Alla P Toropova

List of Publications by Year
in descending order

254	5,456	100601	198040
papers	citations	38 h-index	52 g-index

264	264	264	2142
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Quasi-SMILES as a basis to build up models of endpoints for nanomaterials. Environmental Technology (United Kingdom), 2023, 44, 4460-4467.	1.2	2
2	SARS-CoV M^{pro} inhibitory activity of aromatic disulfide compounds: QSAR model. Journal of Biomolecular Structure and Dynamics, 2022, 40, 780-786.	2.0	23
3	Paradox of â€˜ideal correlationsâ€™: improved model for air half-life of persistent organic pollutants. Environmental Technology (United Kingdom), 2022, 43, 2510-2515.	1.2	7
4	QSAR models for soil ecotoxicity: Development and validation of models to predict reproductive toxicity of organic chemicals in the collembola Folsomia candida. Journal of Hazardous Materials, 2022, 423, 127236.	6.5	22
5	The system of self-consistent QSPR-models for refractive index of polymers. Structural Chemistry, 2022, 33, 617-624.	1.0	6
6	The system of self-consistent models for vapour pressure. Chemical Physics Letters, 2022, 790, 139354.	1.2	9
7	The development of nano-QSPR models for viscosity of nanofluids using the index of ideality of correlation and the correlation intensity index. Chemometrics and Intelligent Laboratory Systems, 2022, 222, 104500.	1.8	10
8	How fullerene derivatives (FDs) act on therapeutically important targets associated with diabetic diseases. Computational and Structural Biotechnology Journal, 2022, 20, 913-924.	1.9	9
9	Nanomaterials: Quasi-SMILES as a flexible basis for regulation and environmental risk assessment. Science of the Total Environment, 2022, 823, 153747.	3.9	22
10	The searching for agents for Alzheimerâ€™s disease treatment via the system of self-consistent models. Toxicology Mechanisms and Methods, 2022, , 1-9.	1.3	13
11	A regression-based QSAR-model to predict acute toxicity of aromatic chemicals in tadpoles of the Japanese brown frog (Rana japonica): Calibration, validation, and future developments to support risk assessment of chemicals in amphibians. Science of the Total Environment, 2022, 830, 154795.	3.9	10
12	Use of quasi-SMILES to build models based on quantitative results from experiments with nanomaterials. Chemosphere, 2022, 303, 135086.	4.2	10
13	Carcinogenicity prediction using the index of ideality of correlation. SAR and QSAR in Environmental Research, 2022, 33, 419-428.	1.0	4
14	Monte Carlo Models for Sub-Chronic Repeated-Dose Toxicity: Systemic and Organ-Specific Toxicity. International Journal of Molecular Sciences, 2022, 23, 6615.	1.8	6
15	Pesticides, cosmetics, drugs: identical and opposite influences of various molecular features as measures of endpoints similarity and dissimilarity. Molecular Diversity, 2021, 25, 1137-1144.	2.1	2
16	Integrated In Silico Models for the Prediction of No-Observed-(Adverse)-Effect Levels and Lowest-Observed-(Adverse)-Effect Levels in Rats for Sub-chronic Repeated-Dose Toxicity. Chemical Research in Toxicology, 2021, 34, 247-257.	1.7	13
17	EFSAâ€™s OpenFoodTox: An open source toxicological database on chemicals in food and feed and its future developments. Environment International, 2021, 146, 106293.	4.8	36
18	Prediction of the selfâ€accelerating decomposition temperature of organic peroxides. Process Safety Progress, 2021, 40, e12189.	0.4	6

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19	Can the Monte Carlo method predict the toxicity of binary mixtures?. Environmental Science and Pollution Research, 2021, 28, 39493-39500.	2.7	4
20	Maintenance, update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0. EFSA Supporting Publications, 2021, 18, 6476E.	0.3	2
21	The Monte Carlo method to build up models of the hydrolysis half-lives of organic compounds. SAR and QSAR in Environmental Research, 2021, 32, 463-471.	1.0	8
22	The self-organizing vector of atom-pairs proportions: use to develop models for melting points. Structural Chemistry, 2021, 32, 967-971.	1.0	7
