Mati Karelson

List of Publications by Year
in descending order

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	1,3-Thiazolbenzamide Derivatives as Chikungunya Virus nsP2 Protease Inhibitors. ACS Omega, 2021, 6, 5786-5794.	3.5	12
2	Small-Molecule Inhibitors of the RNA M6A Demethylases FTO Potently Support the Survival of Dopamine Neurons. International Journal of Molecular Sciences, 2021, 22, 4537.	4.1	20
3	Novel Analogues of the Chikungunya Virus Protease Inhibitor: Molecular Design, Synthesis, and Biological Evaluation. ACS Omega, 2021, 6, 10884-10896.	3.5	8
4	Rational Design of Novel Anticancer Small-Molecule RNA m6A Demethylase ALKBH5 Inhibitors. ACS Omega, 2021, 6, 13310-13320.	3.5	57
5	Epitranscriptomics of Ischemic Heart Diseaseâ€"The IHD-EPITRAN Study Design and Objectives. International Journal of Molecular Sciences, 2021, 22, 6630.	4.1	10
6	HIV Replication Is Increased by RNA Methylation METTL3/METTL14/WTAP Complex Activators. ACS Omega, 2021, 6, 15957-15963.	3.5	13
7	Neuroprotective Potential of a Small Molecule RET Agonist in Cultured Dopamine Neurons and Hemiparkinsonian Rats. Journal of Parkinson's Disease, 2021, 11, 1023-1046.	2.8	8
8	Glial Cell Lineâ€"Derived Neurotrophic Factor Receptor Rearranged During Transfection Agonist Supports Dopamine Neurons In Vitro and Enhances Dopamine Release In Vivo. Movement Disorders, 2020, 35, 245-255.	3.9	24
9	Novel RET agonist for the treatment of experimental neuropathies. Molecular Pain, 2020, 16, 174480692095086.	2.1	12
10	Multitarget Approach to Drug Candidates against Alzheimerâ€™s Disease Related to AChE, SERT, BACE1 and GSK3Î² Protein Targets. Molecules, 2020, 25, 1846.	3.8	10
11	Discovery of Small Molecules that Activate RNA Methylation through Cooperative Binding to the METTL3-14-WTAP Complex Active Site. Cell Reports, 2019, 26, 3762-3771.e5.	6.4	121
12	Small-Molecule Ligands as Potential GDNF Family Receptor Agonists. ACS Omega, 2018, 3, 1022-1030.	3.5	14
13	Molecular Dynamics Simulations of the Interactions between Glial Cell Line-Derived Neurotrophic Factor Family Receptor GFRÎ±1 and Small-Molecule Ligands. ACS Omega, 2018, 3, 11407-11414.	3.5	69
14	Identification of Natural Compounds against Neurodegenerative Diseases Using In Silico Techniques. Molecules, 2018, 23, 1847.	3.8	14
15	Refinement of a Quantitative Structureâ€"Activity Relationship Model for Prediction of Cell-Penetrating Peptide Based Transfection Systems. International Journal of Peptide Research and Therapeutics, 2017, 23, 91-100.	1.9	7
16	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
17	Have artificial neural networks met expectations in drug discovery as implemented in QSAR framework?. Expert Opinion on Drug Discovery, 2016, 11, 627-639.	5.0	30
18	Design and Validation of Novel Chikungunya Virus Protease Inhibitors. Antimicrobial Agents and Chemotherapy, 2016, 60, 7382-7395.	3.2	40

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19	QSAR of Heterocyclic Compounds in Large Descriptor Spaces. Advances in Heterocyclic Chemistry, 2016, 120, 237-273.	1.7	4
20	Indole-like Trk receptor antagonists. European Journal of Medicinal Chemistry, 2016, 121, 541-552.	5.5	6
21	RNA Interference-Guided Targeting of Hepatitis C Virus Replication with Antisense Locked Nucleic Acid-Based Oligonucleotides Containing 8-oxo-dG Modifications. PLoS ONE, 2015, 10, e0128686.	2.5	11
22	Prediction of Cell-Penetrating Peptides. Methods in Molecular Biology, 2015, 1324, 39-58.	0.9	8
23	Topological Fingerprints as an Aid in Finding Structural Patterns for LRRK2 Inhibition. Molecular Informatics, 2014, 33, 269-275.	2.5	6
24	Rational design of a series of novel amphipathic cell-penetrating peptides. International Journal of Pharmaceutics, 2014, 464, 111-116.	5.2	30
