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Principles of QSAR Modeling

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#	Paper	IF	Citations
79	modeling for quick prediction of inhibitory activity against 3CL enzyme in SARS CoV diseases. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020 , 1-27	3.6	15
78	Predicting oxidative stress induced by organic chemicals by using quantitative Structure-Activity relationship methods. <i>Ecotoxicology and Environmental Safety</i> , 2020 , 201, 110817	7	7
77	Prediction of ozonolytic decolorization half-lives of azo dyes in a continuous-flow system using QSPR. <i>Dyes and Pigments</i> , 2021 , 185, 108915	4.6	2
76	QSAR and molecular docking modelling of anti-leishmanial activities of organic selenium and tellurium compounds. <i>SAR and QSAR in Environmental Research</i> , 2021 , 32, 29-50	3.5	3
75	Evaluating the properties of ionic liquid at variable temperatures and pressures by quantitative structure-property relationship (QSPR). <i>Chemical Engineering Science</i> , 2021 , 231, 116326	4.4	4
74	A simple method for assessing the psychotomimetic activity of the substituted phenethylamines. <i>Zeitschrift Fur Anorganische Und Allgemeine Chemie</i> , 2021 , 647, 651-662	1.3	
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72	Predictive classification-based QSTR models for toxicity study of diverse pesticides on multiple avian species. <i>Environmental Science and Pollution Research</i> , 2021 , 28, 17992-18003	5.1	3
71	Application of Quantitative Structure-Property Relationship Predictive Models to Water Treatment: A Critical Review. <i>ACS ES&T Water</i> , 2021 , 1, 498-517		4
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69	In Silico Screening of the DrugBank Database to Search for Possible Drugs against SARS-CoV-2. <i>Molecules</i> , 2021 , 26,	4.8	8
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65	Predictive Global Models of Cruzain Inhibitors with Large Chemical Coverage. <i>ACS Omega</i> , 2021 , 6, 6722-6735	3.3	2
64	QSAR and Pharmacophore Modeling of Nitrogen Heterocycles as Potent Human -Myristoyltransferase (Hs-NMT) Inhibitors. <i>Molecules</i> , 2021 , 26,	4.8	3
63	Identification of Anti-SARS-CoV-2 Compounds from Food Using QSAR-Based Virtual Screening, Molecular Docking, and Molecular Dynamics Simulation Analysis. <i>Pharmaceuticals</i> , 2021 , 14,	5.2	7

62	Understanding structural characteristics of PARP-1 inhibitors through combined 3D-QSAR and molecular docking studies and discovery of new inhibitors by multistage virtual screening. <i>Structural Chemistry</i> , 2021 , 32, 2035-2050	1.8	1
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58	On the use of electronegativity and electron affinity based pseudo-molecular field descriptors in developing correlations for quantitative structure-activity relationship modeling of drug activities. <i>Chemical Biology and Drug Design</i> , 2021 , 98, 258-269	2.9	
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56	Biological Activities Related to Plant Protection and Environmental Effects of Coumarin Derivatives: QSAR and Molecular Docking Studies. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	3
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