analysis Chain for SWATH-MS Based Pharmacoproteomic Quantification. Frontiers in Pharmacology, 2018, 9, 681. | 3.5 | 69 |
| 35 | CMAUP: a database of collective molecular activities of useful plants. Nucleic Acids Research, 2019, 47, D1118-D1127. | 14.5 | 68 |
| 36 | Drug Adverse Reaction Target Database (DART). Drug Safety, 2003, 26, 685-690. | 3.2 | 67 |

| # | Article | IF | Citations |
|---|---|---|---|
| 37 | Efficacy of different protein descriptors in predicting protein functional families. BMC Bioinformatics, 2007, 8, 300. | 2.6 | 66 |
| 38 | Novel synthetic acridine derivatives as potent DNA-binding and apoptosis-inducing antitumor agents. Bioorganic and Medicinal Chemistry, 2013, 21, 4170-4177. | 3.0 | 66 |
| 39 | Identification of the inhibitory mechanism of FDA approved selective serotonin reuptake inhibitors: an insight from molecular dynamics simulation study. Physical Chemistry Chemical Physics, 2016, 18, 3260-3271. | 2.8 | 66 |
| 40 | Out-of-the-box deep learning prediction of pharmaceutical properties by broadly learned knowledge-based molecular representations. Nature Machine Intelligence, 2021, 3, 334-343. | 16.0 | 66 |
| 41 | Olaparib hydroxamic acid derivatives as dual PARP and HDAC inhibitors for cancer therapy. Bioorganic and Medicinal Chemistry, 2017, 25, 4100-4109. | 3.0 | 64 |
| 42 | Exploration of acridine scaffold as a potentially interesting scaffold for discovering novel multi-target VEGFR-2 and Src kinase inhibitors. Bioorganic and Medicinal Chemistry, 2011, 19, 3312-3319. | 3.0 | 62 |
| 43 | Differentiating Physicochemical Properties between Addictive and Nonaddictive ADHD Drugs Revealed by Molecular Dynamics Simulation Studies. ACS Chemical Neuroscience, 2017, 8, 1416-1428. | 3.5 | 61 |
| 44 | Progress and problems in the exploration of therapeutic targets. Drug Discovery Today, 2006, 11, 412-420. | 6.4 | 60 |
| 45 | Computer prediction of drug resistance mutations in proteins. Drug Discovery Today, 2005, 10, 521-529. | 6.4 | 58 |
| 46 | Differentiating physicochemical properties between NDRIs and sNRIs clinically important for the treatment of ADHD. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 2766-2777. | 2.4 | 56 |
| 47 | Drug Discovery Prospect from Untapped Species: Indications from Approved Natural Product Drugs. PLoS ONE, 2012, 7, e39782. | 2.5 | 53 |
| 48 | Co-targeting cancer drug escape pathways confers clinical advantage for multi-target anticancer drugs. Pharmacological Research, 2015, 102, 123-131. | 7.1 | 51 |
| 49 | In silico search of putative adverse drug reaction related proteins as a potential tool for facilitating drug adverse effect prediction. Toxicology Letters, 2006, 164, 104-112. | 0.8 | 49 |
| 50 | Dissipative particle dynamics simulations of electroosmotic flow in nano-fluidic devices. Microfluidics and Nanofluidics, 2008, 4, 219-225. | 2.2 | 47 |
| 51 | What Are Next Generation Innovative Therapeutic Targets? Clues from Genetic, Structural, Physicochemical, and Systems Profiles of Successful Targets. Journal of Pharmacology and Experimental Therapeutics, 2009, 330, 304-315. | 2.5 | 47 |
| 52 | Design, synthesis and anticancer potential of NSC-319745 hydroxamic acid derivatives as DNMT and HDAC inhibitors. European Journal of Medicinal Chemistry, 2017, 134, 281-292. | 5.5 | 47 |
| 53 | Predicting Drug Combination Index and Simulating the Network-Regulation Dynamics by Mathematical Modeling of Drug-Targeted EGFR-ERK Signaling Pathway. Scientific Reports, 2017, 7, 40752. | 3.3 | 46 |