23	The unreliability of the reliability criteria in the estimation of QSAR for skin sensitivity: A pun or a reliable law?. Toxicology Letters, 2021, 340, 133-140.	0.4	11
24	The index of ideality of correlation improves the predictive potential of models of the antioxidant activity of tripeptides from frog skin (Litoria rubella). Computers in Biology and Medicine, 2021, 133, 104370.	3.9	13
25	The System of Self-Consistent of Models: A New Approach to Build Up and Validation of Predictive Models of the Octanol/Water Partition Coefficient for Gold Nanoparticles. International Journal of Environmental Research, 2021, 15, 709-722.	1.1	16
26	Quasi-SMILES as a basis for the development of models for the toxicity of ZnO nanoparticles. Science of the Total Environment, 2021, 772, 145532.	3.9	20
27	The QSAR-search of effective agents towards coronaviruses applying the Monte Carlo method. SAR and QSAR in Environmental Research, 2021, 32, 689-698.	1.0	6
28	Using quasi-SMILES for the predictive modeling of the safety of 574 metal oxide nanoparticles measured in different experimental conditions. Environmental Toxicology and Pharmacology, 2021, 86, 103665.	2.0	19
29	Application of quasi-SMILES to the model of gold-nanoparticles uptake in A549Âcells. Computers in Biology and Medicine, 2021, 136, 104720.	3.9	8
30	Semi-correlations as a tool to model for skin sensitization. Food and Chemical Toxicology, 2021, 157, 112580.	1.8	4
31	The sequence of amino acids as the basis for the model of biological activity of peptides. Theoretical Chemistry Accounts, 2021, 140, 15.	0.5	5
32	The system of self-consistent semi-correlations as one of the tools of cheminformatics for designing antiviral drugs. New Journal of Chemistry, 2021, 45, 20713-20720.	1.4	7
33	The system of self-consistent models for the uptake of nanoparticles in PaCa2 cancer cells. Nanotoxicology, 2021, 15, 995-1004.	1.6	7
34	The index of ideality of correlation: models for flammability of binary liquid mixtures. Chemical Papers, 2020, 74, 601-609.	1.0	18
35	QSAR-Models, Validation, and IIC-Paradox for Drug Toxicity. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 22-43.	1.1	1
36	Use of the index of ideality of correlation to improve aquatic solubility model. Journal of Molecular Graphics and Modelling, 2020, 96, 107525.	1.3	14

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37	Predicting acute contact toxicity of organic binary mixtures in honey bees (A. mellifera) through innovative QSAR models. Science of the Total Environment, 2020, 704, 135302.	3.9	38
38	How the CORAL software can be used to select compounds for efficient treatment of neurodegenerative diseases?. Toxicology and Applied Pharmacology, 2020, 408, 115276.	1.3	6
39	Zebrafish AC modelling: (Q)SAR models to predict developmental toxicity in zebrafish embryo. Ecotoxicology and Environmental Safety, 2020, 202, 110936.	2.9	13
40	QSAR model for pesticides toxicity to Rainbow Trout based on â€œideal correlationsâ€• Aquatic Toxicology, 2020, 227, 105589.	1.9	14
41	Ecosystem ecology: Models for acute toxicity of pesticides towards Daphnia magna. Environmental Toxicology and Pharmacology, 2020, 80, 103459.	2.0	13
42	Advancement of predictive modeling of zeta potentials (Î¶) in metal oxide nanoparticles with correlation intensity index (CII). Journal of Molecular Liquids, 2020, 317, 113929.	2.3	15
43	Applying the Monte Carlo technique to build up models of glass transition temperatures of diverse polymers. Structural Chemistry, 2020, 31, 1739-1743.	1.0	7
44	â€˜Ideal correlationsâ€™ for the predictive toxicity to Tetrahymena pyriformis. Toxicology Mechanisms and Methods, 2020, 30, 605-610.	1.3	6
45	Correlation intensity index: mathematical modeling of cytotoxicity of metal oxide nanoparticles. Nanotoxicology, 2020, 14, 1118-1126.	1.6	34
46	Prediction of No Observed Adverse Effect Concentration for inhalation toxicity using Monte Carlo approach. SAR and QSAR in Environmental Research, 2020, 31, 1-12.	1.0	8
