Viktorya Aviyente

List of Publications by Citations

156 papers	2,530 citations	28 h-index	41 g-index
169 ext. papers	2,794 ext. citations	3.7 avg, IF	5.02 L-index

#	Paper	IF	Citations
156	Role of Chain Transfer Agents in Free Radical Polymerization Kinetics. *Macromolecules*, **2010**, 43, 1823-1835	5.5	144
155	Deamidation of asparagine residues: direct hydrolysis versus succinimide-mediated deamidation mechanisms. *Journal of Physical Chemistry A*, **2009**, 113, 1111-20	2.8	88
154	DFT Study on the Propagation Kinetics of Free-Radical Polymerization of Substituted Acrylates. *Macromolecules*, **2009**, 42, 3033-3041	5.5	66
153	Lewis acid catalysis alters the shapes and products of bis-pericyclic Diels-Alder transition states. *Journal of the American Chemical Society*, **2007**, 129, 4528-9	16.4	66
152	Solvent effects on glycine. I. A supermolecule modeling of tautomerization via intramolecular proton transfer. *Journal of Computational Chemistry*, **2003**, 24, 1789-802	3.5	62
151	Solvent effects on glycine II. Water-assisted tautomerization. *Journal of Computational Chemistry*, **2004**, 25, 690-703	3.5	58
150	Experimental and modeling approach to decolorization of azo dyes by ultrasound: degradation of the hydrazone tautomer. *Journal of Physical Chemistry A*, **2005**, 109, 3506-16	2.8	56
149	Modeling the Oxidative Degradation of Azo Dyes: A Density Functional Theory Study. *Journal of Physical Chemistry A*, **2003**, 107, 4898-4907	2.8	54
148	Effect of Lewis acid catalysts on Diels-Alder and hetero-Diels-Alder cycloadditions sharing a common transition state. *Journal of Organic Chemistry*, **2008**, 73, 7472-80	4.2	52
147	Computational study on nonenzymatic peptide bond cleavage at asparagine and aspartic acid. *Journal of Physical Chemistry A*, **2008**, 112, 8752-61	2.8	51
146	Reaction mechanism of deamidation of asparaginyl residues in peptides: effect of solvent molecules. *Journal of Physical Chemistry A*, **2006**, 110, 8354-65	2.8	50
145	Effect of cooperative hydrogen bonding in azo-hydrazone tautomerism of azo dyes. *Journal of Physical Chemistry A*, **2007**, 111, 13506-14	2.8	47
144	Structures and reactivity of gaseous glycine and its derivatives. *International Journal of Mass Spectrometry*, **2000**, 201, 69-85	1.9	47
143	Analysis of Substituent Effects on the Claisen Rearrangement with Ab Initio and Density Functional Theory. *Journal of Organic Chemistry*, **1997**, 62, 6121-6128	4.2	46
142	Interpretation of hydrogen bonding in the weak and strong regions using conceptual DFT descriptors. *Journal of Physical Chemistry A*, **2006**, 110, 5860-8	2.8	42
141	Elimination of water from the carboxyl group of GlyGlyH+. *Journal of the American Society for Mass Spectrometry*, **2003**, 14, 1192-203	3.5	41
140	Computational Studies on Cinchona Alkaloid-Catalyzed Asymmetric Organic Reactions. *Accounts of Chemical Research*, **2016**, 49, 1250-62	24.3	38

139	Density Functional Theory Study of Free-Radical Polymerization of Acrylates and Methacrylates: Structure–Reactivity Relationship. *Macromolecules*, **2007**, 40, 9590-9602	5.5	37
138	Modeling the Substituent Effect on the Oxidative Degradation of Azo Dyes. *Journal of Physical Chemistry A*, **2004**, 108, 5990-6000	2.8	37
137	Origins of boat or chair preferences in the Ireland-Claisen rearrangements of cyclohexenyl esters: a theoretical study. *Journal of Organic Chemistry*, **2003**, 68, 572-7	4.2	37
136	Cyano, Amino, and Trifluoromethyl Substituent Effects on the Claisen Rearrangement. *Journal of Physical Chemistry A*, **2001**, 105, 383-391	2.8	34
