Andrey Toropov

List of Publications by Year in Descending Order

317 papers	6,116 citations	38 h-index	55 g-index
338 ext. papers	6,652 ext. citations	3.9 avg, IF	6.54 L-index

#	Paper	IF	Citations
317	The system of self-consistent QSPR-models for refractive index of polymers. *Structural Chemistry*, **2022**, 33, 617	1.8	1
316	The system of self-consistent models for vapour pressure. *Chemical Physics Letters*, **2022**, 790, 139354	2.5	2
315	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	3.8	1
314	How fullerene derivatives (FDs) act on therapeutically important targets associated with diabetic diseases.. *Computational and Structural Biotechnology Journal*, **2022**, 20, 913-924	6.8	3
313	Nanomaterials: Quasi-SMILES as a flexible basis for regulation and environmental risk assessment.. *Science of the Total Environment*, **2022**, 823, 153747	10.2	6
312	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	12.8	6
311	In Silico Methods for Environmental Risk Assessment: Principles, Tiered Approaches, Applications, and Future Perspectives.. *Methods in Molecular Biology*, **2022**, 2425, 589-636	1.4	4
310	The searching for agents for Alzheimer's disease treatment via the system of self-consistent models.. *Toxicology Mechanisms and Methods*, **2022**, 1-26	3.6	2
309	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	10.2	0
308	Use of quasi-SMILES to build models based on quantitative results from experiments with nanomaterials. *Chemosphere*, **2022**, 135086	8.4	2
307	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	3.6	2
306	Can the Monte Carlo method predict the toxicity of binary mixtures?. *Environmental Science and Pollution Research*, **2021**, 28, 39493-39500	5.1	3
305	Maintenance, update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0. *EFSA Supporting Publications*, **2021**, 18, 6476E	1.1	1
304	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	3.5	5
303	The self-organizing vector of atom-pairs proportions: use to develop models for melting points. *Structural Chemistry*, **2021**, 32, 967-971	1.8	3
302	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	4.4	4
301	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	7	6

300	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	2.9	6
299	Quasi-SMILES as a basis for the development of models for the toxicity of ZnO nanoparticles. *Science of the Total Environment*, **2021**, 772, 145532	10.2	9
298	The QSAR-search of effective agents towards coronaviruses applying the Monte Carlo method. *SAR and QSAR in Environmental Research*, **2021**, 32, 689-698	3.5	1
297	Pesticides, cosmetics, drugs: identical and opposite influences of various molecular features as measures of endpoints similarity and dissimilarity. *Molecular Diversity*, **2021**, 25, 1137-1144	3.1	2
296	Integrated 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	4	5
295	EFSA's OpenFoodTox: An open source toxicological database on chemicals in food and feed and its future developments. *Environment International*, **2021**, 146, 106293	12.9	19
294	Prediction of the self-accelerating decomposition temperature of organic peroxides. *Process Safety Progress*, **2021**, 40, e12189	1	1
293	Paradox of 'ideal correlations': improved model for air half-life of persistent organic pollutants. *Environmental Technology (United Kingdom)*, **2021**, 1-6	2.6	3
292	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	5.8	7
291	Application of quasi-SMILES to the model of gold-nanoparticles uptake in A549 cells. *Computers in Biology and Medicine*, **2021**, 136, 104720	7	2
290	Semi-correlations as a tool to model for skin sensitization. *Food and Chemical Toxicology*, **2021**, 157, 112580	4.7	0
289	The sequence of amino acids as the basis for the model of biological activity of peptides. *Theoretical Chemistry Accounts*, **2021**, 140, 15	1.9	2
288	The system of self-consistent models for the uptake of nanoparticles in PaCa2 cancer cells. *Nanotoxicology*, **2021**, 15, 995-1004	5.3	4
287	Maintenance,update and further development of EFSA's Chemical Hazards: OpenFoodTox 2.0. *EFSA Supporting Publications*, **2020**, 17, 1822E	1.1	3
286	Integrating QSAR models predicting acute contact toxicity and mode of action profiling in honey bees (A. mellifera): Data curation using open source databases, performance testing and validation. *Science of the Total Environment*, **2020**, 735, 139243	10.2	12
285	QSPR/QSAR: State-of-Art, Weirdness, the Future. *Molecules*, **2020**, 25,	4.8	18
284	Fullerenes C60 and C70: a model for solubility by applying the correlation intensity index. *Fullerenes Nanotubes and Carbon Nanostructures*, **2020**, 28, 900-906	1.8	8
283	Correlation intensity index: Building up models for mutagenicity of silver nanoparticles. *Science of the Total Environment*, **2020**, 737, 139720	10.2	13

