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DOI: 10.1016/s1093-3263(01)00123-1

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2344	Superimposition evaluation of ecdysteroid agonist chemotypes through multidimensional QSAR. <b>2003</b> , 17, 135-53		15
2343	Boosted leave-many-out cross-validation: the effect of training and test set diversity on PLS statistics. <b>2003</b> , 17, 265-75		46
2342	Rational selection of training and test sets for the development of validated QSAR models. <b>2003</b> , 17, 241-53		492
2341	Evaluation of extended parameter sets for the 3D-QSAR technique MaP: implications for interpretability and model quality exemplified by antimalarially active naphthylisoquinoline alkaloids. <b>2003</b> , 17, 347-65		20
2340	Inhibition and substrate recognition--a computational approach applied to HIV protease. <b>2003</b> , 17, 567-81		9
2339	Comparative molecular surface analysis: a novel tool for drug design and molecular diversity studies. <b>2003</b> , 7, 45-59		6

2338	Predicting the NO <sub>3</sub> radical tropospheric degradability of organic pollutants by theoretical molecular descriptors. <b>2003</b> , 37, 3115-3124	34
2337	Cross-validation as the objective function for variable-selection techniques. <b>2003</b> , 22, 395-406	182
2336	Pitfalls in QSAR. <b>2003</b> , 622, 39-51	260
2335	Design of EGFR kinase inhibitors: a ligand-based approach and its confirmation with structure-based studies. <b>2003</b> , 11, 4643-53	24
2334	The Importance of Being Earnest: Validation is the Absolute Essential for Successful Application and Interpretation of QSPR Models. <b>2003</b> , 22, 69-77	1447
2333	QSAR Prediction of Ozone Tropospheric Degradation. <b>2003</b> , 22, 364-373	36
2332	QSAR Modeling of Bioconcentration Factor by theoretical molecular descriptors. <b>2003</b> , 22, 374-385	74
2331	QSAR modeling of alpha-campholenic derivatives with sandalwood odor. <b>2003</b> , 43, 259-66	29
2330	Development and validation of k-nearest-neighbor QSPR models of metabolic stability of drug candidates. <b>2003</b> , 46, 3013-20	134
2329	Modeling toxicity by using supervised kohonen neural networks. <b>2003</b> , 43, 485-92	42
2328	Methods for reliability and uncertainty assessment and for applicability evaluations of classification- and regression-based QSARs. <b>2003</b> , 111, 1361-75	957
2327	Generation of ligand conformations in continuum solvent consistent with protein active site topology: application to thrombin. <b>2003</b> , 46, 1293-305	20
2326	Spectroscopic QSAR methods and self-organizing molecular field analysis for relating molecular structure and estrogenic activity. <b>2003</b> , 43, 1974-81	30
2325	Partial least squares modelling of the acute toxicity of aliphatic compounds to <i>Tetrahymena pyriformis</i> . <b>2003</b> , 14, 265-83	25
2324	Comparative molecular surface analysis (CoMSA) for modeling dye-fiber affinities of the azo and anthraquinone dyes. <b>2003</b> , 43, 1754-62	20
2323	QSAR modeling using chirality descriptors derived from molecular topology. <b>2003</b> , 43, 144-54	89
2322	Structural modeling extends QSAR analysis of antibody-lysozyme interactions to 3D-QSAR. <b>2003</b> , 84, 2264-72	21
2321	VSMP: a novel variable selection and modeling method based on the prediction. <b>2003</b> , 43, 964-9	89

2320	Comparison of MLR, PLS and GA-MLR in QSAR analysis. <b>2003</b> , 14, 433-45	73
2319	Computational studies of chiral catalysts: a comparative molecular field analysis of an asymmetric Diels-Alder reaction with catalysts containing bisoxazoline or phosphinooxazoline ligands. <b>2003</b> , 68, 4648-56	53
2318	Selection of data sets for QSARs: analyses of Tetrahymena toxicity from aromatic compounds. <b>2003</b> , 14, 59-81	48
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2315	Total and Local Quadratic Indices of the Molecular Pseudograph's Atom Adjacency Matrix: Application to Prediction of Caco-2 Permeability of Drugs. <b>2003</b> , 4, 512-536	48
2314	Modelling Aquatic Toxicity with Advanced Computational Techniques: Procedures to Standardize Data and Compare Models. <b>2004</b> , 235-248	3
2313	Protein quadratic indices of the "macromolecular pseudograph's alpha-carbon atom adjacency matrix". 1. Prediction of Arc repressor alanine-mutant's stability. <b>2004</b> , 9, 1124-47	38
2312	Nucleic Acid Quadratic Indices of the Macromolecular Graph's Nucleotides Adjacency Matrix: Modeling of Footprints after the Interaction of Paromomycin with the HIV-1 RNA Packaging Region. <b>2004</b> , 5, 276-293	51
2311	Performance of (consensus) kNN QSAR for predicting estrogenic activity in a large diverse set of organic compounds. <b>2004</b> , 15, 19-32	38
2310	3D-quantitative structure-activity relationship study of organophosphate compounds. <b>2004</b> , 49, 240	1
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2307	Rational design of new antituberculosis agents: receptor-independent four-dimensional quantitative structure-activity relationship analysis of a set of isoniazid derivatives. <b>2004</b> , 47, 3755-64	43
2306	3D-quantitative structure-activity relationship study of organophosphate compounds. <b>2004</b> , 49, 240-245	4
2305	Mapping dye pharmacophores by the Comparative Molecular Surface Analysis (CoMSA): application to heterocyclic monoazo dyes. <b>2004</b> , 62, 61-76	12
2304	3D-QSAR illusions. <b>2004</b> , 18, 587-96	106
2303	Validation tools for variable subset regression. <b>2004</b> , 18, 549-62	58

