Haiying Yu

List of Publications by Year
in descending order

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45 papers	1,113 citations	331670 21 h-index	414414 32 g-index
45 all docs	45 docs citations	45 times ranked	1148 citing authors

#	Article	IF	Citations
1	Computational insight into biotransformation of halophenols by cytochrome P450: Mechanism and reactivity for epoxidation. Chemosphere, 2022, 286, 131708.	8.2	8
2	Computational Investigation of the Bisphenolic Drug Metabolism by Cytochrome P450: What Factors Favor Intramolecular Phenol Coupling. Chemical Research in Toxicology, 2022, 35, 440-449.	3.3	2
3	Polystyrene microplastics sunlight-induce oxidative dissolution, chemical transformation and toxicity enhancement of silver nanoparticles. Science of the Total Environment, 2022, 827, 154180.	8.0	13
4	Using Physical Organic Chemistry Knowledge to Predict Unusual Metabolites of Synthetic Phenolic Antioxidants by Cytochrome P450. Chemical Research in Toxicology, 2022, 35, 840-848.	3.3	3
5	Computational Insight into Biotransformation Profiles of Organophosphorus Flame Retardants to Their Diester Metabolites by Cytochrome P450. Molecules, 2022, 27, 2799.	3.8	2
6	In Silico simulation of Cytochrome P450-Mediated metabolism of aromatic amines: A case study of N-Hydroxylation. Ecotoxicology and Environmental Safety, 2022, 237, 113544.	6.0	4
7	Insights into the electrochemical degradation of triclosan from human urine: Kinetics, mechanism and toxicity. Chemosphere, 2021, 264, 128598.	8.2	22
8	Investigating the molecular mechanism of hydroxylated bromdiphenyl ethers to inhibit the thyroid hormone sulfotransferase SULT1A1. Chemosphere, 2021, 263, 128353.	8.2	7
9	Developing the QSPR model for predicting the storage lipid/water distribution coefficient of organic compounds. Frontiers of Environmental Science and Engineering, 2021, 15, 1.	6.0	3
10	Precision Biotransformation of Emerging Pollutants by Human Cytochrome P450 Using Computationalâ€“Experimental Synergy: A Case Study of Tris(1,3-dichloro-2-propyl) Phosphate. Environmental Science & Technology, 2021, 55, 14037-14050.	10.0	19
11	Role of polystyrene microplastics in sunlight-mediated transformation of silver in aquatic environments: Mechanisms, kinetics and toxicity. Journal of Hazardous Materials, 2021, 419, 126429.	12.4	18
12	Molecular Basis for Metabolic Regioselectivity and Mechanism of Cytochrome P450s toward Carcinogenic 4-(Methylnitrosamino)-(3-pyridyl)-1-butanone. Chemical Research in Toxicology, 2020, 33, 436-447.	3.3	10
13	Understanding and predicting the diffusivity of organic chemicals for diffusive gradients in thin-films using a QSPR model. Science of the Total Environment, 2020, 706, 135691.	8.0	19
14	QSPR models for predicting the adsorption capacity for microplastics of polyethylene, polypropylene and polystyrene. Scientific Reports, 2020, 10, 14597.	3.3	20
15	Biotransformation Mechanism of Pesticides by Cytochrome P450: A DFT Study on Dieldrin. Chemical Research in Toxicology, 2020, 33, 1442-1448.	3.3	15
16	Computational Biotransformation Profile of Emerging Phenolic Pollutants by Cytochromes P450: Phenol-Coupling Mechanism. Environmental Science & Technology, 2020, 54, 2902-2912.	10.0	37
17	Binding and Metabolism of Brominated Flame Retardant Î²-1,2-Dibromo-4-(1,2-dibromoethyl)cyclohexane in Human Microsomal P450 Enzymes: Insights from Computational Studies. Chemical Research in Toxicology, 2020, 33, 1487-1496.	3.3	10
18	In silico study for inhibiting thyroid hormone sulfotransferase activity by halogenated phenolic chemicals. Ecotoxicology and Environmental Safety, 2019, 180, 146-151.	6.0	4

