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Application of Genetic Function Approximation to Quantitative Structure-Activity Relationships and Quantitative Structure-Property Relationships

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916	Genetic algorithms in molecular recognition and design. 1995 , 13, 516-21		90
915	PRO-LIGAND: an approach to de novo molecular design. 3. A genetic algorithm for structure refinement. 1995 , 9, 139-48		51
914	Prediction of the Progesterone Receptor Binding of Steroids using a Combination of Genetic Algorithms and Neural Networks. 1996 , 159-192		4
913	Prediction of the Impact Sensitivity by Neural Networks. <i>Journal of Chemical Information and Computer Sciences</i> , 1996 , 36, 804-810		45
912	Conformational analysis, molecular shape comparison, and pharmacophore identification of different allosteric modulators of muscarinic receptors. <i>Journal of Chemical Information and Computer Sciences</i> , 1996 , 36, 1018-24		34
911	Neural network studies. 2. Variable selection. <i>Journal of Chemical Information and Computer Sciences</i> , 1996 , 36, 794-803		122
910	Prediction of Polymer Glass Transition Temperatures Using a General Quantitative StructureProperty Relationship Treatment. <i>Journal of Chemical Information and Computer Sciences</i> , 1996 , 36, 879-884		75
909	Genetic neural networks for quantitative structure-activity relationships: improvements and application of benzodiazepine affinity for benzodiazepine/GABAA receptors. 1996 , 39, 5246-56		110
908	Evolutionary optimization in quantitative structure-activity relationship: an application of genetic neural networks. 1996 , 39, 1521-30		248
907	Some Theory and Examples of Genetic Function Approximation with Comparison to Evolutionary Techniques. 1996 , 87-107		12
906	Application of Genetic Algorithms to the General QSAR Problem and to Guiding Molecular Diversity Experiments. 1996 , 131-157		7
905	Genetic Algorithms in Computer-Aided Molecular Design. 1996 , 1-34		11
904	Genetic Partial Least Squares in QSAR. 1996 , 109-130		28
903	Evolutionary and genetic methods in drug design. 1996 , 1, 514-521		29
902	The rationale for E2020 as a potent acetylcholinesterase inhibitor. 1996 , 4, 1429-46		106

901	Using multivariate adaptive regression splines to QSAR studies of dihydroartemisinin derivatives. 1996 , 31, 797-803	33
900	Evolutionary algorithms in computer-aided molecular design. 1996 , 10, 337-58	102
899	Protein design automation. 1996 , 5, 895-903	232
898	Solution of the conformation and alignment tensors for the binding of trimethoprim and its analogs to dihydrofolate reductase: 3D-quantitative structure-activity relationship study using molecular shape analysis, 3-way partial least-squares regression, and 3-way factor analysis. 1996 , 39, 4825-32	27
897	New Developments in QSPR/QSAR Modeling Based on Topological Indices. 1997 , 7, 45-62	17
896	Genetic function approximation in the molecular pharmacology of cancer.	1
895	The application of evolutionary computation to selected problems in molecular biology. 1997 , 23-33	1
894	Applications of genetic algorithms to drug design. 1997 , 7, 247-254	10
893	GA strategy for variable selection in QSAR studies: GA-based PLS analysis of calcium channel antagonists. <i>Journal of Chemical Information and Computer Sciences</i> , 1997 , 37, 306-10	199
892	Prediction of ligand-receptor binding thermodynamics by free energy force field (FEFF) 3D-QSAR analysis: application to a set of peptidomimetic renin inhibitors. <i>Journal of Chemical Information and Computer Sciences</i> , 1997 , 37, 792-811	62
891	QSAR and 3D QSAR in drug design Part 2: applications and problems. 1997 , 2, 538-546	156
890	Construction of 3D-QSAR Models Using the 4D-QSAR Analysis Formalism. 1997 , 119, 10509-10524	341
889	The method of frontal polyhedra for conformationally-nonrigid molecules. Quantitative structure-activity relationship in the series of baker triazines. Dihydrofolate reductase inhibitors. 1997 , 31, 147-154	1
888	Molecular modelling of polymers 17. Simulation and QSPR analyses of transport behavior in amorphous polymeric materials. 1997 , 7, 199-214	22
887	Introduction to multi-layer feed-forward neural networks. 1997 , 39, 43-62	698
886	Discrimination of the variety and region of origin of extra virgin olive oils using ¹³ C NMR and multivariate calibration with variable reduction. 1997 , 348, 357-374	82
885	3D QSAR: current state, scope, and limitations. 1998 , 12/14, 3-23	42
884	Recent progress in CoMFA methodology and related techniques. 1998 , 12/14, 25-39	26

883	Receptor surface models. 1998 , 12/14, 117-133	8
882	Mining the NCI anticancer drug discovery databases: genetic function approximation for the QSAR study of anticancer ellipticine analogues. <i>Journal of Chemical Information and Computer Sciences</i> , 1998 , 38, 189-99	100
881	Quasi-atomistic receptor modeling. A bridge between 3D QSAR and receptor fitting. 1998 , 73, 11-8	11
880	Artificial neural networks for computer-based molecular design. 1998 , 70, 175-222	160
879	GA strategy for variable selection in QSAR studies: GAPLS and D-optimal designs for predictive QSAR model. 1998 , 425, 255-262	37
878	Four-dimensional quantitative structure-activity relationship analysis of a series of interphenylene 7-oxabicycloheptane oxazole thromboxane A2 receptor antagonists. <i>Journal of Chemical Information and Computer Sciences</i> , 1998 , 38, 925-38	42
877	Application of Quantitative Structure-Performance Relationship and Neural Network Models for the Prediction of Physical Properties from Molecular Structure. 1998 , 37, 3043-3051	26
876	GA Strategy for Variable Selection in QSAR Studies: GA-Based Region Selection for CoMFA Modeling. <i>Journal of Chemical Information and Computer Sciences</i> , 1998 , 38, 276-282	44
875	Genetic Function Approximation Experimental Design (GFXD): A New Method for Experimental Design. <i>Journal of Chemical Information and Computer Sciences</i> , 1998 , 38, 858-866	7
874	Structure-activity analysis of the interaction of curacin A, the potent colchicine site antimitotic agent, with tubulin and effects of analogs on the growth of MCF-7 breast cancer cells. 1998 , 53, 62-76	245
873	Quantitative Structure-Activity Relationship Studies of Sulfamates RNHSO ₃ Na: Distinction between Sweet, Sweet-Bitter, and Bitter Molecules. 1998 , 46, 3016-3026	35
872	Transfer of Calibrations of Near-Infrared Spectra Using Neural Networks. 1998 , 52, 732-745	31
871	Mining the National Cancer Institute Anticancer Drug Discovery Database: cluster analysis of ellipticine analogs with p53-inverse and central nervous system-selective patterns of activity. 1998 , 53, 241-51	78
870	Three-dimensional quantitative similarity-activity relationships (3D QSiAR) from SEAL similarity matrices. 1998 , 41, 2553-64	219
869	Glossary of Terms Used in Computational Drug Design (IUPAC Recommendations 1997). 1998 , 33, 397-409	15
868	Applications of soft computing in drug design. 1998 , 8, 249-258	18
867	Overview of Rational Drug Design. 1999 , 1-11	7
866	Evolutionary Algorithms in Computer-Aided Molecular Design: A Review of Current Applications and a Look to the Future. 1999 , 255-270	6

865	Quantitative structure-property relationships and neural networks: correlation and prediction of physical properties of pure components and mixtures from molecular structure. 1999 , 158-160, 367-374	24
864	Neural networks in drug discovery: have they lived up to their promise?. 1999 , 34, 195-208	109
863	Heterogeneous catalysis: looking forward with molecular simulation. 1999 , 50, 451-477	18
862	Comparison of three different QSAR/QSPR generation techniques. 1999 , 468, 13-20	13
861	Multivariate Regression Outperforms Several Robust Architectures of Neural Networks in QSAR Modeling. <i>Journal of Chemical Information and Computer Sciences</i> , 1999 , 39, 121-132	107
860	GA strategy for variable selection in QSAR studies: application of GA-based region selection to a 3D-QSAR study of acetylcholinesterase inhibitors. <i>Journal of Chemical Information and Computer Sciences</i> , 1999 , 39, 112-20	69
859	Quantitative structure-activity relationship modeling of dopamine D(1) antagonists using comparative molecular field analysis, genetic algorithms-partial least-squares, and K nearest neighbor methods. 1999 , 42, 3217-26	89
858	Synthesis, pharmacological and biophysical characterization, and membrane-interaction QSAR analysis of cationic amphiphilic model compounds. 1999 , 42, 3874-88	14
857	Applications of genetic algorithms on the structure-activity relationship analysis of some cinnamamides. <i>Journal of Chemical Information and Computer Sciences</i> , 1999 , 39, 775-81	61
856	Development and Validation of a Novel Variable Selection Technique with Application to Multidimensional Quantitative Structure-Activity Relationship Studies. <i>Journal of Chemical Information and Computer Sciences</i> , 1999 , 39, 345-355	85
855	Prediction of Ligand-Receptor Binding Free Energy by 4D-QSAR Analysis: Application to a Set of Glucose Analogue Inhibitors of Glycogen Phosphorylase. <i>Journal of Chemical Information and Computer Sciences</i> , 1999 , 39, 1141-1150	31
854	Construction of a Virtual High Throughput Screen by 4D-QSAR Analysis: Application to a Combinatorial Library of Glucose Inhibitors of Glycogen Phosphorylase. <i>Journal of Chemical Information and Computer Sciences</i> , 1999 , 39, 1151-1160	49
853	Reactivity Prediction Models Applied to the Selection of Novel Candidate Building Blocks for High-Throughput Organic Synthesis of Combinatorial Libraries. <i>Journal of Chemical Information and Computer Sciences</i> , 1999 , 39, 1119-1127	9
852	Designing Diverse and Focused Combinatorial Libraries of Synthetic Polymers. 1999 , 1, 297-306	48
851	Prediction of ligand-receptor binding thermodynamics by free energy force field three-dimensional quantitative structure-activity relationship analysis: applications to a set of glucose analogue inhibitors of glycogen phosphorylase. 1999 , 42, 2169-79	41
850	Quantitative component analysis of mixtures for risk assessment: application to eye irritation. 1999 , 12, 1050-6	4
849	Quantitative Structure-Activity Relationships. 2000 , 71-97	1
848	Multi-conformational Ligand Representation in 4D-QSAR: Reducing the Bias Associated with Ligand Alignment. 2000 , 19, 149-161	19

847	A widely applicable set of descriptors. 2000 , 18, 464-77	251
846	Extraction of pharmacophore information from high-throughput screens. 2000 , 11, 97-103	28
845	Understanding the antifungal activity of terbinafine analogues using quantitative structure-activity relationship (QSAR) models. 2000 , 8, 2487-99	39
844	The use of 'electronic nose' sensor responses to predict the inhibition activity of alcohols on the cytochrome P-450 catalyzed p-hydroxylation of aniline. 2000 , 8, 795-805	9
843	Quantitative structure-property relationships in pharmaceutical research - Part 1. 2000 , 3, 28-35	87
842	Comparison of different data set screening methods for use in QSAR/QSPR generation studies. 2000 , 507, 229-238	3
841	Novel variable selection quantitative structure--property relationship approach based on the k-nearest-neighbor principle. <i>Journal of Chemical Information and Computer Sciences</i> , 2000 , 40, 185-94	378
840	Multi-dimensional QSAR in drug research. 2000 , 105-135	24
839	Three-Dimensional Quantitative Structural Activity Relationship (3D-QSAR) Studies of Some 1,5-Diarylpyrazoles: Analogue Based Design of Selective Cyclooxygenase-2 Inhibitors. 2000 , 5, 945-955	17
838	Chemometrics. 2000 , 99-114	
837	Mining and visualizing large anticancer drug discovery databases. <i>Journal of Chemical Information and Computer Sciences</i> , 2000 , 40, 367-79	83
836	Partial least squares modeling and genetic algorithm optimization in quantitative structure-activity relationships. 2000 , 11, 189-209	38
835	Unsupervised forward selection: a method for eliminating redundant variables. <i>Journal of Chemical Information and Computer Sciences</i> , 2000 , 40, 1160-8	148
834	Multiple-conformation and protonation-state representation in 4D-QSAR: the neurokinin-1 receptor system. 2000 , 43, 4416-27	81
833	Bibliography. 2000 , 524-667	
832	Binary formal inference-based recursive modeling using multiple atom and physicochemical property class pair and torsion descriptors as decision criteria. <i>Journal of Chemical Information and Computer Sciences</i> , 2000 , 40, 668-80	22
831	Quantitative structure-activity relationship studies of progesterone receptor binding steroids. <i>Journal of Chemical Information and Computer Sciences</i> , 2000 , 40, 762-72	29
830	Structurally diverse quantitative structure--property relationship correlations of technologically relevant physical properties. <i>Journal of Chemical Information and Computer Sciences</i> , 2000 , 40, 1-18	218

829	Inhibition of heme detoxification processes underlies the antimalarial activity of terpene isonitrile compounds from marine sponges. 2001 , 44, 873-85	108
828	Application of BCUT metrics and genetic algorithm in binary QSAR analysis. <i>Journal of Chemical Information and Computer Sciences</i> , 2001 , 41, 402-7	51
827	Identification of the descriptor pharmacophores using variable selection QSAR: applications to database mining. 2001 , 7, 599-612	58
826	Retrospective analysis of an experimental high-throughput screening data set by recursive partitioning. 2001 , 3, 267-77	28
825	4D-QSAR analysis of a set of ecdysteroids and a comparison to CoMFA modeling. <i>Journal of Chemical Information and Computer Sciences</i> , 2001 , 41, 1587-604	56
824	Three-dimensional quantitative structure-permeability relationship analysis for a series of inhibitors of rhinovirus replication. <i>Journal of Chemical Information and Computer Sciences</i> , 2001 , 41, 1578-86	41
823	Glass Transition. 2001 ,	
822	Comparison of selection methods of explanatory variables in PLS regression with application to manufacturing process data. 2001 , 58, 171-193	85
821	QSPR studies of PCBs by the combination of genetic algorithms and PLS analysis. 2001 , 25, 197-204	22
820	Three-dimensional quantitative structure-activity relationship (3D-QSAR) of 3-aryloxazolidin-2-one antibacterials. 2001 , 9, 3153-60	40
819	A new molecular simulation software package--Peking University Drug Design System (PKUDDS) for structure-based drug design. 2001 , 19, 455-65, 474-5	5
818	Design of fuel additives using neural networks and evolutionary algorithms. 2001 , 47, 1387-1406	37
817	Approaches to quantitative structure-enantioselectivity relationship modeling of chiral separations using capillary electrophoresis. 2001 , 914, 299-314	20
816	Quantitative structure-antitumor activity relationships of camptothecin analogues: cluster analysis and genetic algorithm-based studies. 2001 , 44, 3254-63	159
815	Molecular modeling, structure-activity relationships and functional antagonism studies of 4-hydroxy-1-methyl-4-(4-methylphenyl)-3-piperidyl 4-methylphenyl ketones as a novel class of dopamine transporter inhibitors. 2001 , 9, 1753-64	18
814	Prediction of eye irritation from organic chemicals using membrane-interaction QSAR analysis. 2001 , 59, 335-45	48
813	Adaptive Splines and Genetic Algorithms. 2002 , 11, 615-638	30
812	The present utility and future potential for medicinal chemistry of QSAR/QSPR with whole molecule descriptors. 2002 , 2, 1333-56	56