25	In Silico Machine Learning Methods in Drug Development. Current Topics in Medicinal Chemistry, 2014, 14, 1913-1922.	2.1	40
26	Subchronic Oral and Inhalation Toxicities: a Challenging Attempt for Modeling and Prediction. Molecular Informatics, 2013, 32, 793-801.	2.5	7
27	Fragment-Based Development of HCV Protease Inhibitors for the Treatment of Hepatitis C. Current Computer-Aided Drug Design, 2012, 8, 55-61.	1.2	13
28	Prediction of peptide IMS cross sections from extended molecular connectivity. International Journal of Mass Spectrometry, 2012, 314, 1-5.	1.5	2
29	Application of the QSPR Approach to the Boiling Points of Azeotropes. Journal of Physical Chemistry A, 2011, 115, 3475-3479.	2.5	26
30	Using artificial neural networks to predict cell-penetrating compounds. Expert Opinion on Drug Discovery, 2011, 6, 783-796.	5.0	20
31	Prediction of Cell-Penetrating Peptides Using Artificial Neural Networks. Current Computer-Aided Drug Design, 2010, 6, 79-89.	1.2	49
32	Quantitative Correlation of Physical and Chemical Properties with Chemical Structure: Utility for Prediction. Chemical Reviews, 2010, 110, 5714-5789.	47.7	460
33	Quantitative structureâ€“activity relationship modeling of bioconcentration factors of polychlorinated biphenyls. Toxicological and Environmental Chemistry, 2010, 92, 1233-1247.	1.2	4
34	Estimating the toxicities of organic chemicals in activated sludge process. Water Research, 2010, 44, 2451-2460.	11.3	18
35	Quantitative Structureâ€“Activity Relationship (QSAR) Modeling of EC₅₀of Aquatic Toxicities forDaphnia magna. Journal of Toxicology and Environmental Health - Part A: Current Issues, 2009, 72, 1181-1190.	2.3	40
36	QSPR study of the first and second critical micelle concentrations of cationic surfactants. Computers and Chemical Engineering, 2009, 33, 321-332.	3.8	27

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37	Computational Chemistry Approaches for Understanding how Structure Determines Properties. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2009, 64, 773-777.	0.7	2
38	QSAR modeling of the antifungal activity against Candida albicans for a diverse set of organic compounds. Bioorganic and Medicinal Chemistry, 2008, 16, 7055-7069.	3.0	22
39	Legitimate Utilization of Large Descriptor Pools for QSPR/QSAR Models. Journal of Chemical Information and Modeling, 2008, 48, 2207-2213.	5.4	25
40	QSPR Study of Critical Micelle Concentrations of Nonionic Surfactants. Industrial & Engineering Chemistry Research, 2008, 47, 9687-9695.	3.7	45
41	Novel computational models for predicting dopamine interactions. Experimental Neurology, 2008, 211, 150-171.	4.1	1
42	QSPR Modeling of the Polarizability of Polyaromatic Hydrocarbons and Fullerenes. Journal of Physical Chemistry C, 2008, 112, 4785-4790.	3.1	18
43	Quantitative Structureâ€“Property Relationship Studies on Ostwald Solubility and Partition Coefficients of Organic Solutes in Ionic Liquids. Journal of Chemical & Engineering Data, 2008, 53, 1085-1092.	1.9	25
44	Structure-based calculation of drug efficiency indices. Bioinformatics, 2007, 23, 2678-2685.	4.1	26
45	QSPR Study of Critical Micelle Concentration of Anionic Surfactants Using Computational Molecular Descriptors. Journal of Chemical Information and Modeling, 2007, 47, 782-793.	5.4	29
46	QSPR Modeling of Solubility of Polyaromatic Hydrocarbons and Fullerene in 1-Octanol and n-Heptane. Journal of Physical Chemistry B, 2007, 111, 9853-9857.	2.6	33
47	Rapid QSPR model development technique for prediction of vapor pressure of organic compounds. Computers and Chemical Engineering, 2007, 31, 1123-1130.	3.8	48
48	QSPR modeling of flash points: An update. Journal of Molecular Graphics and Modelling, 2007, 26, 529-536.	2.4	97