2302	Classification of a large anticancer data set by adaptive fuzzy partition. <b>2004</b> , 18, 577-86		5
2301	Statistical variation in progressive scrambling. <b>2004</b> , 18, 563-76		111
2300	TOMOCOMD-CARDD, a novel approach for computer-aided 'rational' drug design: I. Theoretical and experimental assessment of a promising method for computational screening and in silico design of new anthelmintic compounds. <b>2004</b> , 18, 615-34		54
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2298	Comparison of Different Classification Methods Applied to a Mode of Toxic Action Data Set. <b>2004</b> , 23, 779-791		24
2297	Quantitative structure-activity relationships for phenyl triazolinones of protoporphyrinogen oxidase inhibitors: a density functional theory study. <b>2004</b> , 25, 1827-32		23
2296	3D-chiral quadratic indices of the 'molecular pseudograph's atom adjacency matrix' and their application to central chirality codification: classification of ACE inhibitors and prediction of sigma-receptor antagonist activities. <b>2004</b> , 12, 5331-42		79
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2293	Detecting Bad Regression models: multicriteria fitness functions in regression analysis. <b>2004</b> , 515, 199-208		147
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2290	QSAR analysis of the toxicity of aromatic compounds to <i>Chlorella vulgaris</i> in a novel short-term assay. <b>2004</b> , 44, 258-65		35
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2287	"In silico" design of new uranyl extractants based on phosphoryl-containing podands: QSPR studies, generation and screening of virtual combinatorial library, and experimental tests. <b>2004</b> , 44, 1365-82		39
2286	Combinatorial QSAR of ambergris fragrance compounds. <b>2004</b> , 44, 582-95		84
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2283	Validated QSAR prediction of OH tropospheric degradation of VOCs: splitting into training-test sets and consensus modeling. <b>2004</b> , 44, 1794-802	187
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2276	A comparison of methods for modeling quantitative structure-activity relationships. <b>2004</b> , 47, 5541-54	191
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2273	A topological sub-structural approach to the mutagenic activity in dental monomers. 3. Heterogeneous set of compounds. <b>2005</b> , 46, 2783-2790	20
2272	Non-stochastic and stochastic linear indices of the 'molecular pseudograph's atom adjacency matrix': application to 'in silico' studies for the rational discovery of new antimalarial compounds. <b>2005</b> , 13, 1293-304	62
2271	Atom, atom-type and total molecular linear indices as a promising approach for bioorganic and medicinal chemistry: theoretical and experimental assessment of a novel method for virtual screening and rational design of new lead anthelmintic. <b>2005</b> , 13, 1005-20	84
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2268	Linear indices of the 'macromolecular graph's nucleotides adjacency matrix' as a promising approach for bioinformatics studies. Part 1: prediction of paromomycin's affinity constant with HIV-1 psi-RNA packaging region. <b>2005</b> , 13, 3397-404	41
2267	QSAR study on thiazole and thiadiazole analogues as antagonists for the adenosine A1 and A3 receptors. <b>2005</b> , 13, 5330-7	17

2266	A novel non-stochastic quadratic fingerprints-based approach for the 'in silico' discovery of new antitrypanosomal compounds. <b>2005</b> , 13, 6264-75	41
2265	Application of molecular topology to the prediction of potency and selection of novel insecticides active against malaria vectors. <b>2005</b> , 727, 107-113	1
2264	CoMFA and docking studies on glycogen phosphorylase a inhibitors as antidiabetic agents. <b>2005</b> , 45, 136-45	22
2263	Structure activity relationships and quantitative structure activity relationships for the flavonoid-mediated inhibition of breast cancer resistance protein. <b>2005</b> , 70, 627-39	162
2262	Unbiased descriptor and parameter selection confirms the potential of proteochemometric modelling. <b>2005</b> , 6, 50	30
2261	A new set of amino acid descriptors and its application in peptide QSARs. <b>2005</b> , 80, 775-86	118
2260	Application of 3D-QSAR in the rational design of receptor ligands and enzyme inhibitors. <b>2005</b> , 2, 1438-51	8
2259	Quantitative Structure-Pharmacokinetic Relationships for drug distribution properties by using general regression neural network. <b>2005</b> , 94, 153-68	37
2258	General linearized biexponential model for QSAR data showing bilinear-type distribution. <b>2005</b> , 94, 2355-79	31
2257	Support vector machine applied in QSAR modelling. <b>2005</b> , 50, 2291-2296	14
2256	Characterization of beta3-adrenergic receptor: determination of pharmacophore and 3D QSAR model for beta3 adrenergic receptor agonism. <b>2005</b> , 19, 93-110	24
2255	Quantitative structure-activity relationship analysis of pyridinone HIV-1 reverse transcriptase inhibitors using the k nearest neighbor method and QSAR-based database mining. <b>2005</b> , 19, 229-42	28
2254	3D-chiral atom, atom-type, and total non-stochastic and stochastic molecular linear indices and their applications to central chirality codification. <b>2005</b> , 19, 369-83	27
2253	Genetic neural network modeling of the selective inhibition of the intermediate-conductance Ca <sup>2+</sup> -activated K <sup>+</sup> channel by some triarylmethanes using topological charge indexes descriptors. <b>2005</b> , 19, 771-89	12
2252	A novel in-silico approach for QSAR Studies of Anabolic and Androgenic Activities in the 17 $\beta$ -hydroxy-5 $\alpha$ -androstane Steroid Family. <b>2005</b> , 24, 218-226	21
2251	The Better Predictive Model: High q <sup>2</sup> for the Training Set or Low Root Mean Square Error of Prediction for the Test Set?. <b>2005</b> , 24, 385-396	86
2250	In silico predictions of blood-brain barrier penetration: considerations to "keep in mind". <b>2005</b> , 315, 477-83	100
2249	Ligand-based virtual screening and in silico design of new antimalarial compounds using nonstochastic and stochastic total and atom-type quadratic maps. <b>2005</b> , 45, 1082-100	71