811	Receptor Surface Models. 1998 , 117-133	1
810	Structural requirements for potent anti-human immunodeficiency virus (HIV) and sperm-immobilizing activities of cyclohexenyl thiourea and urea non-nucleoside inhibitors of HIV-1 reverse transcriptase. 2002 , 67, 1959-74	21
809	QSAR Studies on Dipeptides Based on a Combinatorial MHDV-GA-MLR Method. 2002 , 49, 1089-1096	3
808	Optimization of focused chemical libraries using recursive partitioning. 2002 , 5, 125-33	21
807	Genetic Algorithm guided Selection: variable selection and subset selection. <i>Journal of Chemical Information and Computer Sciences</i> , 2002 , 42, 927-36	107
806	Three-dimensional quantitative structure-activity relationship of 1,4-dihydropyridines as antitubercular agents. 2002 , 45, 4858-67	89
805	Combined MEDV-GA-MLR method for QSAR of three panels of steroids, dipeptides, and COX-2 inhibitors. <i>Journal of Chemical Information and Computer Sciences</i> , 2002 , 42, 749-56	42
804	Multiobjective optimization in quantitative structure-activity relationships: deriving accurate and interpretable QSARs. 2002 , 45, 5069-80	80
803	Feature selection for structure-activity correlation using binary particle swarms. 2002 , 45, 1098-107	138
802	Predicting Caco-2 cell permeation coefficients of organic molecules using membrane-interaction QSAR analysis. <i>Journal of Chemical Information and Computer Sciences</i> , 2002 , 42, 331-42	91
801	On the use of neural network ensembles in QSAR and QSPR. <i>Journal of Chemical Information and Computer Sciences</i> , 2002 , 42, 903-11	142
800	Chemical information based scaling of molecular descriptors: a universal chemical scale for library design and analysis. <i>Journal of Chemical Information and Computer Sciences</i> , 2002 , 42, 879-84	11
799	Antitumor agents. 213. Modeling of epipodophyllotoxin derivatives using variable selection k nearest neighbor QSAR method. 2002 , 45, 2294-309	79
798	Prediction of protein retention times in anion-exchange chromatography systems using support vector regression. <i>Journal of Chemical Information and Computer Sciences</i> , 2002 , 42, 1347-57	131
797	4D-QSAR analysis of a set of propofol analogues: mapping binding sites for an anesthetic phenol on the GABA(A) receptor. 2002 , 45, 3210-21	86
796	Recent Progress in CoMFA Methodology and Related Techniques. 1998 , 25-39	5
795	Prediction of skin irritation from organic chemicals using membrane-interaction QSAR analysis. 2002 , 66, 336-46	22
794	Prediction of aqueous solubility of organic compounds using a quantitative structure-property relationship. 2002 , 91, 1838-52	70

793	ADME evaluation in drug discovery. 1. Applications of genetic algorithms to the prediction of blood-brain partitioning of a large set of drugs. 2002 , 8, 337-49	87
792	Analogue based design of MMP-13 (Collagenase-3) inhibitors. 2002 , 12, 2689-93	2
791	QSAR of HIV-1 integrase inhibitors by genetic function approximation method. 2002 , 10, 1483-97	24
790	Enhancement of binary QSAR analysis by a GA-based variable selection method. 2002 , 20, 259-68	25
789	QSAR for dihydrofolate reductase inhibitors with molecular graph structural descriptors. 2002 , 582, 39-51	14
788	Local intersection volume: a new 3D descriptor applied to develop a 3D-QSAR pharmacophore model for benzodiazepine receptor ligands. 2002 , 37, 219-29	26
787	QSAR studies of HIV-1 integrase inhibition. 2002 , 10, 4169-83	55
786	5D-QSAR: the key for simulating induced fit?. 2002 , 45, 2139-49	173
785	3D QSAR: Current State, Scope, and Limitations. 1998 , 3-23	8
784	Predicting blood-brain barrier partitioning of organic molecules using membrane-interaction QSAR analysis. 2002 , 19, 1611-21	110
783	Spline-fitting with a genetic algorithm: a method for developing classification structure-activity relationships. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 1906-15	86
782	QSAR Modeling of Genotoxicity on Non-congeneric Sets of Organic Compounds. 2003 , 20, 13-38	14
781	A simple clustering technique to improve QSAR model selection and predictivity: application to a receptor independent 4D-QSAR analysis of cyclic urea derived inhibitors of HIV-1 protease. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 2180-93	25
780	A quantitative structure-activity relationship and pharmacophore modeling investigation of aryl-X and heterocyclic bisphosphonates as bone resorption agents. 2003 , 46, 2932-44	48
779	Variable selection by an evolution algorithm using modified Cp based on MLR and PLS modeling: QSAR studies of carcinogenicity of aromatic amines. 2003 , 375, 248-54	9
778	Predicting the NO ₃ radical tropospheric degradability of organic pollutants by theoretical molecular descriptors. 2003 , 37, 3115-3124	34
777	Two-step multivariate adaptive regression splines for modeling a quantitative relationship between gas chromatography retention indices and molecular descriptors. 2003 , 998, 155-67	43
776	Prediction of bioconcentration factor using genetic algorithm and artificial neural network. 2003 , 486, 101-108	67

775	Synthesis and QSAR study of the anticancer activity of some novel indane carbocyclic nucleosides. 2003 , 11, 4999-5006	51
774	Cross-validation as the objective function for variable-selection techniques. 2003 , 22, 395-406	182
773	Artificial neural networks and genetic algorithms in QSAR. 2003 , 622, 71-83	128
772	QSAR models in receptor-mediated effects: the nuclear receptor superfamily. 2003 , 622, 113-125	29
771	LigandFit: a novel method for the shape-directed rapid docking of ligands to protein active sites. 2003 , 21, 289-307	732
770	A Combinatorial Approach to the Variable Selection in Multiple Linear Regression: Analysis of Selwood et al. Data Set I A Case Study. 2003 , 22, 583-595	47
769	QSAR Prediction of Ozone Tropospheric Degradation. 2003 , 22, 364-373	36
768	Methods for reliability and uncertainty assessment and for applicability evaluations of classification- and regression-based QSARs. 2003 , 111, 1361-75	957
767	3D-pharmacophores of flavonoid binding at the benzodiazepine GABA(A) receptor site using 4D-QSAR analysis. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 324-36	44
766	Development of quantitative structure-activity relationships and classification models for anticonvulsant activity of hydantoin analogues. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 1028-36	32
765	Toward generating simpler QSAR models: nonlinear multivariate regression versus several neural network ensembles and some related methods. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 1094-102	25
764	Quantitative structure-based design: formalism and application of receptor-dependent RD-4D-QSAR analysis to a set of glucose analogue inhibitors of glycogen phosphorylase. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 1591-607	42
763	4D-QSAR analysis of a series of antifungal p450 inhibitors and 3D-pharmacophore comparisons as a function of alignment. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 2170-9	25
762	Receptor-independent 4D-QSAR analysis of a set of norstatine derived inhibitors of HIV-1 protease. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 1297-307	25
761	Parameters for the Generalized Born Model Consistent with RESP Atomic Partial Charge Assignment Protocol. 2003 , 107, 9071-9078	28
760	A general treatment of solubility. 1. The QSPR correlation of solvation free energies of single solutes in series of solvents. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 1794-805	84
759	3D QSAR in modern drug design. 2003 , 223-41	12
758	Transcriptomic analysis of the NCI-60 cancer cell lines. 2003 , 326, 909-20	40

757	Predicting the carcinogenic potential of pharmaceuticals in rodents using molecular structural similarity and E-state indices. 2003 , 38, 243-59	77
756	VSMP: a novel variable selection and modeling method based on the prediction. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 964-9	89
755	Multimode ligand binding in receptor site modeling: implementation in CoMFA. <i>Journal of Chemical Information and Computer Sciences</i> , 2003 , 43, 2093-105	31
754	Comparison of MLR, PLS and GA-MLR in QSAR analysis. 2003 , 14, 433-45	73
753	Optimum Refrigerant Selection for Low Temperature Engineering. 2003 , 101-118	2
752	Fuzzy structure-activity relationships. 2003 , 14, 41-57	1
751	A Novel Quantitative Structure-Biodegradability Relationship (QSBR) of Substituted Benzenes Based on MHDV Descriptor. 2003 , 50, 319-324	3
750	3D-QSAR Studies of Some [[1-Aryl(or Benzyl)-1-(benzenesulphonamido)methyl] phenyl] Alkanoic Acid Derivatives as Thromboxane A2 Receptor Antagonists. 2003 , 18, 47-51	
749	Applying genetic algorithms and neural networks to chemometric problems. 2003 , 23, 343-375	2
748	Feature Selection Methods Based on Genetic Algorithms for in Silico Drug Design. 2003 , 317-339	1
747	Methods for applying the quantitative structure-activity relationship paradigm. 2004 , 275, 131-214	74
746	Derivation and applications of molecular descriptors based on approximate surface area. 2004 , 275, 261-78	6
745	11. Integration of Modelling at Various Length and Time Scales. 2004 , 223-233	8
744	Modified particle swarm optimization algorithm for variable selection in MLR and PLS modeling: QSAR studies of antagonism of angiotensin II antagonists. 2004 , 22, 145-52	101
743	Molecular polarizability as a single-parameter predictor of vapour pressures and octanol/water partitioning coefficients of non-polar compounds: a priori approach and results. 2004 , 38, 213-225	52
742	Rational design of new antituberculosis agents: receptor-independent four-dimensional quantitative structure-activity relationship analysis of a set of isoniazid derivatives. 2004 , 47, 3755-64	43
741	A method for quantifying and visualizing the diversity of QSAR models. 2004 , 22, 275-84	16
740	Genetic algorithms and self-organizing maps: a powerful combination for modeling complex QSAR and QSPR problems. 2004 , 18, 483-93	14

739	Comparison of commercially available genetic algorithms: gas as variable selection tool. 2004 , 18, 511-21	7
738	Applying data mining techniques to library design, lead generation and lead optimization. 2004 , 8, 264-70	39
737	Multivariate adaptive regression splines—studies of HIV reverse transcriptase inhibitors. 2004 , 72, 27-34	37
736	Detecting Bad—Regression models: multicriteria fitness functions in regression analysis. 2004 , 515, 199-208	147
735	LIV-3D-QSAR models for PGI2 receptor ligands using multiple conformations. 2004 , 39, 359-67	
734	Novel scoring functions comprising QXP, SASA, and protein side-chain entropy terms. <i>Journal of Chemical Information and Computer Sciences</i> , 2004 , 44, 882-93	32
733	Constructing optimum blood brain barrier QSAR models using a combination of 4D-molecular similarity measures and cluster analysis. <i>Journal of Chemical Information and Computer Sciences</i> , 2004 , 44, 2083-98	43
732	Characterization of a ligand-receptor binding event using receptor-dependent four-dimensional quantitative structure-activity relationship analysis. 2004 , 47, 3075-88	24
731	A 3D-QSAR of angiotensin II (AT1) receptor antagonists based on receptor surface analysis. <i>Journal of Chemical Information and Computer Sciences</i> , 2004 , 44, 210-20	19
730	Prediction of HPLC conditions using QSPR techniques: an effective tool to improve combinatorial library design. 2004 , 6, 916-27	29
729	Classification of kinase inhibitors using a Bayesian model. 2004 , 47, 4463-70	276
728	4D-fingerprints, universal QSAR and QSPR descriptors. <i>Journal of Chemical Information and Computer Sciences</i> , 2004 , 44, 1526-39	49
727	Particle swarm optimization and neural network application for QSAR.	3
726	Linear indices of the "molecular pseudograph's atom adjacency matrix": definition, significance-interpretation, and application to QSAR analysis of flavone derivatives as HIV-1 integrase inhibitors. <i>Journal of Chemical Information and Computer Sciences</i> , 2004 , 44, 2010-26	72
725	Chemoinformatics. 2004 ,	22
724	Estimating the safe starting dose in phase I clinical trials and no observed effect level based on QSAR modeling of the human maximum recommended daily dose. 2004 , 40, 185-206	65
723	QSAR studies of multidentate nitrogen ligands used in lanthanide and actinide extraction processes. 2004 , 374, 408-415	20
722	Evaluation of mutual information and genetic programming for feature selection in QSAR. <i>Journal of Chemical Information and Computer Sciences</i> , 2004 , 44, 1686-92	47

721	Enzyme Inhibitors. 2004,	
720	Integromic analysis of the NCI-60 cancer cell lines. 2004, 19, 11-22	36
719	Development of nonlinear quantitative structure-activity relationships using rbf networks and evolutionary computing. 2004, 265-270	1
718	Resolution of Differential Pulse Voltammetric Peaks Using Genetic Algorithm Based Variable Selection-Partial Least Squares and Principal Component-Artificial Neural Networks. 2005, 52, 21-28	14
717	Cluster analysis and three-dimensional QSAR studies of HIV-1 integrase inhibitors. 2005, 23, 317-28	17
716	LigScore: a novel scoring function for predicting binding affinities. 2005, 23, 395-407	281
715	A topological sub-structural approach to the mutagenic activity in dental monomers. 3. Heterogeneous set of compounds. 2005, 46, 2783-2790	20
714	Predicting permeability coefficient in ADMET evaluation by using different membranes-interaction QSAR. 2005, 304, 115-23	11
713	QSTR with extended topochemical atom indices. Part 5: Modeling of the acute toxicity of phenylsulfonyl carboxylates to <i>Vibrio fischeri</i> using genetic function approximation. 2005, 13, 1185-94	34
712	Exploring QSAR of thiazole and thiadiazole derivatives as potent and selective human adenosine A3 receptor antagonists using FA and GFA techniques. 2005, 13, 1159-65	67
711	QSAR by LFER model of cytotoxicity data of anti-HIV 5-phenyl-1-phenylamino-1H-imidazole derivatives using principal component factor analysis and genetic function approximation. 2005, 13, 2967-73	32
710	Application of genetic stochastic resonance algorithm to quantitative structure-activity relationship study. 2005, 75, 181-188	8
709	Molecular modeling of mono- and bis-quaternary ammonium salts as ligands at the alpha4beta2 nicotinic acetylcholine receptor subtype using nonlinear techniques. 2005, 7, E678-85	9
708	Computational Prediction of Blood-brain Barrier Permeation. 2005, 40, 403-415	26
707	Pharmacophore modeling, docking, and principal component analysis based clustering: combined computer-assisted approaches to identify new inhibitors of the human rhinovirus coat protein. 2005, 48, 6250-60	40
706	Predictive model of blood-brain barrier penetration of organic compounds. 2005, 26, 500-12	111
705	QSAR analysis of substituted bis[(acridine-4-carboxamide)propyl]methylamines using optimized block-wise variable combination by particle swarm optimization for partial least squares modeling. 2005, 25, 245-54	13
704	A new set of amino acid descriptors and its application in peptide QSARs. 2005, 80, 775-86	118

703	QSAR of adenosine A3 receptor antagonist 1,2,4-triazolo[4,3-a]quinoxalin-1-one derivatives using chemometric tools. 2005 , 15, 3737-43	25
702	Exploring 3D-QSAR of thiazole and thiadiazole derivatives as potent and selective human adenosine A3 receptor antagonists+. 2005 , 11, 516-24	9
701	Construction of 4D-QSAR models for use in the design of novel p38-MAPK inhibitors. 2005 , 19, 385-400	27
700	Evolutionary Algorithms in Drug Design. 2005 , 4, 177-243	31
699	QSAR Analysis of the Structure-Toxicity Relationship of Aconitum and Delphinium Diterpene Alkaloids. 2005 , 41, 213-219	10
698	Investigation of iminosulfuranes as novel transdermal penetration enhancers: enhancement activity and cytotoxicity. 2005 , 22, 1918-25	39
697	A Quantitative Structure-Activity Relationship (QSAR) Study of the Antioxidant Activity of Flavonoids. 2005 , 24, 1056-1065	77
696	4D-QSAR Models of HOE/BAY-793 Analogues as HIV-1 Protease Inhibitors. 2005 , 24, 240-253	11
695	Mutagenicity of Aromatic and Heteroaromatic Amines and Related Compounds: A QSAR Investigation. 2005 , 24, 831-843	18
694	Docking Versus Pharmacophore Model Generation: A Comparison of High-Throughput Virtual Screening Strategies for the Search of Human Rhinovirus Coat Protein Inhibitors. 2005 , 24, 470-479	19
693	Prediction of Protein Retention Times in Anion-Exchange Chromatography Systems Using Support Vector Regression. 2005 , 111-125	1
692	A comparison of particle swarms techniques for the development of quantitative structure-activity relationship models for drug design.	5
691	A study of the relationship between cornea permeability and eye irritation using membrane-interaction QSAR analysis. 2005 , 88, 434-46	15
690	Particle swarms for drug design.	2
689	Optimized block-wise variable combination by particle swarm optimization for partial least squares modeling in quantitative structure-activity relationship studies. 2005 , 45, 486-93	34
688	Novel ligands for the chemokine receptor-3 (CCR3): a receptor-modeling study based on 5D-QSAR. 2005 , 48, 1515-27	36
687	QSAR analyses of 3-(4-benzylpiperidin-1-yl)-N-phenylpropylamine derivatives as potent CCR5 antagonists. 2005 , 45, 1352-68	37
686	Synthesis of 3-arylpiperazinylalkylpyrrolo[3,2-d]pyrimidine-2,4-dione derivatives as novel, potent, and selective alpha1-adrenoceptor ligands. 2005 , 48, 2420-31	25