49	Comparison Between 2D and 3D-QSAR Approaches to Correlate Inhibitor Activity for a Series of Indole Amide Hydroxamic Acids. QSAR and Combinatorial Science, 2007, 26, 333-345.	1.4	18
50	QSPR modeling of UV absorption intensities. Journal of Computer-Aided Molecular Design, 2007, 21, 371-377.	2.9	15
51	QSPR modeling of hyperpolarizabilities. Journal of Molecular Modeling, 2007, 13, 951-963.	1.8	19
52	QSPR Modelling of Lanthanideâ€Organic Complex Stability Constants. Separation Science and Technology, 2006, 41, 197-216.	2.5	19
53	Skin Permeation Rate as a Function of Chemical Structure. Journal of Medicinal Chemistry, 2006, 49, 3305-3314.	6.4	49
54	Open Computing Grid for Molecular Science and Engineering. Journal of Chemical Information and Modeling, 2006, 46, 953-959.	5.4	32

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55	Combination of a Modified Scoring Function with Two-Dimensional Descriptors for Calculation of Binding Affinities of Bulky, Flexible Ligands to Proteins. Journal of the American Chemical Society, 2006, 128, 1233-1239.	13.7	31
56	Neural Networks Convergence Using Physicochemical Data. Journal of Chemical Information and Modeling, 2006, 46, 1891-1897.	5.4	16
57	Physical, Chemical, and Technological Property Correlation with Chemical Structure: The Potential of QSPR. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2006, 61, 373-384.	0.7	17
58	QSAR modeling of anti-invasive activity of organic compounds using structural descriptors. Bioorganic and Medicinal Chemistry, 2006, 14, 6933-6939.	3.0	12
59	QSAR study of antiplatelet agents. Bioorganic and Medicinal Chemistry, 2006, 14, 7490-7500.	3.0	13
60	QSAR study of mosquito repellents using Codessa Pro. Bioorganic and Medicinal Chemistry Letters, 2006, 16, 2306-2311.	2.2	49
61	Antimalarial activity: A QSAR modeling using CODESSA PRO software. Bioorganic and Medicinal Chemistry, 2006, 14, 2333-2357.	3.0	47
62	QSAR modeling of the inhibition of Glycogen Synthase Kinase-3. Bioorganic and Medicinal Chemistry, 2006, 14, 4987-5002.	3.0	30
63	Correlation of bloodâ€“brain penetration using structural descriptors. Bioorganic and Medicinal Chemistry, 2006, 14, 4888-4917.	3.0	80
64	Reparameterized Austin Model 1 for quantitative structureâ€“property relationships in liquid media. Journal of Molecular Modeling, 2006, 12, 503-512.	1.8	3
65	QSAR treatment of drugs transfer into human breast milk. Bioorganic and Medicinal Chemistry, 2005, 13, 1623-1632.	3.0	41
66	QSAR modeling of blood:air and tissue:air partition coefficients using theoretical descriptors. Bioorganic and Medicinal Chemistry, 2005, 13, 6450-6463.	3.0	40
67	QSAR studies on 1-phenylbenzimidazoles as inhibitors of the platelet-derived growth factor. Bioorganic and Medicinal Chemistry, 2005, 13, 6598-6608.	3.0	24
68	QSPR Treatment of the Soil Sorption Coefficients of Organic Pollutants.. ChemInform, 2005, 36, no.	0.0	0
69	The Classification of Solvents by Combining Classical QSPR Methodology with Principal Component Analysis. Journal of Physical Chemistry A, 2005, 109, 10323-10341.	2.5	81
70	QSPR Treatment of the Soil Sorption Coefficients of Organic Pollutants. Journal of Chemical Information and Modeling, 2005, 45, 94-105.	5.4	41
71	Quantitative Measures of Solvent Polarity. ChemInform, 2004, 35, no.	0.0	0
72	Quantitative Structureâ€”Property Relationship Modeling of Î²-Cyclodextrin Complexation Free Energies.. ChemInform, 2004, 35, no.	0.0	0

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73	QSPR of 3-aryloxazolidin-2-one antibacterials. Bioorganic and Medicinal Chemistry, 2004, 12, 3027-3035.	3.0	25
74	QSPR treatment of rat blood:air, saline:air and olive oil:air partition coefficients using theoretical molecular descriptors. Bioorganic and Medicinal Chemistry, 2004, 12, 4735-4748.	3.0	27