47	QSPR/QSAR: State-of-Art, Weirdness, the Future. Molecules, 2020, 25, 1292.	1.7	42
48	Fullerenes C₆₀ and C₇₀: a model for solubility by applying the correlation intensity index. Fullerenes Nanotubes and Carbon Nanostructures, 2020, 28, 900-906.	1.0	16
49	Correlation intensity index: Building up models for mutagenicity of silver nanoparticles. Science of the Total Environment, 2020, 737, 139720.	3.9	32
50	The using of the Index of Ideality of Correlation (IIC) to improve predictive potential of models of water solubility for pesticides. Environmental Science and Pollution Research, 2020, 27, 13339-13347.	2.7	21
51	The index of ideality of correlation: models of the flash points of ternary mixtures. New Journal of Chemistry, 2020, 44, 4858-4868.	1.4	12
52	QSAR models for biocides: The example of the prediction of Daphnia magna acute toxicity. SAR and QSAR in Environmental Research, 2020, 31, 227-243.	1.0	22
53	The Use of the Index of Ideality of Correlation to Build Up Models for Bioconcentration Factor. Molecular Informatics, 2020, 39, e1900070.	1.4	12
54	The index of ideality of correlation and the variety of molecular rings as a base to improve model of HIV-1 protease inhibitors activity. Structural Chemistry, 2020, 31, 1441-1448.	1.0	6

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55	Correlation Intensity Index (CII) as a criterion of predictive potential: Applying to model thermal conductivity of metal oxide-based ethylene glycol nanofluids. Chemical Physics Letters, 2020, 754, 137614.	1.2	22
56	The Monte Carlo Method as a Tool to Build up Predictive QSPR/QSAR. Current Computer-Aided Drug Design, 2020, 16, 197-206.	0.8	9
57	Medicinal Chemistry and Computational Chemistry: Mutual Influence and Harmonization. Mini-Reviews in Medicinal Chemistry, 2020, 20, 1320-1321.	1.1	0
58	Interpretable SMILES-based QSAR model of inhibitory activity of sirtuins 1 and 2. Combinatorial Chemistry and High Throughput Screening, 2020, 23, .	0.6	1
59	Semi-correlations combined with the index of ideality of correlation: a tool to build up model of mutagenic potential. Molecular and Cellular Biochemistry, 2019, 452, 133-140.	1.4	13
60	Use of the index of ideality of correlation to improve predictive potential for biochemical endpoints. Toxicology Mechanisms and Methods, 2019, 29, 43-52.	1.3	26
61	CORAL: Building up QSAR models for the chromosome aberration test. Saudi Journal of Biological Sciences, 2019, 26, 1101-1106.	1.8	25
62	QSPR as a random event: solubility of fullerenes C[60] and C[70]. Fullerenes Nanotubes and Carbon Nanostructures, 2019, 27, 816-821.	1.0	8
63	QSAR Development for Plasma Protein Binding: Influence of the Ionization State. Pharmaceutical Research, 2019, 36, 28.	1.7	11
64	Idealization of correlations between optimal simplified molecular input-line entry system-based descriptors and skin sensitization. SAR and QSAR in Environmental Research, 2019, 30, 447-455.	1.0	19
65	QSAR as a random event: criteria of predictive potential for a chance model. Structural Chemistry, 2019, 30, 1677-1683.	1.0	32
66	The Correlation Contradictions Index (CCI): Building up reliable models of mutagenic potential of silver nanoparticles under different conditions using quasi-SMILES. Science of the Total Environment, 2019, 681, 102-109.	3.9	29
67	Combinations of graph invariants and attributes of simplified molecular input-line entry system (SMILES) to build up models for sweetness. Food Research International, 2019, 122, 40-46.	2.9	32
68	â€œIdeal correlationsâ€•for biological activity of peptides. BioSystems, 2019, 181, 51-57.	0.9	11
69	The Index of Ideality of Correlation (IIC): model for sweetness. Monatshefte FÃ¼r Chemie, 2019, 150, 617-623.	0.9	5
70	The Index of Ideality of Correlation: QSAR Model of Acute Toxicity for Zebrafish (Danio rerio) Embryo. International Journal of Environmental Research, 2019, 13, 387-394.	1.1	7
