Aleksandar Sabljic

List of Publications by Year
in descending order

68	2,721	159585 30	182427 51
papers	citations	h-index	g-index

68	68	68	1779
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Atmospheric oxidation of halogenated aromatics: comparative analysis of reaction mechanisms and reaction kinetics. Environmental Sciences: Processes and Impacts, 2017, 19, 357-369.	3.5	15
2	Atmospheric oxidation of hexachlorobenzene: New global source of pentachlorophenol. Chemosphere, 2016, 159, 488-495.	8.2	10
3	Reactions of 2-Propanol Radical with Halogenated Organics in Aqueous Solution: Theoretical Evidence for Proton-Coupled Electron Transfer and Competing Mechanisms. Journal of Physical Chemistry B, 2016, 120, 11810-11820.	2.6	9
4	Tropospheric Degradation of Perfluorinated Aromatics: A Case of Hexafluorobenzene. Croatica Chemica Acta, 2015, 88, 547-552.	0.4	2
5	Sorption and Quantitative Structure-Activity Relationship (QSAR). ACS Symposium Series, 2014, , 85-118.	0.5	2
6	Biodegradation and Quantitative Structure-Activity Relationship (QSAR). ACS Symposium Series, 2014, , 57-84.	0.5	8
7	Comments on â€œOzonation of a mixture of estrogens and progestins in aqueous solution: Interpretation of experimental results by computational methodsâ€•by Ekaterina V. Rokhina, Nagarjuna S. Vattikonda, Candice Johnson, Rominder P.S. Suri [Chemosphere 89 (11) (2012) 1323â€“1329]. Chemosphere, 2013, 92, 1062-1063.	8.2	0
8	Theoretical study on the mechanism and kinetics of addition of hydroxyl radicals to fluorobenzene. Journal of Computational Chemistry, 2013, 34, 646-655.	3.3	17
9	Mechanisms and reaction-path dynamics of hydroxyl radical reactions with aromatic hydrocarbons: The case of chlorobenzene. Chemosphere, 2013, 92, 851-856.	8.2	29
10	CASSCF/CASPT2 and TD-DFT Study of Valence and Rydberg Electronic Transitions in Fluorene, Carbazole, Dibenzofuran, and Dibenzothiophene. Journal of Physical Chemistry A, 2011, 115, 4840-4850.	2.5	27
11	Introduction to Larry Needham Issue. Chemosphere, 2011, 85, 141.	8.2	0
12	Bioavailability of Xenobiotics in the Soil Environment. Reviews of Environmental Contamination and Toxicology, 2010, 203, 1-86.	1.3	78
13	Symmetry of rydberg transitions in 1,4-cyclohexadiene: Multiphoton ionization investigation. International Journal of Quantum Chemistry, 2009, 22, 357-362.	2.0	0
14	A surprisingly complex aqueous chemistry of the simplest amino acid. A pulse radiolysis and theoretical study on H/D kinetic isotope effects in the reaction of glycine anions with hydroxyl radicals. Physical Chemistry Chemical Physics, 2009, 11, 2256.	2.8	30
15	Theoretical Study of Structure, Vibrational Frequencies, and Electronic Spectra of Dibenzofuran and Its Polychlorinated Derivatives. Journal of Physical Chemistry A, 2007, 111, 1339-1350.	2.5	11
16	Theoretical Study of Structure, Vibrational Frequencies, and Electronic Spectra of Polychlorinated Dibenzo-p-dioxins. Journal of Physical Chemistry A, 2006, 110, 4524-4534.	2.5	16
17	Fluorocarbonyl oxide: CASSCF/CASPT2 study of structure, cis effect and unimolecular decomposition paths. Chemical Physics, 2005, 309, 157-165.	1.9	15
18	Dibenzo-p-dioxin. An ab Initio CASSCF/CASPT2 Study of the Ï€âˆ—Ï€* and nâˆ—Ï€* Valence Excited States. Journal of Physical Chemistry A, 2005, 109, 8209-8217.	2.5	12