2248	QSPR using MOLGEN-QSPR: the challenge of fluoroalkane boiling points. <b>2005</b> , 45, 74-80	13
2247	General melting point prediction based on a diverse compound data set and artificial neural networks. <b>2005</b> , 45, 581-90	92
2246	MTD-PLS: a PLS variant of the minimal topologic difference method. III. Mapping interactions between estradiol derivatives and the alpha estrogenic receptor. <b>2005</b> , 45, 1275-81	14
2245	Improving binding mode predictions by docking into protein-specifically adapted potential fields. <b>2005</b> , 48, 5466-79	29
2244	Ranking of aquatic toxicity of esters modelled by QSAR. <b>2005</b> , 58, 559-70	40
2243	An all atom energy based computational protocol for predicting binding affinities of protein-ligand complexes. <b>2005</b> , 579, 6659-66	61
2242	In silico screening of chemicals for bacterial mutagenicity using electrotopological E-state indices and MDL QSAR software. <b>2005</b> , 43, 313-23	47
2241	A quantitative structure-activity relationship study for $\beta$ -substituted acetamido-N-benzylacetamide derivatives ? A novel anticonvulsant drug class. <b>2005</b> , 83, 37-45	9
2240	Modeling of cyclin-dependent kinase inhibition by 1H-pyrazolo[3,4-d]pyrimidine derivatives using artificial neural network ensembles. <b>2005</b> , 45, 1884-95	48
2239	Ecdysteroid Agonists and Antagonists. <b>2005</b> , 197-242	18
2238	kappa Nearest neighbors QSAR modeling as a variational problem: theory and applications. <b>2005</b> , 45, 777-85	44
2237	McQSAR: a multiconformational quantitative structure-activity relationship engine driven by genetic algorithms. <b>2005</b> , 45, 1953-61	16
2236	Ligand-based prediction of active conformation by 3D-QSAR flexibility descriptors and their application in 3+3D-QSAR models. <b>2005</b> , 48, 3239-50	21
2235	A perspective on quantitative structure-activity relationships and carbonic anhydrase inhibitors. <b>2006</b> , 2, 113-37	29
2234	Molecular Chemometrics. <b>2006</b> , 36, 189-198	7
2233	Refinement and use of the approximate similarity in QSAR models for benzodiazepine receptor ligands. <b>2006</b> , 46, 2022-9	17
2232	Modeling robust QSAR. <b>2006</b> , 46, 2310-8	73
2231	Chapter 7 Variable Selection QSAR Modeling, Model Validation, and Virtual Screening. <b>2006</b> , 2, 113-126	14



2230	Combinatorial QSAR modeling of P-glycoprotein substrates. <b>2006</b> , 46, 1245-54	124
2229	Computation of relative bond dissociation enthalpies (DeltaBDE) of phenolic antioxidants from quantum topological molecular similarity (QTMS). <b>2006</b> , 110, 6498-503	25
2228	QSAR prediction of estrogen activity for a large set of diverse chemicals under the guidance of OECD principles. <b>2006</b> , 19, 1540-8	108
2227	Chapter 9 Molecular Similarity: Advances in Methods, Applications and Validations in Virtual Screening and QSAR. <b>2006</b> , 2, 141-168	10
2226	On the use of <sup>1</sup> H and <sup>13</sup> C 1D NMR spectra as QSPR descriptors. <b>2006</b> , 46, 487-94	18
2225	Improved CoMFA modeling by optimization of settings. <b>2006</b> , 46, 355-64	18
2224	A novel automated lazy learning QSAR (ALL-QSAR) approach: method development, applications, and virtual screening of chemical databases using validated ALL-QSAR models. <b>2006</b> , 46, 1984-95	187
2223	Development of quantitative structure-binding affinity relationship models based on novel geometrical chemical descriptors of the protein-ligand interfaces. <b>2006</b> , 49, 2713-24	83
2222	A comparative molecular field analysis (CoMFA) and comparative molecular similarity indices analysis (CoMSIA) of anthranilamide derivatives that are multidrug resistance modulators. <b>2006</b> , 49, 7646-60	24
2221	Exploration of a binding mode of benzothiazol-2-yl acetonitrile pyrimidine core based derivatives as potent c-Jun N-terminal kinase-3 inhibitors and 3D-QSAR analyses. <b>2006</b> , 46, 1763-74	15
2220	Development of a chirality-sensitive flexibility descriptor for 3+3D-QSAR. <b>2006</b> , 46, 1431-8	20
2219	Supervised feature ranking using a genetic algorithm optimized artificial neural network. <b>2006</b> , 46, 1604-14	13
2218	Cytotoxicity of organic compounds against ovarian cancer cells: a quantitative structure-activity relationship study. <b>2006</b> , 3, 441-50	18
2217	Virtual screening for aryl hydrocarbon receptor binding prediction. <b>2006</b> , 49, 5702-9	25
2216	Supervised self-organizing maps in drug discovery. 2. Improvements in descriptor selection and model validation. <b>2006</b> , 46, 137-44	14
2215	Computers, Cheminformatics, and the Medicinal Chemist. <b>2006</b> , 301-319	
2214	On Selection of Training and Test Sets for the Development of Predictive QSAR models. <b>2006</b> , 25, 235-251	183
2213	Quantitative Structure-Activity Relationship of the 4,5-Dihydrotestosterone Steroid Family. <b>2006</b> , 25, 881-894	9

2212	A Novel QSAR Model for Evaluating and Predicting the Inhibition Activity of Dipeptidyl Aspartyl Fluoromethylketones. <b>2006</b> , 25, 928-935	27
2211	Ensembles of Bayesian-regularized genetic neural networks for modeling of acetylcholinesterase inhibition by huprines. <b>2006</b> , 68, 201-12	20
2210	QSAR study of 4-phenylpiperidine derivatives as mu opioid agonists by neural network method. <b>2006</b> , 41, 226-32	14
2209	A novel QSAR model for predicting induction of apoptosis by 4-aryl-4H-chromenes. <b>2006</b> , 14, 6686-94	78
2208	Novel ligands for the human histamine H1 receptor: synthesis, pharmacology, and comparative molecular field analysis studies of 2-dimethylamino-5-(6)-phenyl-1,2,3,4-tetrahydronaphthalenes. <b>2006</b> , 14, 6640-58	27
2207	QSAR studies about cytotoxicity of benzophenazines with dual inhibition toward both topoisomerases I and II: 3D-MoRSE descriptors and statistical considerations about variable selection. <b>2006</b> , 14, 7347-58	54
2206	Predicting antitrichomonal activity: a computational screening using atom-based bilinear indices and experimental proofs. <b>2006</b> , 14, 6502-24	48
2205	The cytotoxicity of ortho alkyl substituted 4-X-phenols: a QSAR based on theoretical bond lengths and electron densities. <b>2006</b> , 16, 1249-54	34
2204	Design, synthesis, antibacterial, and QSAR studies of myristic acid derivatives. <b>2006</b> , 16, 3023-9	43
2203	Correlation of antibacterial activity of some N-[5-(2-furanyl)-2-methyl-4-oxo-4H-thieno[2,3-d]pyrimidin-3-yl]-carboxamide and 3-substituted-5-(2-furanyl)-2-methyl-3H-thieno[2,3-d]pyrimidin-4-ones with topological indices using Hansch analysis. <b>2006</b> , 16, 4951-8	21
2202	Improved 3D-QSAR CoMFA of the dopamine transporter blockers with multiple conformations using the genetic algorithm. <b>2006</b> , 16, 6267-72	11
2201	Atom-based 3D-chiral quadratic indices. Part 2: prediction of the corticosteroid-binding globulinbinding affinity of the 31 benchmark steroids data set. <b>2006</b> , 14, 2398-408	32
2200	Prediction of hERG potassium channel affinity by the CODESSA approach. <b>2006</b> , 14, 3153-9	51
2199	2D QSAR of PPARgamma agonist binding and transactivation. <b>2006</b> , 14, 5178-95	25
2198	Quantitative study of the structure-retention index relationship in the imine family. <b>2006</b> , 1102, 238-44	41
2197	Prediction of intrinsic viscosity in polymer/solvent combinations using a QSPR model. <b>2006</b> , 47, 3240-3248	61
2196	Quantitative structure-pharmacokinetic relationships for drug clearance by using statistical learning methods. <i>Journal of Molecular Graphics and Modelling</i> , <b>2006</b> , 24, 383-95	2.8 57
2195	Bayesian-regularized genetic neural networks applied to the modeling of non-peptide antagonists for the human luteinizing hormone-releasing hormone receptor. <i>Journal of Molecular Graphics and Modelling</i> , <b>2006</b> , 25, 410-22	2.8 33

