Andrey Toropov

List of Publications by Citations

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	Using nano-QSAR to predict the cytotoxicity of metal oxide nanoparticles. *Nature Nanotechnology*, **2011**, 6, 175-8	28.7	551
316	QSAR as a random event: modeling of nanoparticles uptake in PaCa2 cancer cells. *Chemosphere*, **2013**, 92, 31-7	8.4	114
315	CORAL: quantitative structure-activity relationship models for estimating toxicity of organic compounds in rats. *Journal of Computational Chemistry*, **2011**, 32, 2727-33	3.5	80
314	Novel application of the CORAL software to model cytotoxicity of metal oxide nanoparticles to bacteria Escherichia coli. *Chemosphere*, **2012**, 89, 1098-102	8.4	78
313	Special Issue on Flexible Molecular Descriptors. *Molecules*, **2004**, 9, 988-988	4.8	78
312	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
311	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
310	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
309	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
308	Quasi-QSAR for mutagenic potential of multi-walled carbon-nanotubes. *Chemosphere*, **2015**, 124, 40-6	8.4	60
307	In silico methods to predict drug toxicity. *Current Opinion in Pharmacology*, **2013**, 13, 802-6	5.1	58
306	Quasi-SMILES and nano-QFAR: united model for mutagenicity of fullerene and MWCNT under different conditions. *Chemosphere*, **2015**, 139, 18-22	8.4	52
305	Optimal descriptor as a translator of eclectic information into the prediction of membrane damage by means of various TiO(2) nanoparticles. *Chemosphere*, **2013**, 93, 2650-5	8.4	51
304	QSAR models for HEPT derivates as NNRTI inhibitors based on Monte Carlo method. *European Journal of Medicinal Chemistry*, **2014**, 77, 298-305	6.8	50
303	SMILES-based QSAR model for arylpiperazines as high-affinity 5-HT(1A) receptor ligands using CORAL. *European Journal of Pharmaceutical Sciences*, **2013**, 48, 532-41	5.1	50
302	Predicting water solubility and octanol water partition coefficient for carbon nanotubes based on the chiral vector. *Computational Biology and Chemistry*, **2007**, 31, 127-8	3.6	48
301	Index of Ideality of Correlation: new possibilities to validate QSAR: a case study. *Structural Chemistry*, **2018**, 29, 33-38	1.8	47

300	CORAL: QSAR modeling of toxicity of organic chemicals towards Daphnia magna. *Chemometrics and Intelligent Laboratory Systems*, **2012**, 110, 177-181	3.8	47
299	Prediction of heteroaromatic amine mutagenicity by means of correlation weighting of atomic orbital graphs of local invariants. *Computational and Theoretical Chemistry*, **2001**, 538, 287-293		47
298	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
297	QSAR modeling of acute toxicity by balance of correlations. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 5999-6008	3.4	46
296	Comprehension of drug toxicity: software and databases. *Computers in Biology and Medicine*, **2014**, 45, 20-5	7	45
295	CORAL: building up the model for bioconcentration factor and defining it's applicability domain. *European Journal of Medicinal Chemistry*, **2011**, 46, 1400-3	6.8	45
294	Large-scale QSAR study of aromatase inhibitors using SMILES-based descriptors. *Chemometrics and Intelligent Laboratory Systems*, **2014**, 138, 120-126	3.8	43
293	Improved model for fullerene C60 solubility in organic solvents based on quantum-chemical and topological descriptors. *Journal of Nanoparticle Research*, **2011**, 13, 3235-3247	2.3	43
292	SMILES as an alternative to the graph in QSAR modelling of bee toxicity. *Computational Biology and Chemistry*, **2007**, 31, 57-60	3.6	43
291	Additive SMILES-based optimal descriptors in QSAR modelling bee toxicity: Using rare SMILES attributes to define the applicability domain. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 4801-9	3.4	43
290	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
289	QSAR modeling of measured binding affinity for fullerene-based HIV-1 PR inhibitors by CORAL. *Journal of Mathematical Chemistry*, **2010**, 48, 959-987	2.1	40
288	SMILES in QSPR/QSAR Modeling: results and perspectives. *Current Drug Discovery Technologies*, **2007**, 4, 77-116	1.5	40
287	QSPR modeling of alkanes properties based on graph of atomic orbitals. *Computational and Theoretical Chemistry*, **2003**, 637, 1-10		40
286	QSPR studies on refractive indices of structurally heterogeneous polymers. *Chemometrics and Intelligent Laboratory Systems*, **2015**, 140, 86-91	3.8	39
285	Comparison of SMILES and molecular graphs as the representation of the molecular structure for QSAR analysis for mutagenic potential of polyaromatic amines. *Chemometrics and Intelligent Laboratory Systems*, **2011**, 109, 94-100	3.8	39
284	Multiplicative SMILES-based optimal descriptors: QSPR modeling of fullerene C60 solubility in organic solvents. *Chemical Physics Letters*, **2008**, 457, 332-336	2.5	39
283	Prediction of aquatic toxicity: use of optimization of correlation weights of local graph invariants. *Journal of Chemical Information and Computer Sciences*, **2003**, 43, 560-7		39