685	kappa Nearest neighbors QSAR modeling as a variational problem: theory and applications. 2005 , 45, 777-85	44
684	McQSAR: a multiconformational quantitative structure-activity relationship engine driven by genetic algorithms. 2005 , 45, 1953-61	16
683	Three-dimensional QSAR using the k-nearest neighbor method and its interpretation. 2006 , 46, 24-31	152
682	Biological activities and 3D QSAR studies of a series of <i>Delisea pulchra</i> (cf. <i>fimbriata</i>) derived natural products. 2006 , 69, 1180-7	29
681	Predicting thermochemical parameters of oxygen-containing heterocycles using simple QSPR models. 2006 , 32, 125-134	5
680	Chapter 7 Variable Selection QSAR Modeling, Model Validation, and Virtual Screening. 2006 , 2, 113-126	14
679	Topological descriptors in modeling the antimalarial activity of 4-(3',5'-disubstituted anilino)quinolines. 2006 , 46, 93-102	33
678	QSAR prediction of estrogen activity for a large set of diverse chemicals under the guidance of OECD principles. 2006 , 19, 1540-8	108
677	Using Voronoi Grid and SVM Linear Regression in Drug Discovery. 2006 ,	1
676	Structure-based QSAR analysis of a set of 4-hydroxy-5,6-dihydropyrone as inhibitors of HIV-1 protease: an application of the receptor-dependent (RD) 4D-QSAR formalism. 2006 , 46, 345-54	26
675	QSAR and QSPR studies of a highly structured physicochemical domain. 2006 , 46, 264-76	48
674	QSAR Studies on Thiazolidines: A Biologically Privileged Scaffold. 161-249	37
673	Flavor release from i-carrageenan matrix: a quantitative structure-property relationships approach. 2006 , 54, 3679-85	19
672	A high dimensional QSAR study on the aldose reductase inhibitory activity of some flavones: topological descriptors in modeling the activity. 2006 , 46, 86-92	26
671	A fixed functional set genetic algorithm (FFSGA) approach for function approximation. 2006 , 8, 193-206	7
670	A genetic-function-approximation-based QSAR model for the affinity of arylpiperazines toward alpha1 adrenoceptors. 2006 , 46, 1466-78	12
669	The Quantitative Structure-Mutagenicity Relationship of Polycyclic Aromatic Hydrocarbon Metabolites. 2006 , 7, 556-570	9
668	Glass Transition. 2006 ,	0

667	Artificial Intelligence and Data Mining for Toxicity Prediction. 2006 , 2, 123-133	8
666	Statistical deconvolution of enthalpic energetic contributions to MHC-peptide binding affinity. 2006 , 6, 5	21
665	QSTR with Extended Topochemical Atom (ETA) Indices 8.a QSAR for the inhibition of substituted phenols on germination rate of Cucumis sativus using chemometric tools. 2006 , 25, 846-859	23
664	Molecular dynamics simulations of a set of isoniazid derivatives bound to InhA, the enoyl-acp reductase from <i>M. tuberculosis</i> . 2006 , 106, 2689-2699	3
663	A QSAR model of HERG binding using a large, diverse, and internally consistent training set. 2006 , 67, 284-96	65
662	Quantitative structure activity relationship of benzoxazinone derivatives as neuropeptide Y Y5 receptor antagonists. 2006 , 41, 552-7	11
661	Quantitative structure activity relationship studies of aryl heterocycle-based thrombin inhibitors. 2006 , 41, 1339-46	30
660	SVRCDSPR model for predicting saturated vapor pressures of pure fluids. 2006 , 246, 39-51	43
659	QSAR analysis of antimicrobial and haemolytic effects of cyclic cationic antimicrobial peptides derived from protegrin-1. 2006 , 14, 6065-74	52
658	Comparative QSAR modeling of CCR5 receptor binding affinity of substituted 1-(3,3-diphenylpropyl)-piperidinyl amides and ureas. 2006 , 16, 4467-74	39
657	Prediction of ozone tropospheric degradation rate constant of organic compounds by using artificial neural networks. 2006 , 556, 355-363	49
656	Studies of relationship between biological activities and HIV Reverse Transcriptase Inhibitors by Multivariate Adaptive Regression Splines with Curds and Whey. 2006 , 82, 24-30	5
655	Effect of cholesterol on DMPC phospholipid membranes and QSAR model construction in membrane-interaction QSAR study through molecular dynamics simulation. 2006 , 14, 2225-34	12
654	Quantitative structure-activity relationship of spirosuccinimide type aldose reductase inhibitors diminishing sorbitol accumulation in vivo. 2006 , 14, 3090-7	7
653	In silico ADME modelling 2: computational models to predict human serum albumin binding affinity using ant colony systems. 2006 , 14, 4118-29	43
652	Application of artificial neural networks and DFT-based parameters for prediction of reaction kinetics of ethylbenzene dehydrogenase. 2006 , 20, 145-57	33
651	Comparative residue interaction analysis (CoRIA): a 3D-QSAR approach to explore the binding contributions of active site residues with ligands. 2006 , 20, 343-60	36
650	Bond-based global and local (bond, group and bond-type) quadratic indices and their applications to computer-aided molecular design. 1. QSPR studies of diverse sets of organic chemicals. 2006 , 20, 685-701	21

649	Molecular similarity and diversity in chemoinformatics: from theory to applications. 2006 , 10, 39-79	180
648	QSTR with extended topochemical atom (ETA) indices. VI. Acute toxicity of benzene derivatives to tadpoles (<i>Rana japonica</i>). 2006 , 12, 306-16	25
647	Computational approaches for modeling human intestinal absorption and permeability. 2006 , 12, 577-89	21
646	Free-energy force-field three-dimensional quantitative structure-activity relationship analysis of a set of p38-mitogen activated protein kinase inhibitors. 2006 , 12, 855-68	12
645	Three-dimensional quantitative structure-activity relationship (3 D-QSAR) and docking studies on (benzothiazole-2-yl) acetonitrile derivatives as c-Jun N-terminal kinase-3 (JNK3) inhibitors. 2006 , 16, 5917-25	28
644	Cluster analysis and two-dimensional quantitative structure-activity relationship (2D-QSAR) of <i>Pseudomonas aeruginosa</i> deacetylase LpxC inhibitors. 2006 , 16, 5136-43	24
643	A new descriptor of amino acids based on the three-dimensional vector of atomic interaction field. 2006 , 51, 524-529	15
642	Consensus scoring for protein-ligand interactions. 2006 , 11, 421-8	183
641	Recent Advances in Chemometric Methodologies for QSAR Studies. 2006 , 2, 255-266	4
640	Quantitative Structure-Uptake Relationship of Metal-Organic Frameworks as Hydrogen Storage Material. 2006 , 927, 1	
639	Correlating Polymer-Carbon Composite Sensor Response with Molecular Descriptors. 2006 , 153, H209	19
638	Approaches to Three-Dimensional Quantitative Structure-Activity Relationships. 2007 , 183-240	11
637	QSAR analyses of skin penetration enhancers. 2007 , 47, 1130-49	18
636	Theoretical and Practical Aspects of Three-Dimensional Quantitative Structure-Activity Relationships. 2007 , 127-182	24
635	Evaluation of <i>Pseudomonas aeruginosa</i> deacetylase LpxC inhibitory activity of dual PDE4-TNFalpha inhibitors: a multiscreening approach. 2007 , 47, 1188-95	9
634	Genetic Algorithms and Their Use in Chemistry. 2007 , 1-73	11
633	Human protein tyrosine phosphatase 1B inhibitors: QSAR by genetic function approximation. 2007 , 22, 267-76, 371-3	16
632	General purpose interactive physico-chemical property exploration. 2007 , 47, 1182-7	3

631	Perspective assessment of COX-1 and COX-2 selectivity of nonsteroidal anti-inflammatory drugs from clinical practice: use of genetic function approximation. 2007 , 47, 635-43	8
630	Exploration of rate-limiting conformational state for 5-[(7-chloro-4-quinolinyl)amino]-3-[(alkylamino)methyl][1,1'-biphenyl]-2-ols and N(omega)-oxides (tebuquine analogues) for antimalarial activity using molecular shape analysis and molecular field analysis studies. 2007 , 47, 1087-96	7
629	An Introduction To Chemoinformatics. 2007 ,	191
628	Modeling robust QSAR. 2. iterative variable elimination schemes for CoMSA: application for modeling benzoic acid pKa values. 2007 , 47, 547-56	35
627	ADME evaluation in drug discovery. 7. Prediction of oral absorption by correlation and classification. 2007 , 47, 208-18	141
626	Random forest models to predict aqueous solubility. 2007 , 47, 150-8	217
625	Treating chemical diversity in QSAR analysis: modeling diverse HIV-1 integrase inhibitors using 4D fingerprints. 2007 , 47, 1945-60	19
624	Predictive Quantitative Structure-Activity Relationship Modeling. 2007 , 149-165	2
623	Combination of genetic algorithm and partial least squares for cloud point prediction of nonionic surfactants from molecular structures. 2007 , 97, 69-83	25
622	A QSPR study on the GC retention times of a series of fatty, dicarboxylic and amino acids by MLR and ANN. 2007 , 97, 925-33	5
621	Computational chemistry development of a unified free energy Markov model for the distribution of 1300 chemicals to 38 different environmental or biological systems. 2007 , 28, 1909-23	67
620	QSAR studies and pharmacophore identification for arylsubstituted cycloalkenecarboxylic acid methyl esters with affinity for the human dopamine transporter. 2007 , 15, 5262-74	9
619	QSAR study of selective ligands for the thyroid hormone receptor beta. 2007 , 15, 5251-61	67
618	Prediction of binding affinities to beta1 isoform of human thyroid hormone receptor by genetic algorithm and projection pursuit regression. 2007 , 17, 2474-82	23
617	QSAR analysis of tyrosine kinase inhibitor using modified ant colony optimization and multiple linear regression. 2007 , 42, 81-6	37
616	A novel range based QSAR study of human neuropeptide Y (NPY) Y5 receptor inhibitors. 2007 , 42, 463-70	15
615	Application of genetic algorithm-kernel partial least square as a novel nonlinear feature selection method: activity of carbonic anhydrase II inhibitors. 2007 , 42, 649-59	57
614	Supervised pattern recognition in food analysis. 2007 , 1158, 196-214	696

613	Quantitative structure-activity relationship (QSAR) of tacrine derivatives against acetylcholinesterase (AChE) activity using variable selections. 2007 , 17, 1082-90	29
612	T-scale as a novel vector of topological descriptors for amino acids and its application in QSARs of peptides. 2007 , 830, 106-115	85
611	Encoding Type and Position in Peptide QSAR: Application to Peptides Binding to Class I MHC Molecule HLA-A*0201. 2007 , 26, 189-203	12
610	Quantitative Structure-Activity Relationship Studies for the Binding Affinities of Imidazobenzodiazepines for the α Benzodiazepine Receptor Isoform Utilizing Optimized Blockwise Variable Combination by Particle Swarm Optimization for Partial Least Squares Modeling. 2007 , 26, 92-101	6
609	In Silico ADME Modeling 3: Computational Models to Predict Human Intestinal Absorption Using Sphere Exclusion and kNN QSAR Methods. 2007 , 26, 653-668	29
608	Comparative Classical QSAR Modeling of Anti-HIV Thiocarbamates. 2007 , 26, 980-990	10
607	Comparison of Shuffling-Adaptive Neuro Fuzzy Inference System (Shuffling-ANFIS) with Conventional ANFIS as Feature Selection Methods for Nonlinear Systems. 2007 , 26, 1046-1059	10
606	Caco-2 cell permeability modelling: a neural network coupled genetic algorithm approach. 2007 , 21, 207-21	20
605	In silico screening of estrogen-like chemicals based on different nonlinear classification models. 2007 , 26, 135-44	32
604	Selectivity-based QSAR approach for screening and evaluation of TRH analogs for TRH-R1 and TRH-R2 receptors subtypes. 2008 , 27, 309-20	2
603	Novel 2D TOMOCOMD-CARDD molecular descriptors: atom-based stochastic and non-stochastic bilinear indices and their QSPR applications. 2008 , 44, 650-673	15
602	A comprehensive analysis of the thermodynamic events involved in ligand-receptor binding using CoRIA and its variants. 2008 , 22, 91-104	18
601	Hierarchical QSAR technology based on the Simplex representation of molecular structure. 2008 , 22, 403-21	119
600	Quantitative Series Enrichment Analysis (QSEA): a novel procedure for 3D-QSAR analysis. 2008 , 22, 541-51	9
599	Considerations and recent advances in QSAR models for cytochrome P450-mediated drug metabolism prediction. 2008 , 22, 843-55	46
598	Some molecular descriptors for non-specific chromosomal genotoxicity based on hydrophobic interactions. 2008 , 82, 333-8	9
597	A novel vector of topological and structural information for amino acids and its QSAR applications for peptides and analogues. 2008 , 51, 946-957	3
596	QSAR study on estrogenic activity of structurally diverse compounds using generalized regression neural network. 2008 , 51, 677-683	8

595	Back-propagation network improved by conjugate gradient based on genetic algorithm in QSAR study on endocrine disrupting chemicals. 2008 , 53, 33-39	15
594	Improvement of bioavailability of water insoluble drugs: Estimation of intrinsic bioavailability (Short Communication). 2008 , 25, 171-175	9
593	Feature Set Selection in QSAR of 1-[(2-Hydroxyethoxy)methyl]-6-(phenylthio)thymine (HEPT) Analogues by Using Swarm Intelligence. 2008 , 139, 197-211	6
592	Modelling the property of compounds from structure: statistical methods for models validation. 2008 , 6, 175-181	21
591	Simultaneous feature selection and parameter optimisation using an artificial ant colony: case study of melting point prediction. 2008 , 2, 21	19
590	In Silico Prediction of BloodBrain Partitioning Using a Chemometric Method Called Genetic Algorithm Based Variable Selection. 2008 , 27, 704-717	17
589	Accurate Prediction of Aquatic Toxicity of Aromatic Compounds Based on Genetic Algorithm and Least Squares Support Vector Machines. 2008 , 27, 850-865	10
588	Prediction of hERG Potassium Channel Blockade Using kNN-QSAR and Local Lazy Regression Methods. 2008 , 27, 1305-1317	14
587	A Novel Approach for the Identification of Selective Anticonvulsants Based on Differential Molecular Properties for TBPS Displacement and Anticonvulsant Activity: An Integrated QSAR Modelling. 2008 , 27, 876-889	2
586	Quantitative structure-antibacterial activity relationship modeling using a combination of piecewise linear regression-discriminant analysis (I): Quantum chemical, topographic, and topological descriptors. 2008 , 108, 1856-1871	5
585	Combined 4D-fingerprint and clustering based membrane-interaction QSAR analyses for constructing consensus Caco-2 cell permeation virtual screens. 2008 , 97, 566-83	10
584	QSAR study of malonyl-CoA decarboxylase inhibitors using GA-MLR and a new strategy of consensus modeling. 2008 , 29, 2636-47	43
583	Application of molecular connectivity and electro-topological indices in quantitative structure-activity analysis of pyrazole derivatives as inhibitors of factor Xa and thrombin. 2008 , 5, 2609-20	3
582	A novel descriptor of amino acids and its application in peptide QSAR. 2008 , 253, 90-7	49
581	Comparative QSTR studies for predicting mutagenicity of nitro compounds. 2008 , 26, 916-34	19
580	Exploring QSTR and toxicophore of hERG K ⁺ channel blockers using GFA and HypoGen techniques. 2008 , 26, 966-76	34
579	Development of predictive in silico model for cyclosporine- and aureobasidin-based P-glycoprotein inhibitors employing receptor surface analysis. 2008 , 27, 439-51	7
578	Molecular structural characteristics as determinants of estrogen receptor selectivity. 2008 , 48, 369-75	17