#	Article	IF	Citations
19	Ozonolysis of Fluoroethene:Â Theoretical Study of Unimolecular Decomposition Paths of Primary and Secondary Fluorozonide. Journal of Physical Chemistry A, 2005, 109, 2381-2393.	2.5	12
20	Evaluation of Artificial Intelligence Based Models for Chemical Biodegradability Prediction. Molecules, 2004, 9, 989-1003.	3.8	28
21	Systematic CASPT2 analysis of the geometry and force field of ozone with extrapolation to the infinite basis set. Chemical Physics Letters, 2004, 385, 214-219.	2.6	16
22	Theoretical Study of the Mechanism and Kinetics of Gas-Phase Ozone Additions to Ethene, Fluoroethene, and Chloroethene:Â A Multireference Approach. Journal of Physical Chemistry A, 2002, 106, 4745-4757.	2.5	81
23	QSAR models for estimating properties of persistent organic pollutants required in evaluation of their environmental fate and risk. Chemosphere, 2001, 43, 363-375.	8.2	108
24	Reliable QSAR for estimating Koc for persistent organic pollutants: correlation with molecular connectivity indices. Chemosphere, 2001, 45, 213-221.	8.2	56
25	IUPAC and UNESCO efforts towards sustainable development. Environmental Science and Pollution Research, 2000, 7, 185-187.	5.3	1
26	The IUPAC symposium â€œdegradation processes in the environmentâ€•24â€“28 May 1998, Dubrovnik (Cavtat), Croatia. Chemosphere, 1999, 38, xi-xii.	8.2	0
27	Reactivity and Regioselectivity of Hydroxyl Radical Addition to Halogenated Ethenes. Journal of Physical Chemistry A, 1998, 102, 1583-1594.	2.5	81
28	Reaction-Path Dynamics of Hydroxyl Radical Reactions with Ethane and Haloethanes. Journal of Physical Chemistry A, 1997, 101, 4245-4253.	2.5	43
29	The role of complexes in hydrogen abstraction from haloethanes by the hydroxyl radical. A case of guided reactions. Chemical Physics Letters, 1997, 272, 353-360.	2.6	40
30	Applications of expertsâ€™ judgement to derive structure-biodegradation relationships. Environmental Science and Pollution Research, 1996, 3, 224-228.	5.3	22
31	Comparative QSAR study on hydroxyl radical reactivity with unsaturated hydrocarbons: PLS versus MLR. Journal of Chemometrics, 1996, 10, 135-147.	1.3	35
32	An ab Initio Study on Reactivity of Fluoroethane with Hydroxyl Radical:â€‰ Application of G2 Theory. The Journal of Physical Chemistry, 1996, 100, 6212-6224.	2.9	39
33	Quantitative structure-activity relationships for N-(indol-3-ylacetyl)amino acids used as sources of auxin in plant tissue culture. Plant Growth Regulation, 1995, 16, 141-152.	3.4	13
34	QSAR study of 4-hydroxypyridine derivatives as inhibitors of the HILL reaction. Pest Management Science, 1995, 45, 133-141.	0.4	6
35	An ab initio investigation on transition states and reactivity of chloroethane with OH radical. Journal of Chemical Physics, 1995, 102, 7504-7518.	3.0	42
36	Predicting Tropospheric Degradation of Chemicals: From Estimation to Computation. SAR and QSAR in Environmental Research, 1995, 4, 197-209.	2.2	43