| 54 | Exploration of (S)-3-aminopyrrolidine as a potentially interesting scaffold for discovery of novel Abl and PI3K dual inhibitors. European Journal of Medicinal Chemistry, 2011, 46, 1404-1414. | 5.5 | 45 |

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| 55 | Design, synthesis and evaluation of acridine derivatives as multi-target Src and MEK kinase inhibitors for anti-tumor treatment. Bioorganic and Medicinal Chemistry, 2016, 24, 261-269. | 3.0 | 45 |
| 56 | Synthesis and investigation of novel 6-(1,2,3-triazol-4-yl)-4-aminoquinazolin derivatives possessing hydroxamic acid moiety for cancer therapy. Bioorganic and Medicinal Chemistry, 2017, 25, 27-37. | 3.0 | 45 |
| 57 | SNORD89 promotes stemness phenotype of ovarian cancer cells by regulating Notch1-c-Myc pathway. Journal of Translational Medicine, 2019, 17, 259. | 4.4 | 43 |
| 58 | Revealing vilazodone's binding mechanism underlying its partial agonism to the 5-HT<sub>1A</sub> receptor in the treatment of major depressive disorder. Physical Chemistry Chemical Physics, 2017, 19, 28885-28896. | 2.8 | 41 |
| 59 | Histopathology classification and localization of colorectal cancer using global labels by weakly supervised deep learning. Computerized Medical Imaging and Graphics, 2021, 88, 101861. | 5.8 | 41 |
| 60 | Novel multi-substituted benzyl acridone derivatives as survivin inhibitors for hepatocellular carcinoma treatment. European Journal of Medicinal Chemistry, 2017, 129, 337-348. | 5.5 | 38 |
| 61 | Computational characterization of the selective inhibition of human norepinephrine and serotonin transporters by an escitalopram scaffold. Physical Chemistry Chemical Physics, 2018, 20, 29513-29527. | 2.8 | 37 |
| 62 | Development of a versatile DNMT and HDAC inhibitor C02S modulating multiple cancer hallmarks for breast cancer therapy. Bioorganic Chemistry, 2019, 87, 200-208. | 4.1 | 37 |
| 63 | ConSIG: consistent discovery of molecular signature from OMIC data. Briefings in Bioinformatics, 2022, 23, . | 6.5 | 37 |
| 64 | Assessing the Performances of Protein Function Prediction Algorithms from the Perspectives of Identification Accuracy and False Discovery Rate. International Journal of Molecular Sciences, 2018, 19, 183. | 4.1 | 35 |
| 65 | Nature's contribution to today's pharmacopeia. Nature Biotechnology, 2014, 32, 979-980. | 17.5 | 32 |
| 66 | Expression signature of sixâ€snoRNA serves as novel nonâ€invasive biomarker for diagnosis and prognosis prediction of renal clear cell carcinoma. Journal of Cellular and Molecular Medicine, 2020, 24, 2215-2228. | 3.6 | 32 |
| 67 | Tannic Acid, a Potent Inhibitor of Epidermal Growth Factor Receptor Tyrosine Kinase. Journal of Biochemistry, 2006, 139, 495-502. | 1.7 | 31 |
| 68 | Simulation of the regulation of EGFR endocytosis and EGFRâ€ERK signaling by endophilinâ€mediated RhoAâ€EGFR crosstalk. FEBS Letters, 2008, 582, 2283-2290. | 2.8 | 31 |
| 69 | Design, synthesis and evaluation of azaacridine derivatives as dual-target EGFR and Src kinase inhibitors for antitumor treatment. European Journal of Medicinal Chemistry, 2017, 136, 372-381. | 5.5 | 31 |
| 70 | Learning the drug targetâ€likeness of a protein. Proteomics, 2007, 7, 4255-4263. | 2.2 | 29 |
| 71 | Simulation of crosstalk between small GTPase RhoA and EGFR-ERK signaling pathway via MEKK1. Bioinformatics, 2009, 25, 358-364. | 4.1 | 29 |
| 72 | MASI: microbiotaâ€”active substance interactions database. Nucleic Acids Research, 2021, 49, D776-D782. | 14.5 | 28 |