2194	3D-QSAR studies on cannabinoid CB1 receptor agonists: G-protein activation as biological data. <b>2006</b> , 49, 554-66	22
2193	An overlooked property of plot methods. <b>2006</b> , 39, 475-484	15
2192	Novel approach to evolutionary neural network based descriptor selection and QSAR model development. <b>2005</b> , 19, 835-55	4
2191	Investigation of substituent effect of 1-(3,3-diphenylpropyl)-piperidinyl phenylacetamides on CCR5 binding affinity using QSAR and virtual screening techniques. <b>2006</b> , 20, 83-95	32
2190	A novel RBF neural network training methodology to predict toxicity to <i>Vibrio fischeri</i> . <b>2006</b> , 10, 213-21	27
2189	A novel simple QSAR model for the prediction of anti-HIV activity using multiple linear regression analysis. <b>2006</b> , 10, 405-14	49
2188	Non-stochastic and stochastic linear indices of the molecular pseudograph's atom-adjacency matrix: a novel approach for computational in silico screening and "rational" selection of new lead antibacterial agents. <b>2006</b> , 12, 255-71	48
2187	A novel QSPR model for predicting $T_c$ (lower critical solution temperature) in polymer solutions using molecular descriptors. <b>2007</b> , 13, 55-64	25
2186	New tyrosinase inhibitors selected by atomic linear indices-based classification models. <b>2006</b> , 16, 324-30	48
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2184	Structure-permeation relationships for the non-invasive transdermal delivery of cationic peptides by iontophoresis. <b>2006</b> , 29, 53-9	24
2183	Integrated approach using protein and ligand information to analyze selectivity- and affinity-determining features of carbonic anhydrase isozymes. <b>2006</b> , 1, 839-53	16
2182	Prediction of chromatographic relative retention time of polychlorinated biphenyls from the molecular electronegativity distance vector. <b>2006</b> , 29, 296-301	30
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2179	Chapter 8 Machine Learning in Computational Chemistry. <b>2006</b> , 2, 127-140	26
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1460	Exploring the role of water molecules for docking and receptor guided 3D-QSAR analysis of naphthyridine derivatives as spleen tyrosine kinase (Syk) inhibitors. <b>2012</b> , 52, 2619-30		12
1459	Structural analysis of structurally diverse $\beta$ -glucosidase inhibitors for active site feature analysis. <b>2012</b> , 27, 649-57		5
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1457	Towards Model-Based Identification of Biofuels for Compression Ignition Engines. <b>2012</b> , 5, 990-1003		17