282	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	5.1	16
281	The index of ideality of correlation: models of the flash points of ternary mixtures. *New Journal of Chemistry*, **2020**, 44, 4858-4868	3.6	9
280	QSAR models for biocides: The example of the prediction of acute toxicity. *SAR and QSAR in Environmental Research*, **2020**, 31, 227-243	3.5	18
279	The Use of the Index of Ideality of Correlation to Build Up Models for Bioconcentration Factor. *Molecular Informatics*, **2020**, 39, e1900070	3.8	8
278	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	1.8	2
277	The Monte Carlo Method as a Tool to Build up Predictive QSPR/QSAR. *Current Computer-Aided Drug Design*, **2020**, 16, 197-206	1.4	5
276	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	2.5	11
275	QSAR-Models, Validation, and IIC-Paradox for Drug Toxicity. *International Journal of Quantitative Structure-Property Relationships*, **2020**, 5, 22-43	1.2	1
274	Exploring QSAR modeling of toxicity of chemicals on earthworm. *Ecotoxicology and Environmental Safety*, **2020**, 190, 110067	7	16
273	Use of the index of ideality of correlation to improve aquatic solubility model. *Journal of Molecular Graphics and Modelling*, **2020**, 96, 107525	2.8	11
272	First report on a classification-based QSAR model for chemical toxicity to earthworm. *Journal of Hazardous Materials*, **2020**, 386, 121660	12.8	14
271	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	10.2	21
270	How the CORAL software can be used to select compounds for efficient treatment of neurodegenerative diseases?. *Toxicology and Applied Pharmacology*, **2020**, 408, 115276	4.6	6
269	Zebrafish AC modelling: (Q)SAR models to predict developmental toxicity in zebrafish embryo. *Ecotoxicology and Environmental Safety*, **2020**, 202, 110936	7	5
268	QSAR model for pesticides toxicity to Rainbow Trout based on "ideal correlations". *Aquatic Toxicology*, **2020**, 227, 105589	5.1	8
267	Ecosystem ecology: Models for acute toxicity of pesticides towards Daphnia magna. *Environmental Toxicology and Pharmacology*, **2020**, 80, 103459	5.8	6
266	Advancement of predictive modeling of zeta potentials (ζ) in metal oxide nanoparticles with correlation intensity index (CII). *Journal of Molecular Liquids*, **2020**, 317, 113929	6	9
265	Applying the Monte Carlo technique to build up models of glass transition temperatures of diverse polymers. *Structural Chemistry*, **2020**, 31, 1739-1743	1.8	3

264	'Ideal correlations' for the predictive toxicity to. *Toxicology Mechanisms and Methods*, **2020**, 30, 605-610	3.6	5
263	Correlation intensity index: mathematical modeling of cytotoxicity of metal oxide nanoparticles. *Nanotoxicology*, **2020**, 14, 1118-1126	5.3	20
262	SARS-CoV M inhibitory activity of aromatic disulfide compounds: QSAR model. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-7	3.6	13
261	Prediction of No Observed Adverse Effect Concentration for inhalation toxicity using Monte Carlo approach. *SAR and QSAR in Environmental Research*, **2020**, 31, 1-12	3.5	6
260	The index of ideality of correlation: models for flammability of binary liquid mixtures. *Chemical Papers*, **2020**, 74, 601-609	1.9	13
259	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	3.5	16
258	QSAR as a random event: criteria of predictive potential for a chance model. *Structural Chemistry*, **2019**, 30, 1677-1683	1.8	20
257	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	10.2	19
256	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	7	17
255	"Ideal correlations" for biological activity of peptides. *BioSystems*, **2019**, 181, 51-57	1.9	7
254	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	2.9	7
253	Does the Index of Ideality of Correlation Detect the Better Model Correctly?. *Molecular Informatics*, **2019**, 38, e1800157	3.8	36
252	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	4.2	10
251	Use of the index of ideality of correlation to improve predictive potential for biochemical endpoints. *Toxicology Mechanisms and Methods*, **2019**, 29, 43-52	3.6	24
250	CORAL: Building up QSAR models for the chromosome aberration test. *Saudi Journal of Biological Sciences*, **2019**, 26, 1101-1106	4	15
249	QSPR as a random event: solubility of fullerenes C[60] and C[70]. *Fullerenes Nanotubes and Carbon Nanostructures*, **2019**, 27, 816-821	1.8	5
248	Investigating combined toxicity of binary mixtures in bees: Meta-analysis of laboratory tests, modelling, mechanistic basis and implications for risk assessment. *Environment International*, **2019**, 133, 105256	12.9	33
247	Application of the Monte Carlo Method for the Prediction of Behavior of Peptides. *Current Protein and Peptide Science*, **2019**, 20, 1151-1157	2.8	3