71	Does the Index of Ideality of Correlation Detect the Better Model Correctly?. Molecular Informatics, 2019, 38, e1800157.	1.4	41
72	Estimation of 2D autocorrelation descriptors and 2D Monte Carlo descriptors as a tool to build up predictive models for acetylcholinesterase (AChE) inhibitory activity. Chemometrics and Intelligent Laboratory Systems, 2019, 184, 14-21.	1.8	18

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73	Semi-correlations as a tool to build up categorical (active/inactive) model of GABAA receptor modulator activity. Structural Chemistry, 2019, 30, 853-861.	1.0	7
74	The study of the index of ideality of correlation as a new criterion of predictive potential of QSPR/QSAR-models. Science of the Total Environment, 2019, 659, 1387-1394.	3.9	43
75	QSPR and nano-QSPR: What is the difference?. Journal of Molecular Structure, 2019, 1182, 141-149.	1.8	48
76	Quasi-SMILES: quantitative structureâ€“activity relationships to predict anticancer activity. Molecular Diversity, 2019, 23, 403-412.	2.1	15
77	The index of ideality of correlation: improvement of models for toxicity to algae. Natural Product Research, 2019, 33, 2200-2207.	1.0	22
78	Application of the Monte Carlo Method for the Prediction of Behavior of Peptides. Current Protein and Peptide Science, 2019, 20, 1151-1157.	0.7	5
79	Whether the Validation of the Predictive Potential of Toxicity Models is a Solved Task?. Current Topics in Medicinal Chemistry, 2019, 19, 2643-2657.	1.0	5
80	Virtual Screening of Anti-Cancer Compounds: Application of Monte Carlo Technique. Anti-Cancer Agents in Medicinal Chemistry, 2019, 19, 148-153.	0.9	4
81	Mutagenicity, anticancer activity and blood brain barrier: similarity and dissimilarity of molecular alerts. Toxicology Mechanisms and Methods, 2018, 28, 321-327.	1.3	12
82	QSPR analysis of threshold of odor for the large number of heterogenic chemicals. Molecular Diversity, 2018, 22, 397-403.	2.1	3
83	CORAL: QSAR models for carcinogenicity of organic compounds for male and female rats. Computational Biology and Chemistry, 2018, 72, 26-32.	1.1	23
84	Use of quasi-SMILES to model biological activity of â€œmicelleâ€“polymerâ€•samples. Structural Chemistry, 2018, 29, 1213-1223.	1.0	10
85	Application of the Monte Carlo method for building up models for octanol-water partition coefficient of platinum complexes. Chemical Physics Letters, 2018, 701, 137-146.	1.2	16
86	The application of new HARD-descriptor available from the CORAL software to building up NOAEL models. Food and Chemical Toxicology, 2018, 112, 544-550.	1.8	33
87	Index of Ideality of Correlation: new possibilities to validate QSAR: a case study. Structural Chemistry, 2018, 29, 33-38.	1.0	61
88	Predicting Cytotoxicity of 2-Phenylindole Derivatives Against Breast Cancer Cells Using Index of Ideality of Correlation. Anticancer Research, 2018, 38, 6189-6194.	0.5	29
89	Use of the index of ideality of correlation to improve models of eco-toxicity. Environmental Science and Pollution Research, 2018, 25, 31771-31775.	2.7	27
90	The index of ideality of correlation: hierarchy of Monte Carlo models for glass transition temperatures of polymers. Journal of Polymer Research, 2018, 25, 1.	1.2	12

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91	Design and development of novel antibiotics based on FtsZ inhibition â€“ in silico studies. New Journal of Chemistry, 2018, 42, 10976-10982.	1.4	27
92	Prediction of antimicrobial activity of large pool of peptides using quasi-SMILES. BioSystems, 2018, 169-170, 5-12.	0.9	13
93	SAR for gastro-intestinal absorption and blood-brain barrier permeation of pesticides. Chemico-Biological Interactions, 2018, 290, 1-5.	1.7	10
94	CORAL: Predictive models for cytotoxicity of functionalized nanozeolites based on quasi-SMILES. Chemosphere, 2018, 210, 52-56.	4.2	15
95	Prediction of Biochemical Endpoints by the CORAL Software: Prejudices, Paradoxes, and Results. Methods in Molecular Biology, 2018, 1800, 573-583.	0.4	6