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1450	Analysis of van der Waals surface area properties for human ether-a-go-go-related gene blocking activity: computational study on structurally diverse compounds. <b>2012</b> , 23, 521-36	20
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1430	Synthesis and structure-activity analysis of new phosphonium salts with potent activity against African trypanosomes. <b>2012</b> , 55, 2606-22	37
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1419	Structure-based prediction of protein-protein binding affinity with consideration of allosteric effect. <b>2012</b> , 43, 531-43	40
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1413	Study of indole derivative inhibitors of Cytosolic phospholipase A2 based on Quantitative Structure Activity Relationship. <b>2012</b> , 114, 1-9	2
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1398	Revealing interaction mode between HIV-1 protease and mannitol analog inhibitor. <b>2012</b> , 79, 916-25		
1397	A segmented principal component analysis--regression approach to QSAR study of peptides. <b>2012</b> , 305, 37-44		11
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1352	Prediction of tyrosinase inhibition for drug design using the genetic algorithm multiple linear regressions. <b>2013</b> , 22, 5453-5465	4
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1347	Activity landscape analysis, CoMFA and CoMSIA studies of pyrazole CB1 antagonists. <b>2013</b> , 22, 4133-4145	7
1346	Molecular modeling studies on 3,4-dihydroquinazolines as trypanothione reductase inhibitors using 3D-QSAR and docking approaches. <b>2013</b> , 22, 3541-3555	2
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1338	Design equations for prediction of pressuremeter soil deformation moduli utilizing expression programming systems. <b>2013</b> , 23, 1771-1786	43
1337	New design equations for assessment of load carrying capacity of castellated steel beams: a machine learning approach. <b>2013</b> , 23, 119-131	14
1336	Quantitative Structure-Retention Relationships of Polychlorinated Biphenyls (PCBs) Gas Chromatographic Retention Times: A Quantum Similarity Approach. <b>2013</b> , 76, 837-847	4
1335	Integration of ligand and structure-based virtual screening for identification of leading anabolic steroids. <b>2013</b> , 138, 348-58	3
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1329	A docking-based receptor library of antibiotics and its novel application in predicting chronic mixture toxicity for environmental risk assessment. <b>2013</b> , 185, 4513-27	19
1328	Modeling of CCR5 antagonists as anti HIV agents using combined genetic algorithm and adaptive neuro-fuzzy inference system (GANNFIS). <b>2013</b> , 22, 4423-4436	6
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1326	Identification of putative estrogen receptor-mediated endocrine disrupting chemicals using QSAR- and structure-based virtual screening approaches. <b>2013</b> , 272, 67-76	65
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1324	An evolutionary approach for modeling of shear strength of RC deep beams. <b>2013</b> , 46, 2109-2119	127
1323	QSPR prediction of thermal decomposition property of non-vinyl polymers having amino acids moieties. <b>2013</b> , 70, 715-732	6
1322	Modified particle swarm optimization method for variable selection in QSAR/QSPR studies. <b>2013</b> , 24, 1401-1409	14
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1320	Formulation of soil angle of shearing resistance using a hybrid GP and OLS method. <b>2013</b> , 29, 37-53	10
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1317	The effect of different log P algorithms on the modeling of the soil sorption coefficient of nonionic pesticides. <b>2013</b> , 47, 5751-9	14
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1307	Scoring functions for protein-protein interactions. <b>2013</b> , 23, 862-7	66
1306	3D QSAR kNN-MFA studies on 6-substituted benzimidazoles derivatives as Nonpeptide Angiotensin II Receptor Antagonists: A rational approach to antihypertensive agents. <b>2013</b> , 17, 167-176	35
1305	Leak location of pipelines based on transient model and PSO-SVM. <b>2013</b> , 26, 1085-1093	43
1304	Molecular modeling of the ideal gas enthalpy of formation of hydrocarbons. <b>2013</b> , 360, 423-434	14
1303	Hands-off linear interaction energy approach to binding mode and affinity estimation of estrogens. <b>2013</b> , 53, 2681-8	9
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1300	What are the ideal properties for functional food peptides with antihypertensive effect? A computational peptidology approach. <b>2013</b> , 141, 2967-73	93
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1298	First report on exploring structural requirements of 1,2,3,4- tetrahydroacridin-9(10H)-one analogs as antimalarials using multiple QSAR approaches: descriptor-based QSAR, CoMFA-CoMSIA 3DQSAR, HQSAR and G-QSAR approaches. <b>2013</b> , 16, 7-21	15
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1291	Criterion for evaluating the predictive ability of nonlinear regression models without cross-validation. <b>2013</b> , 53, 2341-8	16
1290	Prediction of retention indices for frequently reported compounds of plant essential oils using multiple linear regression, partial least squares, and support vector machine. <b>2013</b> , 36, 2464-71	14
1289	QSPR models for prediction of gas-to-heptane and gas-to-hexadecane solvation enthalpies of organic compounds from theoretical molecular descriptors. <b>2013</b> , 24, 1799-1810	10
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1109	3D-QSAR and molecular fragment replacement study on diaminopyrimidine and pyrrolotriazine ALK inhibitors. <b>2014</b> , 1067, 127-137	9
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1068	Ontology of core data mining entities. <b>2014</b> , 28, 1222-1265	27
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939	Combining radial basis function neural network with genetic algorithm to QSPR modeling of adsorption on multi-walled carbon nanotubes surface. <b>2015</b> , 1098, 191-198		13
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881	Explicit formulation of bearing capacity of shallow foundations on rock masses using artificial neural networks: application and supplementary studies. <b>2015</b> , 73, 3417-3431		31

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590	Synthesis, characterization, in vitro antimicrobial, DNA binding activity and QSAR studies of diorganotin(IV) complexes of Schiff bases derived from 2-benzoyl-1H-indene-1,3(2H)-dione and 4-substituted benzoic acid hydrazides. <b>2021</b> , 196, 133-145	1
589	Foodinformatic prediction of the retention time of pesticide residues detected in fruits and vegetables using UHPLC/ESI Q-Orbitrap. <b>2021</b> , 342, 128354	6
588	Structure activity relationships (SAR) study to design and synthesize new tubulin inhibitors with enhanced anti-tubulin activity: In silico and in vitro analysis. <b>2021</b> , 1223, 129204	2
587	Alkylacrylic-carboxyalkylacrylic random copolymers as demulsifiers for heavy crude oils. <b>2021</b> , 256, 117850	5
586	Drug design of new sigma-1 antagonists against neuropathic pain: A QSAR study using partial least squares and artificial neural networks. <b>2021</b> , 1223, 129156	2
585	The experimental and theoretical assessment of biopartitioning micellar liquid chromatography to mimic the drug-protein binding of some pain-relief drugs. <b>2021</b> , 68, 298-305	1
584	Structure-activity relationship and molecular docking analysis of cysteine-containing dipeptides as antioxidant and ACE inhibitory. <b>2021</b> , 56, 2789-2803	1
583	Suspect screening of environmental contaminants by UHPLC-HRMS and transposable Quantitative Structure-Retention Relationship modelling. <b>2021</b> , 409, 124652	3
582	Quantitative structure-property relationship for melting and freezing points of deep eutectic solvents. <b>2021</b> , 321, 114744	7
581	A selectivity study of polysubstituted pyridinylimidazoles as dual inhibitors of JNK3 and p38 $\beta$ MAPK based on 3D-QSAR, molecular docking, and molecular dynamics simulation. <b>2021</b> , 32, 819-834	3
580	Structural investigation of isatin-based benzenesulfonamides as carbonic anhydrase isoform IX inhibitors endowed with anticancer activity using molecular modeling approaches. <b>2021</b> , 1229, 129735	2
579	Synergistic and Antagonistic Drug Combinations against SARS-CoV-2. <b>2021</b> , 29, 873-885	29
578	The simplest method for reliable prediction of autoignition temperature of organic hydroxyl compounds to assess their process safety in industrial applications. <b>2021</b> , 148, 283-290	4
577	Microwave assisted synthesis, characterization and biological activities of ferrocenyl chalcones and their QSAR analysis: Part II. <b>2021</b> , 56, 82-97	1
576	A hybrid genetic algorithm-neural network model for power spectral density compatible ground motion prediction. <b>2021</b> , 142, 106528	1
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569	Combined remediation of polychlorinated naphthalene-contaminated soil under multiple scenarios: An integrated method of genetic engineering and environmental remediation technology. <b>2021</b> , 405, 124139	9
568	A simple model for the assessment of the agonistic activity of dibenzazepine derivatives by molecular moieties. <b>2021</b> , 30, 215-225	
567	Identification of good and bad fragments of tricyclic triazinone analogues as potential PKC- $\alpha$ inhibitors through SMILES-based QSAR and molecular docking. <b>2021</b> , 32, 149-165	13
566	DeepDSC: A Deep Learning Method to Predict Drug Sensitivity of Cancer Cell Lines. <b>2021</b> , 18, 575-582	27
565	Experimental and Modelling Study of Ultra-Fine Grained ZK60 Magnesium Alloy with Simultaneously Improved Strength and Ductility Processed by Parallel Tubular Channel Angular Pressing. <b>2021</b> , 27, 277-297	6
564	Use of size-dependent electron configuration fingerprint to develop general prediction models for nanomaterials.. <b>2021</b> , 21, 100298	5
563	Computer-aided identification of a series of novel ligands showing high potency as hepatitis C virus NS3/4A protease inhibitors. <b>2021</b> , 45,	0
562	design of novel FAK inhibitors using integrated molecular docking, 3D-QSAR and molecular dynamics simulation studies. <b>2021</b> , 1-19	3
561	Monte-Carlo method-based QSAR model to discover phytochemical urease inhibitors using SMILES and GRAPH descriptors. <b>2021</b> , 1-10	1
560	Molecular modeling and design of some amino alcohol grafted 1,4,5-trisubstituted 1,2,3-triazoles derivatives against chloroquine sensitive, 3D7 strain of. <b>2021</b> , 7, e05924	2
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558	Current computer-aided drug design methodologies in discovery of novel drug candidates for neuropsychiatric and inflammatory diseases. <b>2021</b> , 71, 225-256	
557	A computational approach for designing novel SARS-CoV-2 Mpro inhibitors: combined QSAR, molecular docking, and molecular dynamics simulation techniques.	4

