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	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
2	Synthesis, Complexation Properties, and Evaluation of New Aminodiphosphonic Acids as Vector Molecules for 68Ga Radiopharmaceuticals. Molecules, 2021, 26, 2357.	3.8	2
3	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
4	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
5	QSPR Modeling of Potentiometric Mg²⁺/Ca²⁺ Selectivity for PVCâ€plasticized Sensor Membranes. Electroanalysis, 2020, 32, 792-798.	2.9	9
6	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
7	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
8	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
9	QSPR modeling of potentiometric sensitivity towards heavy metal ions for polymeric membrane sensors. Sensors and Actuators B: Chemical, 2019, 301, 126941.	7.8	11
10	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
11	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
12	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
13	Predictive Models for HOMO and LUMO Energies of Nâ€Đonor Heterocycles as Ligands for Lanthanides Separation. Molecular Informatics, 2018, 37, e1800025.	2.5	6
14	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
15	Predictive cartography of metal binders using generative topographic mapping. Journal of Computer-Aided Molecular Design, 2017, 31, 701-714.	2.9	6
16	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
17	Predictive Models for Halogenâ€bond Basicity of Binding Sites of Polyfunctional Molecules. Molecular Informatics, 2016, 35, 70-80.	2.5	12
18	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

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19	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
20	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
21	Individual Hydrogenâ€Bond Strength QSPR Modelling with ISIDA Local Descriptors: a Step Towards Polyfunctional Molecules. Molecular Informatics, 2014, 33, 477-487.	2.5	19
22	QSPR ensemble modelling of alkaline-earth metal complexation. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2013, 76, 159-171.	1.6	21
23	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
24	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
25	Interpretability of SAR/QSAR Models of any Complexity by Atomic Contributions. Molecular Informatics, 2012, 31, 639-642.	2.5	32
26	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
27	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
28	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
29	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
30	Computer-aided design of new metal binders. Radiochimica Acta, 2008, 96, 505-511.	1.2	13
31	ISIDA - Platform for Virtual Screening Based on Fragment and Pharmacophoric Descriptors. Current Computer-Aided Drug Design, 2008, 4, 191-198.	1.2	173
32	QSPR Modeling of the AmIII/EuIIISeparation Factor: How Far Can we Predict ?. Solvent Extraction and Ion Exchange, 2007, 25, 1-26.	2.0	21
33	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
34	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
35	Successful â€œIn Silicoâ€•Design of New Efficient Uranyl Binders. Solvent Extraction and Ion Exchange, 2007, 25, 433-462.	2.0	24
36	Skin Permeation Rate as a Function of Chemical Structure. Journal of Medicinal Chemistry, 2006, 49, 3305-3314.	6.4	49

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37	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
38	Correlation of bloodâ€"brain penetration using structural descriptors. Bioorganic and Medicinal Chemistry, 2006, 14, 4888-4917.	3.0	80
39	Structure-property modelling of complex formation of strontium with organic ligands in water. Journal of Structural Chemistry, 2006, 47, 298-311.	1.0	16
40	QSAR modeling of blood:air and tissue:air partition coefficients using theoretical descriptors. Bioorganic and Medicinal Chemistry, 2005, 13, 6450-6463.	3.0	40
41	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
42	“In Silico” Design of Potential Anti-HIV Actives Using Fragment Descriptors. Combinatorial Chemistry and High Throughput Screening, 2005, 8, 403-416.	1.1	18
43	Structureâ€"property modeling of metal binders using molecular fragments. Russian Chemical Bulletin, 2004, 53, 1434-1445.	1.5	27
44	Quantitative Structureâ€"Property Relationship Modeling of Î²-Cyclodextrin Complexation Free Energies.. ChemInform, 2004, 35, no.	0.0	0
45	Quantitative Structureâ^'Property Relationship Modeling ofÎ²-Cyclodextrin Complexation Free Energies. Journal of Chemical Information and Computer Sciences, 2004, 44, 529-541.	2.8	66
46	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
47	Coordination Numbers of Central Atoms in Coordination Compounds. Russian Journal of Coordination Chemistry/Koordinatsionnaya Khimiya, 2003, 29, 660-668.	1.0	13
48	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
49	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
50	TOWARDS AN INFORMATION SYSTEM ON SOLVENT EXTRACTION. Solvent Extraction and Ion Exchange, 2001, 19, 791-837.	2.0	22
51	Modeling of Ion Complexation and Extraction Using Substructural Molecular Fragments. Journal of Chemical Information and Computer Sciences, 2000, 40, 847-858.	2.8	76
52	Crown Etherâ€"Ammonium Complexes: Binding Mechanisms and Solvent Effects. European Journal of Organic Chemistry, 1999, 1999, 1847-1856.	2.4	72
53	Steric and Stereoelectronic Effects in Aza Crown Ether Complexes[1]. European Journal of Organic Chemistry, 1998, 1998, 1379-1389.	2.4	28
54	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

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55	Solvent Effects on Crown Ether Complexations1. Journal of Organic Chemistry, 1996, 61, 5221-5226.	3.2	69
56	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
57	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
58	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
59	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
60	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
61	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
62	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
63	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
64	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
65	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
66	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
67	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
68	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