246	Whether the Validation of the Predictive Potential of Toxicity Models is a Solved Task?. *Current Topics in Medicinal Chemistry*, **2019**, 19, 2643-2657	3	4
245	Virtual Screening of Anti-Cancer Compounds: Application of Monte Carlo Technique. *Anti-Cancer Agents in Medicinal Chemistry*, **2019**, 19, 148-153	2.2	3
244	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	3.8	13
243	Semi-correlations as a tool to build up categorical (active/inactive) model of GABAA receptor modulator activity. *Structural Chemistry*, **2019**, 30, 853-861	1.8	6
242	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	10.2	32
241	QSPR and nano-QSPR: What is the difference?. *Journal of Molecular Structure*, **2019**, 1182, 141-149	3.4	38
240	Quasi-SMILES: quantitative structure-activity relationships to predict anticancer activity. *Molecular Diversity*, **2019**, 23, 403-412	3.1	12
239	The index of ideality of correlation: improvement of models for toxicity to algae. *Natural Product Research*, **2019**, 33, 2200-2207	2.3	19
238	QSAR Development for Plasma Protein Binding: Influence of the Ionization State. *Pharmaceutical Research*, **2018**, 36, 28	4.5	8
237	Mutagenicity, anticancer activity and blood brain barrier: similarity and dissimilarity of molecular alerts. *Toxicology Mechanisms and Methods*, **2018**, 28, 321-327	3.6	8
236	QSPR analysis of threshold of odor for the large number of heterogenic chemicals. *Molecular Diversity*, **2018**, 22, 397-403	3.1	3
235	CORAL: QSAR models for carcinogenicity of organic compounds for male and female rats. *Computational Biology and Chemistry*, **2018**, 72, 26-32	3.6	19
234	Use of quasi-SMILES to model biological activity of micelle polymer samples. *Structural Chemistry* , **2018**, 29, 1213-1223	1.8	7
233	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	2.5	14
232	The application of new HARD-descriptor available from the CORAL software to building up NOAEL models. *Food and Chemical Toxicology*, **2018**, 112, 544-550	4.7	26
231	Index of Ideality of Correlation: new possibilities to validate QSAR: a case study. *Structural Chemistry*, **2018**, 29, 33-38	1.8	47
230	Quasi-SMILES as a tool to predict removal rates of pharmaceuticals and dyes in sewage. *Chemical Engineering Research and Design*, **2018**, 118, 227-233	5.5	9
229	Towards the Development of Global Nano-Quantitative Structure-Property Relationship Models: Zeta Potentials of Metal Oxide Nanoparticles. *Nanomaterials*, **2018**, 8,	5.4	22

