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List of Publications by Citations

76 papers	2,095 citations	28 h-index	44 g-index
81 ext. papers	2,294 ext. citations	4.5 avg, IF	4.76 L-index

#	Paper	IF	Citations
76	Refractive indices, molar volumes and molar refractions of binary liquid mixtures: concepts and correlations. *Physical Chemistry Chemical Physics*, **2003**, 5, 550-557	3.6	257
75	Molecular Dynamics Simulations of Phosphatidylcholine Membranes: A Comparative Force Field Study. *Journal of Chemical Theory and Computation*, **2012**, 8, 4593-609	6.4	154
74	Surface tensions and refractive indices of (tetrahydrofuran +n -alkanes) atT =298.15 K. *Journal of Chemical Thermodynamics*, **1999**, 31, 931-942	2.9	91
73	Heat Capacities, Excess Enthalpies, and Volumes of Mixtures Containing Cyclic Ethers. 4. Binary Systems 1,4-Dioxane + 1-Alkanols. *Journal of Chemical & Engineering Data*, **1999**, 44, 948-954	2.8	91
72	On the characterization of host-guest complexes: surface tension, calorimetry, and molecular dynamics of cyclodextrins with a non-ionic surfactant. *Journal of Physical Chemistry B*, **2007**, 111, 4383-92	3.4	89
71	Prediction of Excess Volumes and Excess Surface Tensions from Experimental Refractive Indices. *Physics and Chemistry of Liquids*, **2000**, 38, 251-260	1.5	73
70	Refractive Indexes of Binary Mixtures of Tetrahydrofuran with 1-Alkanols at 25°C and Temperature Dependence of n and for the Pure Liquids. *Journal of Solution Chemistry*, **2002**, 31, 369-380	1.8	66
69	Molecular dynamics simulations reveal insights into key structural elements of adenosine receptors. *Biochemistry*, **2011**, 50, 4194-208	3.2	60
68	Extended Langmuir Isotherm for Binary Liquid Mixtures. *Langmuir*, **2001**, 17, 4261-4266	4	60
67	Excess Molar Enthalpies of Tetrahydrofuran or Diisopropyl Ether + 1-Alkanols at 298.15 K, Using a Newly Designed Flow Mixing Cell for an Isothermal Microcalorimeter. *Journal of Chemical & Engineering Data*, **2001**, 46, 1274-1279	2.8	53
66	Heat Capacities, Excess Enthalpies, and Volumes of Mixtures Containing Cyclic Ethers. 5. Binary Systems {1,3-Dioxolane + 1-Alkanols}. *Journal of Chemical & Engineering Data*, **1999**, 44, 1341-1347	2.8	51
65	Multiscale molecular dynamics simulations of micelles: coarse-grain for self-assembly and atomic resolution for finer details. *Soft Matter*, **2012**, 8, 9005	3.6	50
64	Similarities and differences between cyclodextrin-sodium dodecyl sulfate host-guest complexes of different stoichiometries: molecular dynamics simulations at several temperatures. *Journal of Physical Chemistry B*, **2010**, 114, 12455-67	3.4	46
63	AFFINImeter: A software to analyze molecular recognition processes from experimental data. *Analytical Biochemistry*, **2019**, 577, 117-134	3.1	44
62	Excess volumes and isobaric heat capacities of diisopropyl ether with several alkanols at 298.15 K: Application of the symmetrical extended real associated solution model. *Fluid Phase Equilibria*, **2004**, 216, 245-256	2.5	44
61	A comprehensive approach to the surface tension of binary liquid mixtures. *Fluid Phase Equilibria*, **2001**, 182, 337-352	2.5	42
60	Thermodynamics of Mixtures Involving Some Linear or Cyclic Ketones and Cyclic Ethers. 1. Systems Containing Tetrahydrofuran. *Journal of Chemical & Engineering Data*, **2002**, 47, 351-358	2.8	42