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555	Quantitative Structure-Activity Relationships (QSARs) Study for KCNQ Genes (Kv7) and Drug Discovery. <b>2021</b> , 61-70	0
554	Predictive retention study of $\beta$ -blockers in different chromatographic systems as potential tool for lipophilicity screening based on QSRR approach. <b>2021</b> , 44, 12-24	1
553	A Protocol to Use Comparative Binding Energy Analysis to Estimate Drug-Target Residence Time. <b>2021</b> , 2266, 171-186	1
552	Prediction of Catenary Action Capacity of RC Beam-Column Substructures under a Missing Column Scenario Using Evolutionary Algorithm. <b>2021</b> , 25, 891-905	24
551	Fragment-Based Drug Design of Selective HDAC6 Inhibitors. <b>2021</b> , 2266, 155-170	0
550	Machine learning field 3D-QSAR models for serotonin 2A receptor psychoactive substances identification.. <b>2021</b> , 11, 14587-14595	1
549	Structural, QSAR, machine learning and molecular docking studies of 5-thiophen-2-yl pyrazole derivatives as potent and selective cannabinoid-1 receptor antagonists.	1
548	Statistical methods and parameters: Tools to generate and evaluate theoretical in silico models. <b>2021</b> , 333-350	
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546	Prediction Models on p and Base-Catalyzed Hydrolysis Kinetics of Parabens: Experimental and Quantum Chemical Studies. <b>2021</b> , 55, 6022-6031	6
545	An evolutionary-based predictive soft computing model for the prediction of electricity consumption using multi expression programming. <b>2021</b> , 283, 125287	14
544	Novel and Predictive QSAR Model for Steroidal and Nonsteroidal 5 $\beta$ -Reductase Type II Inhibitors. <b>2021</b> , 18, 317-332	
543	In Silico Based Structural and Fingerprint Analysis of Structurally Diverse AT1 inhibitors. <b>2021</b> , 18, 93-103	0
542	Cross-validation strategies in QSPR modelling of chemical reactions. <b>2021</b> , 32, 207-219	2
541	Molecular dynamics-guided receptor-dependent 4D-QSAR studies of HDACs inhibitors. <b>2021</b> , 1	1
540	Designing new hybrid artificial intelligence model for CFST beam flexural performance prediction. 1	4
539	Support Vector Machine Method for Developing Ground Motion Models for Earthquakes in Western Part of China. 1-16	1

538	Review on the Use of Artificial Intelligence to Predict Fire Performance of Construction Materials and Their Flame Retardancy. <b>2021</b> , 26,	5
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533	In silico guided design of non-covalent inhibitors of DprE1: synthesis and biological evaluation. <b>2021</b> , 32, 333-352	3
532	Machine Learning-Based Modeling with Optimization Algorithm for Predicting Mechanical Properties of Sustainable Concrete. <b>2021</b> , 2021, 1-15	9
531	Prediction of potential inhibitors of SARS-CoV-2 using 3D-QSAR, molecular docking modeling and ADMET properties. <b>2021</b> , 7, e06603	7
530	QSAR study of unsymmetrical aromatic disulfides as potent avian SARS-CoV main protease inhibitors using quantum chemical descriptors and statistical methods. <b>2021</b> , 210, 104266	12
529	Design, Synthesis, and Evaluation of Novel 3-Carboranyl-1,8-Naphthalimide Derivatives as Potential Anticancer Agents. <b>2021</b> , 22,	8
528	Quantitative structure-critical micelle concentration modeling of anionic gemini surfactants, comparison of MLR, PLS, WNN, and ANFIS models with eigenvalue and correlation ranking methods. <b>2021</b> , 18, 2703-2711	2
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525	Pyrazoles and fused pyrimidines: Synthesis, structure elucidation, antitubercular activity and molecular docking study. <b>2021</b> ,	1
524	Consolidation parameters conceptualization using regression analysis and genetic programming for Addis Ababa red clay soils. 1	0
523	Understanding the Molecular Basis of 5-HT Receptor Partial Agonists through 3D-QSAR Studies. <b>2021</b> , 22,	2
522	Systematic Comparison and Comprehensive Evaluation of 80 Amino Acid Descriptors in Peptide QSAR Modeling. <b>2021</b> , 61, 1718-1731	24
521	Dynamic characterization of recycled glass-recycled concrete blends using experimental analysis and artificial neural network modeling. <b>2021</b> , 142, 106544	16

520	Concentration Addition, Independent Action, and Quantitative Structure-Activity Relationships for Chemical Mixture Toxicities of the Disinfection By products of Haloacetic Acids on the Green Alga <i>Raphidocelis subcapitata</i> . <b>2021</b> , 40, 1431-1442	1
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518	Predictive Global Models of Cruzain Inhibitors with Large Chemical Coverage. <b>2021</b> , 6, 6722-6735	2
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514	Modeling and Toxicity Profiling of a Set of Quinoline Derivatives as c-MET Inhibitors in the treatment of Human Tumors.. <b>2021</b> , 18, 738-743	1
513	QSPR modelling for intrinsic viscosity in polymer-solvent combinations based on density functional theory. <b>2021</b> , 32, 379-393	2
512	New D2R partial agonist candidates: an in silico approach from statistical models, molecular docking, and ADME/Tox properties. <b>2021</b> , 32, 2019-2033	0
511	Molecular insights into a mechanism of resveratrol action using hybrid computational docking/CoMFA and machine learning approach. <b>2021</b> , 1-15	3
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508	QSAR models for insecticidal properties of plant essential oils on the housefly ( <i>L.</i> ). <b>2021</b> , 32, 395-410	
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503	Machine Learning in Discovery of New Antivirals and Optimization of Viral Infections Therapy. <b>2021</b> , ,	1