577	Exploring molecular shape analysis of styrylquinoline derivatives as HIV-1 integrase inhibitors. 2008 , 43, 81-92	40
576	Quantitative structure activity relationship studies on thiourea analogues as influenza virus neuraminidase inhibitors. 2008 , 43, 293-9	30
575	3D-QSAR studies of triazafluorenone inhibitors of metabotropic glutamate receptor subtype 1. 2008 , 43, 1025-34	2
574	A novel quantitative structure-activity relationship method to predict the affinities of MT3 melatonin binding site. 2008 , 43, 2861-9	13
573	Quantitative structure-activity relationship studies on 1-aryl-tetrahydroisoquinoline analogs as active anti-HIV agents. 2008 , 18, 5381-6	24
572	Impact of topological and electronic descriptors in the QSAR of pyrazine containing thiazolines and thiazolidinones as antitubercular and antibacterial agents. 2008 , 71, 447-463	15
571	Exploring QSARs for binding affinity of azoles with CYP2B and CYP3A enzymes using GFA and G/PLS techniques. 2008 , 71, 464-473	5
570	QSTR with extended topochemical atom indices. 10. Modeling of toxicity of organic chemicals to humans using different chemometric tools. 2008 , 72, 383-94	19
569	Comparative QSAR studies of CYP1A2 inhibitor flavonoids using 2D and 3D descriptors. 2008 , 72, 370-82	47
568	Estimating forage biomass and quality in a mixed sown pasture based on partial least squares regression with waveband selection. 2008 , 54, 131-145	71
567	Combined ligand and structure based approaches for narrowing on the essential physicochemical characteristics for CDK4 inhibition. 2008 , 48, 1325-36	12
566	Membrane-interaction quantitative structure--activity relationship (MI-QSAR) analyses of skin penetration enhancers. 2008 , 48, 1238-56	17
565	Using molecular docking, 3D-QSAR, and cluster analysis for screening structurally diverse data sets of pharmacological interest. 2008 , 48, 2054-65	14
564	Prediction of the logarithmic of partition coefficients (log P) of some organic compounds by least square-support vector machine (LS-SVM). 2008 , 106, 2525-2535	15
563	DNA-damaging activity and mutagenicity of 16 newly synthesized thiazolo[5,4-a]acridine derivatives with high photo-inducible cytotoxicity. 2008 , 650, 104-14	13
562	An updated steroid benchmark set and its application in the discovery of novel nanomolar ligands of sex hormone-binding globulin. 2008 , 51, 2047-56	38
561	The effect of nitroaromatics' composition on their toxicity in vivo: novel, efficient non-additive 1D QSAR analysis. 2008 , 72, 1373-80	44
560	Quantitative Approaches to Structure-Activity Relationships. 2008 , 491-513	6

559	Development of linear and nonlinear predictive QSAR models and their external validation using molecular similarity principle for anti-HIV indolyl aryl sulfones. 2008 , 23, 980-95	30
558	Using quantitative structure-activity relationships (QSAR) to predict toxic endpoints for polycyclic aromatic hydrocarbons (PAH). 2008 , 71, 1073-84	11
557	Variable selection methods in QSAR: an overview. 2008 , 8, 1606-27	136
556	Partition Coefficient Prediction of a Large Set of Various Drugs and Poisons by a Genetic Algorithm and Artificial Neural Network. 2008 , 55, 345-355	12
555	QSAR in Drug Design. 2008 , 1532-1554	11
554	Comparative QSAR studies of nitrofuranyl amide derivatives using theoretical structural properties. 2009 , 35, 1185-1200	18
553	Exploring the structural requirements for jasmonates and related compounds as novel plant growth regulators: a current computational perspective. 2009 , 4, 1007-9	2
552	Quantitative Structure-Activity Relationship Studies on Some Novel Anti- HIV Thiourea Derivatives with Cytotoxicity Data (CC50) in MT-4 Cells. 2009 , 6, 193-200	1
551	Quantitative Structure Activity Relationship of Indole-Carbaldehyde Derivatives as Cannabinoid Receptor 2 Agonists. 2009 , 6, 599-619	1
550	QSAR modeling for quinoxaline derivatives using genetic algorithm and simulated annealing based feature selection. 2009 , 16, 4032-48	42
549	QSTR with extended topochemical atom (ETA) indices. 11. Comparative QSAR of acute NSAID cytotoxicity in rat hepatocytes using chemometric tools. 2009 , 35, 648-659	18
548	Optimal functional forms for estimation of missing precipitation data. 2009 , 374, 106-115	42
547	Cluster Analysis and QSAR Study of Some Anti-hepatitis B Virus Agents Comprising 4-Aryl-6-chloro-quinolin-2-ones and 5-Aryl-7-chloro-1,4-benzodiazepines. 2009 , 27, 2352-2358	1
546	QSAR of antilipid peroxidative activity of substituted benzodioxoles using chemometric tools. 2009 , 30, 2712-22	12
545	A new strategy to improve the predictive ability of the local lazy regression and its application to the QSAR study of melanin-concentrating hormone receptor 1 antagonists. 2010 , 31, 973-85	3
544	Quantitative structure migration relationship modeling of migration factor for some benzene derivatives in micellar electrokinetic chromatography. 2009 , 32, 1934-40	4
543	Exploring the binding of HIV-1 integrase inhibitors by comparative residue interaction analysis (CoRIA). 2009 , 15, 233-45	28
542	In silico quantitative prediction of peptides binding affinity to human MHC molecule: an intuitive quantitative structure-activity relationship approach. 2009 , 36, 535-54	71

541	An improved QSPR study of the toxicity of aliphatic carboxylic acids using genetic algorithm. 2009 , 18, 143-157	8
540	QSAR analysis of N-myristoyltransferase inhibitors: antifungal activity of benzofurans. 2009 , 18, 206-220	9
539	Exploring 2D and 3D QSARs of 2,4-Diphenyl-1,3-oxazolines for Ovicidal Activity Against <i>Tetranychus urticae</i> . 2009 , 28, 406-425	46
538	QSAR Approach to Correlate TRPV1 Antagonist Activity for a Series of Heteroaromatic Urea. 2009 , 28, 1098-1111	3
537	Predicting the Androgenicity of Structurally Diverse Compounds from Molecular Structure Using Different Classifiers. 2009 , 28, 542-550	4
536	Quantitative Structure-Activity Relationship Analysis of Some Thiourea Derivatives with Activities Against HIV-1 (IIIB). 2009 , 28, 89-97	10
535	Consensus QSAR Modeling of Phosphor-Containing Chiral AChE Inhibitors. 2009 , 28, 664-677	32
534	Molecular Modeling and Receptor-Dependent (RD) 3D-QSAR Approach to a Set of Antituberculosis Derivatives. 2009 , 28, 1455-1464	3
533	Is Feature Selection Essential for ANN Modeling?. 2009 , 28, 1487-1499	18
532	Quantitative structure-property relationship studies on amino acid conjugates of jasmonic acid as defense signaling molecules. 2009 , 51, 581-92	4
531	Quantitative structure-activity relationship modeling of antioxidant activities of hydroxybenzalacetones using quantum chemical, physicochemical and spatial descriptors. 2009 , 73, 526-36	29
530	Molecular shape analysis of antioxidant and squalene synthase inhibitory activities of aromatic tetrahydro-1,4-oxazine derivatives. 2009 , 74, 507-16	12
529	Predicting the auto-ignition temperatures of organic compounds from molecular structure using support vector machine. 2009 , 164, 1242-9	42
528	Dissipative particle dynamics study on the phase morphologies of the ultrahigh molecular weight polyethylene/polypropylene/poly(ethylene glycol) blends. 2009 , 50, 336-346	38
527	Quantitative structure-activity relationship (QSAR) of aryl alkenyl amides/imines for bacterial efflux pump inhibitors. 2009 , 44, 229-38	33
526	Predictive QSAR modeling of HIV reverse transcriptase inhibitor TIBO derivatives. 2009 , 44, 1509-24	32
525	Comparative chemometric modeling of cytochrome 3A4 inhibitory activity of structurally diverse compounds using stepwise MLR, FA-MLR, PLS, GFA, G/PLS and ANN techniques. 2009 , 44, 2913-22	96
524	Quantitative structure activity relationship (QSAR) of piperine analogs for bacterial NorA efflux pump inhibitors. 2009 , 44, 4128-35	32

523	Quantitative structure-activity relationship analysis of aryl alkanol piperazine derivatives with antidepressant activities. 2009 , 44, 4367-75	19
522	Validated quantitative structure-activity relationship analysis of a series of 2-aminothiazole based p56(Lck) inhibitors. 2009 , 631, 29-39	8
521	A segmented principal component analysis-regression approach to quantitative structure-activity relationship modeling. 2009 , 646, 30-8	18
520	An efficient variable selection method based on the use of external memory in ant colony optimization. Application to QSAR/QSPR studies. 2009 , 646, 39-46	44
519	QSAR studies of CYP2D6 inhibitor aryloxypropanolamines using 2D and 3D descriptors. 2009 , 73, 442-55	66
518	Structural analysis of carboline derivatives as inhibitors of MAPKAP K2 using 3D QSAR and docking studies. 2009 , 49, 53-67	23
517	Automated procedure for candidate compound selection in GC-MS metabolomics based on prediction of Kovats retention index. 2009 , 25, 787-94	33
516	Mixed-model QSAR at the human mineralocorticoid receptor: predicting binding mode and affinity of anabolic steroids. 2009 , 189, 219-24	9
515	Current mathematical methods used in QSAR/QSPR studies. 2009 , 10, 1978-98	123
514	Bibliography. 2009 , 1-241	1
513	Combinatorial library enumeration and lead hopping using comparative interaction fingerprint analysis and classical 2D QSAR methods for seeking novel GABA(A) alpha(3) modulators. 2009 , 49, 2498-511	15
512	Local indices for similarity analysis (LISA)-a 3D-QSAR formalism based on local molecular similarity. 2009 , 49, 2695-707	8
511	Predictive QSAR modeling of CCR5 antagonist piperidine derivatives using chemometric tools. 2009 , 24, 205-23	11
510	Pharmacophore modeling, quantitative structure-activity relationship analysis, and shape-complemented in silico screening allow access to novel influenza neuraminidase inhibitors. 2009 , 49, 978-96	49
509	On two novel parameters for validation of predictive QSAR models. 2009 , 14, 1660-701	363
508	3D pharmacophore mapping using 4D QSAR analysis for the cytotoxicity of lamellarins against human hormone-dependent T47D breast cancer cells. 2009 , 49, 2312-22	16
507	Rational design and 3D-pharmacophore mapping of 5'-thiourea-substituted alpha-thymidine analogues as mycobacterial TMPK inhibitors. 2009 , 49, 1070-8	29
506	The use of machine learning and nonlinear statistical tools for ADME prediction. 2009 , 5, 149-69	28

505	Predicting multiple binding modes using a kernel method based on a vector space model molecular descriptor. 2009 , 2, 58-80	3
504	Review on lazy learning regressors and their applications in QSAR. 2009 , 12, 440-50	4
503	Bayesian modeling in virtual high throughput screening. 2009 , 12, 469-83	16
502	4D-QSAR: perspectives in drug design. 2010 , 15, 3281-94	68
501	A QSAR study for modeling of 8-azaadenine analogues proposed as A1 adenosine receptor antagonists using genetic algorithm coupling adaptive neuro-fuzzy inference system (ANFIS). 2010 , 26, 897-902	9
500	Exploring quantitative structure-activity relationship studies of antioxidant phenolic compounds obtained from traditional Chinese medicinal plants. 2010 , 36, 1067-1079	221
499	Quantitative correlation of physical and chemical properties with chemical structure: utility for prediction. 2010 , 110, 5714-89	372
498	In silico binary classification QSAR models based on 4D-fingerprints and MOE descriptors for prediction of hERG blockage. 2010 , 50, 1304-18	60
497	Two- and three-dimensional QSAR studies on benzyl amide-ketoacid inhibitors of HIV integrase and their reduced analogues. 2010 , 19, 1106-1120	4
496	Functionalized aurones as inducers of NAD(P)H:quinone oxidoreductase 1 that activate AhR/XRE and Nrf2/ARE signaling pathways: synthesis, evaluation and SAR. 2010 , 45, 2957-71	63
495	Molecular docking and QSAR study on steroidal compounds as aromatase inhibitors. 2010 , 45, 5612-20	40
494	Global and local prediction of protein folding rates based on sequence autocorrelation information. 2010 , 264, 1159-68	7
493	Docking and 3D QSAR studies of protoporphyrinogen oxidase inhibitor 3H-pyrazolo[3,4-d][1,2,3]triazin-4-one derivatives. 2010 , 16, 137-53	26
492	Molecular modelling and QSAR analysis of some structurally diverse N-type calcium channel blockers. 2010 , 16, 629-44	15
491	New molecular scaffolds for the design of Mycobacterium tuberculosis type II dehydroquinase inhibitors identified using ligand and receptor based virtual screening. 2010 , 16, 693-712	15
490	Docking and 3D-QSAR studies of acetohydroxy acid synthase inhibitor sulfonylurea derivatives. 2010 , 16, 951-64	21
489	Docking and 3D-QSAR studies of diverse classes of human aromatase (CYP19) inhibitors. 2010 , 16, 1597-616	27
488	ST-scale as a novel amino acid descriptor and its application in QSAM of peptides and analogues. 2010 , 38, 805-16	41

487	Synthesis, characterization, ab initio calculations, thermal behaviour and thermodynamics of some oxovanadium(IV) complexes involving O,O- and N,N-donor moieties. 2010 , 122, 539-548	10
486	3D-Pharmacophore mapping of thymidine-based inhibitors of TMPK as potential antituberculosis agents. 2010 , 24, 157-72	15
485	Bond-based linear indices of the non-stochastic and stochastic edge-adjacency matrix. 1. Theory and modeling of ChemPhys properties of organic molecules. 2010 , 14, 731-53	11
484	The importance of molecular structures, endpoints' values, and predictivity parameters in QSAR research: QSAR analysis of a series of estrogen receptor binders. 2010 , 14, 687-96	30
483	Predicting logarithmic values of the subcooled liquid vapor pressure of halogenated persistent organic pollutants with QSPR: How different are chlorinated and brominated congeners?. 2010 , 44, 1428-1436 ²⁹	
482	First report on interspecies quantitative correlation of ecotoxicity of pharmaceuticals. 2010 , 81, 738-47	57
481	Retention/Release equilibrium of aroma compounds in polysaccharide gels: study by quantitative structure/Activity/property relationships approach. 2010 , 25, 431-442	21
480	A combined molecular modeling study on gelatinases and their potent inhibitors. 2010 , 31, 24-42	15
479	QSAR modeling of a set of pyrazinoate esters as antituberculosis prodrugs. 2010 , 343, 91-7	5
478	Quantitative structure-property relationship modeling of water-to-wet butyl acetate partition coefficient of 76 organic solutes using multiple linear regression and artificial neural network. 2010 , 33, 3800-10	11
477	QSAR modeling of toxicity of diverse organic chemicals to <i>Daphnia magna</i> using 2D and 3D descriptors. 2010 , 177, 344-51	76
476	QSPR prediction of flash point of esters by means of GFA and ANFIS. 2010 , 179, 715-20	45
475	QSTR with extended topochemical atom (ETA) indices. 14. QSAR modeling of toxicity of aromatic aldehydes to <i>Tetrahymena pyriformis</i> . 2010 , 183, 913-22	23
474	3D QSAR study, synthesis, and in vitro evaluation of (+)-5-FBVM as potential PET radioligand for the vesicular acetylcholine transporter (VACHT). 2010 , 18, 7659-67	22
473	Chemometric modeling, docking and in silico design of triazolopyrimidine-based dihydroorotate dehydrogenase inhibitors as antimalarials. 2010 , 45, 4645-56	45
472	Chemometric modeling of free radical scavenging activity of flavone derivatives. 2010 , 45, 5071-9	23
471	QSAR studies on aminothiazole derivatives as aurora a kinase inhibitors. 2010 , 76, 527-37	3
470	Development of predictive quantitative structure-activity relationship models of epipodophyllotoxin derivatives. 2010 , 15, 1194-203	2

469	Predicting mutagenicity of aromatic amines by various machine learning approaches. 2010 , 116, 498-513	31
468	Exploring QSAR of hydroxyphenylureas as antioxidants using physicochemical and electrotopological state atom parameters. 2010 , 36, 484-492	4
467	Variable selection in nonlinear modeling based on RBF networks and evolutionary computation. 2010 , 20, 365-79	29
466	Prediction of skin sensitization potential using D-optimal design and GA-kNN classification methods. 2010 , 21, 305-35	3
465	Classical and 3D-QSAR studies of cytochrome 17 inhibitor imidazole-substituted biphenyls. 2010 , 36, 311-325	6
464	Exploring QSAR for CYP11B2 binding affinity and CYP11B2/CYP11B1 selectivity of diverse functional compounds using GFA and G/PLS techniques. 2010 , 25, 354-69	6
463	Computer tools in the discovery of HIV-1 integrase inhibitors. 2010 , 2, 1123-40	13
462	3D-QSAR in drug design--a review. 2010 , 10, 95-115	481
461	A QSPR model for the prediction of the "fish-tail" temperature of C(i)E4/water/polar hydrocarbon oil systems. 2010 , 26, 7962-70	26
460	Jackknife-based selection of Gram-Schmidt orthogonalized descriptors in QSAR. 2010 , 50, 2055-66	11
459	A novel structure-based multimode QSAR method affords predictive models for phosphodiesterase inhibitors. 2010 , 50, 240-50	9
458	Quantitative structure-reactivity modeling of copper-catalyzed atom transfer radical polymerization. 2010 , 1, 922	15
457	Per aspera ad astra: application of Simplex QSAR approach in antiviral research. 2010 , 2, 1205-26	52
456	Dissipative Particle Dynamics and Flory-Edwards Theories for Predicting the Rheological Behavior of Ultrahigh Molecular Weight Polyethylene Blends. 2010 , 49, 11369-11379	15
455	Chemometric modelling of antimalarial activity of aryltriazolylhydroxamates. 2010 , 36, 939-952	15
454	EMBM - a new enzyme mechanism-based method for rational design of chemical sites of covalent inhibitors. 2010 , 50, 2256-65	7
453	Molecular interaction fields and 3D-QSAR studies of p53-MDM2 inhibitors suggest additional features of ligand-target interaction. 2010 , 50, 1451-65	11
452	Molecular docking and QSAR studies of aromatase inhibitor androstenedione derivatives. 2010 , 62, 1717-28	33