282	QSPR study on solubility of fullerene C60 in organic solvents using optimal descriptors calculated with SMILES. *Chemical Physics Letters*, **2007**, 441, 119-122	2.5	38
281	A new approach to the characterization of nanomaterials: Predicting Young modulus by correlation weighting of nanomaterials codes. *Chemical Physics Letters*, **2006**, 433, 125-129	2.5	38
280	QSAR modeling of toxicity on optimization of correlation weights of Morgan extended connectivity. *Computational and Theoretical Chemistry*, **2002**, 578, 129-134		38
279	QSPR and nano-QSPR: What is the difference?. *Journal of Molecular Structure*, **2019**, 1182, 141-149	3.4	38
278	SMILES-based optimal descriptors: QSAR analysis of fullerene-based HIV-1 PR inhibitors by means of balance of correlations. *Journal of Computational Chemistry*, **2010**, 31, 381-92	3.5	37
277	QSAR models for Daphnia toxicity of pesticides based on combinations of topological parameters of molecular structures. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 2779-88	3.4	37
276	Does the Index of Ideality of Correlation Detect the Better Model Correctly?. *Molecular Informatics*, **2019**, 38, e1800157	3.8	36
275	QSAR as a random event: a case of NOAEL. *Environmental Science and Pollution Research*, **2015**, 22, 8264-71	5.1	36
274	QSPR modeling of octanol/water partition coefficient for vitamins by optimal descriptors calculated with SMILES. *European Journal of Medicinal Chemistry*, **2008**, 43, 714-40	6.8	36
273	SMILES-based optimal descriptors: QSAR modeling of carcinogenicity by balance of correlations with ideal slopes. *European Journal of Medicinal Chemistry*, **2010**, 45, 3581-7	6.8	35
272	QSPR modeling of the enthalpy of formation from elements by means of correlation weighting of local invariants of atomic orbital molecular graphs. *Chemical Physics Letters*, **2000**, 330, 612-623	2.5	35
271	Additive SMILES-based carcinogenicity models: Probabilistic principles in the search for robust predictions. *International Journal of Molecular Sciences*, **2009**, 10, 3106-27	6.3	34
270	Additive SMILES based optimal descriptors: QSPR modeling of fullerene C60 solubility in organic solvents. *Chemical Physics Letters*, **2007**, 444, 209-214	2.5	34
269	Nano-QSAR: Model of mutagenicity of fullerene as a mathematical function of different conditions. *Ecotoxicology and Environmental Safety*, **2016**, 124, 32-36	7	33
268	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
267	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
266	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
265	Co-evolutions of correlations for QSAR of toxicity of organometallic and inorganic substances: An unexpected good prediction based on a model that seems untrustworthy. *Chemometrics and Intelligent Laboratory Systems*, **2011**, 105, 215-219	3.8	33