75	Quantitative Structureâ^'Property Relationship Modeling ofÎ²-Cyclodextrin Complexation Free Energies. Journal of Chemical Information and Computer Sciences, 2004, 44, 529-541.	2.8	66
76	Quantitative Measures of Solvent Polarity. Chemical Reviews, 2004, 104, 175-198.	47.7	385
77	A Quantitative Structureâ^'Property Relationship Study of Lithium Cation Basicities. Journal of Physical Chemistry A, 2004, 108, 4812-4818.	2.5	31
78	The Present Utility and Future Potential for Medicinal Chemistry of QSAR/QSPR with Whole Molecule Descriptors. ChemInform, 2003, 34, no.	0.0	0
79	Nitrobenzene toxicity: QSAR correlations and mechanistic interpretations. Journal of Physical Organic Chemistry, 2003, 16, 811-817.	1.9	48
80	A Comprehensive Docking Study on the Selectivity of Binding of Aromatic Compounds to Proteins. Journal of Chemical Information and Computer Sciences, 2003, 43, 1576-1583.	2.8	13
81	Quantum-Chemical Descriptors in QSAR. , 2003, , .		2
82	The Present Utility and Future Potential for Medicinal Chemistry of QSAR / QSPR with Whole Molecule Descriptors. Current Topics in Medicinal Chemistry, 2002, 2, 1333-1356.	2.1	70
83	Prediction of Ultraviolet Spectral Absorbance Using Quantitative Structureâ^'Property Relationships. Journal of Chemical Information and Computer Sciences, 2002, 42, 830-840.	2.8	30
84	General and Class Specific Models for Prediction of Soil Sorption Using Various Physicochemical Descriptors. Journal of Chemical Information and Computer Sciences, 2002, 42, 1450-1459.	2.8	12
85	Correlation of the Melting Points of Potential Ionic Liquids (Imidazolium Bromides and) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 Computer Sciences, 2002, 42, 225-231.	2.8	196
86	QSPR Correlation of the Melting Point for Pyridinium Bromides, Potential Ionic Liquids. Journal of Chemical Information and Computer Sciences, 2002, 42, 71-74.	2.8	170
87	Theoretical study of the effect of counterions on the structure of pyrrole oligomers. International Journal of Quantum Chemistry, 2002, 88, 296-301.	2.0	17
88	QSPR models derived for the kinetic data of the gas-phase homolysis of the carbonâ€"methyl bond. Computers & Chemistry, 2002, 26, 237-243.	1.2	8
89	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
90	A General QSPR Treatment for Dielectric Constants of Organic Compounds. Journal of Chemical Information and Computer Sciences, 2002, 42, 360-367.	2.8	42

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91	Correlation of liquid viscosity with molecular structure for organic compounds using different variable selection methods. Arkivoc, 2002, 2002, 45-59.	0.5	16
92	Interpretation of Quantitative Structureâ^'Property and â^'Activity Relationships. Journal of Chemical Information and Computer Sciences, 2001, 41, 679-685.	2.8	110
93	QSRR Correlation of Free-Radical Polymerization Chain-Transfer Constants for Styrene. Journal of Chemical Information and Computer Sciences, 2001, 41, 295-299.	2.8	23
94	Perspective on the Relationship between Melting Points and Chemical Structure. Crystal Growth and Design, 2001, 1, 261-265.	3.0	167
95	QSPR Analysis of Flash Points. Journal of Chemical Information and Computer Sciences, 2001, 41, 1521-1530.	2.8	144
96	A QSPR model for the prediction of the gas-phase free energies of activation of rotation around the Nî—¸C(O) bond. Computers & Chemistry, 2001, 25, 171-176.	1.2	4
97	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
98	Quantitative Relationship between Rate Constants of the Gas-Phase Homolysis of Câ^'X Bonds and Molecular Descriptors. Journal of Chemical Information and Computer Sciences, 2000, 40, 1062-1071.	2.8	14
