

# Mati Karelson

## List of Publications by Year in descending order

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145  
papers

8,980  
citations

50276

46  
h-index

42399

92  
g-index

156  
all docs

156  
docs citations

156  
times ranked

6943  
citing authors

#	ARTICLE	IF	CITATIONS
1	Quantum-Chemical Descriptors in QSAR/QSPR Studies. <i>Chemical Reviews</i> , 1996, 96, 1027-1044.	47.7	1,375
2	QSPR: the correlation and quantitative prediction of chemical and physical properties from structure. <i>Chemical Society Reviews</i> , 1995, 24, 279.	38.1	474
3	Quantitative Correlation of Physical and Chemical Properties with Chemical Structure: Utility for Prediction. <i>Chemical Reviews</i> , 2010, 110, 5714-5789.	47.7	460
4	Quantitative Measures of Solvent Polarity. <i>Chemical Reviews</i> , 2004, 104, 175-198.	47.7	385
5	Aromaticity as a Quantitative Concept. 7. Aromaticity Reaffirmed as a Multidimensional Characteristic. <i>Journal of Organic Chemistry</i> , 1998, 63, 5228-5231.	3.2	289
6	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.	2.8	238
7	Correlation of Boiling Points with Molecular Structure. 1. A Training Set of 298 Diverse Organics and a Test Set of 9 Simple Inorganics. <i>The Journal of Physical Chemistry</i> , 1996, 100, 10400-10407.	2.9	227
8	Correlation of the Melting Points of Potential Ionic Liquids (Imidazolium Bromides and) <i>Journal of Chemical Information and Computer Sciences</i> , 2002, 42, 225-231.	2.8	196
9	Prediction of Gas Chromatographic Retention Times and Response Factors Using a General Qualitative Structure-Property Relationships Treatment. <i>Analytical Chemistry</i> , 1994, 66, 1799-1807.	6.5	187
10	Prediction of Critical Micelle Concentration Using a Quantitative Structure-Property Relationship Approach. 1. Nonionic Surfactants. <i>Langmuir</i> , 1996, 12, 1462-1470.	3.5	174
11	QSPR Correlation of the Melting Point for Pyridinium Bromides, Potential Ionic Liquids. <i>Journal of Chemical Information and Computer Sciences</i> , 2002, 42, 71-74.	2.8	170
12	Perspective on the Relationship between Melting Points and Chemical Structure. <i>Crystal Growth and Design</i> , 2001, 1, 261-265.	3.0	167
13	QSPR Studies on Vapor Pressure, Aqueous Solubility, and the Prediction of Water-Air Partition Coefficients. <i>Journal of Chemical Information and Computer Sciences</i> , 1998, 38, 720-725.	2.8	152
14	AM1 calculations of reaction field effects on the tautomeric equilibria of nucleic acid pyrimidine and purine bases and their 1-methyl analogs. <i>Journal of the American Chemical Society</i> , 1991, 113, 1561-1566.	13.7	148
15	QSPR Analysis of Flash Points. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 1521-1530.	2.8	144
16	Quantitative Structure-Property Relationship (QSPR) Correlation of Glass Transition Temperatures of High Molecular Weight Polymers. <i>Journal of Chemical Information and Computer Sciences</i> , 1998, 38, 300-304.	2.8	124
17	Discovery of Small Molecules that Activate RNA Methylation through Cooperative Binding to the METTL3-14-WTAP Complex Active Site. <i>Cell Reports</i> , 2019, 26, 3762-3771.e5.	6.4	121
18	Correlation and Prediction of the Refractive Indices of Polymers by QSPR. <i>Journal of Chemical Information and Computer Sciences</i> , 1998, 38, 1171-1176.	2.8	118