96	Quasi-SMILES as a tool to predict removal rates of pharmaceuticals and dyes in sewage. Chemical Engineering Research and Design, 2018, 118, 227-233.	2.7	11
97	Towards the Development of Global Nano-Quantitative Structureâ€“Property Relationship Models: Zeta Potentials of Metal Oxide Nanoparticles. Nanomaterials, 2018, 8, 243.	1.9	31
98	Editorial; Impact of Drug Metabolism and its Relevance upon Drug Discovery. Current Drug Metabolism, 2018, 18, 1070-1070.	0.7	0
99	CORAL: Monte Carlo Method to Predict Endpoints for Medical Chemistry. Mini-Reviews in Medicinal Chemistry, 2018, 18, 382-391.	1.1	20
100	Blood Brain Barrier and Alzheimerâ€™s Disease: Similarity and Dissimilarity of Molecular Alerts. Current Neuropharmacology, 2018, 16, 769-785.	1.4	19
101	Quantitative Structure-activity Relationship Study of Betulinic Acid Derivatives Against HIV using SMILES-based Descriptors. Current Computer-Aided Drug Design, 2018, 14, 152-159.	0.8	6
102	CORAL: Binary classifications (active/inactive) for drug-induced liver injury. Toxicology Letters, 2017, 268, 51-57.	0.4	38
103	Large-scale classification of P-glycoprotein inhibitors using SMILES-based descriptors. SAR and QSAR in Environmental Research, 2017, 28, 1-16.	1.0	18
104	Nano-QSAR in cell biology: Model of cell viability as a mathematical function of available eclectic data. Journal of Theoretical Biology, 2017, 416, 113-118.	0.8	36
105	CORAL and Nano-QFAR: Quantitative feature â€“ Activity relationships (QFAR) for bioavailability of nanoparticles (ZnO, CuO, Co 3 O 4 , and TiO 2). Ecotoxicology and Environmental Safety, 2017, 139, 404-407.	2.9	29
106	The index of ideality of correlation: A criterion of predictability of QSAR models for skin permeability?. Science of the Total Environment, 2017, 586, 466-472.	3.9	92
107	QSAR model for blood-brain barrier permeation. Journal of Pharmacological and Toxicological Methods, 2017, 88, 7-18.	0.3	33
108	The index of ideality of correlation: A criterion of predictive potential of QSPR/QSAR models?. Mutation Research - Genetic Toxicology and Environmental Mutagenesis, 2017, 819, 31-37.	0.9	107

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109	QSAR models for predicting acute toxicity of pesticides in rainbow trout using the CORAL software and EFSAâ€™s OpenFoodTox database. Environmental Toxicology and Pharmacology, 2017, 53, 158-163.	2.0	52
110	Hybrid optimal descriptors as a tool to predict skin sensitization in accordance to OECD principles. Toxicology Letters, 2017, 275, 57-66.	0.4	38
111	Prediction of gas chromatographic retention indices based on Monte Carlo method. Talanta, 2017, 168, 257-262.	2.9	11
112	Developing innovative in silico models with EFSA's OpenFoodTox database. EFSA Supporting Publications, 2017, 14, 1206E.	0.3	10
113	QSAR of antimycobacterial activity of benzoxazoles by optimal SMILES-based descriptors. Medicinal Chemistry Research, 2017, 26, 3203-3208.	1.1	6
114	Quasi-SMILES as a Novel Tool for Prediction of Nanomaterialsâ€² Endpoints. , 2017, , 191-221.		5
115	CORAL Software: Analysis of Impacts of Pharmaceutical Agents Upon Metabolism via the Optimal Descriptors. Current Drug Metabolism, 2017, 18, 500-510.	0.7	10
116	Utilization of the Monte Carlo Method to Build up QSAR Models for Hemolysis and Cytotoxicity of Antimicrobial Peptides. Current Drug Discovery Technologies, 2017, 14, 229-243.	0.6	17
117	Quasi-SMILES for Nano-QSAR Prediction of Toxic Effect of Al2O3 Nanoparticles. , 2017, , 1573-1584.		0
118	QSPR/QSAR Analyses by Means of the CORAL Software. , 2017, , 929-955.		0
119	Quasi-SMILES for Nano-QSAR Prediction of Toxic Effect of Al2O3 Nanoparticles. , 2017, , 1624-1635.		0
120	Quasi-SMILES for Nano-QSAR Prediction of Toxic Effect of Al2O3 Nanoparticles. Journal of Nanotoxicology and Nanomedicine, 2016, 1, 17-28.	0.7	6
121	QSAR as a Random Event: Selecting of the Molecular Structure for Potential Anti-tuberculosis Agents. Anti-Infective Agents, 2016, 14, 3-10.	0.1	7