59	Extending ITC to Kinetics with kinITC. *Methods in Enzymology*, **2016**, 567, 157-80	1.7	41
58	Cyclodextrin-based self-assembled nanotubes at the water/air interface. *Journal of Physical Chemistry B*, **2007**, 111, 12625-30	3.4	39
57	Activity Coefficients at Infinite Dilution from Surface Tension Data. *Langmuir*, **2002**, 18, 3604-3608	4	37
56	The "true" affinities of metal cations to p-sulfonatocalix[4]arene: a thermodynamic study at neutral pH reveals a pitfall due to salt effects in microcalorimetry. *Chemistry - A European Journal*, **2013**, 19, 17809-20	4.8	36
55	Functional and structural roles of conserved cysteine residues in the carboxyl-terminal domain of the follicle-stimulating hormone receptor in human embryonic kidney 293 cells. *Biology of Reproduction*, **2008**, 78, 869-82	3.9	36
54	Re-examination and symmetrization of the adjustable parameters of the ERAS model. *Fluid Phase Equilibria*, **2000**, 173, 211-239	2.5	34
53	Lipid Bilayer Membrane Perturbation by Embedded Nanopores: A Simulation Study. *ACS Nano*, **2016**, 10, 3693-701	16.7	31
52	Modeling and molecular dynamics simulation of the human gonadotropin-releasing hormone receptor in a lipid bilayer. *Journal of Physical Chemistry B*, **2008**, 112, 10704-13	3.4	31
51	A critical approach to the thermodynamic characterization of inclusion complexes: multiple-temperature isothermal titration calorimetric studies of native cyclodextrins with sodium dodecyl sulfate. *Journal of Physical Chemistry B*, **2011**, 115, 14381-96	3.4	30
50	Surface adsorption and bulk aggregation of cyclodextrins by computational molecular dynamics simulations as a function of temperature: □CD vs □CD. *Journal of Physical Chemistry B*, **2014**, 118, 6999-7011	3.4	28
49	Cooperative assembly of discrete stacked aggregates driven by supramolecular host-guest complexation. *Journal of Organic Chemistry*, **2013**, 78, 9113-9	4.2	28
48	Application of the Extended Langmuir model to surface tension data of binary liquid mixtures. *Fluid Phase Equilibria*, **2005**, 237, 140-151	2.5	26
47	The Lord of the NanoRings: Cyclodextrins and the battle against SARS-CoV-2. *International Journal of Pharmaceutics*, **2020**, 588, 119689	6.5	24
46	Molecular dynamics study of triosephosphate isomerase from Trypanosoma cruzi in water/decane mixtures. *Journal of Physical Chemistry B*, **2008**, 112, 3529-39	3.4	23
45	A molecular dynamics study of the formation, stability, and oligomerization state of two designed coiled coils: possibilities and limitations. *Biophysical Journal*, **2005**, 89, 3701-13	2.9	23
44	Thermodynamics of Mixtures Involving Some Linear or Cyclic Ketones and Cyclic Ethers. 2. Systems Containing Tetrahydropyran. *Journal of Chemical & Engineering Data*, **2003**, 48, 712-719	2.8	21
43	STAND: Surface Tension for Aggregation Number Determination. *Langmuir*, **2016**, 32, 3917-25	4	19
42	Interplay between Protein Thermal Flexibility and Kinetic Stability. *Structure*, **2017**, 25, 167-179	5.2	18

41	A proposal for the estimation of binary mixture activity coefficients from surface tension measurements throughout the entire concentration range. *Fluid Phase Equilibria*, **2007**, 260, 343-353	2.5	17
40	Thermodynamics of Mixtures Involving Some Linear or Cyclic Ketones and Cyclic Ethers. 4. Systems Containing 1,3-Dioxolane. *Journal of Chemical & Engineering Data*, **2004**, 49, 647-657	2.8	16
39	Key structural arrangements at the C-terminus domain of CETP suggest a potential mechanism for lipid-transfer activity. *Journal of Structural Biology*, **2014**, 186, 19-27	3.4	15
38	A small molecular size system giving unexpected surface effects: alpha-Cyclodextrin + sodium dodecyl sulfate in water. *Journal of Colloid and Interface Science*, **2008**, 328, 391-5	9.3	15
37	Hydrogenated/fluorinated catanionic surfactants as potential templates for nanostructure design. *Langmuir*, **2011**, 27, 9719-28	4	14
36	Complex Behavior of Aqueous Cyclodextrin Solutions. Interfacial Morphologies Resulting from Bulk Aggregation. *Langmuir*, **2016**, 32, 6682-90	4	13
35	Conformational effects of Lys191 in the human GnRH receptor: mutagenesis and molecular dynamics simulations studies. *Journal of Endocrinology*, **2009**, 201, 297-307	4.7	13
34	Surface films of short fluorocarbon-hydrocarbon diblocks studied by molecular dynamics simulations: Spontaneous formation of elongated hemimicelles. *Journal of Colloid and Interface Science*, **2009**, 329, 351-6	9.3	13
33	AFFINImeter Software: from its Beginnings to Future Trends- A Literature review. *Journal of Applied Bioanalysis*, **2018**, 4, 124-139	1.3	11
32	Langmuir monolayers of a hydrogenated/fluorinated catanionic surfactant: from the macroscopic to the nanoscopic size scale. *Langmuir*, **2009**, 25, 8075-82	4	9
31	Thermodynamics of the interaction between hydroxypropyl-cyclodextrin and alkanols in aqueous solutions. *Thermochimica Acta*, **2003**, 405, 109-115	2.9	9
30	Thermodynamics of Mixtures Involving Some Linear or Cyclic Ketones and Cyclic Ethers. 3. Systems Containing 1,4-Dioxane. *Journal of Chemical & Engineering Data*, **2003**, 48, 1055-1061	2.8	9
29	An immersive journey to the molecular structure of SARS-CoV-2: Virtual reality in COVID-19. *Computational and Structural Biotechnology Journal*, **2020**, 18, 2621-2628	6.8	9
28	Highly viscoelastic films at the water/air interface: Cyclodextrin with anionic surfactants. *Journal of Colloid and Interface Science*, **2020**, 565, 601-613	9.3	8
27	Testing the effect of the cavity size and the number of molecular substitutions in host guest complexes formed by 2-hydroxypropyl-cyclodextrins and n-octyl-d-glucopyranoside. *Journal of Chemical Thermodynamics*, **2013**, 67, 112-119	2.9	7
26	On the self-assembly of a highly selective benzothiazole-based TIM inhibitor in aqueous solution. *Langmuir*, **2010**, 26, 16681-9	4	7
25	Rings, Hexagons, Hetals, and Dipolar Moment Sink-Sources: The Fanciful Behavior of Water around Cyclodextrin Complexes. *Biomolecules*, **2020**, 10,	5.9	6
24	Exploring the conformational dynamics and membrane interactions of PorB from C. glutamicum: a multi-scale molecular dynamics simulation study. *Biochimica Et Biophysica Acta - Biomembranes*, **2011**, 1808, 1746-52	3.8	6