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| 73 | MHC-BPS: MHC-binder prediction server for identifying peptides of flexible lengths from sequence-derived physicochemical properties. Immunogenetics, 2006, 58, 607-613. | 2.4 | 27 |
| 74 | Realistic simulations of combined DNA electrophoretic flow and EOF in nanoâ€fluidic devices. Electrophoresis, 2008, 29, 4880-4886. | 2.4 | 27 |
| 75 | A Preclinical Evaluation of SKLB261, a Multikinase Inhibitor of EGFR/Src/VEGFR2, as a Therapeutic Agent against Pancreatic Cancer. Molecular Cancer Therapeutics, 2015, 14, 407-418. | 4.1 | 27 |
| 76 | Fluorescence Analysis of Circulating Exosomes for Breast Cancer Diagnosis Using a Sensor Array and Deep Learning. ACS Sensors, 2022, 7, 1524-1532. | 7.8 | 27 |
| 77 | Identification of small molecule aggregators from large compound libraries by support vector machines. Journal of Computational Chemistry, 2010, 31, 752-763. | 3.3 | 26 |
| 78 | Synthesis and Cytotoxic Activity of Some Novel N-Pyridinyl-2-(6-phenylimidazo[2,1-b]thiazol-3-yl)acetamide Derivatives. Molecules, 2012, 17, 4703-4716. | 3.8 | 25 |
| 79 | Molecular design, synthesis and biological research of novel pyridyl acridones as potent DNA-binding and apoptosis-inducing agents. European Journal of Medicinal Chemistry, 2015, 93, 214-226. | 5.5 | 25 |
| 80 | The interprotein scoring noises in glide docking scores. Proteins: Structure, Function and Bioinformatics, 2012, 80, 169-183. | 2.6 | 24 |
| 81 | Discovery of indolylpiperazinylpyrimidines with dual-target profiles at adenosine A2A and dopamine D2 receptors for Parkinson's disease treatment. PLoS ONE, 2018, 13, e0188212. | 2.5 | 23 |
| 82 | A Two-Step Target Binding and Selectivity Support Vector Machines Approach for Virtual Screening of Dopamine Receptor Subtype-Selective Ligands. PLoS ONE, 2012, 7, e39076. | 2.5 | 22 |
| 83 | Continuum transport model of Ogston sieving in patterned nanofilter arrays for separation of rodâ€like biomolecules. Electrophoresis, 2008, 29, 329-339. | 2.4 | 21 |
| 84 | Antiproliferative activities of the second-generation antipsychotic drug sertindole against breast cancers with a potential application for treatment of breast-to-brain metastases. Scientific Reports, 2018, 8, 15753. | 3.3 | 21 |
| 85 | The Therapeutic Target Database: an Internet resource for the primary targets of approved, clinical trial and experimental drugs. Expert Opinion on Therapeutic Targets, 2011, 15, 903-912. | 3.4 | 20 |
| 86 | Clustered Distribution of Natural Product Leads of Drugs in the Chemical Space as Influenced by the Privileged Target-Sites. Scientific Reports, 2015, 5, 9325. | 3.3 | 20 |
| 87 | Exploration of 1-(3-chloro-4-(4-oxo-4H-chromen-2-yl)phenyl)-3-phenylurea derivatives as selective dual inhibitors of Raf1 and JNK1 kinases for anti-tumor treatment. Bioorganic and Medicinal Chemistry, 2013, 21, 824-831. | 3.0 | 19 |
| 88 | Physicochemical Profiles of the Marketed Agrochemicals and Clues for Agrochemical Lead Discovery and Screening Library Development. Molecular Informatics, 2015, 34, 331-338. | 2.5 | 19 |
| 89 | Database and Bioinformatics Studies of Probiotics. Journal of Agricultural and Food Chemistry, 2017, 65, 7599-7606. | 5.2 | 18 |
| 90 | Exploration of N-(2-aminoethyl)piperidine-4-carboxamide as a potential scaffold for development of VEGFR-2, ERK-2 and Abl-1 multikinase inhibitor. Bioorganic and Medicinal Chemistry, 2013, 21, 5694-5706. | 3.0 | 17 |