228	CORAL: Monte Carlo Method to Predict Endpoints for Medical Chemistry. *Mini-Reviews in Medicinal Chemistry*, **2018**, 18, 382-391	3.2	15
227	Blood Brain Barrier and Alzheimer's Disease: Similarity and Dissimilarity of Molecular Alerts. *Current Neuropharmacology*, **2018**, 16, 769-785	7.6	13
226	Quantitative Structure-activity Relationship Study of Betulinic Acid Derivatives Against HIV using SMILES-based Descriptors. *Current Computer-Aided Drug Design*, **2018**, 14, 152-159	1.4	6
225	Improved Model for Biodegradability of Organic Compounds: The Correlation Contributions of Rings. *Methods in Pharmacology and Toxicology*, **2018**, 147-183	1.1	6
224	Predicting Cytotoxicity of 2-Phenylindole Derivatives Against Breast Cancer Cells Using Index of Ideality of Correlation. *Anticancer Research*, **2018**, 38, 6189-6194	2.3	22
223	Use of the index of ideality of correlation to improve models of eco-toxicity. *Environmental Science and Pollution Research*, **2018**, 25, 31771-31775	5.1	24
222	The index of ideality of correlation: hierarchy of Monte Carlo models for glass transition temperatures of polymers. *Journal of Polymer Research*, **2018**, 25, 1	2.7	11
221	Design and development of novel antibiotics based on FtsZ inhibition In silico studies. *New Journal of Chemistry*, **2018**, 42, 10976-10982	3.6	19
220	Prediction of antimicrobial activity of large pool of peptides using quasi-SMILES. *BioSystems*, **2018**, 169-170, 5-12	1.9	6
219	SAR for gastro-intestinal absorption and blood-brain barrier permeation of pesticides. *Chemico-Biological Interactions*, **2018**, 290, 1-5	5	7
218	CORAL: Predictive models for cytotoxicity of functionalized nanozeolites based on quasi-SMILES. *Chemosphere*, **2018**, 210, 52-56	8.4	9
217	Prediction of Biochemical Endpoints by the CORAL Software: Prejudices, Paradoxes, and Results. *Methods in Molecular Biology*, **2018**, 1800, 573-583	1.4	3
216	CORAL: Binary classifications (active/inactive) for drug-induced liver injury. *Toxicology Letters*, **2017**, 268, 51-57	4.4	29
215	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	2.3	33
214	CORAL and Nano-QFAR: Quantitative feature - Activity relationships (QFAR) for bioavailability of nanoparticles (ZnO, CuO, CoO, and TiO). *Ecotoxicology and Environmental Safety*, **2017**, 139, 404-407	7	25
213	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	10.2	68
212	QSAR model for blood-brain barrier permeation. *Journal of Pharmacological and Toxicological Methods*, **2017**, 88, 7-18	1.7	23
211	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	3	77

210	QSAR models for predicting acute toxicity of pesticides in rainbow trout using the CORAL software and EFSA's OpenFoodTox database. *Environmental Toxicology and Pharmacology*, **2017**, 53, 158-163	5.8	42
209	Hybrid optimal descriptors as a tool to predict skin sensitization in accordance to OECD principles. *Toxicology Letters*, **2017**, 275, 57-66	4.4	27
208	Prediction of gas chromatographic retention indices based on Monte Carlo method. *Talanta*, **2017**, 168, 257-262	6.2	9
207	Quasi-SMILES as a Novel Tool for Prediction of Nanomaterials? Endpoints **2017**, 191-221		3
206	Developing innovative in silico models with EFSA's OpenFoodTox database. *EFSA Supporting Publications*, **2017**, 14, 1206E	1.1	8
205	QSAR of antimycobacterial activity of benzoxazoles by optimal SMILES-based descriptors. *Medicinal Chemistry Research*, **2017**, 26, 3203-3208	2.2	4
204	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	1.5	16
203	Development of Monte Carlo Approaches in Support of Environmental Research. *Challenges and Advances in Computational Chemistry and Physics*, **2017**, 453-469	0.7	2
202	Quasi-SMILES for Nano-QSAR Prediction of Toxic Effect of Al2O3 Nanoparticles **2017**, 1573-1584		
201	QSPR/QSAR Analyses by Means of the CORAL Software **2017**, 929-955		
200	Quasi-SMILES for Nano-QSAR Prediction of Toxic Effect of Al2O3 Nanoparticles **2017**, 1624-1635		
199	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	1.8	7
198	Nano-QSAR: Model of mutagenicity of fullerene as a mathematical function of different conditions. *Ecotoxicology and Environmental Safety*, **2016**, 124, 32-36	7	33
197	Odor threshold prediction by means of the Monte Carlo method. *Ecotoxicology and Environmental Safety*, **2016**, 133, 390-4	7	8
196	Assessment of nano-QSPR models of organic contaminant absorption by carbon nanotubes for ecological impact studies. *Materials Discovery*, **2016**, 4, 22-28		5
195	Quantitative structure□ctivity relationship models for bee toxicity. *Toxicological and Environmental Chemistry*, **2016**, 1-12	1.4	2
194	Monte Carlo-based quantitative structure-activity relationship models for toxicity of organic chemicals to Daphnia magna. *Environmental Toxicology and Chemistry*, **2016**, 35, 2691-2697	3.8	21
193	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, 135-45	5.8	21