122	Evolution of Optimal Descriptors. International Journal of Quantitative Structure-Property Relationships, 2016, 1, 52-71.	1.1	0
123	Towards predicting the solubility of CO₂and N₂in different polymers using a quasi-SMILES based QSPR approach. SAR and QSAR in Environmental Research, 2016, 27, 293-301.	1.0	11
124	Improved building up a model of toxicity towards Pimephales promelas by the Monte Carlo method. Environmental Toxicology and Pharmacology, 2016, 48, 278-285.	2.0	8
125	A quasi-SMILES based QSPR Approach towards the prediction of adsorption energy of Ziegler â˜’ Natta catalysts for propylene polymerization. Materials Discovery, 2016, 5, 22-28.	3.3	13
126	QSAR Model for Cytotoxicity of Silica Nanoparticles on Human Embryonic Kidney Cells1. Materials Today: Proceedings, 2016, 3, 847-854.	0.9	10

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127	Quasi-SMILES as a tool to utilize eclectic data for predicting the behavior of nanomaterials. NanoImpact, 2016, 1, 60-64.	2.4	24
128	Development of the Latest Tools for Building up â€œNano-QSARâ€• Quantitative Featuresâ€”Property/Activity Relationships (QFPRs/QFARs). , 2016, , 353-396.		0
129	The Monte Carlo technique as a tool to predict LOAEL. European Journal of Medicinal Chemistry, 2016, 116, 71-75.	2.6	34
130	Quasi-SMILES and nano-QFPR: The predictive model for zeta potentials of metal oxide nanoparticles. Chemical Physics Letters, 2016, 660, 107-110.	1.2	36
131	Odor threshold prediction by means of the Monte Carlo method. Ecotoxicology and Environmental Safety, 2016, 133, 390-394.	2.9	9
132	Assessment of nano-QSPR models of organic contaminant absorption by carbon nanotubes for ecological impact studies. Materials Discovery, 2016, 4, 22-28.	3.3	5
133	Monte Carloâ€“based quantitative structureâ€“activity relationship models for toxicity of organic chemicals to Daphnia magna. Environmental Toxicology and Chemistry, 2016, 35, 2691-2697.	2.2	24
134	Building up a QSAR model for toxicity toward Tetrahymena pyriformis by the Monte Carlo method: A case of benzene derivatives. Environmental Toxicology and Pharmacology, 2016, 42, 135-145.	2.0	23
135	Model for electrochemical parameters for 4-(benzylsulfanyl)pyridines calculated from the molecular structure. Journal of Electroanalytical Chemistry, 2016, 766, 24-29.	1.9	2
136	QSAR model for predicting cell viability of human embryonic kidney cells exposed to SiO2 nanoparticles. Chemosphere, 2016, 144, 995-1001.	4.2	40
137	QSPR models for estimating retention in HPLC with the p solute polarity parameter based on the Monte Carlo method. Structural Chemistry, 2016, 27, 821-828.	1.0	7
138	Nano-QSAR: Model of mutagenicity of fullerene as a mathematical function of different conditions. Ecotoxicology and Environmental Safety, 2016, 124, 32-36.	2.9	40
139	QSPR Model for Dispersibility of Graphene in Various Solvents. Letters in Drug Design and Discovery, 2016, 13, 514-520.	0.4	1
140	Editorial (Thematic Issue: From Chemoinformatics to Nanoinformatics: New Tools for Drug Discovery) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 1767-1767.	1.0	3
141	A quasi-QSPR modelling for the photocatalytic decolourization rate constants and cellular viability (CV%) of nanoparticles by CORAL. SAR and QSAR in Environmental Research, 2015, 26, 29-40.	1.0	23
142	QSAR model as a random event: A case of rat toxicity. Bioorganic and Medicinal Chemistry, 2015, 23, 1223-1230.	1.4	36
143	Quasi-SMILES and nano-QFAR: United model for mutagenicity of fullerene and MWCNT under different conditions. Chemosphere, 2015, 139, 18-22.	4.2	66
144	QSAR models for 1,2,4-benzotriazines as Src inhibitors based on Monte Carlo method. Medicinal Chemistry Research, 2015, 24, 283-290.	1.1	5

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145	Large-scale structure-activity relationship study of hepatitis C virus NS5B polymerase inhibition using SMILES-based descriptors. Molecular Diversity, 2015, 19, 955-964.	2.1	13