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19	QSPR as a means of predicting and understanding chemical and physical properties in terms of structure. <i>Pure and Applied Chemistry</i> , 1997, 69, 245-248.	1.9	114
20	Heterocyclic Aromaticity. <i>Heterocycles</i> , 1991, 32, 127.	0.7	114
21	Interpretation of Quantitative Structure~Property and ~Activity Relationships. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 679-685.	2.8	110
22	A New Efficient Approach for Variable Selection Based on Multiregression:~ Prediction of Gas Chromatographic Retention Times and Response Factors. <i>Journal of Chemical Information and Computer Sciences</i> , 1999, 39, 610-621.	2.8	104
23	On the n-pi.* blue shift accompanying solvation. <i>Journal of the American Chemical Society</i> , 1990, 112, 9405-9406.	13.7	101
24	QSPR modeling of flash points: An update. <i>Journal of Molecular Graphics and Modelling</i> , 2007, 26, 529-536.	2.4	97
25	Prediction of Polymer Glass Transition Temperatures Using a General Quantitative Structure~Property Relationship Treatment. <i>Journal of Chemical Information and Computer Sciences</i> , 1996, 36, 879-884.	2.8	88
26	The Classification of Solvents by Combining Classical QSPR Methodology with Principal Component Analysis. <i>Journal of Physical Chemistry A</i> , 2005, 109, 10323-10341.	2.5	81
27	Normal Boiling Points for Organic Compounds:~ Correlation and Prediction by a Quantitative Structure~Property Relationship. <i>Journal of Chemical Information and Computer Sciences</i> , 1998, 38, 28-41.	2.8	80
28	Correlation of blood~brain penetration using structural descriptors. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 4888-4917.	3.0	80
29	Prediction of Melting Points for the Substituted Benzenes:~ A QSPR Approach. <i>Journal of Chemical Information and Computer Sciences</i> , 1997, 37, 913-919.	2.8	70
30	QSPR and QSAR Models Derived Using Large Molecular Descriptor Spaces. A Review of CODESSA Applications. <i>Collection of Czechoslovak Chemical Communications</i> , 1999, 64, 1551-1571.	1.0	70
31	The Present Utility and Future Potential for Medicinal Chemistry of QSAR / QSPR with Whole Molecule Descriptors. <i>Current Topics in Medicinal Chemistry</i> , 2002, 2, 1333-1356.	2.1	70
32	Molecular Dynamics Simulations of the Interactions between Glial Cell Line-Derived Neurotrophic Factor Family Receptor GFR~1 and Small-Molecule Ligands. <i>ACS Omega</i> , 2018, 3, 11407-11414.	3.5	69
33	Multicavity reaction field method for the solvent effect description in flexible molecular systems. <i>The Journal of Physical Chemistry</i> , 1993, 97, 11901-11907.	2.9	67
34	A QSPR Study of the Solubility of Gases and Vapors in Water. <i>Journal of Chemical Information and Computer Sciences</i> , 1996, 36, 1162-1168.	2.8	66
35	Quantitative Structure~Property Relationship Modeling of~2-Cyclodextrin Complexation Free Energies. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 529-541.	2.8	66
36	A Comprehensive QSAR Treatment of the Genotoxicity of Heteroaromatic and Aromatic Amines. <i>QSAR and Combinatorial Science</i> , 1999, 18, 03-10.	1.2	65

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37	Aromaticity as a Quantitative Concept. 6. Aromaticity Variation with Molecular Environment. Journal of Organic Chemistry, 1996, 61, 1619-1623.	3.2	60
38	Rational Design of Novel Anticancer Small-Molecule RNA m6A Demethylase ALKBH5 Inhibitors. ACS Omega, 2021, 6, 13310-13320.	3.5	57
39	Reaction field effects on the electronic structure of carbon radical and ionic centers. International Journal of Quantum Chemistry, 1990, 37, 1-13.	2.0	53
40	Six-membered cyclic ureas as HIV-1 protease inhibitors: A QSAR study based on CODESSA PRO approach. Bioorganic and Medicinal Chemistry Letters, 2002, 12, 3453-3457.	2.2	53
41	Prediction of liquid viscosity for organic compounds by a quantitative structure-property relationship. Journal of Physical Organic Chemistry, 2000, 13, 80-86.	1.9	51
42	Skin Permeation Rate as a Function of Chemical Structure. Journal of Medicinal Chemistry, 2006, 49, 3305-3314.	6.4	49
43	QSAR study of mosquito repellents using Codessa Pro. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 2306-2311.	2.2	49
44	Prediction of Cell-Penetrating Peptides Using Artificial Neural Networks. Current Computer-Aided Drug Design, 2010, 6, 79-89.	1.2	49
45	Nitrobenzene toxicity: QSAR correlations and mechanistic interpretations. Journal of Physical Organic Chemistry, 2003, 16, 811-817.	1.9	48
46	Rapid QSPR model development technique for prediction of vapor pressure of organic compounds. Computers and Chemical Engineering, 2007, 31, 1123-1130.	3.8	48
47	Antimalarial activity: A QSAR modeling using CODESSA PRO software. Bioorganic and Medicinal Chemistry, 2006, 14, 2333-2357.	3.0	47
48	General Quantitative Structure-Property Relationship Treatment of the Refractive Index of Organic Compounds. Journal of Chemical Information and Computer Sciences, 1998, 38, 840-844.	2.8	46
49	QSPR Study of Critical Micelle Concentrations of Nonionic Surfactants. Industrial & Engineering Chemistry Research, 2008, 47, 9687-9695.	3.7	45
50	A Novel Small Molecule GDNF Receptor RET Agonist, BT13, Promotes Neurite Growth from Sensory Neurons in Vitro and Attenuates Experimental Neuropathy in the Rat. Frontiers in Pharmacology, 2017, 8, 365.	3.5	45
51	QSPR Treatment of Solvent Scales. Journal of Chemical Information and Computer Sciences, 1999, 39, 684-691.	2.8	43
52	A General QSPR Treatment for Dielectric Constants of Organic Compounds. Journal of Chemical Information and Computer Sciences, 2002, 42, 360-367.	2.8	42
53	A Unified Treatment of Solvent Properties. Journal of Chemical Information and Computer Sciences, 1999, 39, 692-698.	2.8	41
54	QSAR treatment of drugs transfer into human breast milk. Bioorganic and Medicinal Chemistry, 2005, 13, 1623-1632.	3.0	41