264	Improved molecular descriptors to calculate boiling points based on the optimization of correlation weights of local graph invariants. *Computational and Theoretical Chemistry*, **2001**, 542, 107-113		32
263	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
262	QSAR model as a random event: A case of rat toxicity. *Bioorganic and Medicinal Chemistry*, **2015**, 23, 1223-30	3.4	31
261	QSAR model for predicting cell viability of human embryonic kidney cells exposed to SiO□ nanoparticles. *Chemosphere*, **2016**, 144, 995-1001	8.4	30
260	CORAL: QSPR model of water solubility based on local and global SMILES attributes. *Chemosphere*, **2013**, 90, 877-80	8.4	30
259	Modeling of acyclic carbonyl compounds normal boiling points by correlation weighting of nearest neighboring codes. *Computational and Theoretical Chemistry*, **2002**, 581, 11-15		30
258	CORAL: Binary classifications (active/inactive) for drug-induced liver injury. *Toxicology Letters*, **2017**, 268, 51-57	4.4	29
257	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
256	SMILES-based QSAR models for the calcium channel-antagonistic effect of 1,4-dihydropyridines. *Archiv Der Pharmazie*, **2013**, 346, 134-9	4.3	29
255	coral Software: QSAR for Anticancer Agents. *Chemical Biology and Drug Design*, **2011**, 77, 471-6	2.9	29
254	QSPR modeling for enthalpies of formation of organometallic compounds by means of SMILES-based optimal descriptors. *Chemical Physics Letters*, **2008**, 461, 343-347	2.5	29
253	Searching therapeutic agents for treatment of Alzheimer disease using the Monte Carlo method. *Computers in Biology and Medicine*, **2015**, 64, 148-54	7	28
252	Additive InChI-based optimal descriptors: QSPR modeling of fullerene C 60 solubility in organic solvents. *Journal of Mathematical Chemistry*, **2009**, 46, 1232-1251	2.1	28
251	QSAR Modeling of Acute Toxicity for Nitrobenzene Derivatives Towards Rats: Comparative Analysis by MLRA and Optimal Descriptors. *QSAR and Combinatorial Science*, **2007**, 26, 686-693		28
250	Hybrid optimal descriptors as a tool to predict skin sensitization in accordance to OECD principles. *Toxicology Letters*, **2017**, 275, 57-66	4.4	27
249	CORAL: QSPR models for solubility of [C60] and [C70] fullerene derivatives. *Molecular Diversity*, **2011**, 15, 249-56	3.1	27
248	A new bioconcentration factor model based on SMILES and indices of presence of atoms. *European Journal of Medicinal Chemistry*, **2010**, 45, 4399-402	6.8	27
247	QSPR modeling of lipid-water partition coefficient by optimization of correlation weights of local graph invariants. *Journal of Chemical Information and Computer Sciences*, **2004**, 44, 179-86		27