#	Article	IF	Citations
37	Assessment of QSARS for Predicting Fate and Effects of Chemicals in the Environment: An International European Project. SAR and QSAR in Environmental Research, 1995, 3, 223-236.	2.2	40
38	QSAR modelling of soil sorption. Improvements and systematics of log KOC vs. log KOW correlations. Chemosphere, 1995, 31, 4489-4514.	8.2	401
39	Calculation of retention indices by molecular topology. Journal of Chromatography A, 1993, 628, 69-79.	3.7	15
40	Herbicidal selectivity of (E)-3-(2,4-dichlorophenoxy)acrylates: QSAR study with molecular connectivity indices. Pest Management Science, 1993, 39, 245-250.	0.4	6
41	GRAPH III: A computer program for calculating molecular connectivity indices on microcomputers. Journal of Chemical Information and Computer Sciences, 1993, 33, 292-295.	2.8	34
42	Modeling octanol/water partition coefficients by molecular topology: chlorinated benzenes and biphenyls. Environmental Science & Technology, 1993, 27, 1394-1402.	10.0	71
43	A novel efficient and accurate method to calculate n-octanol/water partition coefficients of highly hydrophobic chemicals. Science of the Total Environment, 1993, 134, 1373-1381.	8.0	2
44	Soil sorption and chemical topology. Journal of Mathematical Chemistry, 1992, 11, 271-280.	1.5	15
45	Quantitative modeling of environmental fate and impact of commercial chemicals. Environmental Toxicology and Chemistry, 1992, 11, 961-972.	4.3	28
46	QUANTITATIVE MODELING OF ENVIRONMENTAL FATE AND IMPACT OF COMMERCIAL CHEMICALS. Environmental Toxicology and Chemistry, 1992, 11, 961.	4.3	3
47	Modelling N-octanol/water partition coefficients by molecular topology: polycyclic aromatic hydrocarbons and their alkyl derivatives. Chemosphere, 1991, 23, 199-213.	8.2	30
48	Chemical topology and ecotoxicology. Science of the Total Environment, 1991, 109-110, 197-220.	8.0	35
49	Modeling plant uptake of airborne organic chemicals. 1. Plant cuticle/water partitioning and molecular connectivity. Environmental Science & Technology, 1990, 24, 1321-1326.	10.0	84
50	Predicting the night-time NO3 radical reactivity in the troposphere. Atmospheric Environment Part A General Topics, 1990, 24, 73-78.	1.3	79
51	Inhibition of Hill Reaction by 2-Azido-s-triazine Derivatives: QSAR Study with Molecular Connectivity Indices. Zeitschrift Fur Naturforschung - Section C Journal of Biosciences, 1989, 44, 255-261.	1.4	8
52	Quantitative Modeling of Soil Sorption for Xenobiotic Chemicals. Environmental Health Perspectives, 1989, 83, 179.	6.0	11
53	Expert systems survey on biodegradation of xenobiotic chemicals. Ecotoxicology and Environmental Safety, 1989, 18, 252-267.	6.0	41
54	Predicting Henry's law constants for polychlorinated biphenyls. Chemosphere, 1989, 19, 1503-1511.	8.2	27

#	Article	IF	Citations
55	Quantitative structure-activity relationships of acute toxicity of commercial chemicals on fathead minnows: effect of molecular size. Aquatic Toxicology, 1989, 14, 47-64.	4.0	46
56	Screening-level model for aerobic biodegradability based on a survey of expert knowledge. Environmental Science & Technology, 1989, 23, 672-679.	10.0	89
57	A rational selection of graph-theoretical indices in the QSAR. International Journal of Quantum Chemistry, 1988, 34, 267-285.	2.0	18
58	Application of Molecular Topology for the Estimation of Physical Data for Environmental Chemicals. , 1988, , 335-348.		4
59	On the prediction of soil sorption coefficients of organic pollutants from molecular structure: application of molecular topology model. Environmental Science & Technology, 1987, 21, 358-366.	10.0	215
60	Nonempirical Modeling of Environmental Distribution and Toxicity of Major Organic Pollutants. , 1987, , 309-332.		21
61	Calculation of retention indices by molecular topology: chlorinated alkanes. Journal of Chromatography A, 1984, 314, 1-12.	3.7	46
62	Predictions of the nature and strength of soil sorption of organic pollutants by molecular topology. Journal of Agricultural and Food Chemistry, 1984, 32, 243-246.	5.2	116
63	Anthocyanin Degradation in the Presence of Furfural and 5-Hydroxymethylfurfural. Journal of Food Science, 1983, 48, 411-416.	3.1	65
64	Quantitative structure-toxicity relationship of chlorinated compounds: A molecular connectivity investigation. Bulletin of Environmental Contamination and Toxicology, 1983, 30, 80-83.	2.7	41
65	Application of photoelectron spectroscopy to biologically active molecules and their constituent parts. IX. 1,4-Benzodiazepin-2-ones. International Journal of Quantum Chemistry, 1983, 23, 1667-1676.	2.0	7
66	Chemistry of excited states. Part 13. Assignment of lowest Ï€-ionizations in photoelectron spectra of thiophen, furan, and pyrrole. Journal of the Chemical Society Perkin Transactions II, 1982, , 539-543.	0.9	51
67	Relationship between molecular connectivity indices and soil sorption coefficients of polycyclic aromatic hydrocarbons. Bulletin of Environmental Contamination and Toxicology, 1982, 28, 162-165.	2.7	56
68	Molecular connectivity: A novel method for prediction of bioconcentration factor of hazardous chemicals. Chemico-Biological Interactions, 1982, 42, 301-310.	4.0	69