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55	QSPR Treatment of the Soil Sorption Coefficients of Organic Pollutants. <i>Journal of Chemical Information and Modeling</i> , 2005, 45, 94-105.	5.4	41
56	QSAR modeling of blood:air and tissue:air partition coefficients using theoretical descriptors. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 6450-6463.	3.0	40
57	Quantitative Structure-Activity Relationship (QSAR) Modeling of EC <sub>50</sub> of Aquatic Toxicities for <i>Daphnia magna</i> . <i>Journal of Toxicology and Environmental Health - Part A: Current Issues</i> , 2009, 72, 1181-1190.	2.3	40
58	Design and Validation of Novel Chikungunya Virus Protease Inhibitors. <i>Antimicrobial Agents and Chemotherapy</i> , 2016, 60, 7382-7395.	3.2	40
59	In Silico Machine Learning Methods in Drug Development. <i>Current Topics in Medicinal Chemistry</i> , 2014, 14, 1913-1922.	2.1	40
60	QSPR Modeling of Solubility of Polyaromatic Hydrocarbons and Fullerene in 1-Octanol and <i>n</i> -Heptane. <i>Journal of Physical Chemistry B</i> , 2007, 111, 9853-9857.	2.6	33
61	Open Computing Grid for Molecular Science and Engineering. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 953-959.	5.4	32
62	A Quantitative Structure-Property Relationship Study of Lithium Cation Basicities. <i>Journal of Physical Chemistry A</i> , 2004, 108, 4812-4818.	2.5	31
63	Combination of a Modified Scoring Function with Two-Dimensional Descriptors for Calculation of Binding Affinities of Bulky, Flexible Ligands to Proteins. <i>Journal of the American Chemical Society</i> , 2006, 128, 1233-1239.	13.7	31
64	Prediction of Ultraviolet Spectral Absorbance Using Quantitative Structure-Property Relationships. <i>Journal of Chemical Information and Computer Sciences</i> , 2002, 42, 830-840.	2.8	30
65	QSAR modeling of the inhibition of Glycogen Synthase Kinase-3. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 4987-5002.	3.0	30
66	Rational design of a series of novel amphipathic cell-penetrating peptides. <i>International Journal of Pharmaceutics</i> , 2014, 464, 111-116.	5.2	30
67	Have artificial neural networks met expectations in drug discovery as implemented in QSAR framework?. <i>Expert Opinion on Drug Discovery</i> , 2016, 11, 627-639.	5.0	30
68	QSPR Study of Critical Micelle Concentration of Anionic Surfactants Using Computational Molecular Descriptors. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 782-793.	5.4	29
69	QSPR treatment of rat blood:air, saline:air and olive oil:air partition coefficients using theoretical molecular descriptors. <i>Bioorganic and Medicinal Chemistry</i> , 2004, 12, 4735-4748.	3.0	27
70	QSPR study of the first and second critical micelle concentrations of cationic surfactants. <i>Computers and Chemical Engineering</i> , 2009, 33, 321-332.	3.8	27
71	Structure-based calculation of drug efficiency indices. <i>Bioinformatics</i> , 2007, 23, 2678-2685.	4.1	26
72	Application of the QSPR Approach to the Boiling Points of Azeotropes. <i>Journal of Physical Chemistry A</i> , 2011, 115, 3475-3479.	2.5	26