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498	An Artificial Neural Network for Predicting the Near-fault Directivity-pulse Period. 1-20	2
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493	Development of an a priori computational approach for brain uptake of compounds in an insect model system. <b>2021</b> , 40, 127930	1
492	Simple method to assess autoignition temperature of organic ether compounds with high reliability for process safety. 1	
491	Prediction of Ground Motion Intensity Measures Using an Artificial Neural Network. <b>2021</b> , 178, 2025-2058	4
490	A quantitative structure-activity relationship study on CXL017 derivatives as effective drugs for cancer treatment.	0
489	Prediction of organic compounds adsorbed by polyethylene and chlorinated polyethylene microplastics in freshwater using QSAR. <b>2021</b> , 197, 111001	4
488	Synthesis and 4D-QSAR Studies of Alanine Hydroxamic Acid Derivatives as Aminopeptidase N Inhibitors. <b>2021</b> , 17, 658-666	1
487	Docking-Based 3D-QSAR Studies for 1,3,4-oxadiazol-2-one Derivatives as FAAH Inhibitors. <b>2021</b> , 22,	4
486	Quantitative structure-activity relationship and machine learning studies of 2-thiazolylhydrazone derivatives with anti- activity. <b>2021</b> , 1-12	1
485	Integrated 3D-QSAR, molecular docking, and molecular dynamics simulation studies on 1,2,3-triazole based derivatives for designing new acetylcholinesterase inhibitors. <b>2021</b> , 45, 647-660	6

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483	In Silico Studies of Oxadiazole Derivatives as Potent Dengue Virus Inhibitors. 1	1
482	Quantitative Structure-Activity Relationship (QSAR) study of a series of 2-thioarylalkyl benzimidazole derivatives by The Density Functional Theory (DFT). <b>2021</b> , 001-007	
481	Genetic programming to formulate viscoelastic behavior of modified asphalt binder. <b>2021</b> , 286, 122954	3
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478	The index of ideality of correlation: QSAR studies of hepatitis C virus NS3/4A protease inhibitors using SMILES descriptors. <b>2021</b> , 32, 495-520	8
477	Effects of Phthalate Esters (PAEs) on Cell Viability and Nrf2 of HepG2 and 3D-QSAR Studies. <b>2021</b> , 9,	1
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475	Environmental assessment based surface water quality prediction using hyper-parameter optimized machine learning models based on consistent big data. <b>2021</b> , 151, 324-340	9
474	Nondestructive prediction of rutting resistance of in-service middle asphalt layer based on gene expression programming. <b>2021</b> , 293, 123481	5
473	The Psychonauts' Benzodiazepines; Quantitative Structure-Activity Relationship (QSAR) Analysis and Docking Prediction of Their Biological Activity. <b>2021</b> , 14,	2
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467	Improved machine learning scoring functions for identification of <i>Electrophorus electricus</i> 's acetylcholinesterase inhibitors. <b>2021</b> , 1	1

466	QSAR modeling and pharmacoinformatics of SARS coronavirus 3C-like protease inhibitors. <b>2021</b> , 134, 104483	2
465	Double focus in the modelling of anti-influenza properties of 2-iminobenzimidazolines: pharmacology and toxicology. <b>2021</b> , 32, 643-654	2
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462	Catalytic Performance of Cycloalkyl-Fused Aryliminopyridyl Nickel Complexes toward Ethylene Polymerization by QSPR Modeling. <b>2021</b> , 11, 920	0
461	Evolutionary artificial intelligence approach for performance prediction of bio-composites. <b>2021</b> , 290, 123254	4
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459	Data Science Meets Physical Organic Chemistry. <b>2021</b> ,	12
458	Mechanistic elucidation of the oral pungency of capsaicin-related dietary components: Spatial structural insights. <b>2021</b> , 353, 129429	2
457	2D-QSAR modeling and two-fold classification of 1,2,4-triazole derivatives for antitubercular potency against the dormant stage of Mycobacterium tuberculosis. <b>2021</b> , 1	1
456	QSAR-Based Computational Approaches to Accelerate the Discovery of Sigma-2 Receptor (S2R) Ligands as Therapeutic Drugs. <b>2021</b> , 26,	1
455	Multivariate adaptive regression splines model for reinforced soil foundations. <b>2021</b> , 28, 368-390	25
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451	Modeling polyurethane foam (PUF)-air partition coefficients for persistent organic pollutants using linear and non-linear chemometric methods. <b>2021</b> , 9, 105615	
450	Sustainable utilization of foundry waste: Forecasting mechanical properties of foundry sand based concrete using multi-expression programming. <b>2021</b> , 780, 146524	27
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444	A partial least squares and artificial neural network study for a series of arylpiperazines as antidepressant agents. <b>2021</b> , 27, 297	1
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442	Molecular design, molecular docking and ADMET study of cyclic sulfonamide derivatives as SARS-CoV-2 inhibitors. <b>2021</b> , 49, 63-63	1
441	Theoretical design and process control of neonicotinoids insecticides suitable for synergistic degradation with the rubisco enzyme from rhizobia and carbon-fixing bacteria in soil. <b>2021</b> , 1	0
440	Prediction of power conversion efficiency of phenothiazine-based dye-sensitized solar cells using Monte Carlo method with index of ideality of correlation. <b>2021</b> , 32, 817-834	10
439	Density of Deep Eutectic Solvents: The Path Forward Cheminformatics-Driven Reliable Predictions for Mixtures. <b>2021</b> , 26,	5
438	Recent Development in Electricity Price Forecasting Based on Computational Intelligence Techniques in Deregulated Power Market. <b>2021</b> , 14, 6104	2
437	Identification of novel acetylcholinesterase inhibitors through 3D-QSAR, molecular docking, and molecular dynamics simulation targeting Alzheimer's disease. <b>2021</b> , 27, 302	6
436	Machine learning-based constitutive models for cement-grouted coal specimens under shearing. <b>2021</b> , 31, 813-813	14
435	Multigene Expression Programming Based Forecasting the Hardened Properties of Sustainable Bagasse Ash Concrete. <b>2021</b> , 14,	5
434	Combined 4D-QSAR and target-based approaches for the determination of bioactive Isatin derivatives. <b>2021</b> , 32, 769-792	1
433	Hormetic dose-responses for silver antibacterial compounds, quorum sensing inhibitors, and their binary mixtures on bacterial resistance of Escherichia coli. <b>2021</b> , 786, 147464	2
432	Metabolic characteristics of plasma bile acids in patients with intrahepatic cholestasis of pregnancy-mass spectrometric study. <b>2021</b> , 17, 93	0
431	Generating accurate in silico predictions of acute aquatic toxicity for a range of organic chemicals: Towards similarity-based machine learning methods. <b>2021</b> , 280, 130681	4