135	Modeling the Solvent Effect on the Tacticity in the Free Radical Polymerization of Methyl Methacrylate. *Macromolecules*, **2010**, 43, 5602-5610	5.5	33
134	Photophysical and Photochemical Studies of Novel Thioxanthone-Functionalized Methacrylates through LED Excitation. *Macromolecular Chemistry and Physics*, **2016**, 217, 1501-1512	2.6	32
133	Transition-state switchings for single potential well ionic dissociations. *The Journal of Physical Chemistry*, **1991**, 95, 9298-9302		31
132	Design of donor-acceptor copolymers for organic photovoltaic materials: a computational study. *Physical Chemistry Chemical Physics*, **2018**, 20, 3581-3591	3.6	30
131	Cyclopolymerization reactions of diallyl monomers: exploring electronic and steric effects using DFT reactivity indices. *Journal of Physical Chemistry A*, **2009**, 113, 8704-11	2.8	30
130	Sonochemical degradation of diclofenac: byproduct assessment, reaction mechanisms and environmental considerations. *Environmental Science and Pollution Research*, **2014**, 21, 5929-39	5.1	29
129	Peptide nanotube formation: a crystal growth process. *Soft Matter*, **2012**, 8, 7463	3.6	29
128	Assessing One- and Two-Photon Optical Properties of Boron Containing Arenes. *Journal of Physical Chemistry C*, **2016**, 120, 17916-17926	3.8	28
127	Computational study of factors controlling the boat and chair transition states of Ireland-Claisen rearrangements. *Journal of Organic Chemistry*, **2010**, 75, 2115-8	4.2	28
126	Modeling the deamidation of asparagine residues via succinimide intermediates. *Journal of Molecular Modeling*, **2001**, 7, 147-160	2	28
125	Efficient Free-Radical Cyclopolymerization of Oriented Styrenic Difunctional Monomers. *Macromolecules*, **2009**, 42, 1860-1866	5.5	27
124	Mechanism and selectivity of cinchona alkaloid catalyzed [1,3]-shifts of allylic trichloroacetimidates. *Journal of Organic Chemistry*, **2009**, 74, 6944-52	4.2	27
123	Modeling the free radical polymerization of acrylates. *International Journal of Quantum Chemistry*, **2005**, 103, 176-189	2.1	27
122	Detection of Nitroaromatic Explosives Based on Fluorescence Quenching of Silafluorene- and Silole-Containing Polymers: A Time-Dependent Density Functional Theory Study. *Journal of Physical Chemistry C*, **2014**, 118, 23946-23953	3.8	26

121	Modelling the hydrolysis of succinimide: formation of aspartate and reversible isomerization of aspartic acid via succinimide. *Organic and Biomolecular Chemistry*, **2003**, 1, 2290-7	3.9	26
120	Theoretical study of hydrogen abstraction from dimethyl ether and methyl tert-butyl ether by hydroxyl radical. *Physical Chemistry Chemical Physics*, **2002**, 4, 1797-1806	3.6	26
119	Theoretical Study on the Alkaline and Neutral Hydrolysis of Succinimide Derivatives in Deamidation Reactions. *Journal of Physical Chemistry A*, **2002**, 106, 11205-11214	2.8	25
118	Origins of the solvent effect on the propagation kinetics of acrylic acid and methacrylic acid. *Journal of Polymer Science Part A*, **2013**, 51, 2024-2034	2.5	23
117	Conformational properties of amphotericin B amide derivatives--impact on selective toxicity. *Journal of Computer-Aided Molecular Design*, **2000**, 14, 689-703	4.2	21
116	Controlling the tacticity in the polymerization of N-isopropylacrylamide: A computational study. *Polymer*, **2011**, 52, 5503-5512	3.9	20