246	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
245	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
244	QSAR modeling of endpoints for peptides which is based on representation of the molecular structure by a sequence of amino acids. *Structural Chemistry*, **2012**, 23, 1891-1904	1.8	26
243	3D weighting of molecular descriptors for QSPR/QSAR by the method of ideal symmetry (MIS). 1. Application to boiling points of alkanes. *Computational and Theoretical Chemistry*, **1998**, 424, 237-247		26
242	QSAR models of quail dietary toxicity based on the graph of atomic orbitals. *Bioorganic and Medicinal Chemistry Letters*, **2006**, 16, 1941-3	2.9	26
241	QSAR modelling of aldehyde toxicity by means of optimisation of correlation weights of nearest neighbouring codes. *Computational and Theoretical Chemistry*, **2004**, 676, 165-169		26
240	The Monte Carlo technique as a tool to predict LOAEL. *European Journal of Medicinal Chemistry*, **2016**, 116, 71-75	6.8	26
239	Monte Carlo method for predicting of cardiac toxicity: hERG blocker compounds. *Toxicology Letters*, **2016**, 250-251, 42-6	4.4	26
238	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
237	QSPR modeling bioconcentration factor (BCF) by balance of correlations. *European Journal of Medicinal Chemistry*, **2009**, 44, 2544-51	6.8	25
236	InChI-based optimal descriptors: QSAR analysis of fullerene[C60]-based HIV-1 PR inhibitors by correlation balance. *European Journal of Medicinal Chemistry*, **2010**, 45, 1387-94	6.8	25
235	Maximum Topological Distances Based Indices as Molecular Descriptors for QSPR. 4. Modeling the Enthalpy of Formation of Hydrocarbons from Elements. *International Journal of Molecular Sciences*, **2001**, 2, 121-132	6.3	25
234	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
233	QSAR models for ACE-inhibitor activity of tri-peptides based on representation of the molecular structure by graph of atomic orbitals and SMILES. *Structural Chemistry*, **2012**, 23, 1873-1878	1.8	24
232	Analysis of the co-evolutions of correlations as a tool for QSAR-modeling of carcinogenicity: an unexpected good prediction based on a model that seems untrustworthy. *Open Chemistry*, **2011**, 9, 165-174	1.6	24
231	Mutagenicity: QSAR - quasi-QSAR - nano-QSAR. *Mini-Reviews in Medicinal Chemistry*, **2015**, 15, 608-21	3.2	24
230	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
229	QSAR model for blood-brain barrier permeation. *Journal of Pharmacological and Toxicological Methods*, **2017**, 88, 7-18	1.7	23

228	Towards the Development of Global Nano-Quantitative Structure-Property Relationship Models: Zeta Potentials of Metal Oxide Nanoparticles. *Nanomaterials*, **2018**, 8,	5.4	22
227	Optimal descriptor as a translator of eclectic information into the prediction of membrane damage: the case of a group of ZnO and TiO2 nanoparticles. *Ecotoxicology and Environmental Safety*, **2014**, 108, 203-9	7	22
226	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
225	Predicting thermal conductivity of nanomaterials by correlation weighting technological attributes codes. *Materials Letters*, **2007**, 61, 4777-4780	3.3	22
224	QSPR modeling of the half-wave potentials of benzoxazines by optimal descriptors calculated with the SMILES. *Computational Biology and Chemistry*, **2006**, 30, 434-7	3.6	22
223	Correlation weighting of valence shells in QSAR analysis of toxicity. *Bioorganic and Medicinal Chemistry*, **2006**, 14, 3923-8	3.4	22
222	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
221	Monte carlo method-based QSAR modeling of penicillins binding to human serum proteins. *Archiv Der Pharmazie*, **2015**, 348, 62-7	4.3	21
220	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
219	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
218	SMILES-based quantitative structure-property relationships for half-wave potential of N-benzylsalicylthioamides. *European Journal of Medicinal Chemistry*, **2013**, 67, 111-4	6.8	21
217	CORAL: Models of toxicity of binary mixtures. *Chemometrics and Intelligent Laboratory Systems*, **2012**, 119, 39-43	3.8	21
216	SMILES-based QSAR approaches for carcinogenicity and anticancer activity: comparison of correlation weights for identical SMILES attributes. *Anti-Cancer Agents in Medicinal Chemistry*, **2011**, 11, 974-82	2.2	21
215	Optimisation of correlation weights of SMILES invariants for modelling oral quail toxicity. *European Journal of Medicinal Chemistry*, **2007**, 42, 606-13	6.8	21
214	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
213	QSAR as a random event: criteria of predictive potential for a chance model. *Structural Chemistry*, **2019**, 30, 1677-1683	1.8	20
212	CORAL: Predictions of rate constants of hydroxyl radical reaction using representation of the molecular structure obtained by combination of SMILES and Graph approaches. *Chemometrics and Intelligent Laboratory Systems*, **2012**, 112, 65-70	3.8	20
211	Improved Molecular Descriptors Based on the Optimization of Correlation Weights of Local Graph Invariants. *International Journal of Molecular Sciences*, **2001**, 2, 57-65	6.3	20