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| 91 | What Does It Take to Synergistically Combine Sub-Potent Natural Products into Drug-Level Potent Combinations?. PLoS ONE, 2012, 7, e49969. | 2.5 | 17 |
| 92 | Synthesis and biological research of novel azaacridine derivatives as potent DNA-binding ligands and topoisomerase II inhibitors. Bioorganic and Medicinal Chemistry, 2017, 25, 3437-3446. | 3.0 | 16 |
| 93 | Development of Ligandâ€based Big Data Deep Neural Network Models for Virtual Screening of Large Compound Libraries. Molecular Informatics, 2018, 37, e1800031. | 2.5 | 16 |
| 94 | Databases for the targeted COVIDâ€19 therapeutics. British Journal of Pharmacology, 2020, 177, 4999-5001. | 5.4 | 16 |
| 95 | The Assessment of the Readiness of Molecular Biomarker-Based Mobile Health Technologies for Healthcare Applications. Scientific Reports, 2015, 5, 17854. | 3.3 | 15 |
| 96 | Transport of biomolecules in asymmetric nanofilter arrays. Analytical and Bioanalytical Chemistry, 2009, 394, 427-435. | 3.7 | 14 |
| 97 | Discovery of 1-(3-aryl-4-chlorophenyl)-3-( p -aryl)urea derivatives against breast cancer by inhibiting PI3K/Akt/mTOR and Hedgehog signalings. European Journal of Medicinal Chemistry, 2017, 141, 721-733. | 5.5 | 14 |
| 98 | The Antipsychotic Agent Sertindole Exhibited Antiproliferative Activities by Inhibiting the STAT3 Signaling Pathway in Human Gastric Cancer Cells. Journal of Cancer, 2020, 11, 849-857. | 2.5 | 14 |
| 99 | Does Drug-target Have a Likeness?. Methods of Information in Medicine, 2007, 46, 360-366. | 1.2 | 13 |
| 100 | Multitarget inhibitors derived from crosstalk mechanism involving VEGFR2. Future Medicinal Chemistry, 2014, 6, 1771-1789. | 2.3 | 13 |
| 101 | A benchmarking study on virtual ligand screening against homology models of human GPCRs. Proteins: Structure, Function and Bioinformatics, 2018, 86, 978-989. | 2.6 | 13 |
| 102 | Fluorescence array-based sensing of nitroaromatics using conjugated polyelectrolytes. Analyst, The, 2016, 141, 3242-3245. | 3.5 | 12 |
| 103 | The pros and cons of traditional Chinese medicines in the treatment of COVID-19. Pharmacological Research, 2020, 157, 104873. | 7.1 | 12 |
| 104 | Analysis of bypass signaling in EGFR pathway and profiling of bypass genes for predicting response to anticancer EGFR tyrosine kinase inhibitors. Molecular BioSystems, 2012, 8, 2645. | 2.9 | 11 |
| 105 | Discovery of novel dual VEGFR2 and Src inhibitors using a multistep virtual screening approach. Future Medicinal Chemistry, 2017, 9, 7-24. | 2.3 | 11 |
| 106 | Prognostic relevance of miRâ€137 and its liver microenvironment regulatory target gene AFM in hepatocellular carcinoma. Journal of Cellular Physiology, 2019, 234, 11888-11899. | 4.1 | 11 |
| 107 | Databases for facilitating mechanistic investigations of traditional Chinese medicines against COVID-19. Pharmacological Research, 2020, 159, 104989. | 7.1 | 11 |
| 108 | Simulating EGFR-ERK Signaling Control by Scaffold Proteins KSR and MP1 Reveals Differential Ligand-Sensitivity Co-Regulated by Cbl-CIN85 and Endophilin. PLoS ONE, 2011, 6, e22933. | 2.5 | 9 |

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|---|---|---|---|
| 109 | AggMapNet: enhanced and explainable low-sample omics deep learning with feature-aggregated multi-channel networks. Nucleic Acids Research, 2022, 50, e45-e45. | 14.5 | 9 |
| 110 | Prediction of Functional Class of Proteins and Peptides Irrespective of Sequence Homology by Support Vector Machines. Bioinformatics and Biology Insights, 2007, 1, BBI.S315. | 2.0 | 8 |