115	Theoretical study of factors controlling rates of cyclization of radical intermediates from diallylamine and diallylammonium monomers in radical polymerizations. *Journal of Organic Chemistry*, **2002**, 67, 5068-75	4.2	19
114	Causation in a cascade: the origins of selectivities in intramolecular nitrone cycloadditions. *Journal of the American Chemical Society*, **2012**, 134, 12010-5	16.4	18
113	Tandem mass spectrometry studies of acetone and acetone/water cluster ions. *Journal of the American Society for Mass Spectrometry*, **1991**, 2, 113-9	3.5	18
112	Hydroxyl radical-mediated degradation of diclofenac revisited: a computational approach to assessment of reaction mechanisms and by-products. *Environmental Science and Pollution Research*, **2017**, 24, 18458-18469	5.1	17
111	Free radical polymerization of ethyl methacrylate and ethyl 2-hydroxy methacrylate: A computational approach to the propagation kinetics. *Polymer*, **2012**, 53, 3211-3219	3.9	17
110	Origins of the diastereoselectivity in hydrogen bonding directed Diels-Alder reactions of chiral dienes with achiral dienophiles: a computational study. *Organic and Biomolecular Chemistry*, **2011**, 9, 8079-88	3.9	17
109	A Theoretical Study of the Mechanism of the Desymmetrization of Cyclic meso-Anhydrides by Chiral Amino Alcohols. *ChemCatChem*, **2010**, 2, 1122-1129	5.2	17
108	Nickel(II)–PPh3 Complexes of S,N-Substituted Thiosemicarbazones – Structure, DFT Study, and Catalytic Efficiency. *European Journal of Inorganic Chemistry*, **2016**, 2016, 538-544	2.3	16
107	Solvent effects on free-radical copolymerization of styrene and 2-hydroxyethyl methacrylate: a DFT study. *New Journal of Chemistry*, **2014**, 38, 170-178	3.6	16
106	Theoretical investigation of thiol-ene click reactions: A DFT perspective. *European Polymer Journal*, **2019**, 110, 211-220	5.2	16
105	Structure-reactivity relationships of novel monomeric photoinitiators. *Journal of Photochemistry and Photobiology A: Chemistry*, **2016**, 329, 77-87	4.7	15
104	Insertion of Amines and Alcohols into Proton-Bound Dimers. A Density Functional Study. *Journal of Physical Chemistry A*, **1997**, 101, 2597-2606	2.8	15

103	Structures and energetics of proton-bound formic acid–water clusters, (HCOOH)n(H2O)H+. *International Journal of Mass Spectrometry and Ion Processes*, **1997**, 161, 123-132		15
102	Exploring the Photophysics of Polyfluorinated Phthalocyanine Derivatives as Potential Theranostic Agents. *Journal of Physical Chemistry C*, **2019**, 123, 24417-24425	3.8	14
101	The origin of exo-stereoselectivity of norbornene in hetero Diels-Alder reactions. *Organic and Biomolecular Chemistry*, **2014**, 12, 8079-86	3.9	14
100	Computational Insight into the Explosive Detection Mechanisms in Silafluorene- and Silole-Containing Photoluminescent Polymers. *Journal of Physical Chemistry C*, **2014**, 118, 6385-6397	3.8	14
99	A theoretical study on the mechanism of the cyclopolymerization of diallyl monomers. *Journal of Organic Chemistry*, **2003**, 68, 6369-74	4.2	14
98	Why does Asn71 deamidate faster than Asn15 in the enzyme triosephosphate isomerase? Answers from microsecond molecular dynamics simulation and QM/MM free energy calculations. *Biochemistry*, **2015**, 54, 1429-39	3.2	13
97	Barriers to internal rotation around the C-N bond in 3-(o-aryl)-5-methyl-rhodanines using NMR spectroscopy and computational studies. Electron density topological analysis of the transition states. *Organic and Biomolecular Chemistry*, **2004**, 2, 2426-36	3.9	13
96	Synthesis and modeling of new phosphorus-containing acrylates. *Journal of Polymer Science Part A*, **2005**, 43, 2574-2583	2.5	13