451	Pharmacophore mapping, molecular docking and QSAR studies of structurally diverse compounds as CYP2B6 inhibitors. 2010 , 36, 887-905	14
450	Chemometric Methods and Theoretical Molecular Descriptors in Predictive QSAR Modeling of the Environmental Behavior of Organic Pollutants. 2010 , 327-366	10
449	Insights for predicting blood-brain barrier penetration of CNS targeted molecules using QSPR approaches. 2010 , 50, 1123-33	54
448	Recent Advances in QSAR Studies. 2010 ,	82
447	Advances in computational methods to predict the biological activity of compounds. 2010 , 5, 633-54	128
446	Replacement method and enhanced replacement method versus the genetic algorithm approach for the selection of molecular descriptors in QSPR/QSAR theories. 2010 , 50, 1542-8	73
445	Ranking chemical structures for drug discovery: a new machine learning approach. 2010 , 50, 716-31	80
444	Stroke prevention by traditional Chinese medicine? A genetic algorithm, support vector machine and molecular dynamics approach. 2011 , 7, 4001	52
443	Traditional Chinese medicine, a solution for reducing dual stroke risk factors at once?. 2011 , 7, 2711-9	39
442	In silico pharmacology suggests ginger extracts may reduce stroke risks. 2011 , 7, 2702-10	42
441	Artificial neural network-based QSPR study on absorption maxima of organic dyes for dye-sensitised solar cells. 2011 , 37, 1-10	12
440	Quantitative StructureProperty Relationship for Flash Points of Alcohols. 2011 , 50, 11337-11342	19
439	A comprehensive support vector machine binary hERG classification model based on extensive but biased end point hERG data sets. 2011 , 24, 934-49	33
438	Quantitative Structure Property Relationship Studies for Predicting Dust Explosibility Characteristics (K _{st} ,P _{max}) of Organic Chemical Dusts. 2011 , 50, 2373-2379	23
437	Exploring molecular docking and QSAR studies of plasmepsin-II inhibitor di-tertiary amines as potential antimalarial compounds. 2011 , 37, 779-803	5
436	Review of the quantitative structureactivity relationship modelling methods on estimation of formation constants of macrocyclic compounds with different guest molecules. 2011 , 23, 614-629	20
435	Allosteric inhibition of the hepatitis C virus NS5B polymerase: in silico strategies for drug discovery and development. 2011 , 3, 1027-55	35
434	Descriptors for antimicrobial peptides. 2011 , 6, 171-84	22

433	Computational ligand-based rational design: Role of conformational sampling and force fields in model development. 2011 , 2, 356-370	58
432	QSPR of antioxidant phenolic compounds using quantum chemical descriptors. 2011 , 37, 394-413	8
431	Development of a minimal kinase ensemble receptor (MKER) for surrogate AutoShim. 2011 , 51, 2697-705	2
430	Solubility Parameters of Nonelectrolyte Organic Compounds: Determination Using Quantitative StructureProperty Relationship Strategy. 2011 , 50, 11382-11395	86
429	Modeling corrosion inhibition of iron in acid medium by genetic function approximation method: A QSAR model. 2011 , 53, 3457-3465	50
428	ADME evaluation in drug discovery. 9. Prediction of oral bioavailability in humans based on molecular properties and structural fingerprints. 2011 , 8, 841-51	83
427	Robust scoring functions for protein-ligand interactions with quantum chemical charge models. 2011 , 51, 2528-37	41
426	Using artificial neural networks to predict cell-penetrating compounds. 2011 , 6, 783-96	15
425	Strategies of multi-objective optimization in drug discovery and development. 2011 , 6, 871-84	25
424	QSAR models for CXCR2 receptor antagonists based on the genetic algorithm for data preprocessing prior to application of the PLS linear regression method and design of the new compounds using in silico virtual screening. 2011 , 16, 1928-55	35
423	In silico predictions of ADME-Tox properties: drug absorption. 2011 , 14, 339-61	32
422	Investigation into potent inflammation inhibitors from traditional Chinese medicine. 2011 , 78, 679-88	50
421	Improved in silico prediction of carcinogenic potency (TD50) and the risk specific dose (RSD) adjusted Threshold of Toxicological Concern (TTC) for genotoxic chemicals and pharmaceutical impurities. 2011 , 59, 133-41	15
420	Handling a very large data set for determination of surface tension of chemical compounds using Quantitative StructureProperty Relationship strategy. 2011 , 66, 4991-5023	40
419	Comparative QSARs for antimalarial endochins: Importance of descriptor-thinning and noise reduction prior to feature selection. 2011 , 109, 146-161	162
418	On various metrics used for validation of predictive QSAR models with applications in virtual screening and focused library design. 2011 , 14, 450-74	159
417	Toward better QSAR/QSPR modeling: simultaneous outlier detection and variable selection using distribution of model features. 2011 , 25, 67-80	22
416	Predicting Infinite Dilution Activity Coefficients of Chlorinated Organic Compounds in Aqueous Solution Based on Three-Dimensional WHIM and GETAWAY Descriptors. 2011 , 40, 118-130	5

415	An integrated drug-likeness study for bicyclic privileged structures: from physicochemical properties to in vitro ADME properties. 2011 , 15, 857-76		17
414	Quantitative structure-property relationship prediction of liquid thermal conductivity for some alcohols. <i>Structural Chemistry</i> , 2011 , 22, 1315-1323	1.8	16
413	Molecular modeling and QSAR studies of a set of indole and benzimidazole derivatives as H ₁ receptor antagonists. 2011 , 17, 921-8		8
412	Mosquito larvicidal studies of some chalcone analogues and their derived products: structure-activity relationship analysis. 2011 , 20, 184-191		33
411	Synthesis, antioxidant evaluation, and quantitative structure-activity relationship studies of chalcones. 2011 , 20, 482-492		79
410	QSAR modeling of the inhibition of reverse transcriptase enzyme with benzimidazolone analogs. 2011 , 20, 1530-1541		8
409	QSAR study of a series of acyl coenzyme A (CoA): cholesterol acyltransferase inhibitors using genetic function approximation. 2011 , 20, 1573-1580		6
408	Receptor-dependent (RD) 3D-QSAR approach of a series of benzylpiperidine inhibitors of human acetylcholinesterase (HuAChE). 2011 , 46, 39-51		29
407	Interpretation of QSAR Models Based on Random Forest Methods. 2011 , 30, 593-603		47
406	Molecular Docking Guided Comparative GFA, G/PLS, SVM and ANN Models of Structurally Diverse Dual Binding Site Acetylcholinesterase Inhibitors. 2011 , 30, 689-706		12
405	Deciphering the Structural Requirements of Nucleoside Bisubstrate Analogues for Inhibition of MtbA in Mycobacterium tuberculosis: A FB-QSAR Study and Combinatorial Library Generation for Identifying Potential Hits. 2011 , 30, 863-72		2
404	Application of a Novel Ant Algorithm Termed Continuous Gridded in Aided Drug Design. 2011 , 29, 2019-2026		
403	Quantitative structure-property relationship for surface tension of some common alcohols. 2011 , 25, 333-339		19
402	Differentiating serine and cysteine protease mechanisms by new covalent QSAR descriptors. 2011 , 12, 1023-6		15
401	Further exploring rm2 metrics for validation of QSPR models. 2011 , 107, 194-205		407
400	Quantitative structure-activity relationship analysis of a novel series of chemicals antagonizing WT and MT AR. 2011 , 107, 283-289		
399	QSAR of adenosine receptor antagonists: Exploring physicochemical requirements for binding of pyrazolo[4,3-e]-1,2,4-triazolo[1,5-c]pyrimidine derivatives with human adenosine A(3) receptor subtype. 2011 , 21, 818-23		35
398	QSAR study of natural estrogen-like isoflavonoids and diphenolics from Thai medicinal plants. 2011 , 29, 784-94		18

397	QSPR modeling of nonionic surfactant cloud points: an update. 2011 , 358, 202-7	13
396	Treat Alzheimer's disease by traditional Chinese medicine?. 2011 , 37, 923-931	2
395	QSPR Study on Electric Spark Sensitivity of Nitro Arenes. 2011 , 284-286, 197-200	2
394	QSAR study of a series of cholesteryl ester transfer protein inhibitors. 2011 , 76, 803-813	3
393	Reviewing ligand-based rational drug design: the search for an ATP synthase inhibitor. 2011 , 12, 5304-18	39
392	Two birds with one stone? Possible dual-targeting H1N1 inhibitors from traditional Chinese medicine. 2011 , 7, e1002315	72
391	Structural Insights into the Active Site of Human Sodium Dependent Glucose Co-Transporter 2: Homology Modelling, Molecular Docking, and 3D - QSAR Studies. 2012 , 65, 1314	18
390	Feature selection methods in QSAR studies. 2012 , 95, 636-51	79
389	QSAR applications during last decade on inhibitors of acetylcholinesterase in Alzheimer's disease. 2012 , 12, 936-46	12
388	QSAR and QM/MM approaches applied to drug metabolism prediction. 2012 , 12, 573-82	18
387	The use of Bayesian nonlinear regression techniques for the modelling of the retention behaviour of volatile components of Artemisia species. 2012 , 23, 461-83	
386	Target prediction of small molecules with information of key molecular interactions. 2012 , 12, 1903-10	6
385	A QSAR study of biphenyl analogues of 2-nitroimidazo-[2, 1-b] [1, 3]-oxazines as antitubercular agents using genetic function approximation. 2012 , 8, 717-26	7
384	QSAR studies of PTP1B inhibitors: recent advances and perspectives. 2012 , 19, 4208-17	9
383	Derivatives in discrete mathematics: a novel graph-theoretical invariant for generating new 2/3D molecular descriptors. I. Theory and QSPR application. 2012 , 26, 1229-46	13
382	Computational studies of novel chymase inhibitors against cardiovascular and allergic diseases: mechanism and inhibition. 2012 , 80, 862-75	5
381	Application of modified particle swarm optimization as an efficient variable selection strategy in QSAR/QSPR studies. 2012 , 26, 598-603	9
380	Prediction of hERG Potassium Channel Blocking Actions Using Combination of Classification and Regression Based Models: A Mixed Descriptors Approach. 2012 , 31, 879-94	4

379	The imidazolidone analogs as phospholipase D1 inhibitors: analysis of the three-dimensional quantitative structure–activity relationship. 2012 , 21, 2517-2525	1
378	Computational approaches to enhance activity of taxanes as antimitotic agent. 2012 , 21, 2557-2570	1
377	Quantitative structure–property relationship for thermal decomposition temperature of ionic liquids. 2012 , 84, 557-563	31
376	Introduction of rm2(rank) metric incorporating rank-order predictions as an additional tool for validation of QSAR/QSPR models. 2012 , 118, 200-210	55
375	WITHDRAWN: A comprehensive structure–activity analysis of 5-Carboxyl Imidazolyl biphenyl Sulfonylureas derivatives angiotensin AT1 receptor antagonists: 2D- and 3D-QSAR approach. 2012 ,	13
374	Development of classification and regression models for <i>Vibrio fischeri</i> toxicity of ionic liquids: green solvents for the future. 2012 , 1, 186	39
373	Quantitative Structure–Property Relationship Prediction of Gas Heat Capacity for Organic Compounds. 2012 , 51, 13490-13495	4
372	Quantitative Structure–Property Relationship Prediction of Liquid Heat Capacity at 298.15 K for Organic Compounds. 2012 , 51, 6251-6255	7
371	Predictive Quantitative Structure–Property Relationship Model for the Estimation of Ionic Liquid Viscosity. 2012 , 51, 2470-2477	47
370	Determination of the glass transition temperature of ionic liquids: A molecular approach. 2012 , 543, 88-95	23
369	QSTR with extended topochemical atom (ETA) indices. 15. Development of predictive models for toxicity of organic chemicals against fathead minnow using second-generation ETA indices. 2012 , 23, 125-40	19
368	QSPR with extended topochemical atom (ETA) indices, 3: Modeling of critical micelle concentration of cationic surfactants. 2012 , 81, 169-178	13
367	Development of classification and regression based QSAR models to predict rodent carcinogenic potency using oral slope factor. 2012 , 82, 85-95	15
366	Cheminformatics and chemical genomics: potential utility of in silico methods. 2012 , 32, 880-9	21
365	Mold2 Molecular Descriptors for QSAR. 2012 , 65-109	3
364	Partial-Order Ranking and Linear Modeling: Their Use in Predictive QSAR/QSPR Studies. 2012 , 149-174	
363	Computer-aided molecular modeling study on antibody recognition of small molecules: an immunoassay for triazine herbicides. 2012 , 60, 10486-93	18
362	Cellular quantitative structure–activity relationship (Cell-QSAR): conceptual dissection of receptor binding and intracellular disposition in antifilarial activities of Selwood antimycins. 2012 , 55, 3699-712	6

361	Ionic liquids: Prediction of melting point by molecular-based model. 2012 , 549, 17-34	27
360	QSAR analysis of selectivity in flotation of chalcopyrite from pyrite for xanthate derivatives: Xanthogen formates and thionocarbamates. 2012 , 39, 140-148	13
359	Poster abstracts. 2012 , 44, 36-152	4
358	Determination of Diffusion Coefficient of Organic Compounds in Water Using a Simple Molecular-Based Method. 2012 , 51, 2797-2803	25
357	Prediction of enzyme activity with neural network models based on electronic and geometrical features of substrates. 2012 , 64, 761-81	14
356	QSAR study and the hydrolysis activity prediction of three alkaline lipases from different lipase-producing microorganisms. 2012 , 11, 124	3
355	Application of 4D-QSAR studies to a series of raloxifene analogs and design of potential selective estrogen receptor modulators. 2012 , 17, 7415-39	9
354	Residue-ligand interaction energy (ReLIE) on a receptor-dependent 3D-QSAR analysis of S- and NH-DABOs as non-nucleoside reverse transcriptase inhibitors. 2012 , 17, 7666-94	5
353	In silico development, validation and comparison of predictive QSAR models for lipid peroxidation inhibitory activity of cinnamic acid and caffeic acid derivatives using multiple chemometric and cheminformatics tools. 2012 , 18, 3951-67	11
352	Comparative Occupancy Analysis (CoOAn) - A Straightforward and Directly Applicable 3D-QSAR Formalism to Extract Molecular Features Obligatory for Designing Potent Leads. 2012 , 31, 431-42	2
351	Benchmarking Variable Selection in QSAR. 2012 , 31, 173-9	19
350	Predictive toxicology modeling: protocols for exploring hERG classification and Tetrahymena pyriformis end point predictions. 2012 , 52, 1660-73	19
349	Application of GA-MLR method in QSPR modeling of stability constants of diverse 15-crown-5 complexes with sodium cation. 2012 , 74, 57-66	14
348	Novel algorithm to select basis functions in spline regression: applications in quantitative structure-activity relationship studies. 2012 , 26, 85-94	2
347	Protein-ligand-based pharmacophores: generation and utility assessment in computational ligand profiling. 2012 , 52, 943-55	94
346	Quantitative structure-retention relationship study of analgesic drugs by application of combined data splitting-feature selection strategy and genetic algorithm-partial least square. 2012 , 9, 53-60	13
345	Molecular modeling of the Toxoplasma gondii adenosine kinase inhibitors. 2012 , 21, 590-600	20
344	QSAR studies on substituted 3- or 4-phenyl-1,8-naphthyridine derivatives as antimicrobial agents. 2012 , 21, 788-795	8

