Vitaly Solovyov

List of Publications by Year
in descending order

68	1,851	257450 24	265206 42
papers	citations	h-index	g-index

71	71	71	1443
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	ISIDA - Platform for Virtual Screening Based on Fragment and Pharmacophoric Descriptors. Current Computer-Aided Drug Design, 2008, 4, 191-198.	1.2	173
2	Substructural fragments: an universal language to encode reactions, molecular and supramolecular structures. Journal of Computer-Aided Molecular Design, 2005, 19, 693-703.	2.9	166
3	Exhaustive QSPR Studies of a Large Diverse Set of Ionic Liquids:â€‰ How Accurately Can We Predict Melting Points?. Journal of Chemical Information and Modeling, 2007, 47, 1111-1122.	5.4	129
4	Correlation of bloodâ€“brain penetration using structural descriptors. Bioorganic and Medicinal Chemistry, 2006, 14, 4888-4917.	3.0	80
5	Modeling of Ion Complexation and Extraction Using Substructural Molecular Fragments. Journal of Chemical Information and Computer Sciences, 2000, 40, 847-858.	2.8	76
6	Crown Etherâ€“Ammonium Complexes: Binding Mechanisms and Solvent Effects. European Journal of Organic Chemistry, 1999, 1999, 1847-1856.	2.4	72
7	Solvent Effects on Crown Ether Complexations1. Journal of Organic Chemistry, 1996, 61, 5221-5226.	3.2	69
8	Benchmarking of Linear and Nonlinear Approaches for Quantitative Structureâ^'Property Relationship Studies of Metal Complexation with Ionophores. Journal of Chemical Information and Modeling, 2006, 46, 808-819.	5.4	68
9	Quantitative Structureâ^'Property Relationship Modeling ofÎ²-Cyclodextrin Complexation Free Energies. Journal of Chemical Information and Computer Sciences, 2004, 44, 529-541.	2.8	66
10	Determination of Successive Complexation Constants in an Ionic Liquid: Complexation of UO₂²⁺ with NO₃^{â^'} in C₄-mimTf₂N Studied by UVâ^'Vis Spectroscopy. Journal of Physical Chemistry B, 2010, 114, 4276-4282.	2.6	60
11	Skin Permeation Rate as a Function of Chemical Structure. Journal of Medicinal Chemistry, 2006, 49, 3305-3314.	6.4	49
12	â€œIn Silicoâ€•Design of New Uranyl Extractants Based on Phosphoryl-Containing Podands:â€‰ QSPR Studies, Generation and Screening of Virtual Combinatorial Library, and Experimental Tests. Journal of Chemical Information and Computer Sciences, 2004, 44, 1365-1382.	2.8	44
13	Assessment of the Macrocyclic Effect for the Complexation of Crown-Ethers with Alkali Cations Using the Substructural Molecular Fragments Method. Journal of Chemical Information and Computer Sciences, 2002, 42, 812-829.	2.8	41
14	QSAR modeling of blood:air and tissue:air partition coefficients using theoretical descriptors. Bioorganic and Medicinal Chemistry, 2005, 13, 6450-6463.	3.0	40
15	Anti-HIV Activity of HEPT, TIBO, and Cyclic Urea Derivatives:â€‰ Structureâ^'Property Studies, Focused Combinatorial Library Generation, and Hits Selection Using Substructural Molecular Fragments Method. Journal of Chemical Information and Computer Sciences, 2003, 43, 1703-1719.	2.8	39
16	The impact of alicyclic substituents on the extraction ability of new family of 1,10-phenanthroline-2,9-diamides. RSC Advances, 2020, 10, 26022-26033.	3.6	34
17	Complexation of phosphoryl-containing mono-, bi- and tri-podands with alkali cations in acetonitrile. Structure of the complexes and binding selectivity. Journal of the Chemical Society Perkin Transactions II, 1998, , 1489-1498.	0.9	33
18	Stochastic versus Stepwise Strategies for Quantitative Structureâ^'Activity Relationship GenerationHow Much Effort May the Mining for Successful QSAR Models Take?. Journal of Chemical Information and Modeling, 2007, 47, 927-939.	5.4	32