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73	Relationships of Critical Temperatures to Calculated Molecular Properties. <i>Journal of Chemical Information and Computer Sciences</i> , 1998, 38, 293-299.	2.8	25
74	QSPR of 3-aryloxazolidin-2-one antibacterials. <i>Bioorganic and Medicinal Chemistry</i> , 2004, 12, 3027-3035.	3.0	25
75	Legitimate Utilization of Large Descriptor Pools for QSPR/QSAR Models. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 2207-2213.	5.4	25
76	Quantitative Structure-Property Relationship Studies on Ostwald Solubility and Partition Coefficients of Organic Solutes in Ionic Liquids. <i>Journal of Chemical &amp; Engineering Data</i> , 2008, 53, 1085-1092.	1.9	25
77	AM1, PM3, and MNDO calculations of radical formation energies in the gas phase and in solution. <i>Journal of Organic Chemistry</i> , 1991, 56, 134-137.	3.2	24
78	QSAR studies on 1-phenylbenzimidazoles as inhibitors of the platelet-derived growth factor. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 6598-6608.	3.0	24
79	Glial Cell Line-Derived Neurotrophic Factor Receptor Rearranged During Transfection Agonist Supports Dopamine Neurons <i>in Vitro</i> and Enhances Dopamine Release <i>in Vivo</i> . <i>Movement Disorders</i> , 2020, 35, 245-255.	3.9	24
80	Semiempirical study of the solvent effect on the Menshutkin reaction. <i>Journal of the Chemical Society Perkin Transactions II</i> , 1994, , 2445.	0.9	23
81	QSRR Correlation of Free-Radical Polymerization Chain-Transfer Constants for Styrene. <i>Journal of Chemical Information and Computer Sciences</i> , 2001, 41, 295-299.	2.8	23
82	QSAR modeling of the antifungal activity against <i>Candida albicans</i> for a diverse set of organic compounds. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 7055-7069.	3.0	22
83	QSPR Treatment of the Unified Nonspecific Solvent Polarity Scale. <i>Journal of Chemical Information and Computer Sciences</i> , 1997, 37, 756-761.	2.8	21
84	Using artificial neural networks to predict cell-penetrating compounds. <i>Expert Opinion on Drug Discovery</i> , 2011, 6, 783-796.	5.0	20
85	Small-Molecule Inhibitors of the RNA M6A Demethylases FTO Potently Support the Survival of Dopamine Neurons. <i>International Journal of Molecular Sciences</i> , 2021, 22, 4537.	4.1	20
86	Insights into Sulfur Vulcanization from QSPR Quantitative Structure-Property Relationships Studies. <i>Rubber Chemistry and Technology</i> , 1999, 72, 318-333.	1.2	19
87	QSPR Modelling of Lanthanide-Organic Complex Stability Constants. <i>Separation Science and Technology</i> , 2006, 41, 197-216.	2.5	19
88	QSPR modeling of hyperpolarizabilities. <i>Journal of Molecular Modeling</i> , 2007, 13, 951-963.	1.8	19
89	Theoretical study of the keto-enol tautomerism in aqueous solutions. <i>Tetrahedron</i> , 1996, 52, 11325-11328.	1.9	18
90	Comparison Between 2D and 3D-QSAR Approaches to Correlate Inhibitor Activity for a Series of Indole Amide Hydroxamic Acids. <i>QSAR and Combinatorial Science</i> , 2007, 26, 333-345.	1.4	18