343	Predicting 3H-1,2,4-triazolinones as angiotensin II receptor antagonists: 2D and 3D QSAR by kNN-molecular field analysis approach. 2012 , 21, 1166-1178	2
342	Three-dimensional quantitative structure-activity relationship (3D-QSAR) analysis and molecular docking of ATP-competitive triazine analogs of human mTOR inhibitors. 2012 , 21, 1207-1217	10
341	De novo design of 7-aminocoumarin derivatives as novel falcipain-3 inhibitors. 2012 , 18, 1481-93	3
340	Metastable region of phase diagram: optimum parameter range for processing ultrahigh molecular weight polyethylene blends. 2012 , 18, 2501-12	8
339	QSPR with extended topochemical atom (ETA) indices: Modeling of critical micelle concentration of non-ionic surfactants. 2012 , 73, 86-98	28
338	QSPR molecular approach for representation/prediction of very large vapor pressure dataset. 2012 , 76, 99-107	26
337	A QSPR model for prediction of diffusion coefficient of non-electrolyte organic compounds in air at ambient condition. 2012 , 86, 959-66	28
336	First report on development of quantitative interspecies structure-carcinogenicity relationship models and exploring discriminatory features for rodent carcinogenicity of diverse organic chemicals using OECD guidelines. 2012 , 87, 339-55	34
335	An accurate model for the prediction of the glass transition temperature of ammonium based ionic liquids: A QSPR approach. 2012 , 324, 50-63	24
334	QSPR prediction of surface tension of refrigerants from their molecular structures. 2012 , 35, 150-159	20
333	QSAR study and synthesis of new phenyltropanes as ligands of the dopamine transporter (DAT). 2012 , 20, 1388-95	8
332	Identification of novel HIV-1 integrase inhibitors using shape-based screening, QSAR, and docking approach. 2012 , 79, 835-49	20
331	Receptor-dependent 4D-QSAR analysis of peptidomimetic inhibitors of Trypanosoma cruzi trypanothione reductase with receptor-based alignment. 2012 , 79, 740-8	14
330	Functional polymer thin films designed for antifouling materials and biosensors. 2012 , 66,	44
329	Diffusion coefficient prediction of acids in water at infinite dilution by QSPR method. <i>Structural Chemistry</i> , 2012 , 23, 399-406	1.8 13
328	The great descriptor melting pot: mixing descriptors for the common good of QSAR models. 2012 , 26, 39-43	32
327	Elucidation of specific aspects of dielectric constants of conjugated organic compounds: a QSPR approach. 2012 , 18, 251-6	4
326	Estimation of the Heat Capacity of Ionic Liquids: A Quantitative StructureProperty Relationship Approach. 2013 , 52, 13217-13221	19

325	Clustering of variables in regression analysis: a comparative study between different algorithms. 2013 , 27, 306-317		15
324	Prediction of mono-, bi-, and trivalent metal cation relative toxicity to the seaweed <i>Gracilaria domingensis</i> (Gracilariales, Rhodophyta) in synthetic seawater. 2013 , 32, 2571-5		7
323	Uninformative variable elimination assisted by Gram-Schmidt Orthogonalization/successive projection algorithm for descriptor selection in QSAR. 2013 , 128, 56-65		8
322	Pro-apoptotic properties of parthenin analogs: a quantitative structure-activity relationship study. 2013 , 22, 2303-2311		6
321	Quantification of contributions of different molecular fragments for antioxidant activity of coumarin derivatives based on QSAR analyses. 2013 , 91, 428-441		10
320	QSAR studies for the computational prediction of HMG-CoA reductase inhibitors by genetic function approximation technique. 2013 , 91, 263-274		5
319	Modified particle swarm optimization method for variable selection in QSAR/QSPR studies. <i>Structural Chemistry</i> , 2013 , 24, 1401-1409	1.8	14
318	QSPR with extended topochemical atom (ETA) indices. 4. Modeling aqueous solubility of drug like molecules and agrochemicals following OECD guidelines. <i>Structural Chemistry</i> , 2013 , 24, 303-331	1.8	16
317	An integral strategy toward the rapid identification of analogous nontarget compounds from complex mixtures. 2013 , 1303, 39-47		27
316	Structure-Activity Relationship Analysis of the Thermal Stabilities of Nitroaromatic Compounds Following Different Decomposition Mechanisms. 2013 , 32, 193-202		5
315	Development and evaluation of an integrated virtual screening strategy by combining molecular docking and pharmacophore searching based on multiple protein structures. 2013 , 53, 2743-56		53
314	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. 2013 , 16, 7-21		15
313	Structural requirements of 3-carboxyl-4(1H)-quinolones as potential antimalarials from 2D and 3D QSAR analysis. 2013 , 44, 266-77		20
312	Combination of pharmacophore hypothesis, genetic function approximation model, and molecular docking to identify novel inhibitors of S6K1. 2013 , 17, 767-72		5
311	Elaborate ligand-based modeling coupled with QSAR analysis and in silico screening reveal new potent acetylcholinesterase inhibitors. 2013 , 27, 1075-92		28
310	HomoSAR: bridging comparative protein modeling with quantitative structural activity relationship to design new peptides. 2013 , 34, 2635-46		6
309	Exploring QSAR and pharmacophore mapping of structurally diverse selective matrix metalloproteinase-2 inhibitors. 2013 , 65, 1541-54		28
308	A predictive quantitative structure-property relationship for glass transition temperature of 1,3-dialkyl imidazolium ionic liquids. 2013 , 111, 235-246		22

307	Environmental toxicological fate prediction of diverse organic chemicals based on steady-state compartmental chemical mass ratio using quantitative structure-fate relationship (QSFR) models. 2013 , 92, 600-7	5
306	First report on exploring structural requirements of β - and γ -thymidine analogs for PFTMPK inhibitory activity using in silico studies. 2013 , 113, 177-95	7
305	QSPR with extended topochemical atom (ETA) indices: Exploring effects of hydrophobicity, branching and electronic parameters on logCMC values of anionic surfactants. 2013 , 87, 141-151	12
304	Prediction of surface tension of ionic liquids by molecular approach. 2013 , 179, 78-87	25
303	Predictive chemometric modeling of DPPH free radical-scavenging activity ofazole derivatives using 2D- and 3D-quantitative structure-activity relationship tools. 2013 , 5, 261-80	5
302	Predictive QSPR modelling for the olfactory threshold of a series of pyrazine derivatives. 2013 , 28, 102-117	7
301	Preliminary studies on model development for rodent toxicity and its interspecies correlation with aquatic toxicities of pharmaceuticals. 2013 , 90, 375-81	16
300	Review of quantitative structure-activity/property relationship studies of dyes: recent advances and perspectives. 2013 , 129, 173-186	14
299	Dependence of QSAR models on the selection of trial descriptor sets: a demonstration using nanotoxicity endpoints of decorated nanotubes. 2013 , 53, 142-58	40
298	Some case studies on application of "r(m) ² " metrics for judging quality of quantitative structure-activity relationship predictions: emphasis on scaling of response data. 2013 , 34, 1071-82	288
297	QSTR with extended topochemical atom (ETA) indices. 16. Development of predictive classification and regression models for toxicity of ionic liquids towards Daphnia magna. 2013 , 254-255, 166-178	42
296	QSPR analysis for melting point of fatty acids using genetic algorithm based multiple linear regression (GA-MLR). 2013 , 353, 15-21	25
295	Modeling compound-target interaction network of traditional Chinese medicines for type II diabetes mellitus: insight for polypharmacology and drug design. 2013 , 53, 1787-803	34
294	QSAR methods for the discovery of new inflammatory bowel disease drugs. 2013 , 8, 933-49	7
293	Prediction of Flash Points for Fuel Mixtures Using Machine Learning and a Novel Equation. 2013 , 27, 3811-3820	44
292	Descriptor selection methods in quantitative structure-activity relationship studies: a review study. 2013 , 113, 8093-103	132
291	From QSAR to QSIR: searching for enhanced computational toxicology models. 2013 , 930, 53-65	12
290	Elaborate ligand-based modeling coupled with multiple linear regression and k nearest neighbor QSAR analyses unveiled new nanomolar mTOR inhibitors. 2013 , 53, 2587-612	36

- 289 Development and validation of regression-based QSAR models for quantification of contributions of molecular fragments to skin sensitization potency of diverse organic chemicals. **2013**, 24, 1009-23 12
- 288 Predictive Chemometric Modeling and Three-Dimensional Toxicophore Mapping of Diverse Organic Chemicals Causing Bioluminescent Repression of the Bacterium Genus *Pseudomonas*. **2013**, 52, 17648-17657 5
- 287 New strategy for receptor-based pharmacophore query construction: a case study for 5-HT₁ receptor ligands. **2013**, 53, 3233-43 22
- 286 Relations frequency hypermatrices in mutual, conditional and joint entropy-based information indices. **2013**, 34, 259-74 23
- 285 Synthesis, antifungal activity, and QSAR studies of 1,6-dihydropyrimidine derivatives. **2013**, 5, 277-89 8
- 284 Topological Features in Profiling the Antimalarial Activity Landscape of Anilinoquinolines: A Multipronged QSAR Study. **2013**, 2013, 1-14
- 283 Bio-inspired approach to solve chemical equations. **2013**, 1 1
- 282 A novel integrated framework and improved methodology of computer-aided drug design. **2013**, 13, 965-88 53
- 281 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. **2013**, 16, 7-21 5
- 280 Recent advances in multidimensional QSAR (4D-6D): a critical review. **2014**, 14, 35-55 59
- 279 Application of 4D-QSAR studies to a series of benzothiophene analogs. **2014**, 20, 2420 6
- 278 In Silico Identification of Potent PPAR- α Agonists from Traditional Chinese Medicine: A Bioactivity Prediction, Virtual Screening, and Molecular Dynamics Study. **2014**, 2014, 192452 10
- 277 Lead screening for HIV-1 integrase (IN) inhibited by traditional Chinese medicine. **2014**, 2014, 479367 4
- 276 In silico investigation of traditional Chinese medicine compounds to inhibit human histone deacetylase 2 for patients with Alzheimer's disease. **2014**, 2014, 769867 9
- 275 In Silico Investigation of Cytochrome P450 2C9 in relation to Aging Using Traditional Chinese Medicine. **2014**, 2014, 404505 1
- 274 Quantitative Structure-Activity Relationships: A Novel Approach of Drug Design and Discovery. **2014**, 1, 219-232 12
- 273 Chemometric modelling of triphenylmethyl derivatives as potent anticancer agents. **2014**, 40, 1218-1235
- 272 Predicting Novel Antitumor Agents: 3D-Pharmacophore Mapping of β -N-biaryl Ether Sulfonamide-Based Hydroxamates as Potentially MMP-2 Inhibitors. **2014**, 33, 573-87 5

271	Treatment of cardiovascular disease by traditional Chinese medicine against pregnane X receptor. 2014 , 2014, 950191	15
270	Quantification of contributions of molecular fragments for eye irritation of organic chemicals using QSAR study. 2014 , 48, 102-8	4
269	Application of self organizing maps and GA-MLR for the estimation of stability constant of 18-crown-6 ether derivatives with sodium cation. 2014 , 79, 141-149	14
268	Exploring the physicochemical properties of oxime-reactivation therapeutics for cyclosarin, sarin, tabun, and VX inactivated acetylcholinesterase. 2014 , 27, 99-110	14
267	Prediction of new bioactive molecules using a Bayesian belief network. 2014 , 54, 30-6	18
266	Modeling bioconcentration factor (BCF) using mechanistically interpretable descriptors computed from open source tool "PaDEL-Descriptor". 2014 , 21, 2955-65	11
265	A chemical structure based model for the determination of speed of sound in ionic liquids. 2014 , 196, 7-13	8
264	A quantitative structure-property relationship approach to determine the essential molecular functionalities of potent odorants. 2014 , 29, 157-165	4
263	Exploring QSTR modeling and toxicophore mapping for identification of important molecular features contributing to the chemical toxicity in Escherichia coli. 2014 , 28, 265-72	6
262	Development of a group contribution method for the estimation of heat capacities of ionic liquids. 2014 , 115, 1863-1882	36
261	Computational methods in drug discovery. 2014 , 66, 334-95	953
260	Quantitative Structure Relative Volatility Relationship Model for Extractive Distillation of Ethylbenzene/p-Xylene Mixtures. 2014 , 53, 11159-11166	8
259	A chemical structure based model for the estimation of refractive indices of organic compounds. 2014 , 384, 1-13	6
258	Quantitative Structure-Property Relationship Analysis of Drugs-Pharmacokinetics Within the Framework of Biopharmaceutics Classification System Using Simplex Representation of Molecular Structure. 2014 , 461-499	2
257	Design, synthesis and exploring the quantitative structure-activity relationship of some antioxidant flavonoid analogues. 2014 , 24, 5050-4	40
256	Identification and pharmacological characterization of 3,6-diazabicyclo[3.1.1]heptane-3-carboxamides as novel ligands for the $\alpha 4$ and $\beta 2/\beta 3$ nicotinic acetylcholine receptors (nAChRs). 2014 , 86, 60-74	4
255	Phase Behavior of Biomass Components in Supercritical Water. 2014 , 41-68	0
254	Integrative and personalized QSAR analysis in cancer by kernelized Bayesian matrix factorization. 2014 , 54, 2347-59	67

253	Near-critical and Supercritical Water and Their Applications for Biorefineries. 2014 ,	16
252	Global Performance and Trend of QSAR/QSPR Research: A Bibliometric Analysis. 2014 , 33, 655-68	18
251	Designing quantitative structure activity relationships to predict specific toxic endpoints for polybrominated diphenyl ethers in mammalian cells. 2014 , 25, 527-49	3
250	Quantitative structure-activity relationship (QSAR) studies as strategic approach in drug discovery. 2014 , 23, 4991-5007	41
249	Quantitative structure-property relationship study on the intercalation of anticancer drugs with ct-DNA. 2014 , 23, 1148-1161	17
248	A chemical structure-based model for estimating speed of sound in liquids. 2014 , 116, 529-538	4
247	Predictive in silico Modeling of Ionic Liquids toward Inhibition of the Acetyl Cholinesterase Enzyme of Electrophorus electricus: A Predictive Toxicology Approach. 2014 , 53, 1020-1032	22
246	Predictive modeling studies for the ecotoxicity of ionic liquids towards the green algae <i>Scenedesmus vacuolatus</i> . 2014 , 104, 170-6	51
245	Exploring structural requirements of leads for improving activity and selectivity against CDK5/p25 in Alzheimer's disease: an in silico approach. 2014 , 4, 6702-6709	20
244	Kinetics and quantitative structure-activity relationship study on the degradation reaction from perfluorooctanoic acid to trifluoroacetic acid. 2014 , 15, 14153-65	6
243	Combining spatial and chemical information for clustering pharmacophores. 2014 , 15 Suppl 16, S5	5
242	Virtual screening and prediction of the molecular mechanism of bioactive compounds in silico. 2015 , 371-394	1
241	Developing hypothetical inhibition mechanism of novel urea transporter B inhibitor. 2014 , 4, 5775	14
240	Modeling the flammability characteristics of polymers using quantitative structure-property relationships (QSPR). 2015 , 55, 1553-1559	12
239	3D QSAR Analysis on Isatin Derivatives as Carboxyl Esterase Inhibitors Using K-Nearest Neighbor Molecular Field Analysis. 2015 , 02,	
238	Aqueous Molecular Dynamics Simulations of the <i>M. tuberculosis</i> Enoyl-ACP Reductase-NADH System and Its Complex with a Substrate Mimic or Diphenyl Ethers Inhibitors. 2015 , 16, 23695-722	13
237	Quantitative Structure-Activity Relationships Study on the Rate Constants of Polychlorinated Dibenzo-p-Dioxins with OH Radical. 2015 , 16, 18812-24	2
236	New triazolothiadiazole and triazolothiadiazine derivatives as kinesin Eg5 and HIV inhibitors: synthesis, QSAR and modeling studies. 2015 , 70, 47-58	11