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19	Interpretability of SAR/QSAR Models of any Complexity by Atomic Contributions. Molecular Informatics, 2012, 31, 639-642.	2.5	32
20	Conformation of 18-Crown-5 and Its Influence on Complexation with Alkali and Ammonium Cations:Â Why 18-Crown-5 Binds More Than 1000 Times Weaker Than 18C6. Journal of Organic Chemistry, 1996, 61, 8113-8116.	3.2	29
21	Steric and Stereoelectronic Effects in Aza Crown Ether Complexes[1]. European Journal of Organic Chemistry, 1998, 1998, 1379-1389.	2.4	28
22	Structureâ€"property modeling of metal binders using molecular fragments. Russian Chemical Bulletin, 2004, 53, 1434-1445.	1.5	27
23	Quantitative Structureâ€"Property Relationship (QSPR) Modeling of Normal Boiling Point Temperature and Composition of Binary Azeotropes. Industrial & Engineering Chemistry Research, 2011, 50, 14162-14167.	3.7	25
24	Successful â€œIn Silicoâ€•Design of New Efficient Uranyl Binders. Solvent Extraction and Ion Exchange, 2007, 25, 433-462.	2.0	24
25	Mining Chemical Reactions Using Neighborhood Behavior and Condensed Graphs of Reactions Approaches. Journal of Chemical Information and Modeling, 2012, 52, 2325-2338.	5.4	24
26	Supramolecular complexes: Determination of stability constants on the basis of various experimental methods. Protection of Metals and Physical Chemistry of Surfaces, 2015, 51, 1-35.	1.1	23
27	TOWARDS AN INFORMATION SYSTEM ON SOLVENT EXTRACTION. Solvent Extraction and Ion Exchange, 2001, 19, 791-837.	2.0	22
28	QSPR Modeling of the AmIII/EuIIISeparation Factor: How Far Can we Predict ?. Solvent Extraction and Ion Exchange, 2007, 25, 1-26.	2.0	21
29	QSPR ensemble modelling of alkaline-earth metal complexation. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2013, 76, 159-171.	1.6	21
30	New Approach for Accurate QSPR Modeling of Metal Complexation: Application to Stability Constants of Complexes of Lanthanide Ions Ln3+, Ag+, Zn2+, Cd2+ and Hg2+ with Organic Ligands in Water. Macroheterocycles, 2012, 5, 404-410.	0.5	21
31	Stability constants of complexes of Zn2+, Cd2+, and Hg2+ with organic ligands: QSPR consensus modeling and design of new metal binders. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2012, 72, 309-321.	1.6	19
32	QSPR ensemble modelling of the 1:1 and 1:2 complexation of Co2+, Ni2+, and Cu2+ with organic ligands: relationships between stability constants. Journal of Computer-Aided Molecular Design, 2014, 28, 549-564.	2.9	19
33	Individual Hydrogenâ€Bond Strength QSPR Modelling with ISIDA Local Descriptors: a Step Towards Polyfunctional Molecules. Molecular Informatics, 2014, 33, 477-487.	2.5	19
34	“In Silico” Design of Potential Anti-HIV Actives Using Fragment Descriptors. Combinatorial Chemistry and High Throughput Screening, 2005, 8, 403-416.	1.1	18
35	The complexation of metal ions with various organic ligands in water: prediction of stability constants by QSPR ensemble modelling. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2015, 83, 89-101.	1.6	17
36	Structure-property modelling of complex formation of strontium with organic ligands in water. Journal of Structural Chemistry, 2006, 47, 298-311.	1.0	16