99	Structurally Diverse Quantitative Structureâ^'Property Relationship Correlations of Technologically Relevant Physical Properties. Journal of Chemical Information and Computer Sciences, 2000, 40, 1-18.	2.8	238
100	Prediction of liquid viscosity for organic compounds by a quantitative structureâ€“property relationship. , 2000, 13, 80.		1
101	Insights into Sulfur Vulcanization from QSPR Quantitative Structure-Property Relationships Studies. Rubber Chemistry and Technology, 1999, 72, 318-333.	1.2	19
102	Dynamic processes in N-acylated 1,2-dihydro-2,2,4-trimethylbenzo(h)quinoline: A comparative study by NMR spectroscopy and quantum chemistry. Tetrahedron, 1999, 55, 5227-5238.	1.9	6
103	QSPR and QSAR Models Derived Using Large Molecular Descriptor Spaces. A Review of CODESSA Applications. Collection of Czechoslovak Chemical Communications, 1999, 64, 1551-1571.	1.0	70
104	A quantum-mechanical study of oxidized oligopyrroles. International Journal of Quantum Chemistry, 1999, 71, 101-109.	2.0	8
105	A Comprehensive QSAR Treatment of the Genotoxicity of Heteroaromatic and Aromatic Amines. QSAR and Combinatorial Science, 1999, 18, 03-10.	1.2	65
106	A New Efficient Approach for Variable Selection Based on Multiregression:â€‰ Prediction of Gas Chromatographic Retention Times and Response Factors. Journal of Chemical Information and Computer Sciences, 1999, 39, 610-621.	2.8	104
107	A Unified Treatment of Solvent Properties. Journal of Chemical Information and Computer Sciences, 1999, 39, 692-698.	2.8	41
108	QSPR Treatment of Solvent Scales. Journal of Chemical Information and Computer Sciences, 1999, 39, 684-691.	2.8	43

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109	Quantitative Structureâ^'Property Relationship (QSPR) Correlation of Glass Transition Temperatures of High Molecular Weight Polymers. Journal of Chemical Information and Computer Sciences, 1998, 38, 300-304.	2.8	124
110	Aromaticity as a Quantitative Concept. 7. Aromaticity Reaffirmed as a Multidimensional Characteristicâ€. Journal of Organic Chemistry, 1998, 63, 5228-5231.	3.2	289
111	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. Rapid Communications in Mass Spectrometry, 1998, 12, 1845-1858.	1.5	6
112	Quantum chemical modelling of the effect of proline residues on peptide conformation. , 1998, 66, 391-396.		5
113	Theoretical study of aminoalkylation in the Mannich reaction of furan with methyleneimminium salt. International Journal of Quantum Chemistry, 1998, 67, 359-366.	2.0	2
114	General Quantitative Structureâ^'Property Relationship Treatment of the Refractive Index of Organic Compounds. Journal of Chemical Information and Computer Sciences, 1998, 38, 840-844.	2.8	46
115	QSPR Studies on Vapor Pressure, Aqueous Solubility, and the Prediction of Waterâ^'Air Partition Coefficients. Journal of Chemical Information and Computer Sciences, 1998, 38, 720-725.	2.8	152
116	Relationships of Critical Temperatures to Calculated Molecular Properties. Journal of Chemical Information and Computer Sciences, 1998, 38, 293-299.	2.8	25
117	Correlation and Prediction of the Refractive Indices of Polymers by QSPR. Journal of Chemical Information and Computer Sciences, 1998, 38, 1171-1176.	2.8	118
118	Normal Boiling Points for Organic Compounds:â€‰ Correlation and Prediction by a Quantitative Structureâ^'Property Relationship. Journal of Chemical Information and Computer Sciences, 1998, 38, 28-41.	2.8	80
119	QSPR as a means of predicting and understanding chemical and physical properties in terms of structure. Pure and Applied Chemistry, 1997, 69, 245-248.	1.9	114
120	Quantum Chemical Treatment of Molecules in Condensed Disordered Media. Advances in Quantum Chemistry, 1997, 28, 141-157.	0.8	10
121	Prediction of Melting Points for the Substituted Benzenes:â€‰ A QSPR Approach. Journal of Chemical Information and Computer Sciences, 1997, 37, 913-919.	2.8	70