192	Model for electrochemical parameters for 4-(benzylsulfanyl)pyridines calculated from the molecular structure. *Journal of Electroanalytical Chemistry*, **2016**, 766, 24-29	4.1	0
191	QSAR model for predicting cell viability of human embryonic kidney cells exposed to SiO nanoparticles. *Chemosphere*, **2016**, 144, 995-1001	8.4	30
190	The Utilization of the Monte Carlo Technique for Rational Drug Discovery. *Combinatorial Chemistry and High Throughput Screening*, **2016**, 19, 676-687	1.3	14
189	Quasi-SMILES for Nano-QSAR Prediction of Toxic Effect of Al2O3 Nanoparticles. *Journal of Nanotoxicology and Nanomedicine*, **2016**, 1, 17-28		6
188	QSAR as a Random Event: Selecting of the Molecular Structure for Potential Anti-tuberculosis Agents. *Anti-Infective Agents*, **2016**, 14, 3-10	0.6	6
187	Evolution of Optimal Descriptors. *International Journal of Quantitative Structure-Property Relationships*, **2016**, 1, 52-71	1.2	
186	Towards predicting the solubility of CO2 and N2 in different polymers using a quasi-SMILES based QSPR approach. *SAR and QSAR in Environmental Research*, **2016**, 27, 293-301	3.5	7
185	Improved building up a model of toxicity towards Pimephales promelas by the Monte Carlo method. *Environmental Toxicology and Pharmacology*, **2016**, 48, 278-285	5.8	7
184	A quasi-SMILES based QSPR Approach towards the prediction of adsorption energy of Ziegler Natta catalysts for propylene polymerization. *Materials Discovery*, **2016**, 5, 22-28		10
183	QSAR Model for Cytotoxicity of Silica Nanoparticles on Human Embryonic Kidney Cells1. *Materials Today: Proceedings*, **2016**, 3, 847-854	1.4	9
182	Quasi-SMILES as a tool to utilize eclectic data for predicting the behavior of nanomaterials. *NanoImpact*, **2016**, 1, 60-64	5.6	18
181	Development of the Latest Tools for Building up Nano-QSAR Quantitative Features roperty/Activity Relationships (QFPRs/QFARs) **2016**, 353-396		
180	The Monte Carlo technique as a tool to predict LOAEL. *European Journal of Medicinal Chemistry*, **2016**, 116, 71-75	6.8	26
179	Monte Carlo method for predicting of cardiac toxicity: hERG blocker compounds. *Toxicology Letters*, **2016**, 250-251, 42-6	4.4	26
178	Quasi-SMILES and nano-QFPR: The predictive model for zeta potentials of metal oxide nanoparticles. *Chemical Physics Letters*, **2016**, 660, 107-110	2.5	27
177	QSAR models for 1,2,4-benzotriazines as Src inhibitors based on Monte Carlo method. *Medicinal Chemistry Research*, **2015**, 24, 283-290	2.2	5
176	Searching therapeutic agents for treatment of Alzheimer disease using the Monte Carlo method. *Computers in Biology and Medicine*, **2015**, 64, 148-54	7	28
175	Large-scale structure-activity relationship study of hepatitis C virus NS5B polymerase inhibition using SMILES-based descriptors. *Molecular Diversity*, **2015**, 19, 955-64	3.1	11