95	Modeling Proton-Bound Methanol, Ammonia, and Amine Complexes of 12-Crown-4-Ether and Dimethoxyethane (Glyme) Using Density Functional Theory. *Journal of Physical Chemistry A*, **1998**, 102, 6357-6365	2.8	13
94	Solvent Effects on Thiol-Ene Kinetics and Reactivity of Carbon and Sulfur Radicals. *Journal of Physical Chemistry A*, **2020**, 124, 2580-2590	2.8	12
93	Quorum-sensing inhibitor potential of trans-anethole aganist Pseudomonas aeruginosa. *Journal of Applied Microbiology*, **2018**, 125, 731-739	4.7	12
92	A DFT study of carbonyl oxide and its methyl-substituted analogues in solution. *Chemical Physics Letters*, **1998**, 288, 669-676	2.5	12
91	Claisen rearrangement of aliphatic allyl vinyl ethers in the presence of copper(II) bisoxazoline. *Journal of Organic Chemistry*, **2008**, 73, 4800-9	4.2	12
90	Modeling the stereoselectivity of the Johnson-Claisen rearrangements in the Danishefsky synthesis of gelsemine. *Journal of Organic Chemistry*, **2005**, 70, 7028-34	4.2	12
89	Modeling the effect of substitution on the Pb(OAc)4 mediated oxidative cleavage of steroidal 1,2-diols. *Journal of Organic Chemistry*, **2005**, 70, 7080-6	4.2	12
88	A Computational Study on the Substituent Effect of Diallylamine Monomers in Their Cyclopolymerization Reactions. *Journal of Physical Chemistry A*, **2002**, 106, 8184-8190	2.8	12
87	Photophysical, kinetic and thermodynamic study of one-component Type II thioxanthone acetic acid photoinitiators. *European Polymer Journal*, **2020**, 136, 109909	5.2	12
86	Cinchona Alkaloid Catalyzed Asymmetric Desymmetrization of meso-Cyclic Anhydrides: The Origins of Stereoselectivity. *ChemCatChem*, **2015**, 7, 4173-4179	5.2	11

85	Solvent-catalyzed ring-chain-ring tautomerization in axially chiral compounds. *Chemistry - A European Journal*, **2012**, 18, 12725-32	4.8	11
84	Understanding the stereoselection induced by chiral anthracene templates in Diels-Alder cycloaddition: a DFT study. *Journal of Organic Chemistry*, **2009**, 74, 2328-36	4.2	11
83	Lead tetraacetate mediated one-pot multistage transformations: theoretical studies on the diverging behavior in the Hajos-Parrish and Wieland-Miescher series. *Journal of Organic Chemistry*, **2002**, 67, 2447-52	4.2	11
82	Theoretical study of isomeric clusters of protonated acetone. *Computational and Theoretical Chemistry*, **1992**, 277, 285-292		11
81	A quantum mechanical approach to the kinetics of the hydrogen abstraction reaction H2O2 + ⁻OH -p HO2 + H2O. *International Journal of Chemical Kinetics*, **2005**, 37, 502-514	1.4	10
80	Conformational equilibria of α-substituted carbonyl compounds. Study of solvent effects. *Computational and Theoretical Chemistry*, **1993**, 280, 169-179		10
79	Kinetic energy release measurements with an ion trapping device and time-resolved ion momentum spectrometry (trims). *International Journal of Mass Spectrometry and Ion Processes*, **1986**, 70, 67-77		10
78	Rationalizing the regioselectivity of cationic ring-opening polymerization of benzoxazines. *European Polymer Journal*, **2018**, 105, 61-67	5.2	10
77	Understanding the Impact of Thiophene/Furan Substitution on Intrinsic Charge-Carrier Mobility. *Journal of Physical Chemistry C*, **2017**, 121, 25682-25690	3.8	9
76	Multiscale modeling of poly(2-isopropyl-2-oxazoline) chains in aqueous solution. *European Polymer Journal*, **2017**, 88, 594-604	5.2	9