23	GADDLE Maps: General Algorithm for Discrete Object Deformations Based on Local Exchange Maps. *Journal of Chemical Theory and Computation*, **2018**, 14, 466-478	6.4	5
22	Cyclo-lib: a database of computational molecular dynamics simulations of cyclodextrins. *Bioinformatics*, **2016**, 32, 3371-3373	7.2	5
21	Thermodynamics of Mixing Tetrahydropyran with 1-Alkanols and Excess Enthalpies of Homomorphy-Related Systems. *Journal of Chemical & Engineering Data*, **2007**, 52, 429-437	2.8	5
20	Thermodynamic and Kinetic Analysis of Isothermal Titration Calorimetry Experiments by Using KinITC in AFFINImeter. *Methods in Molecular Biology*, **2019**, 1964, 225-239	1.4	4
19	Remdesivir interactions with sulphobutylether-□cyclodextrins: A case study using selected substitution patterns. *Journal of Molecular Liquids*, **2021**, 346, 117157	6	4
18	Inverse Conformational Selection in Lipid-Protein Binding. *Journal of the American Chemical Society*, **2021**, 143, 13701-13709	16.4	4
17	Intermediate structures for higher level arrangements: catching disk-like micelles in decane phosphonic acid aqueous solutions. *Journal of Physical Chemistry B*, **2013**, 117, 6231-40	3.4	3
16	Thermodynamics of Mixing Tetrahydrofuran with 1-Alkanols and Excess Enthalpies of Homomorphy-Related Systems. *Journal of Chemical & Engineering Data*, **2007**, 52, 2298-2305	2.8	3
15	The standard Gibbs energy of adsorption from the bulk at the surface of liquid mixtures: reinterpretation of Traube□s ruleAnalysis of the □dsG0 contributions under the Extended Langmuir model. *Fluid Phase Equilibria*, **2004**, 225, 115-123	2.5	3
14	Calorimetric Methods to Characterize the Forces Driving Macromolecular Association and Folding Processes **2013**, 139-177		2
13	Delving Into the Origin of Destructive Inflammation in COVID-19: A Betrayal of Natural Host Defense Peptides?. *Frontiers in Immunology*, **2020**, 11, 610024	8.4	2
12	Fluid interface calorimetry. *Journal of Colloid and Interface Science*, **2021**, 596, 119-129	9.3	2
11	Aggregation versus inclusion complexes to solubilize drugs with cyclodextrins. A case study using sulphobutylether-□cyclodextrins and remdesivir. *Journal of Molecular Liquids*, **2021**, 343, 117588	6	2
10	A strategy based on thermal flexibility to design triosephosphate isomerase proteins with increased or decreased kinetic stability. *Biochemical and Biophysical Research Communications*, **2018**, 503, 3017-3022	3.4	1
9	Atomistic and Coarse-Grained Molecular Dynamics Simulations of Membrane Proteins **2013**, 193-206		1
8	Natural Fibrous Proteins: Structural Analysis, Assembly, and Applications **2013**, 219-232		1
7	Effect of ionization on the behavior of n-eicosanephosphonic acid monolayers at the air/water interface. Experimental determinations and molecular dynamics simulations. *Langmuir*, **2015**, 31, 2269-80	4	1
6	The standard Gibbs energy of adsorption from the bulk at the surface of liquid mixtures: reinterpretation of Traube□s rule. *Fluid Phase Equilibria*, **2004**, 225, 115-123	2.5	1

5	Cyclodextrin dimers: A versatile approach to optimizing encapsulation and their application to therapeutic extraction of toxic oxysterols. *International Journal of Pharmaceutics*, **2021**, 606, 120522	6.5	1
4	Unsupervised bubble calorimetry analysis: Surface tension from isothermal titration calorimetry. *Journal of Colloid and Interface Science*, **2022**, 606, 1823-1832	9.3	1
3	SuPepMem: A database of innate immune system peptides and their cell membrane interactions.. *Computational and Structural Biotechnology Journal*, **2022**, 20, 874-881	6.8	0
2	Transmembrane Self-Assembled Cyclic Peptide Nanotubes Based on Residues and Cyclic Amino Acids: A Computational Study. *Frontiers in Chemistry*, **2021**, 9, 704160	5	0
1	Simple ApproximaTion for Aggregation Number Determination by Isothermal Titration Calorimetry: STAND-ITC. *Langmuir*, **2021**, 37, 11781-11792	4	0