210	Correlation intensity index: mathematical modeling of cytotoxicity of metal oxide nanoparticles. *Nanotoxicology*, **2020**, 14, 1118-1126	5.3	20
209	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
208	CORAL: QSAR models for carcinogenicity of organic compounds for male and female rats. *Computational Biology and Chemistry*, **2018**, 72, 26-32	3.6	19
207	The definition of the molecular structure for potential anti-malaria agents by the Monte Carlo method. *Structural Chemistry*, **2013**, 24, 1369-1381	1.8	19
206	Structure Toxicity Relationships for Aliphatic Compounds Based on Correlation Weighting of Local Graph Invariants. *International Journal of Molecular Sciences*, **2003**, 4, 272-283	6.3	19
205	The index of ideality of correlation: improvement of models for toxicity to algae. *Natural Product Research*, **2019**, 33, 2200-2207	2.3	19
204	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
203	Design and development of novel antibiotics based on FtsZ inhibition In silico studies. *New Journal of Chemistry*, **2018**, 42, 10976-10982	3.6	19
202	QSPR/QSAR: State-of-Art, Weirdness, the Future. *Molecules*, **2020**, 25,	4.8	18
201	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
200	QSAR modelling of carcinogenicity by balance of correlations. *Molecular Diversity*, **2009**, 13, 367-73	3.1	18
199	Comparison of QSPR models of octanol/water partition coefficient for vitamins and non vitamins. *European Journal of Medicinal Chemistry*, **2006**, 41, 1271-8	6.8	18
198	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
197	QSAR models for anti-malarial activity of 4-aminoquinolines. *Current Computer-Aided Drug Design*, **2014**, 10, 75-82	1.4	18
196	Quasi-SMILES as a tool to utilize eclectic data for predicting the behavior of nanomaterials. *NanoImpact*, **2016**, 1, 60-64	5.6	18
195	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
194	QSAR model for cytotoxicity of SiO2 nanoparticles on human lung fibroblasts. *Journal of Nanoparticle Research*, **2014**, 16, 1	2.3	17
193	CORAL: QSAR models for acute toxicity in fathead minnow (Pimephales promelas). *Journal of Computational Chemistry*, **2012**, 33, 1218-23	3.5	17

192	CORAL: Monte Carlo Method as a Tool for the Prediction of the Bioconcentration Factor of Industrial Pollutants. *Molecular Informatics*, **2013**, 32, 145-54	3.8	17
191	Simplified molecular input line entry system-based optimal descriptors: quantitative structure-activity relationship modeling mutagenicity of nitrated polycyclic aromatic hydrocarbons. *Chemical Biology and Drug Design*, **2009**, 73, 515-25	2.9	17
190	QSPR Modeling of the Reactivity Parameters of Monomers in Radical Copolymerizations. *Journal of Structural Chemistry*, **2004**, 45, 945-950	0.9	17
189	QSAR modelling of aldehyde toxicity against a protozoan, Tetrahymena pyriformis by optimization of correlation weights of nearest neighboring codes. *Computational and Theoretical Chemistry*, **2004**, 679, 225-228		17
188	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
187	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
186	QSAR models for toxicity of organic substances to Daphnia magna built up by using the CORAL freeware. *Chemical Biology and Drug Design*, **2012**, 79, 332-8	2.9	16
185	Modeling of lipophilicity by means of correlation weighting of local graph invariants. *Computational and Theoretical Chemistry*, **2001**, 538, 197-199		16
184	Maximum topological distances based indices as molecular descriptors for QSPR: 2--application to aromatic hydrocarbons. *Computers & Chemistry*, **2000**, 24, 571-6		16
183	Maximum topological distances based indices as molecular descriptors for QSPR. Part 1. Application to alkyl benzenes boiling points. *Computational and Theoretical Chemistry*, **2000**, 501-502, 419-425		16
182	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
181	Exploring QSAR modeling of toxicity of chemicals on earthworm. *Ecotoxicology and Environmental Safety*, **2020**, 190, 110067	7	16
180	CORAL: model for no observed adverse effect level (NOAEL). *Molecular Diversity*, **2015**, 19, 563-75	3.1	15
179	CORAL: prediction of binding affinity and efficacy of thyroid hormone receptor ligands. *European Journal of Medicinal Chemistry*, **2015**, 101, 452-61	6.8	15
178	In silico prediction of the Ecyclodextrin complexation based on Monte Carlo method. *International Journal of Pharmaceutics*, **2015**, 495, 404-409	6.5	15
177	CORAL: Building up QSAR models for the chromosome aberration test. *Saudi Journal of Biological Sciences*, **2019**, 26, 1101-1106	4	15
176	QSAR-modeling of toxicity of organometallic compounds by means of the balance of correlations for InChI-based optimal descriptors. *Molecular Diversity*, **2010**, 14, 183-92	3.1	15
175	Improved QSPR analysis of standard entropy of acyclic and aromatic compounds using optimized correlation weights of linear graph invariants. *Computers & Chemistry*, **2002**, 26, 327-32		15