174	CORAL: Model for octanol/water partition coefficient. *Fluid Phase Equilibria*, **2015**, 397, 44-49	2.5	10
173	CORAL: model for no observed adverse effect level (NOAEL). *Molecular Diversity*, **2015**, 19, 563-75	3.1	15
172	Amino substituted nitrogen heterocycle ureas as kinase insert domain containing receptor (KDR) inhibitors: Performance of structure-activity relationship approaches. *Journal of Food and Drug Analysis*, **2015**, 23, 168-175	7	7
171	Prediction of retention characteristics of heterocyclic compounds. *Analytical and Bioanalytical Chemistry*, **2015**, 407, 9185-9	4.4	2
170	QSAR modeling of the antimicrobial activity of peptides as a mathematical function of a sequence of amino acids. *Computational Biology and Chemistry*, **2015**, 59 Pt A, 126-30	3.6	29
169	Prediction of the Q-e parameters from structures of transfer chain agents. *Journal of Polymer Research*, **2015**, 22, 1	2.7	2
168	CORAL: prediction of binding affinity and efficacy of thyroid hormone receptor ligands. *European Journal of Medicinal Chemistry*, **2015**, 101, 452-61	6.8	15
167	In silico prediction of the Ecyclodextrin complexation based on Monte Carlo method. *International Journal of Pharmaceutics*, **2015**, 495, 404-409	6.5	15
166	Monte carlo method-based QSAR modeling of penicillins binding to human serum proteins. *Archiv Der Pharmazie*, **2015**, 348, 62-7	4.3	21
165	QSAR as a random event: a case of NOAEL. *Environmental Science and Pollution Research*, **2015**, 22, 8264-71	5.1	36
164	Quasi-QSAR for mutagenic potential of multi-walled carbon-nanotubes. *Chemosphere*, **2015**, 124, 40-6	8.4	60
163	QSPR studies on refractive indices of structurally heterogeneous polymers. *Chemometrics and Intelligent Laboratory Systems*, **2015**, 140, 86-91	3.8	39
162	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, 745-57	5.1	33
161	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	7	70
160	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	3.5	22
159	QSAR model as a random event: A case of rat toxicity. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 1223-30	3.4	31
158	Quasi-SMILES and nano-QFAR: united model for mutagenicity of fullerene and MWCNT under different conditions. *Chemosphere*, **2015**, 139, 18-22	8.4	52
157	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, 376-86	1.3	7

156	Mutagenicity: QSAR - quasi-QSAR - nano-QSAR. *Mini-Reviews in Medicinal Chemistry*, **2015**, 15, 608-21	3.2	24
155	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, 1837-44	3	18
154	QSPR/QSAR Analyses by Means of the CORAL Software. *Advances in Chemical and Materials Engineering Book Series*, **2015**, 560-585	0.2	6
153	Optimal descriptors as a tool to predict the thermal decomposition of polymers. *Journal of Mathematical Chemistry*, **2014**, 52, 1171-1181	2.1	13
152	CORAL software: prediction of carcinogenicity of drugs by means of the Monte Carlo method. *European Journal of Pharmaceutical Sciences*, **2014**, 52, 21-5	5.1	65
151	Conformation-independent QSAR on c-Src tyrosine kinase inhibitors. *Chemometrics and Intelligent Laboratory Systems*, **2014**, 134, 47-52	3.8	9
150	Comprehension of drug toxicity: software and databases. *Computers in Biology and Medicine*, **2014**, 45, 20-5	7	45
149	Optimal descriptor as a translator of eclectic data into endpoint prediction: mutagenicity of fullerene as a mathematical function of conditions. *Chemosphere*, **2014**, 104, 262-4	8.4	46
148	QSAR model for cytotoxicity of SiO2 nanoparticles on human lung fibroblasts. *Journal of Nanoparticle Research*, **2014**, 16, 1	2.3	17
147	Aconitum and delphinium diterpenoid alkaloids of local anesthetic activity: comparative QSAR analysis based on GA-MLRA/PLS and optimal descriptors approach. *Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews*, **2014**, 32, 213-38	4.5	11
146	Large-scale QSAR study of aromatase inhibitors using SMILES-based descriptors. *Chemometrics and Intelligent Laboratory Systems*, **2014**, 138, 120-126	3.8	43
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