235	Interspecies quantitative structure-toxicity-toxicity (QSTTR) relationship modeling of ionic liquids. Toxicity of ionic liquids to <i>V. fischeri</i> , <i>D. magna</i> and <i>S. vacuolatus</i> . 2015 , 122, 497-520	26
234	QSPR study on solubility of some fullerenes derivatives using the genetic algorithms [Multiple linear regression. 2015 , 204, 162-169	23
233	QSAR analysis for nano-sized layered manganese-calcium oxide in water oxidation: An application of chemometric methods in artificial photosynthesis. 2015 , 152, 146-55	8
232	Prediction of refractive indices of ionic liquids [A quantitative structure-property relationship based model. 2015 , 52, 165-180	19
231	Exploring possible mechanisms of action for the nanotoxicity and protein binding of decorated nanotubes: interpretation of physicochemical properties from optimal QSAR models. 2015 , 288, 52-62	12
230	Exploring simple, transparent, interpretable and predictive QSAR models for classification and quantitative prediction of rat toxicity of ionic liquids using OECD recommended guidelines. 2015 , 139, 163-73	18
229	Chemometrics tools in QSAR/QSPR studies: A historical perspective. 2015 , 149, 177-204	85
228	Novel global and local 3D atom-based linear descriptors of the Minkowski distance matrix: theory, diversity[variability analysis and QSPR applications. 2015 , 53, 2028-2064	9
227	Computational study of the effects of cations and anions to the cytotoxicity of diverse ionic liquids by supervised machine learning. 2015 , 144, 138-147	12
226	Molecular dynamics simulated validation of anti-cancerous alkaloids as Topo II[inhibitors screened by QSAR, pharmacophore and molecular docking approaches. 2015 , 24, 2972-2985	1
225	Combining docking-based comparative intermolecular contacts analysis and k-nearest neighbor correlation for the discovery of new check point kinase 1 inhibitors. 2015 , 29, 561-81	17
224	QSAR based docking studies of marine algal anticancer compounds as inhibitors of protein kinase B (PKB) 2015 , 76, 110-8	15
223	Selected Statistical Methods in QSAR. 2015 , 191-229	15
222	Prediction of Alternative Gasoline Sorption in a Semicrystalline Poly(ethylene). 2015 , 17, 631-40	4
221	Multivariate statistical analysis methods in QSAR. 2015 , 5, 104635-104665	46
220	CoRILISA: a local similarity based receptor dependent QSAR method. 2015 , 55, 194-205	4
219	Comparative validated molecular modeling of p53-HDM2 inhibitors as antiproliferative agents. 2015 , 90, 860-75	23
218	Predicting the ecotoxicity of ionic liquids towards <i>Vibrio fischeri</i> using genetic function approximation and least squares support vector machine. 2015 , 283, 591-8	53

217	Predictive QSAR modelling of algal toxicity of ionic liquids and its interspecies correlation with Daphnia toxicity. 2015 , 22, 6634-41		34
216	Quantifying ligand-receptor interactions for gorge-spanning acetylcholinesterase inhibitors for the treatment of Alzheimer's disease. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015 , 33, 1107-25	3.6	10
215	Predicting dual-targeting anti-influenza agents using multi-models. 2015 , 19, 123-34		4
214	QSAR modeling of antimalarial activity of urea derivatives using genetic algorithm-multiple linear regressions. 2016 , 20, 282-290		30
213	Prediction of perception using structure-activity models. 2016 , 181-200		1
212	AN ACTIVITY PREDICTION MODEL USING SHAPE-BASED DESCRIPTOR METHOD. 2016 , 78,		
211	Quantitative Structure-Activity Relationship Studies for Potential Rho-Associated Protein Kinase Inhibitors. 2016 , 2016, 1-12		10
210	Finding a Potential Dipeptidyl Peptidase-4 (DPP-4) Inhibitor for Type-2 Diabetes Treatment Based on Molecular Docking, Pharmacophore Generation, and Molecular Dynamics Simulation. 2016 , 17,		22
209	Quantitative Characterization of the Interaction Space of the Mammalian Carbonic Anhydrase Isoforms I, II, VII, IX, XII, and XIV and their Inhibitors, Using the Proteochemometric Approach. 2016 , 88, 341-53		14
208	Temperature-dependent structure-property modeling of viscosity for ionic liquids. 2016 , 427, 9-17		26
207	A stepwise protocol for neural network modeling of persistent postoperative facial pain in chronic rhinosinusitis. 2016 , 12,		0
206	Discovery of potent adenosine A2a antagonists as potential anti-Parkinson disease agents. Non-linear QSAR analyses integrated with pharmacophore modeling. 2016 , 254, 93-101		14
205	QSPR approaches to elucidate the stability constants between Cyclodextrin and some organic compounds: Docking based 3D conformer. 2016 , 219, 1036-1043		4
204	Characterization, in Vivo Evaluation, and Molecular Modeling of Different Propofol-Cyclodextrin Complexes To Assess Their Drug Delivery Potential at the Blood-Brain Barrier Level. 2016 , 56, 1914-1922		27
203	Computer-aided discovery of new FGFR-1 inhibitors followed by in vitro validation. 2016 , 8, 1841-1869		14
202	Development of predictive QSAR models for toxicity of ionic liquids and their true external and experimental validation tests. 2016 , 5, 1388-1399		24
201	D-sorbitol-induced phase control of TiO ₂ nanoparticles and its application for dye-sensitized solar cells. 2016 , 6, 20103		67
200	Steps Toward a Virtual Rat: Predictive Absorption, Distribution, Metabolism, and Toxicity Models. 2016 , 283-329		1

199	Revealing the morphological architecture of a shape memory polyurethane by simulation. 2016 , 6, 29180	15
198	Acute to chronic estimation of toxicity within the QSAAR framework. 2016 , 27, 833-850	8
197	Constructing and Validating 3D-pharmacophore Models to a Set of MMP-9 Inhibitors for Designing Novel Anti-melanoma Agents. 2016 , 35, 238-52	6
196	Phenylphthalazines as small-molecule inhibitors of urea transporter UT-B and their binding model. 2016 , 37, 973-83	9
195	Multi-level structure-based pharmacophore modelling of caspase-3-non-peptide complexes: Extracting essential pharmacophore features and its application to virtual screening. 2016 , 254, 207-20	10
194	QSAR Models Guided by Molecular Dynamics Applied to Human Glucokinase Activators. 2016 , 87, 455-66	18
193	Type (I, II) errors variable selection in quantitative structure activity relationships. 2016 , 152, 10-17	
192	Discovery of new selective cytotoxic agents against Bcl-2 expressing cancer cells using ligand-based modeling. 2016 , 250, 12-26	11
191	Molecular modeling of Plasmodium falciparum peptide deformylase and structure-based pharmacophore screening for inhibitors. 2016 , 6, 29466-29485	8
190	Computation of chromatographic lipophilicity parameter log _k 0 of ionic liquid cations from ETAP descriptors: Application in modeling of toxicity of ionic liquids to pathogenic bacteria. 2016 , 216, 754-763	14
189	Residue-based design of small molecule inhibitor for H1N1, H5N1 and H7N1 mutants. 2016 , 22, 4	
188	Exploration of interaction zones of β -tubulin colchicine binding domain of helminths and binding mechanism of anthelmintics. 2017 , 68, 78-91	8
187	In silico modelling of thiazolidine derivatives with antioxidant potency: Models quantify the degree of contribution of molecular fragments towards the free radical scavenging ability. 2017 , 1138, 17-26	4
186	Prediction of N-Methyl-D-Aspartate Receptor GluN1-Ligand Binding Affinity by a Novel SVM-Pose/SVM-Score Combinatorial Ensemble Docking Scheme. 2017 , 7, 40053	14
185	Design and combinatorial library generation of 1H 1,4 benzodiazepine 2,5 diones as photosystem-II inhibitors: A public QSAR approach. 2017 , 6, 219-231	1
184	Development of a temperature dependent 2D-QSPR model for viscosity of diverse functional ionic liquids. 2017 , 240, 454-467	12
183	Exploring the origin of phosphodiesterase inhibition via proteochemometric modeling. 2017 , 7, 28056-28068	7
182	Toll-like receptor 2 antagonists identified through virtual screening and experimental validation. 2017 , 284, 2264-2283	8

181	QSAR model for prediction of the therapeutic potency of N-benzylpiperidine derivatives as AChE inhibitors. 2017 , 28, 471-489	10
180	Unsupervised pharmacophore modeling combined with QSAR analyses revealed novel low micromolar SIRT2 inhibitors. 2017 , 30, e2623	4
179	In silico prediction of the mutagenicity of nitroaromatic compounds using a novel two-QSAR approach. 2017 , 40, 102-114	13
178	Molecular dynamics-assisted pharmacophore modeling of caspase-3-isatin sulfonamide complex: Recognizing essential intermolecular contacts and features of sulfonamide inhibitor class for caspase-3 binding. 2017 , 71, 117-128	9
177	Ecotoxicological modelling of cosmetics for aquatic organisms: A QSTR approach. 2017 , 28, 567-594	28
176	QSAR modeling and in silico design of small-molecule inhibitors targeting the interaction between E3 ligase VHL and HIF-1 β . 2017 , 21, 719-739	1
175	SCRAMBLE'N'GAMBLE: a tool for fast and facile generation of random data for statistical evaluation of QSAR models. 2017 , 71, 2217-2232	13
174	Proteochemometric Modeling of the Interaction Space of Carbonic Anhydrase and its Inhibitors: An Assessment of Structure-based and Sequence-based Descriptors. 2017 , 36, 1600102	10
173	The QSPR models to predict the solubility of CO ₂ in ionic liquids based on least-squares support vector machines and genetic algorithm-multi linear regression. 2017 , 225, 521-530	25
172	Architectural evolution of phase domains in shape memory polyurethanes by dissipative particle dynamics simulations. 2017 , 8, 260-271	22
171	Discovery of potent NEK2 inhibitors as potential anticancer agents using structure-based exploration of NEK2 pharmacophoric space coupled with QSAR analyses. 2017 , 21, 187-200	6
170	QSAR and docking studies of coumarin derivatives as potent HIV-1 integrase inhibitors. 2017 , 10, S1081-S1094	14
169	Multilayered Variable Selection in QSPR. 2017 , 2, 106-124	9
168	Toxicity of Selected Imidazolium-based Ionic Liquids on <i>Caenorhabditis elegans</i> : a Quantitative Structure-Activity Relationship Study. 2017 , 30, 423-428	11
167	Theoretical study on the reactions of a series of polybromobenzenes with OH radicals: mechanism, kinetics, and QSAR. 2018 , 96, 436-446	
166	Chemometric modeling of odor threshold property of diverse aroma components of wine.. 2018 , 8, 4750-4760	8
165	PLS regression-based chemometric modeling of odorant properties of diverse chemical constituents of black tea and coffee.. 2018 , 8, 2293-2304	11
164	Ligand-based computer aided drug design reveals new tropomyosin receptor kinase a (TrkA) inhibitors. 2018 , 80, 327-352	8

163	Proteochemometric modeling of the origin of thymidylate synthase inhibition. 2018 , 91, 1007-1016	7
162	Optimization of the anticonvulsant activity of 2-acetamido-N-benzyl-2-(5-methylfuran-2-yl) acetamide using QSAR modeling and molecular docking techniques. 2018 , 7, 430-440	10
161	Identification of novel hits as highly prospective dual agonists for mu and kappa opioid receptors: an integrated in silico approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2018 , 36, 279-301	3.6 5
160	Multi-objective Optimization of Benzamide Derivatives as Rho Kinase Inhibitors. 2018 , 37, 1700080	4
159	Experimental and QSAR study on the surface activities of alkyl imidazoline surfactants. 2018 , 1156, 164-171	8
158	Strategies of Virtual Screening in Medicinal Chemistry. 2018 , 3, 134-160	5
157	Theoretical modeling and molecular docking simulation for investigating and evaluating some active compounds as potent anti-tubercular agents against MTB CYP121 receptor. 2018 , 4, 284-295	11
156	CoDe-DTI: Collaborative Deep Learning-based Drug-Target Interaction Prediction. 2018 ,	4
155	Computational studies on aminoacetamide derivatives with anticonvulsant activities. 2018 , 7, 709-718	4
154	QSPR modelling for prediction of glass transition temperature of diverse polymers. 2018 , 29, 935-956	10
153	QSAR and Classification Study on Prediction of Acute Oral Toxicity of -Nitroso Compounds. 2018 , 19,	25
152	Straightforward Design for Phenoxy-Imine Catalytic Activity in Ethylene Polymerization: Theoretical Prediction. 2018 , 8, 422	5
151	Chemometric modeling of aquatic toxicity of contaminants of emerging concern (CECs) in <i>Dugesia japonica</i> and its interspecies correlation with daphnia and fish: QSTR and QSTTR approaches. 2018 , 166, 92-101	31
150	Binding Kinetics Survey of the Drugged Kinome. 2018 , 140, 15774-15782	35
149	Theoretical Prediction of the Complex P-Glycoprotein Substrate Efflux Based on the Novel Hierarchical Support Vector Regression Scheme. 2018 , 23,	12
148	Drug Discovery: An In Silico Approach. 2018 , 307-328	1
147	Prediction of viscosity index and pour point in ester lubricants using quantitative structure-property relationship (QSPR). 2018 , 183, 59-78	11
146	Current approaches for choosing feature selection and learning algorithms in quantitative structure-activity relationships (QSAR). 2018 , 13, 1075-1089	44

145	Development of models to predict fish early-life stage toxicity from acute <i>Daphnia magna</i> toxicity. 2018 , 29, 725-742	5
144	Chemometrics in forensic science. 2018 , 105, 191-201	93
143	QSAR: What Else?. 2018 , 1800, 79-105	10
142	Toxicity of polyhalogenated dibenzo-p-furans in the light of nucleic acid bases interaction. 2018 , 76, 225-231	2
141	Multi-Pharmacophore Modeling of Caspase-3 Inhibitors using Crystal, Dock and Flexible Conformation Schemes. 2018 , 21, 26-40	3
140	The Design, Synthesis, and Characterizations of Spore Germination Inhibitors Effective against an Epidemic Strain of <i>Clostridium difficile</i> . 2018 , 61, 6759-6778	10
139	Machine learning and molecular design of self-assembling -conjugated oligopeptides. 2018 , 44, 930-945	18
138	Identification of PfENR inhibitors: A hybrid structure-based approach in conjunction with molecular dynamics simulations. 2018 , 119, 8490-8500	8
137	New insights into the selective inhibition of the β -carbonic anhydrases of pathogenic bacteria <i>Burkholderia pseudomallei</i> and <i>Francisella tularensis</i> : a proteochemometrics study. 2019 , 23, 263-273	4
136	QSPR modeling of azeotropic temperatures and compositions for binary azeotropes containing lower alcohols using a genetic function approximation. 2019 , 27, 835-844	1
135	Hit identification of SMYD3 enzyme inhibitors using structure-based pharmacophore modeling. 2019 , 11, 1107-1117	4
134	Investigation of Geometric Landscape and Structure-Property Relations for Colloidal Superstructures Using Genetic Algorithm. 2019 , 123, 7445-7454	1
133	Synthesis, anti-HIV activity, molecular modeling study and QSAR of new designed 2-(2-arylidenehydrazinyl)-4-arylthiazoles. 2019 , 1198, 126866	8
132	Quantitative Relationship between CO ₂ Absorption Capacity and Amine Water System: DFT, Statistical, and Experimental Study. 2019 , 58, 13848-13857	4
131	In Silico Prediction of PAMPA Effective Permeability Using a Two-QSAR Approach. 2019 , 20,	16
130	Development of QSAAR and QAAR models for predicting fish early-life stage toxicity with a focus on industrial chemicals. 2019 , 30, 825-846	4
129	Four Methods to Estimate Minimum Miscibility Pressure of CO ₂ -Oil Based on Machine Learning. 2019 , 37, 1271-1278	8
128	Multi-Target Chemometric Modelling, Fragment Analysis and Virtual Screening with ERK Inhibitors as Potential Anticancer Agents. 2019 , 24,	11

127	Development of Multi-Target Chemometric Models for the Inhibition of Class I PI3K Enzyme Isoforms: A Case Study Using QSAR-Co Tool. 2019 , 20,	12
126	Making use of available and emerging data to predict the hazards of engineered nanomaterials by means of in silico tools: A critical review. 2019 , 13, 76-99	33
125	Discovery of novel Flt3 inhibitory chemotypes through extensive ligand-based and new structure-based pharmacophore modelling methods. 2019 , 88, 128-151	9
124	Predictive quantitative structure-property relationship (QSPR) modeling for adsorption of organic pollutants by carbon nanotubes (CNTs). 2019 , 6, 224-247	17
123	Discovery of new JNK3 inhibitory chemotypes via QSAR-Guided selection of docking-based pharmacophores and comparison with other structure-based pharmacophore modeling methods. 2019 , 91, 30-51	10
122	Molecular Modelling of Potential Candidates for the Treatment of Depression. 2019 , 38, e1900024	1
121	Aqueous extract from bark protects cells from oxidative stress caused by electron beam radiation: approach. 2019 , 5, e01749	2
120	QSAR-Co: An Open Source Software for Developing Robust Multitasking or Multitarget Classification-Based QSAR Models. 2019 , 59, 2538-2544	40
119	A novel mechanism of irinotecan targeting MDM2 and Bcl-xL. 2019 , 514, 518-523	9
118	Computational Simulations Identified Two Candidate Inhibitors of Cdk5/p25 to Abrogate Tau-associated Neurological Disorders. 2019 , 17, 579-590	18
117	Identification of antiproliferative emodin analogues as inhibitors of epidermal growth factor receptor in cancer. 2019 , 43, 1281-1288	4
116	Natural barrigenol-like triterpenoids: A comprehensive review of their contributions to medicinal chemistry. 2019 , 161, 41-74	26
115	Construction of a Quantitative Structure Activity Relationship (QSAR) Model to Predict the Absorption of Cephalosporins in Zebrafish for Toxicity Study. 2019 , 10, 31	9
114	Theoretical QSAR modelling and molecular docking studies of some 4-hydroxyphenylpyruvate dioxygenase (HPPD) enzyme inhibitors potentially used as herbicides. 2019 , 5, e02859	3
113	Predictive models for designing potent tyrosine kinase inhibitors in chronic myeloid leukemia for understanding its molecular mechanism of resistance by molecular docking and dynamics simulations. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019 , 37, 4747-4766	3.6 6
112	Ciprofloxacin and Clinafloxacin Antibodies for an Immunoassay of Quinolones: Quantitative Structure-Activity Analysis of Cross-Reactivities. 2019 , 20,	4
111	Molecular modelling and design of lubricant additives and their molecular dynamic simulations studies of Diamond-Like-Carbon (DLC) and steel surface coating. 2019 , 28, 111-115	8
110	In silico study on anticonvulsant activity of isoxazole and thiazole derivatives active in subcutaneous pentylenetetrazole animal model. 2020 , 32, 116-124	3