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429	Predicting Marshall parameters of flexible pavement using support vector machine and genetic programming. <b>2021</b> , 306, 124924		5
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427	Hidden in its color: A molecular-level analysis of the beer's Maillard reaction network. <b>2021</b> , 361, 130112		4
426	Ground motion intensity measures for New Zealand. <b>2021</b> , 150, 106928		3
425	Structural optimization for pyrimidine analogues inhibitors against MAP kinase interacting serine/threonine kinase 1(MNK1) based on molecular simulation. <b>2021</b> , 1243, 130688		1
424	Classical and quantum regression analysis for the optoelectronic performance of NTCDA/p-Si UV photodiode. <b>2021</b> , 246, 167793		8
423	Chemical structure-based models for prediction of density of ammonium and phosphonium-based deep eutectic solvents. <b>2021</b> , 343, 117595		1
422	QSAR-guided pharmacophoric modeling reveals important structural requirements for Polo kinase 1 (Plk1) inhibitors. <i>Journal of Molecular Graphics and Modelling</i> , <b>2021</b> , 109, 108022	2.8	2
421	Artificial intelligence assisted technoeconomic optimization scenarios of hybrid energy systems for water management of an isolated community. <b>2021</b> , 48, 101561		1
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419	Computational strategies towards developing novel SARS-CoV-2 M inhibitors against COVID-19. <b>2021</b> , 131378		3
418	Surface functional groups determine adsorption of pharmaceuticals and personal care products on polypropylene microplastics. <b>2022</b> , 423, 127131		6
417	Multi-algorithm based machine learning and structural pattern studies for hERG ion channel blockers mediated cardiotoxicity prediction. <b>2021</b> , 208, 104213		0
416	Recent advances in quantitative structure-activity relationship models of antimalarial drugs. <b>2021</b> , 16, 659-695		7
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214	Synthesis, molecular docking, and 2D-QSAR modeling of quinoxaline derivatives as potent anticancer agents against triple-negative breast cancer.. <b>2022</b> ,	1
213	MIA-QSAR study of the structural merging of (thio)benzamide herbicides with photosynthetic system II inhibitory activities.. <b>2022</b> , 1-7	
212	Target based structural optimization of substituted pyrazolopyrimidine analogues as inhibitor for IRAK4 by 3D-QSAR and molecular simulation. 1	0
211	QSAR Modeling of Styrylquinoline Derivatives as HIV-1 integrase inhibitors. <b>2022</b> , 16,	
210	Molecular descriptors and QSSR models in asymmetric catalysis. <b>2022</b> , 19,	
209	Insight into the structural requirements of gelatinases (MMP-2 and MMP-9) inhibitors by multiple validated molecular modelling approaches: Part II.. <b>2022</b> , 33, 167-192	1
208	Computer-Assisted Improvement of Sulfonylureas with Antifungal Properties and Limited Herbicidal Activity: Potential Application in Forage Conservation.. <b>2022</b> ,	0
207	A novel evolutionary learning to prepare sustainable concrete mixtures with supplementary cementitious materials. 1	2
206	Prediction reliability of QSAR models: an overview of various validation tools.. <b>2022</b> , 1	5
205	Predicting Marshall Flow and Marshall Stability of Asphalt Pavements Using Multi Expression Programming. <b>2022</b> , 12, 314	0
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199	Development of an in silico consensus model for the prediction of the phospholipogenic potential of small molecules. <b>2022</b> , 22, 100226	
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175	Enhancing the tree-boosting-based pedotransfer function for saturated hydraulic conductivity using data preprocessing and predictor importance using game theory. <b>2022</b> , 420, 115864	0
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167	Design, Synthesis, and Molecular Modeling Studies of a Novel Benzimidazole as an Aromatase Inhibitor.. <b>2022</b> , 7, 16152-16163	4
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165	Advanced Machine Learning Modeling Approach for Prediction of Compressive Strength of FRP Confined Concrete Using Multiphysics Genetic Expression Programming.. <b>2022</b> , 14,	1
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71	PepQSAR: a comprehensive data source and information platform for peptide quantitative structure-activity relationships.	0



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69	Discovery of anti-colon cancer agents targeting wild-type and mutant p53 using computer-aided drug design. 1-19	0
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47	Obstructing <i>Salmonella typhi</i> 's virulence in eukaryotic cells through design of its SipB protein antagonists. <b>2022</b> ,	0
46	Synthesis and Phytotoxic Evaluation of Isatin Derivatives Supported by 3D-QSAR Study. <b>2023</b> , 71, 255-266	0
45	QSAR Studies, Molecular Docking, Molecular Dynamics, Synthesis, and Biological Evaluation of Novel Quinolinone-Based Thiosemicarbazones against <i>Mycobacterium tuberculosis</i> . <b>2023</b> , 12, 61	1
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43	Dronabinol as an answer to flavivirus infections: an in-silico investigation. 1-12	0
42	Ground motion model for Peninsular India using an artificial neural network. <b>2023</b> , 39, 596-633	0
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39	Design, Biological Evaluation, and Computer-Aided Analysis of Dihydrothiazepines as Selective Antichlamydial Agents. <b>2023</b> , 66, 2116-2142	0
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37	Quantum Chemical GA-MLR, Cluster Model, and Conceptual DFT Descriptors Studies on the Binding Interaction of Estrogen Receptor Alpha with Endocrine Disrupting Chemicals. <b>2023</b> , 13, 228	0
36	Application of chemometrics tools for removal of crystal violet and methylene blue in binary solution by eco-friendly magnetic adsorbent modified on <i>Heracleum persicum</i> waste. <b>2023</b> , 292, 122415	0
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