146	CORAL: Model for octanol/water partition coefficient. Fluid Phase Equilibria, 2015, 397, 44-49.	1.4	15
147	CORAL: model for no observed adverse effect level (NOAEL). Molecular Diversity, 2015, 19, 563-575.	2.1	20
148	Prediction of retention characteristics of heterocyclic compounds. Analytical and Bioanalytical Chemistry, 2015, 407, 9185-9189.	1.9	2
149	Prediction of the Q-e parameters from structures of transfer chain agents. Journal of Polymer Research, 2015, 22, 1.	1.2	2
150	CORAL: Prediction of binding affinity and efficacy of thyroid hormone receptor ligands. European Journal of Medicinal Chemistry, 2015, 101, 452-461.	2.6	17
151	In silico prediction of the Î²-cyclodextrin complexation based on Monte Carlo method. International Journal of Pharmaceutics, 2015, 495, 404-409.	2.6	21
152	Monte Carlo Methodâ€Based QSAR Modeling of Penicillins Binding to Human Serum Proteins. Archiv Der Pharmazie, 2015, 348, 62-67.	2.1	24
153	QSAR as a random event: a case of NOAEL. Environmental Science and Pollution Research, 2015, 22, 8264-8271.	2.7	43
154	Quasi-QSAR for mutagenic potential of multi-walled carbon-nanotubes. Chemosphere, 2015, 124, 40-46.	4.2	71
155	QSPR studies on refractive indices of structurally heterogeneous polymers. Chemometrics and Intelligent Laboratory Systems, 2015, 140, 86-91.	1.8	50
156	Optimal nano-descriptors as translators of eclectic data into prediction of the cell membrane damage by means of nano metal-oxides. Environmental Science and Pollution Research, 2015, 22, 745-757.	2.7	41
157	Optimal descriptor as a translator of eclectic data into prediction of cytotoxicity for metal oxide nanoparticles under different conditions. Ecotoxicology and Environmental Safety, 2015, 112, 39-45.	2.9	83
158	The Monte Carlo Method Based on Eclectic Data as an Efficient Tool for Predictions of Endpoints for Nanomaterials - Two Examples of Application. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 376-386.	0.6	10
159	Mutagenicity: QSAR - quasi-QSAR - nano-QSAR. Mini-Reviews in Medicinal Chemistry, 2015, 15, 608-621.	1.1	29
160	Use of Quasi-SMILES and Monte Carlo Optimization to Develop Quantitative Feature Property/Activity Relationships (QFPR/QFAR) for Nanomaterials. Current Topics in Medicinal Chemistry, 2015, 15, 1837-1844.	1.0	20
161	QSAR Models for the Reactivation of Sarin Inhibited Acetylcholinesterase by Quaternary Pyridinium Oximes Based on Monte Carlo Method. Current Computer-Aided Drug Design, 2015, 10, 266-273.	0.8	5
162	QSPR/QSAR Analyses by Means of the CORAL Software. Advances in Chemical and Materials Engineering Book Series, 2015, , 560-585.	0.2	10

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163	Discovery of Potential, Nonâ€Toxic Influenza Virus Inhibitor by Computational Techniques. Molecular Informatics, 2014, 33, 559-565.	1.4	6
164	Monte Carlo Method Based QSAR Modeling of Coumarin Derivates as Potent HIVâ€1 Integrase Inhibitors and Molecular Docking Studies of Selected 4â€phenyl Hydroxycoumarins. Acta Facultatis Medicae Naissensis, 2014, 31, 95-103.	0.1	14
165	SMILES-based quantitative structureâ€“retention relationships for RP HPLC of 1-phenyl-5-benzylsulfanyltetrazoles. Structural Chemistry, 2014, 25, 311-317.	1.0	13
166	Building up QSAR model for toxicity of psychotropic drugs by the Monte Carlo method. Structural Chemistry, 2014, 25, 1067-1073.	1.0	7
167	Optimal descriptors as a tool to predict the thermal decomposition of polymers. Journal of Mathematical Chemistry, 2014, 52, 1171-1181.	0.7	15
168	CORAL software: Prediction of carcinogenicity of drugs by means of the Monte Carlo method. European Journal of Pharmaceutical Sciences, 2014, 52, 21-25.	1.9	77
169	Conformation-independent QSAR on c-Src tyrosine kinase inhibitors. Chemometrics and Intelligent Laboratory Systems, 2014, 134, 47-52.	1.8	10
170	Comprehension of drug toxicity: Software and databases. Computers in Biology and Medicine, 2014, 45, 20-25.	3.9	69
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