75	Structure−reactivity relationships of alkyl α-hydroxymethacrylate derivatives. *Journal of Polymer Science Part A*, **2011**, 49, 3058-3068	2.5	9
74	Modeling the cyclopolymerization of diallyl ether and methyl α-[(allyloxy)methyl]acrylate. *International Journal of Quantum Chemistry*, **2007**, 107, 894-906	2.1	9
73	An ab initio study of the formation of alkoxy radicals by reactions of simple alkenes with the OH radical. *Journal of Molecular Modeling*, **2001**, 7, 398-407	2	9
72	A computational approach to the polymerizabilities of diallylamines. *Journal of Molecular Modeling*, **2001**, 7, 257-264	2	9
71	The Interaction of Protonated Diglycine with Ammonia: A Density Functional Theory Model Study. *Journal of Physical Chemistry A*, **2000**, 104, 7061-7067	2.8	9
70	Structures, Energetics, and Reactions of Proton-Bound Hydrazine Clusters. *The Journal of Physical Chemistry*, **1995**, 99, 1776-1785		9
69	Medium-Ring Effects on the Endo/Exo Selectivity of the Organocatalytic Intramolecular Diels-Alder Reaction. *Journal of Organic Chemistry*, **2015**, 80, 12058-75	4.2	8
68	Cyclization tendencies in the free radical polymerization of allyl acrylate derivatives: A computational study. *Journal of Polymer Science Part A*, **2011**, 49, 2474-2483	2.5	8

67	AB INITIO STUDY ON THE CONFORMATIONAL BEHAVIOUR OF ETHANE-1,1-DIOL and ETHANE-1,1,2-TRIOL IN SOLUTION. *Journal of Physical Organic Chemistry*, **1997**, 10, 196-206	2.1	8
66	Electrostatic solvent effects on the conversion of substituted carbonyl oxides to dioxiranes. *Journal of Molecular Modeling*, **2001**, 7, 70-79	2	8
65	A blind SAMPL6 challenge: insight into the octanol-water partition coefficients of drug-like molecules via a DFT approach. *Journal of Computer-Aided Molecular Design*, **2020**, 34, 463-470	4.2	7
64	Selectivity in the aggregates of the chiral organolithium N-Boc-2-lithiopiperidine with a chiral ligand: a DFT study. *Molecular Physics*, **2012**, 110, 353-359	1.7	7
63	A Computational Study of the Wallach Rearrangement. *Structural Chemistry*, **1998**, 9, 15-25	1.8	7
62	Origin of diastereoselectivity in the synthesis of chiral bicyclic lactams: pi-facial selective attack of singlet oxygen induced by hindered internal rotation. *Journal of Physical Chemistry A*, **2007**, 111, 5855-63	2.8	7
61	Solvent effect on the synthesis of clarithromycin: a molecular dynamics study. *Journal of Computer-Aided Molecular Design*, **2004**, 18, 145-54	4.2	7
60	Conformational equilibria of 5-substituted 1,3-dioxanes. study of solvent effects. *Computational and Theoretical Chemistry*, **1993**, 287, 185-191		7
59	Hydroxyl radical-mediated degradation of salicylic acid and methyl paraben: an experimental and computational approach to assess the reaction mechanisms. *Environmental Science and Pollution Research*, **2019**, 26, 33125-33134	5.1	6
58	First RAFT polymerization of captodative 2-acetamidoacrylic acid (AAA) monomer: An experimental and theoretical study. *Polymer*, **2013**, 54, 5122-5132	3.9	6
57	A computational study on the reactivity enhancement in the free radical polymerization of alkyl α-hydroxymethacrylate and acrylate derivatives. *Journal of Polymer Science Part A*, **2013**, 51, 880-889	2.5	6
56	Effect of Solvation on Ozonolysis Reaction Intermediates and Transition States. *Journal of Molecular Modeling*, **2000**, 6, 608-617	2	6
55	Oxygen donor potential of carbonyl oxide and dioxirane: a DFT study. *Computational and Theoretical Chemistry*, **1999**, 492, 165-174		6