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91	QSPR Modeling of the Polarizability of Polyaromatic Hydrocarbons and Fullerenes. <i>Journal of Physical Chemistry C</i> , 2008, 112, 4785-4790.	3.1	18
92	Estimating the toxicities of organic chemicals in activated sludge process. <i>Water Research</i> , 2010, 44, 2451-2460.	11.3	18
93	Theoretical study of the effect of counterions on the structure of pyrrole oligomers. <i>International Journal of Quantum Chemistry</i> , 2002, 88, 296-301.	2.0	17
94	Physical, Chemical, and Technological Property Correlation with Chemical Structure: The Potential of QSPR. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2006, 61, 373-384.	0.7	17
95	Neural Networks Convergence Using Physicochemical Data. <i>Journal of Chemical Information and Modeling</i> , 2006, 46, 1891-1897.	5.4	16
96	Correlation of liquid viscosity with molecular structure for organic compounds using different variable selection methods. <i>Arkivoc</i> , 2002, 2002, 45-59.	0.5	16
97	QSPR modeling of UV absorption intensities. <i>Journal of Computer-Aided Molecular Design</i> , 2007, 21, 371-377.	2.9	15
98	Quantitative Relationship between Rate Constants of the Gas-Phase Homolysis of C-X Bonds and Molecular Descriptors. <i>Journal of Chemical Information and Computer Sciences</i> , 2000, 40, 1062-1071.	2.8	14
99	Small-Molecule Ligands as Potential GDNF Family Receptor Agonists. <i>ACS Omega</i> , 2018, 3, 1022-1030.	3.5	14
100	Identification of Natural Compounds against Neurodegenerative Diseases Using In Silico Techniques. <i>Molecules</i> , 2018, 23, 1847.	3.8	14
101	MulticavitySCRF calculation of ion hydration energies. <i>International Journal of Quantum Chemistry</i> , 1994, 52, 339-348.	2.0	13
102	Electron impact ionization mass spectrometry and intramolecular cyclization in 2-substituted pyrimidin-4(3H)-ones. <i>Journal of the American Society for Mass Spectrometry</i> , 1994, 5, 113-119.	2.8	13
103	A Comprehensive Docking Study on the Selectivity of Binding of Aromatic Compounds to Proteins. <i>Journal of Chemical Information and Computer Sciences</i> , 2003, 43, 1576-1583.	2.8	13
104	QSAR study of antiplatelet agents. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 7490-7500.	3.0	13
105	Fragment-Based Development of HCV Protease Inhibitors for the Treatment of Hepatitis C. <i>Current Computer-Aided Drug Design</i> , 2012, 8, 55-61.	1.2	13
106	HIV Replication Is Increased by RNA Methylation METTL3/METTL14/WTAP Complex Activators. <i>ACS Omega</i> , 2021, 6, 15957-15963.	3.5	13
107	General and Class Specific Models for Prediction of Soil Sorption Using Various Physicochemical Descriptors. <i>Journal of Chemical Information and Computer Sciences</i> , 2002, 42, 1450-1459.	2.8	12
108	QSAR modeling of anti-invasive activity of organic compounds using structural descriptors. <i>Bioorganic and Medicinal Chemistry</i> , 2006, 14, 6933-6939.	3.0	12

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109	Novel RET agonist for the treatment of experimental neuropathies. <i>Molecular Pain</i> , 2020, 16, 174480692095086.	2.1	12
110	1,3-Thiazolbenzamide Derivatives as Chikungunya Virus nsP2 Protease Inhibitors. <i>ACS Omega</i> , 2021, 6, 5786-5794.	3.5	12
111	RNA Interference-Guided Targeting of Hepatitis C Virus Replication with Antisense Locked Nucleic Acid-Based Oligonucleotides Containing 8-oxo-dG Modifications. <i>PLoS ONE</i> , 2015, 10, e0128686.	2.5	11
112	Quantum Chemical Treatment of Molecules in Condensed Disordered Media. <i>Advances in Quantum Chemistry</i> , 1997, 28, 141-157.	0.8	10
113	Multitarget Approach to Drug Candidates against Alzheimer's Disease Related to AChE, SERT, BACE1 and GSK3 $\beta$ Protein Targets. <i>Molecules</i> , 2020, 25, 1846.	3.8	10
114	Epitranscriptomics of Ischemic Heart Disease—The IHD-EPITRAN Study Design and Objectives. <i>International Journal of Molecular Sciences</i> , 2021, 22, 6630.	4.1	10
115	A semiempirical study of heterocycle oligomers and polymers in different dielectric media. <i>International Journal of Quantum Chemistry</i> , 1995, 54, 369-379.	2.0	9
116	Study of Radical Merostabilization by Electrospray FTICR/MS. <i>Journal of the American Chemical Society</i> , 1996, 118, 11905-11911.	13.7	8
117	A quantum-mechanical study of oxidized oligopyrroles. <i>International Journal of Quantum Chemistry</i> , 1999, 71, 101-109.	2.0	8
118	QSPR models derived for the kinetic data of the gas-phase homolysis of the carbon-methyl bond. <i>Computers &amp; Chemistry</i> , 2002, 26, 237-243.	1.2	8
119	Novel Analogues of the Chikungunya Virus Protease Inhibitor: Molecular Design, Synthesis, and Biological Evaluation. <i>ACS Omega</i> , 2021, 6, 10884-10896.	3.5	8
120	Neuroprotective Potential of a Small Molecule RET Agonist in Cultured Dopamine Neurons and Hemiparkinsonian Rats. <i>Journal of Parkinson's Disease</i> , 2021, 11, 1023-1046.	2.8	8
121	Prediction of Cell-Penetrating Peptides. <i>Methods in Molecular Biology</i> , 2015, 1324, 39-58.	0.9	8
122	Subchronic Oral and Inhalation Toxicities: a Challenging Attempt for Modeling and Prediction. <i>Molecular Informatics</i> , 2013, 32, 793-801.	2.5	7
123	Refinement of a Quantitative Structure-Activity Relationship Model for Prediction of Cell-Penetrating Peptide Based Transfection Systems. <i>International Journal of Peptide Research and Therapeutics</i> , 2017, 23, 91-100.	1.9	7
124	A comparative AM1 and ab initio study of the intramolecular proton transfer in tautomeric organic compounds. <i>International Journal of Quantum Chemistry</i> , 1996, 60, 1765-1773.	2.0	6
125	Electron impact mass spectrometric studies of 2-methyl, 2-phenyl, 2-(1-piperidyl), 2-(2/3/4-pyridyl), piperidino and pyrido[4,3-d]-pyrimidin-4-ones. <i>Rapid Communications in Mass Spectrometry</i> , 1998, 12, 1845-1858.	1.5	6
126	Dynamic processes in N-acylated 1,2-dihydro-2,2,4-trimethylbenzo(h)quinoline: A comparative study by NMR spectroscopy and quantum chemistry. <i>Tetrahedron</i> , 1999, 55, 5227-5238.	1.9	6