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173	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
172	QSPR calculation of normal boiling points of organic molecules based on the use of correlation weighting of atomic orbitals with extended connectivity of zero- and first-order graphs of atomic orbitals. *Molecules*, **2004**, 9, 1019-33	4.8	14
171	The Utilization of the Monte Carlo Technique for Rational Drug Discovery. *Combinatorial Chemistry and High Throughput Screening*, **2016**, 19, 676-687	1.3	14
170	First report on a classification-based QSAR model for chemical toxicity to earthworm. *Journal of Hazardous Materials*, **2020**, 386, 121660	12.8	14
169	Correlation intensity index: Building up models for mutagenicity of silver nanoparticles. *Science of the Total Environment*, **2020**, 737, 139720	10.2	13
168	Optimal descriptors as a tool to predict the thermal decomposition of polymers. *Journal of Mathematical Chemistry*, **2014**, 52, 1171-1181	2.1	13
167	QSAR modelling toxicity toward rats of inorganic substances by means of CORAL. *Open Chemistry*, **2011**, 9, 75-85	1.6	13
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165	QSPR modeling of octanol/water partition coefficient of antineoplastic agents by balance of correlations. *European Journal of Medicinal Chemistry*, **2010**, 45, 1639-47	6.8	13
164	QSAR modelling of the toxicity to Tetrahymena pyriformis by balance of correlations. *Molecular Diversity*, **2010**, 14, 821-7	3.1	13
163	Prediction of alkane enthalpies by means of correlation weighting of Morgan extended connectivity in molecular graphs. *Chemical Physics Letters*, **2004**, 384, 357-363	2.5	13
162	QSPR Modeling of Complex Stability by Optimization of Correlation Weights of the Hydrogen Bond Index and the Local Graph Invariants. *Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya*, **2002**, 28, 877-880	1.6	13
161	Calculation of total molecular electronic energies from Correlation Weighting of Local Graph Invariants. *Journal of Molecular Modeling*, **2001**, 7, 1-5	2	13
160	Blood Brain Barrier and Alzheimer's Disease: Similarity and Dissimilarity of Molecular Alerts. *Current Neuropharmacology*, **2018**, 16, 769-785	7.6	13
159	SARS-CoV M inhibitory activity of aromatic disulfide compounds: QSAR model. *Journal of Biomolecular Structure and Dynamics*, **2020**, 1-7	3.6	13
158	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
157	The index of ideality of correlation: models for flammability of binary liquid mixtures. *Chemical Papers*, **2020**, 74, 601-609	1.9	13

156	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
155	SMILES-based quantitative structure–retention relationships for RP HPLC of 1-phenyl-5-benzylsulfanyltetrazoles. *Structural Chemistry*, **2014**, 25, 311-317	1.8	12
154	CORAL: binary classifications (active/inactive) for Liver-Related Adverse Effects of Drugs. *Current Drug Safety*, **2012**, 7, 257-61	1.4	12
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150	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
149	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
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