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37	Complexation of Mn²⁺, Fe²⁺, Y³⁺, La³⁺, Pb²⁺, and UO₂²⁺ with Organic Ligands: QSPR Ensemble Modeling of Stability Constants. Industrial & Engineering Chemistry Research, 2012, 51, 13482-13489.	3.7	16
38	Coordination Numbers of Central Atoms in Coordination Compounds. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2003, 29, 660-668.	1.0	13
39	Computer-aided design of new metal binders. Radiochimica Acta, 2008, 96, 505-511.	1.2	13
40	Predictive Models for Halogenâ€bond Basicity of Binding Sites of Polyfunctional Molecules. Molecular Informatics, 2016, 35, 70-80.	2.5	12
41	QSPR modeling of potentiometric sensitivity towards heavy metal ions for polymeric membrane sensors. Sensors and Actuators B: Chemical, 2019, 301, 126941.	7.8	11
42	Complexation of the new tetrakis[methyl(diphenylphosphorylated)] cyclen derivative with transition metals: First examples of octacoordinate zinc(II) and cobalt(II) complexes with cyclen molecules. Inorganica Chimica Acta, 2018, 478, 250-259.	2.4	10
43	2,4,6-Tris[2-(diphenylphosphoryl)-4-ethylphenoxy]-1,3,5-triazine: A new ligand for lithium binding. Inorganica Chimica Acta, 2019, 497, 119095.	2.4	10
44	Predictive Models for the Free Energy of Hydrogen Bonded Complexes with Single and Cooperative Hydrogen Bonds. Molecular Informatics, 2016, 35, 629-638.	2.5	9
45	QSPR Modeling of Potentiometric Mg²⁺/Ca²⁺ Selectivity for PVCâ€plasticized Sensor Membranes. Electroanalysis, 2020, 32, 792-798.	2.9	9
46	Complexation of lithium and sodium cations with Î²-phosphorylate ethers, modelling terminal groups of organophosphorus podands. An experimental and theoretical study. Journal of Molecular Structure, 1992, 271, 311-325.	3.6	8
47	Classification of Metal Binders by NaÃ¯ve Bayes Classifier on the Base of Molecular Fragment Descriptors and Ensemble Modeling. Molecular Informatics, 2019, 38, e1900002.	2.5	8
48	Design of phosphoryl containing podands with Li⁺/Na⁺ selectivity using machine learning. SAR and QSAR in Environmental Research, 2021, 32, 521-539.	2.2	7
49	Predictive cartography of metal binders using generative topographic mapping. Journal of Computer-Aided Molecular Design, 2017, 31, 701-714.	2.9	6
50	Predictive Models for HOMO and LUMO Energies of Nâ€Đonor Heterocycles as Ligands for Lanthanides Separation. Molecular Informatics, 2018, 37, e1800025.	2.5	6
51	Machine learning analysis of microwave dielectric properties for seven structure types: The role of the processing and composition. Journal of Physics and Chemistry of Solids, 2021, 156, 110178.	4.0	6
52	Thermodynamics and selectivity of complexation of lithium and sodium thiocyanates with phosphorus-containing podands and compounds modeling the terminal groups of these podands. Russian Chemical Bulletin, 1994, 43, 1493-1499.	1.5	5
53	Complexation of gallium(III) nitrate with 1,4,7,10-tetraazacyclododecane-1,4,7,10-tetrakis(methylenephosphonic acid). Russian Chemical Bulletin, 2018, 67, 2184-2187.	1.5	5
54	3D molecular fragment descriptors for structureâ€“property modeling: predicting the free energies for the complexation between antipodal guests and Î²-cyclodextrins. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2017, 89, 167-175.	1.6	4

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55	Thermodynamic radii of lanthanide ions derived from metalâ€“ligand complexes stability constants. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2020, 98, 69-78.	1.6	4
56	Determination of the purity, melting point and heat of melting of cyclic polyethers. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1986, 35, 632-633.	0.0	2
57	Phosphorus-containing podands. 6. Calorimetric study of complexation of 1,17-bis (diphenylphosphinyl)-3,6,9,12,15-pentaoxaheptadecane with alkali and alkaline-earth metal salts in acetonitrile. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1991, 40, 497-502.	0.0	2
58	Synthesis, Complexation Properties, and Evaluation of New Aminodiphosphonic Acids as Vector Molecules for 68Ga Radiopharmaceuticals. Molecules, 2021, 26, 2357.	3.8	2
59	Prediction of Stability Constants of metal-ligand Complexes Using Thermodynamic Radii of Metal Ions. Comments on Inorganic Chemistry, 2023, 43, 16-33.	5.2	2
60	Evaluation of the electron-donor and electron-acceptor functions of ionized atoms and groups in biologically active substances on the basis of thermodynamic data. Pharmaceutical Chemistry Journal, 1984, 18, 327-331.	0.8	1
61	Phosphorus-containing podands. 4. Complexation of calcium chloride in alcohol at 298 K by solution calorimetry. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1989, 38, 731-734.	0.0	1
62	Determination of standard enthalpies of complexation of calcium salts with 18-crown-6 by means of scanning calorimetry. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1986, 35, 1591-1593.	0.0	0
63	Calorimetric study of complexation of calcium chloride and nitrate with 18-crown-6 in ethanol at 298.15 K. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1987, 36, 545-547.	0.0	0
64	Calorimetric study of the interaction of calcium salts with some benzo-crown ethers. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1988, 37, 660-662.	0.0	0
65	Equilibrium constants and complexation enthalpies and entropies of lithium, sodium, potassium, ammonium, and calcium thiocyanates with benzo-12-crown-4 in acetonitrile. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1988, 37, 2163-2165.	0.0	0
66	Ternary mixed-ligand complexes of copper(II) with ?-aminoalkylphosphonic acids and amino acids. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1991, 40, 492-496.	0.0	0
67	Thermodynamic study of hydrogen-bond formation by 2-chloro-2-fluoro-2-nitroarylethanols with hexa-methylphosphoric triamide and acetone. Bulletin of the Academy of Sciences of the USSR Division of Chemical Science, 1991, 40, 57-61.	0.0	0
68	Quantitative Structureâ€”Property Relationship Modeling of Î²-Cyclodextrin Complexation Free Energies.. ChemInform, 2004, 35, no.	0.0	0