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127	Topological Fingerprints as an Aid in Finding Structural Patterns for LRRK2 Inhibition. <i>Molecular Informatics</i> , 2014, 33, 269-275.	2.5	6
128	Indole-like Trk receptor antagonists. <i>European Journal of Medicinal Chemistry</i> , 2016, 121, 541-552.	5.5	6
129	Quantum chemical modelling of the effect of proline residues on peptide conformation. , 1998, 66, 391-396.		5
130	A QSPR model for the prediction of the gas-phase free energies of activation of rotation around the N-C(O) bond. <i>Computers &amp; Chemistry</i> , 2001, 25, 171-176.	1.2	4
131	Quantitative structure-activity relationship modeling of bioconcentration factors of polychlorinated biphenyls. <i>Toxicological and Environmental Chemistry</i> , 2010, 92, 1233-1247.	1.2	4
132	QSAR of Heterocyclic Compounds in Large Descriptor Spaces. <i>Advances in Heterocyclic Chemistry</i> , 2016, 120, 237-273.	1.7	4
133	Reparameterized Austin Model 1 for quantitative structure-property relationships in liquid media. <i>Journal of Molecular Modeling</i> , 2006, 12, 503-512.	1.8	3
134	Theoretical study of aminoalkylation in the Mannich reaction of furan with methyleneiminium salt. <i>International Journal of Quantum Chemistry</i> , 1998, 67, 359-366.	2.0	2
135	Computational Chemistry Approaches for Understanding how Structure Determines Properties. <i>Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences</i> , 2009, 64, 773-777.	0.7	2
136	Prediction of peptide IMS cross sections from extended molecular connectivity. <i>International Journal of Mass Spectrometry</i> , 2012, 314, 1-5.	1.5	2
137	Quantum-Chemical Descriptors in QSAR. , 2003, , .		2
138	Molecular Properties and Spectra in Solution. , 1997, , 353-387.		1
139	Models for Simulating Molecular Properties in Condensed Systems. , 1997, , 215-248.		1
140	Novel computational models for predicting dopamine interactions. <i>Experimental Neurology</i> , 2008, 211, 150-171.	4.1	1
141	Prediction of liquid viscosity for organic compounds by a quantitative structure-property relationship. , 2000, 13, 80.		1
142	The Present Utility and Future Potential for Medicinal Chemistry of QSAR/QSPR with Whole Molecule Descriptors. <i>ChemInform</i> , 2003, 34, no.	0.0	0
143	Quantitative Measures of Solvent Polarity. <i>ChemInform</i> , 2004, 35, no.	0.0	0
144	Quantitative Structure-Property Relationship Modeling of $\beta$ -Cyclodextrin Complexation Free Energies.. <i>ChemInform</i> , 2004, 35, no.	0.0	0

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145	QSPR Treatment of the Soil Sorption Coefficients of Organic Pollutants.. ChemInform, 2005, 36, no.	0.0	0