122	Molecular Properties and Spectra in Solution. , 1997, , 353-387.		1
123	Models for Simulating Molecular Properties in Condensed Systems. , 1997, , 215-248.		1
124	QSPR Treatment of the Unified Nonspecific Solvent Polarity Scale. Journal of Chemical Information and Computer Sciences, 1997, 37, 756-761.	2.8	21
125	Prediction of Critical Micelle Concentration Using a Quantitative Structureâ^'Property Relationship Approach. 1. Nonionic Surfactants. Langmuir, 1996, 12, 1462-1470.	3.5	174
126	Study of Radical Merostabilization by Electrospray FTICR/MS. Journal of the American Chemical Society, 1996, 118, 11905-11911.	13.7	8

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127	Prediction of Polymer Glass Transition Temperatures Using a General Quantitative Structureâ''Property Relationship Treatment. Journal of Chemical Information and Computer Sciences, 1996, 36, 879-884.	2.8	88
128	A QSPR Study of the Solubility of Gases and Vapors in Water. Journal of Chemical Information and Computer Sciences, 1996, 36, 1162-1168.	2.8	66
129	Correlation of Boiling Points with Molecular Structure. 1. A Training Set of 298 Diverse Organics and a Test Set of 9 Simple Inorganics. The Journal of Physical Chemistry, 1996, 100, 10400-10407.	2.9	227
130	Aromaticity as a Quantitative Concept. 6. Aromaticity Variation with Molecular Environment. Journal of Organic Chemistry, 1996, 61, 1619-1623.	3.2	60
131	Quantum-Chemical Descriptors in QSAR/QSPR Studies. Chemical Reviews, 1996, 96, 1027-1044.	47.7	1,375
132	Theoretical study of the keto-enol tautomerism in aqueous solutions. Tetrahedron, 1996, 52, 11325-11328.	1.9	18
133	A comparative AM1 and ab initio study of the intramolecular proton transfer in tautomeric organic compounds. International Journal of Quantum Chemistry, 1996, 60, 1765-1773.	2.0	6
134	A semiempirical study of heterocycle oligomers and polymers in different dielectric media. International Journal of Quantum Chemistry, 1995, 54, 369-379.	2.0	9
135	QSPR: the correlation and quantitative prediction of chemical and physical properties from structure. Chemical Society Reviews, 1995, 24, 279.	38.1	474
136	MulticavitySCRF calculation of ion hydration energies. International Journal of Quantum Chemistry, 1994, 52, 339-348.	2.0	13
137	Electron impact ionization mass spectrometry and intramolecular cyclization in 2-substituted pyrimidin-4(3H)-ones. Journal of the American Society for Mass Spectrometry, 1994, 5, 113-119.	2.8	13
138	Prediction of Gas Chromatographic Retention Times and Response Factors Using a General Qualitative Structure-Property Relationships Treatment. Analytical Chemistry, 1994, 66, 1799-1807.	6.5	187
139	Semiempirical study of the solvent effect on the Menshutkin reaction. Journal of the Chemical Society Perkin Transactions II, 1994, , 2445.	0.9	23
140	Multicavity reaction field method for the solvent effect description in flexible molecular systems. The Journal of Physical Chemistry, 1993, 97, 11901-11907.	2.9	67
141	AM1 calculations of reaction field effects on the tautomeric equilibria of nucleic acid pyrimidine and purine bases and their 1-methyl analogs. Journal of the American Chemical Society, 1991, 113, 1561-1566.	13.7	148
142	AM1, PM3, and MNDO calculations of radical formation energies in the gas phase and in solution. Journal of Organic Chemistry, 1991, 56, 134-137.	3.2	24
143	Heterocyclic Aromaticity. Heterocycles, 1991, 32, 127.	0.7	114
144	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

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145	On the n-.pi.* blue shift accompanying solvation. Journal of the American Chemical Society, 1990, 112, 9405-9406.	13.7	101