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19	Developing Predictive Models for Carrying Ability of Micro-Plastics towards Organic Pollutants. Molecules, 2019, 24, 1784.	3.8	27
20	Developing predictive models for toxicity of organic chemicals to green algae based on mode of action. Chemosphere, 2018, 190, 463-470.	8.2	42
21	Mechanistic insights into alginate fouling caused by calcium ions based on terahertz time-domain spectra analyses and DFT calculations. Water Research, 2018, 129, 337-346.	11.3	168
22	Formation of disinfection by-products during chlorination of organic matter from phoenix tree leaves and Chlorella vulgaris. Environmental Pollution, 2018, 243, 1887-1893.	7.5	37
23	Computational Insight into the Activation Mechanism of Carcinogenic Nâ€™-Nitrosonornicotine (NNN) Catalyzed by Cytochrome P450. Environmental Science & Technology, 2018, 52, 11838-11847.	10.0	7
24	Cytotoxicity induced by iodinated haloacetamides via ROS accumulation and apoptosis in HepG-2â€cells. Environmental Pollution, 2018, 242, 191-197.	7.5	35
25	Development and evaluation of predictive model for bovine serum albumin-water partition coefficients of neutral organic chemicals. Ecotoxicology and Environmental Safety, 2017, 138, 92-97.	6.0	6
26	In silico investigation of gas/particle partitioning equilibrium of polybrominated diphenyl ethers (PBDEs). Chemosphere, 2017, 188, 110-118.	8.2	13
27	Physicochemical correlations between membrane surface hydrophilicity and adhesive fouling in membrane bioreactors. Journal of Colloid and Interface Science, 2017, 505, 900-909.	9.4	56
28	Novel indicators for thermodynamic prediction of interfacial interactions related with adhesive fouling in a membrane bioreactor. Journal of Colloid and Interface Science, 2017, 487, 320-329.	9.4	43
29	Developing QSPR model of gas/particle partition coefficients of neutral poly-/perfluoroalkyl substances. Atmospheric Environment, 2016, 143, 270-277.	4.1	10
30	Modeling three-dimensional surface morphology of biocake layer in a membrane bioreactor based on fractal geometry. Bioresource Technology, 2016, 222, 478-484.	9.6	24
31	Using regression models to evaluate the formation of trihalomethanes and haloacetonitriles via chlorination of source water with low SUVA values in the Yangtze River Delta region, China. Environmental Geochemistry and Health, 2016, 38, 1303-1312.	3.4	30
32	Comparison of prediction methods for octanol-air partition coefficients of diverse organic compounds. Chemosphere, 2016, 148, 118-125.	8.2	21
33	In Silico Investigation of the Thyroid Hormone Activity of Hydroxylated Polybrominated Diphenyl Ethers. Chemical Research in Toxicology, 2015, 28, 1538-1545.	3.3	22
34	Modeling and predicting pKa values of mono-hydroxylated polychlorinated biphenyls (HO-PCBs) and polybrominated diphenyl ethers (HO-PBDEs) by local molecular descriptors. Chemosphere, 2015, 138, 829-836.	8.2	14
35	Electrochemical determination of bisphenol A with a glassy carbon electrode modified with gold nanodendrites. Mikrochimica Acta, 2015, 182, 703-709.	5.0	30
36	Use of multiple regression models to evaluate the formation of halonitromethane via chlorination/chloramination of water from Tai Lake and the Qiantang River, China. Chemosphere, 2015, 119, 540-546.	8.2	39

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37	Effects of ionic strength on membrane fouling in a membrane bioreactor. Bioresource Technology, 2014, 156, 35-41.	9.6	35
38	Membrane fouling in a submerged membrane bioreactor with focus on surface properties and interactions of cake sludge and bulk sludge. Bioresource Technology, 2014, 169, 213-219.	9.6	27
39	Experimental evidence for osmotic pressure-induced fouling in a membrane bioreactor. Bioresource Technology, 2014, 158, 119-126.	9.6	22
40	Thermodynamic analysis of membrane fouling in a submerged membrane bioreactor and its implications. Bioresource Technology, 2013, 146, 7-14.	9.6	83
41	Factors affecting formation of haloacetonitriles and haloketones during chlorination/monochloramination of Jinlan Reservoir water. Water Science and Technology: Water Supply, 2013, 13, 1123-1129.	2.1	9
42	Prediction of the Dissociation Constant pK_a of Organic Acids from Local Molecular Parameters of Their Electronic Ground State. Journal of Chemical Information and Modeling, 2011, 51, 2336-2344.	5.4	15
43	Comparative Analysis of QSAR Models for Predicting pKa of Organic Oxygen Acids and Nitrogen Bases from Molecular Structure. Journal of Chemical Information and Modeling, 2010, 50, 1949-1960.	5.4	28
44	Estimation of Soil Organic Carbon Normalized Sorption Coefficient (K_{oc}) Using Least Squaresâ€Support Vector Machine. QSAR and Combinatorial Science, 2009, 28, 561-567.	1.4	27
45	Progress and perspectives of quantitative structure-activity relationships used for ecological risk assessment of toxic organic compounds. Science in China Series B: Chemistry, 2008, 51, 593.	0.8	27