109	Prediction of the auto-ignition temperature of binary liquid mixtures based on the quantitative structure-property relationship approach. 2020 , 140, 397-409		5
108	Quantitative structure property relationship for relative volatility of isopropanol and water mixture. 2020 , 55, 3252-3259		2
107	Application of Authentication Evaluation Techniques of Ethnobotanical Medicinal Plant Genus : A Review. 2020 , 50, 405-423		11
106	In-silico molecular design and dynamic binding energy assessments of some multifunctional lubricating oil additives. 2020 , 32, 78-84		1
105	Ecotoxicological assessment of pharmaceuticals and personal care products using predictive toxicology approaches. 2020 , 22, 1458-1516		36
104	Quantitative structure-activity relationship between the toxicity of amine surfactant and its molecular structure. 2020 , 702, 134593		13
103	A robust model for estimating thermal conductivity of liquid alkyl halides. 2020 , 31, 73-85		6
102	Integrating Machine Learning-Based Virtual Screening With Multiple Protein Structures and Bio-Assay Evaluation for Discovery of Novel GSK3 β Inhibitors. 2020 , 11, 566058		4
101	In Silico Modeling, Prediction, and Designing of Some Anti-wear Lubricant Additives. 2020 , 6, 1		0
100	Evolutionary chemical binding similarity approach integrated with 3D-QSAR method for effective virtual screening. 2020 , 21, 309		5
99	Synthesis, In Vitro Anti-HIV Activity, Cytotoxicity, and Computational Studies of Some New Steroids and Their Pyrazoline and Oxime Analogues. <i>Russian Journal of Bioorganic Chemistry</i> , 2020 , 46, 822-836	1	1
98	Mechanism discovery and model identification using genetic feature extraction and statistical testing. 2020 , 140, 106900		5
97	Insight into potent leads for alzheimer's disease by using several artificial intelligence algorithms. 2020 , 129, 110360		2
96	Prediction of Standard Enthalpies of Formation Based on Hydrocarbon Molecular Descriptors and Active Subspace Methodology. 2020 , 59, 4785-4791		7
95	Structural insights into the origin of phosphoinositide 3-kinase inhibition. <i>Structural Chemistry</i> , 2020 , 31, 1505-1522	1.8	3
94	Identification of Human Leukotriene A4 Hydrolase Inhibitors Using Structure-Based Pharmacophore Modeling and Molecular Docking. 2020 , 25,		2
93	Pharmacophore modeling of JAK1: A target infested with activity-cliffs. 2020 , 99, 107615		5
92	Fullerene Derivatives as Lung Cancer Cell Inhibitors: Investigation of Potential Descriptors Using QSAR Approaches. 2020 , 15, 2485-2499		7

91	Minimum Ignition Energy (MIE) prediction models for ignition sensitive fuels using machine learning methods. 2021 , 69, 104343		2
90	Quantitative structure-property relationship for melting and freezing points of deep eutectic solvents. 2021 , 321, 114744		7
89	Towards a universal digital chemical space for pure component properties prediction. 2021 , 527, 112829		1
88	QSPR models for water solubility of ammonium hexafluorosilicates: analysis of the effects of hydrogen bonds. <i>Structural Chemistry</i> , 2021 , 32, 309-319	1.8	3
87	A combined structure-based pharmacophore modeling and 3D-QSAR study on a series of N-heterocyclic scaffolds to screen novel antagonists as human DHFR inhibitors. <i>Structural Chemistry</i> , 2021 , 32, 1571-1588	1.8	
86	Development of a Hierarchical Support Vector Regression-Based In Silico Model for Caco-2 Permeability. 2021 , 13,		1
85	Virtual screening of epalrestat mimicking selective ALR2 inhibitors from natural product database: auto pharmacophore, ADMET prediction and molecular dynamics approach. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 1-19	3.6	0
84	Statistical methods and parameters: Tools to generate and evaluate theoretical in silico models. 2021 , 333-350		
83	QSAR-Co-X: an open source toolkit for multitarget QSAR modelling. 2021 , 13, 29		6
82	QSPR modelling for intrinsic viscosity in polymer-solvent combinations based on density functional theory. 2021 , 32, 379-393		2
81	Stand-Alone Function Approximation Using Fractional Order Techniques. 2021 ,		0
80	DFT based Computational Methodology of IC Prediction. 2021 , 17, 244-253		0
79	Development of QSAR models for prediction of fish bioconcentration factors using physicochemical properties and molecular descriptors with machine learning algorithms. 2021 , 63, 101285		2
78	Study on quantitative structure-biodegradability relationships of amine collectors by GFA-ANN method. 2021 , 415, 125628		0
77	QSAR-guided pharmacophoric modeling reveals important structural requirements for Polo kinase 1 (Plk1) inhibitors. 2021 , 109, 108022		2
76	Identification of potential descriptors of water-soluble fullerene derivatives responsible for antitumor effects on lung cancer cells via QSAR analysis. 2021 , 19, 812-825		5
75	Recent advances in quantitative structure-activity relationship models of antimalarial drugs. 2021 , 16, 659-695		7
74	Genetic Algorithms: Introduction and Applications.		6

73	Genetic and Evolutionary Algorithms.	14
72	Recent Trends in Quantitative Structure-Activity Relationships. 2003 , 49-76	22
71	Chemical Sensor Array Response Modeling Using Quantitative Structure-Activity Relationships Technique. 2009 , 167-192	3
70	Virtual Screening and Molecular Design Based on Hierarchical Qsar Technology. 2010 , 127-176	17
69	Genetic Function Approximation: Evolutionary Construction of Novel, Interpretable, Nonlinear Models of Experimental Data. 1999 , 163-189	1
68	Application of GFA-MLR and G/PLS Techniques in QSAR/QSPR Studies with Application in Medicinal Chemistry and Predictive Toxicology. 2015 , 501-529	1
67	Therapeutic Potential of N-Type Voltage-Gated Ca ²⁺ Channel. 2011 , 289-308	1
66	QUANTITATIVE APPROACHES TO STRUCTURE-ACTIVITY RELATIONSHIPS. 2003 , 351-369	3
65	The Integrated Use of Alternative Approaches for Predicting Toxic Hazard: The Report and Recommendations of ECVAM Workshop 81,2. 1995 , 23, 410-429	42
64	General Introduction to QSAR. 2003 ,	6
63	Overview and Recent Advances in QSAR Studies. 2016 , 1-32	0
62	Cyclotide structure-activity relationships: qualitative and quantitative approaches linking cytotoxic and anthelmintic activity to the clustering of physicochemical forces. 2014 , 9, e91430	15
61	Quantitative structure-property relationship (QSPR) modeling of drug-loaded polymeric micelles via genetic function approximation. 2015 , 10, e0119575	24
60	Ensemble learning method for the prediction of new bioactive molecules. 2018 , 13, e0189538	16
59	Quantitative structure-retention relationship (QSRR) models for predicting the GC retention times of essential oil components. 2010 , 22, 357-373	1
58	A novel QSAR model for designing, evaluating, and predicting the anti-MES activity of new 1H-pyrazole-5-carboxylic acid derivatives. 739-774	4
57	Sugars and Sweeteners: Structure, Properties and In Silico Modeling. 2020 , 27, 5-22	1
56	PTML Multi-Label Algorithms: Models, Software, and Applications. 2020 , 20, 2326-2337	3

55	Molecular Docking and QSAR Studies of Coumarin Derivatives as NMT Inhibitors: Simple Structural Features as Potential Modulators of Antifungal Activity. 2020 , 17, 1293-1308	1
54	Identification of Hydroxamic Acid Based Selective HDAC1 Inhibitors: Computer Aided Drug Design Studies. 2019 , 15, 145-166	5
53	Prediction of anti-cancer activity of 1,8-naphthyridin derivatives by using of genetic algorithm-stepwise multiple linear regression. 2018 , 28, 181-194	1
52	In Silico Prediction of Intestinal Permeability by Hierarchical Support Vector Regression. 2020 , 21,	5
51	Quantitative Structure Activity Relationship Analysis of N-(mercaptoalkanoyl)- and [(acylthio)alkanoyl] Glycine Derivatives as ACE Inhibitors. 2011 , 1, 85-104	5
50	An Intelligent Approach for Virtual Chemistry Laboratory. 2019 , 454-488	1
49	On Extended Topochemical Atom (ETA) Indices for QSPR Studies. 380-411	5
48	Molecular Modeling of Small Molecules as BVDV RNA-Dependent RNA Polymerase Allosteric Inhibitors. 2013 , 34, 837-850	6
47	Pharmacophore Based Design Of Probable Fgfr-1 Inhibitors From The 3d Crystal Structure Of Infigratinib - A Drug Used In The Treatment Of Cholangiocarcinomas. 2021 , 18,	
46	Multivariate Regression Excels Neural Networks, Genetic Algorithm and Partial Least-Squares in Qsar Modeling. 2000 , 288-289	
45	Computer Aided Drug Design. 2001 ,	1
44	Quantitative StructureProperty Relationships (QSPR).	
43	Quantitative StructureActivity Relationships in Drug Design.	
42	Three-dimensional Structure Searching.	
41	2D QSAR Models. 2003 ,	4
40	In Silico Prediction Models for Blood-Brain Barrier Permeation. 403-428	
39	3D- and nD-QSAR Methods. 1576-1603	
38	Advances in StructureActivity Relationship Studies on Potassium Channel Modulators. 2011 , 241-264	

- 37 2D-QSAR Study of a Series of Pyrazoline-Based Anti-Tubercular Agents Using Genetic Function Approximation. **2015**, 03, 45-53 1
- 36 QSAR Models towards Cholinesterase Inhibitors for the Treatment of Alzheimer's Disease. **2015**, 354-399
- 35 An Intelligent Approach for Virtual Chemistry Laboratory. **2016**, 483-517
- 34 QSAR Models towards Cholinesterase Inhibitors for the Treatment of Alzheimer's Disease. **2017**, 591-636
- 33 Denetimli İntan ve Gİa Analizlerinde Uygulamalar 429-438
- 32 New Antagonists of the Membrane Androgen Receptor OXER1 from the ZINC Natural Product Database. **2021**, 6, 29664-29674 2
- 31 Predictive Quantitative Structure-Activity Relationship Modeling of the Antifungal and Antibiotic Properties of Triazolothiadiazine Compounds. **2020**, 4,
- 30 Strategies of Virtual Screening in Medicinal Chemistry. **2020**, 194-225 0
- 29 On Extended Topochemical Atom (ETA) Indices for QSPR Studies. 841-873
- 28 Computational approaches for modeling human intestinal absorption and permeability. 577-589 0
- 27 INSIGHT INTO THE STRUCTURAL REQUIREMENTS OF SULFONYL DERIVATIVES BASED ON TWO AND THREE-DIMENSIONAL DESCRIPTORS: QSAR STUDIES. **2019**, 56, 81-86
- 26 Exploiting activity cliffs for building pharmacophore models and comparison with other pharmacophore generation methods: sphingosine kinase 1 as case study.. **2022**, 36, 39 1
- 25 The design of TOPK inhibitors using structure-based pharmacophore modeling and molecular docking based on an MD-refined homology model.. **2022**, 1
- 24 Computer Aided Drug Design. 563-572
- 23 DataSheet_1.docx. **2020**,
- 22 In Silico Prediction of Skin Permeability Using a Two-QSAR Approach. **2022**, 14, 961
- 21 Discovery of new PKN2 inhibitory chemotypes via QSAR-guided selection of docking-based pharmacophores.. **2022**, 1 4
- 20 Computer Aided Drug Design. **2022**, 505-541 0

19	Friction sensitivity of nitramine energetic materials: a prediction based on genetic function approximation. <i>FirePhysChem</i> , 2022 ,		
18	Structure-guided pharmacophore based virtual screening, docking, and molecular dynamics to discover repurposed drugs as novel inhibitors against endoribonuclease Nsp15 of SARS-CoV-2. <i>Journal of Biomolecular Structure and Dynamics</i> , 1-11	3.6	1
17	Quantitative structure-activity relationship modeling of hydroxylated polychlorinated biphenyls as constitutive androstane receptor agonists. <i>Structural Chemistry</i> ,	1.8	0
16	Quantitative Characterization of the Chemical Space Governed by Human Carbonic Anhydrases and selenium-containing derivatives of sulfonamides. <i>Brazilian Journal of Pharmaceutical Sciences</i> , 58,	1.8	
15	Pharmacophore mapping and modeling approaches for drug development. 2022 , 171-189		
14	Quantitative Structure-Activity Relationship, Structure-Based Design, And ADMET Studies of Pyrimethamine and Cycloquanil Analogues Inhibitors of Plasmodium Falciparum Dihydrofolate Reductase-Thymidylate Synthase (Pf-DHFR-TS). <i>SSRN Electronic Journal</i> ,	1	
13	Synthesis and QSAR of Novel Ketoprofen-Chalcone-Amide Hybrides as Acetylcholinesterase (AChE) Inhibitors for Possible Treatment of Alzheimer Disease. <i>Russian Journal of Bioorganic Chemistry</i> ,	1	
12	Prediction of Aquatic Toxicity of Energetic Materials using Genetic Function Approximation. <i>FirePhysChem</i> , 2022 ,		1
11	A REVIEW OF GROUP CONTRIBUTION MODELS TO CALCULATE THERMODYNAMIC PROPERTIES OF IONIC LIQUIDS FOR PROCESS SYSTEMS ENGINEERING. <i>Chemical Engineering Research and Design</i> , 2022 ,	5.5	
10	Pharmacophore Modeling of Targets Infested with Activity Cliffs via Molecular Dynamics Simulation Coupled with QSAR and Comparison with other Pharmacophore Generation Methods: KDR as Case Study.		0
9	Virtual Screening in the Identification of Sirtuins Activity Modulators. 2022 , 27, 5641		0
8	Chemical similarity and machine learning-based approaches for the prediction of aquatic toxicity of binary and multicomponent pharmaceutical and pesticide mixtures against <i>Aliivibrio fischeri</i> . 2022 , 308, 136463		0
7	Chemical Similarity and Machine Learning-Based Approaches for the Prediction of Aquatic Toxicity of Binary and Multicomponent Pharmaceutical Mixtures Against <i>Aliivibrio Fischeri</i> .		0
6	Regression analysis for predicting the elasticity of liquid crystal elastomers. 2022 , 12,		0
5	Discovery of new potent lysine specific histone demethylase-1 inhibitors (LSD-1) using structure based and ligand based molecular modelling and machine learning. 2022 , 12, 35873-35895		1
4	Identification of Novel 5-Lipoxygenase-Activating Protein (FLAP) Inhibitors by an Integrated Method of Pharmacophore Virtual Screening, Docking, QSAR and ADMET Analyses. 1-21		0
3	Development and Validation of Predictive QSAR Models for Estrogenic Activities of Hydroxylated Polychlorinated Biphenyls.		0
2	2D QSAR ANALYSIS OF CARBONITRILE BASED INHIBITORS OF CATHEPSIN S AS POTENTIAL ANTIRHEUMATIC AGENTS. 2023 , 60, 15-35		0

- 1 Highly selective butyrylcholinesterase inhibitors related to Amaryllidaceae alkaloids - Design, synthesis, and biological evaluation. **2023**, 252, 115301

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