| 111 | Cancer informatics for the clinician: An interaction database for chemotherapy regimens and antiepileptic drugs. Seizure: the Journal of the British Epilepsy Association, 2010, 19, 59-67. | 2.0 | 8 |
| 112 | Advances in Exploration of Machine Learning Methods for Predicting Functional Class and Interaction Profiles of Proteins and Peptides Irrespective of Sequence Homology. Current Bioinformatics, 2007, 2, 95-112. | 1.5 | 7 |
| 113 | Analytical description of Ogston-regime biomolecule separation using nanofilters and nanopores. Physical Review E, 2009, 80, 041911. | 2.1 | 7 |
| 114 | Pathway sensitivity analysis for detecting proâ€proliferation activities of oncogenes and tumor suppressors of epidermal growth factor receptorâ€extracellular signalâ€regulated protein kinase pathway at altered protein levels. Cancer, 2009, 115, 4246-4263. | 4.1 | 7 |
| 115 | Genome-scale search of tumor-specific antigens by collective analysis of mutations, expressions and T-cell recognition. Molecular Immunology, 2009, 46, 1824-1829. | 2.2 | 7 |
| 116 | MILITARY VEHICLE CLASSIFICATION VIA ACOUSTIC AND SEISMIC SIGNALS USING STATISTICAL LEARNING METHODS. International Journal of Modern Physics C, 2006, 17, 197-212. | 1.7 | 6 |
| 117 | CFam: a chemical families database based on iterative selection of functional seeds and seed-directed compound clustering. Nucleic Acids Research, 2015, 43, D558-D565. | 14.5 | 6 |
| 118 | A sensitive polymeric dark quencher-based sensing platform for fluorescence â€œturn onâ€•detection of proteins. RSC Advances, 2016, 6, 42443-42446. | 3.6 | 6 |
| 119 | Current QSAR Techniques for Toxicology. , 0, , 217-238. | | 5 |
| 120 | Advances in Machine Learning Prediction of Toxicological Properties and Adverse Drug Reactions of Pharmaceutical Agents. Current Drug Safety, 2008, 3, 100-114. | 0.6 | 5 |
| 121 | Dispersive transport of biomolecules in periodic energy landscapes with application to nanofilter sieving arrays. Electrophoresis, 2011, 32, 506-517. | 2.4 | 5 |
| 122 | Identification of DNA adduct formation of small molecules by molecular descriptors and machine learning methods. Molecular Simulation, 2012, 38, 259-273. | 2.0 | 5 |
| 123 | Metabolic network analysis revealed distinct routes of deletion effects between essential and non-essential genes. Molecular BioSystems, 2012, 8, 1179. | 2.9 | 5 |
| 124 | An imprinted dopamine receptor for discovery of highly potent and selective D 3 analogues with neuroprotective effects. Process Biochemistry, 2015, 50, 1537-1556. | 3.7 | 5 |
| 125 | East meets West in COVID-19 therapeutics. Pharmacological Research, 2020, 159, 105008. | 7.1 | 5 |
| 126 | Toxicogenomic Analysis Suggests Chemical-Induced Sexual Dimorphism in the Expression of Metabolic Genes in Zebrafish Liver. PLoS ONE, 2012, 7, e51971. | 2.5 | 4 |

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| 127 | An insight into the opening path to semi-open conformation of HIV-1 protease by molecular dynamics simulation. Aids, 2010, 24, 1121-1125. | 2.2 | 3 |
| 128 | Effect of training data size and noise level on support vector machines virtual screening of genotoxic compounds from large compound libraries. Journal of Computer-Aided Molecular Design, 2011, 25, 455-467. | 2.9 | 3 |
| 129 | Development and experimental test of support vector machines virtual screening method for searching Src inhibitors from large compound libraries. Chemistry Central Journal, 2012, 6, 139. | 2.6 | 3 |