54	Solvent effect on the conformational behavior of substituted spiro[4.5]decanes and spiro[5.5]undecanes. *Canadian Journal of Chemistry*, **1995**, 73, 703-709	0.9	6
53	1,3-Dipolar Cycloaddition Reactions of Low-Valent Rhodium and Iridium Complexes with Arylnitrile N-Oxides. *Journal of Organic Chemistry*, **2017**, 82, 5096-5101	4.2	5
52	Local vibrational mode analysis of ion-solvent and solvent-solvent interactions for hydrated Ca clusters. *Journal of Chemical Physics*, **2020**, 153, 224303	3.9	5
51	Bismuth nitrate-promoted disproportionative condensation of indoles with cyclohexanone: a new-type azafulvenium reactivity of indole. *New Journal of Chemistry*, **2017**, 41, 9674-9687	3.6	5
50	Conformational behavior of 2-dimethylamino-1,3-dithiane in solution. *Journal of the Chemical Society Perkin Transactions II*, **1997**, 1835-1838		5

49	Theoretical Approach to the Wear and Tear Mechanism in Triosephoshate Isomerase: A QM/MM Study. *Journal of Physical Chemistry B*, **2004**, 108, 3925-3934	3.4	5
48	Coupling of structural fluctuations to deamidation reaction in triosephosphate isomerase by Gaussian network model. *Proteins: Structure, Function and Bioinformatics*, **2006**, 62, 715-27	4.2	5
47	Time-dependent mass spectra and breakdown graphs. 11. Time-resolved ion momentum spectrometry of anisole. *The Journal of Physical Chemistry*, **1988**, 92, 6548-6553		5
46	Electronic Structure of Atomically Dispersed Supported Iridium Catalyst Controls Iridium Aggregation. *ACS Catalysis*, **2020**, 10, 12354-12358	13.1	5
45	Activity of Topotecan toward the DNA/Topoisomerase I Complex: A Theoretical Rationalization. *Biochemistry*, **2018**, 57, 1542-1551	3.2	4
44	The efficient cyclopolymerization of silyl-tethered styrenic difunctional monomers. *Journal of Polymer Science Part A*, **2018**, 56, 1593-1599	2.5	4
43	Organocatalysts in Ring-Opening Polymerization: Revealing Their Effect on Stereochemistry. *European Polymer Journal*, **2019**, 121, 109291	5.2	4
42	How substitution tunes the electronic and transport properties of oligothiophenes, oligoselenophenes and oligotellurophenes. *Synthetic Metals*, **2015**, 210, 236-244	3.6	4
41	Molecular Docking Study Based on Pharmacophore Modeling for Novel PhosphodiesteraseIV Inhibitors. *Molecular Informatics*, **2012**, 31, 459-71	3.8	4
40	A computational approach to the free radical polymerization kinetics of alkyl □hydroxymethacrylate monomers: A structure□reactivity relationship. *Journal of Polymer Science Part A*, **2013**, 51, 2375-2384	2.5	4
39	Modeling the selective methylation in the synthesis of clarithromycin. *Perkin Transactions II RSC*, **2002**, 670-675		4
38	How does the OH group affect the conversion of carbonyl oxide to dioxirane?. *Computational and Theoretical Chemistry*, **2000**, 530, 97-107		4
37	Protonated aldehyde clusters: a semiempirical approach. *Journal of Molecular Structure*, **1993**, 299, 191-195	3.4	4
36	Analysis of the kinetics of the thermal decomposition of pentafluoroethane. *Canadian Journal of Chemistry*, **1990**, 68, 1332-1337	0.9	4
35	Initiation of the reaction of deamidation in triosephosphate isomerase: investigations by means of molecular dynamics simulations. *Journal of Physical Chemistry B*, **2012**, 116, 6288-301	3.4	3
34	Understanding the mode of action of ThDP in benzoylformate decarboxylase. *Biopolymers*, **2010**, 93, 32-46	2.2	3
33	Conformational analysis of 2-substituted-l,3-diheteroanes. A theoretical study of solvent effects. *Computational and Theoretical Chemistry*, **1997**, 418, 41-47		3