| 130 | Prediction of human major histocompatibility complex class II binding peptides by continuous kernel discrimination method. Artificial Intelligence in Medicine, 2012, 55, 107-115. | 6.5 | 3 |
| 131 | Towards cheminformatics-based estimation of drug therapeutic index: Predicting the protective index of anticonvulsants using a new quantitative structure-index relationship approach. Journal of Molecular Graphics and Modelling, 2016, 67, 102-110. | 2.4 | 3 |
| 132 | Molecularly imprinted polymer microprobes for manipulating neurological function by regulating temperature-dependent molecular interactions. Process Biochemistry, 2016, 51, 142-157. | 3.7 | 3 |
| 133 | Predicting the Enzymatic Hydrolysis Halfâ€lives of New Chemicals Using Support Vector Regression Models Based on Stepwise Feature Elimination. Molecular Informatics, 2017, 36, 1600153. | 2.5 | 3 |
| 134 | Naphthalimide-containing conjugated polyelectrolytes with different chain configurations. Organic and Biomolecular Chemistry, 2019, 17, 2635-2639. | 2.8 | 3 |
| 135 | Immunometabolism and potential targets in severe COVID-19 peripheral immune responses. Asian Journal of Pharmaceutical Sciences, 2021, 16, 665-667. | 9.1 | 3 |
| 136 | Protein music of enhanced musicality by music style guided exploration of diverse amino acid properties. Heliyon, 2021, 7, e07933. | 3.2 | 3 |
| 137 | HEROD: a human ethnic and regional specific omics database. Bioinformatics, 2017, 33, 3276-3282. | 4.1 | 3 |
| 138 | Super Paramagnetic Clustering of DNA Sequences. Journal of Biological Physics, 2006, 32, 11-25. | 1.5 | 2 |
| 139 | Density Functional Theory Studies on Structure, Spectra, and Electronic Properties of 3,7-Dinitrodibenzobromolium Cation and Chloride. Journal of Physical Chemistry A, 2004, 108, 7596-7602. | 2.5 | 1 |
| 140 | Prediction of Putative Adverse Drug Reaction-Related Proteins from Primary Sequence by Support Vector Machines. Pharmaceutical Medicine, 2005, 19, 317-322. | 0.4 | 1 |
| 141 | Virtual screening prediction of new potential organocatalysts for direct aldol reactions. Journal of Molecular Catalysis A, 2010, 319, 114-118. | 4.8 | 1 |
| 142 | In Silico Prediction of Adverse Drug Reactions and Toxicities Based on Structural, Biological and Clinical Data. Current Drug Safety, 2012, 7, 225-237. | 0.6 | 1 |
| 143 | Pharmacological relationships and ligand discovery of G protein-coupled receptors revealed by simultaneous ligand and receptor clustering. Journal of Molecular Graphics and Modelling, 2017, 76, 136-142. | 2.4 | 1 |
| 144 | Metabolic Profiling of Amino Acids by Liquid Chromatographyâ€“Tandem Mass Spectrometry (LCâ€“MS) to Characterize the Significance of Glutamine in Triple-Negative Breast Cancer (TNBC). Analytical Letters, 2019, 52, 1068-1082. | 1.8 | 1 |

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|---|---|---|---|
| 145 | Drug sales confirm clinical advantage of multiâ€target inhibition of drug escapes by anticancer kinase inhibitors. Drug Development Research, 2019, 80, 246-252. | 2.9 | 1 |
| 146 | Computational model of VEGF, thrombin and histamine signalling network. , 2010, , . | | 0 |
| 147 | Design, Synthesis and Evaluation of New Indolylpyrimidylpiperazines for Gastrointestinal Cancer Therapy. Molecules, 2019, 24, 3661. | 3.8 | 0 |
| 148 | Cover Image, Volume 80, Issue 2. Drug Development Research, 2019, 80, i. | 2.9 | 0 |
| 149 | Combining kinase inhibitors for optimally coâ€targeting cancer and drug escape by exploitation of drug target promiscuities. Drug Development Research, 2021, 82, 133-142. | 2.9 | 0 |