32	A computational approach to the synthesis of dirithromycin. *Journal of Molecular Modeling*, **2004**, 10, 94-101	2	3

31	Conformational analysis of 2-cyano-1,1-dihydroxyethane in solution. *Journal of Physical Organic Chemistry*, **1996**, 9, 119-127	2.1	3
30	SAMPL7 blind challenge: quantum-mechanical prediction of partition coefficients and acid dissociation constants for small drug-like molecules. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 841-851	4.2	3
29	Using Atomic Charges to Describe the p of Carboxylic Acids. *Journal of Chemical Information and Modeling*, **2021**, 61, 2733-2743	6.1	3
28	Effect of Lewis acids on the stereoregularity of N,N-dimethyl acrylamide: A computational approach. *European Polymer Journal*, **2016**, 83, 67-76	5.2	3
27	Influence of odd-even effect and intermolecular interactions in 2D molecular layers of bisamide organogelators.. *RSC Advances*, **2018**, 8, 35195-35204	3.7	3
26	Relationship Between the Free Radical Polymerization Rates of Methacrylates and the Chemical Properties of their Monomeric Radicals. *Macromolecular Chemistry and Physics*, **2015**, 216, 334-343	2.6	2
25	Elucidation of the atroposelectivity in the synthesis of axially chiral thiohydantoin derivatives. *Organic and Biomolecular Chemistry*, **2020**, 18, 2233-2241	3.9	2
24	Conformational equilibria of 5-substituted-1,3-dithianes. Study of solvent effects. *Computational and Theoretical Chemistry*, **1997**, 418, 113-118		2
23	Hybrid Usage of Computational Tools in Drug Synthesis. *Current Computer-Aided Drug Design*, **2007**, 3, 149-159	1.4	2
22	Theoretical study of selective methylation in the synthesis of azithromycin. *Journal of Computer-Aided Molecular Design*, **2004**, 18, 1-11	4.2	2
21	Computational study of alkyllithium/pyridine derivative systems as initiators for the living anionic polymerization of methyl methacrylates. *Journal of Polymer Science Part A*, **2005**, 43, 455-467	2.5	2
20	Photophysical Properties of Benzophenone-Based TADF Emitters in Relation to Their Molecular Structure.. *Journal of Physical Chemistry A*, **2022**,	2.8	2
19	Elucidation of the Mechanism of Silver-Catalyzed Inverse Electron-Demand Diels-Alder (IEDDA) Reaction of 1,2-Diazines and Siloxy Alkynes. *ChemCatChem*, **2020**, 12, 366-372	5.2	2
18	Pyrolysis of Alkanes: A Computational Approach. *Journal of Physical Chemistry A*, **2020**, 124, 5700-5708	2.8	1
17	Role of the n+1 amino acid residue on the deamidation of asparagine in pentapeptides. *Molecular Physics*, **2015**, 113, 3839-3848	1.7	1
16	Elucidating the Structural Isomerism of Fluorescent Strigolactone Analogue CISA-1. *European Journal of Organic Chemistry*, **2015**, 2015, 1211-1217	3.2	1
15	Computational study of the synthesis of benzoin derivatives from benzil. *International Journal of Quantum Chemistry*, **2006**, 106, 1596-1610	2.1	1
14	2-Nitroethanal conformations in solution: AnAb initio SCRF study. *Structural Chemistry*, **1994**, 5, 357-360	1.8	1

13	A semiempirical study of protonated ammonia–triethylamine clusters. *Computational and Theoretical Chemistry*, **1994**, 312, 85-91		1
12	Tandem mass spectrometry by time-resolved Ion momentum spectrometry. *Biological Mass Spectrometry*, **1988**, 16, 249-251		1
11	Binding of self-etching monomers to hydroxyapatite: A computational approach. *European Polymer Journal*, **2020**, 122, 109344	5.2	1
10	Oxidative decomposition and mineralization of caffeine by advanced oxidation processes: The effect of hybridization. *Ultrasonics Sonochemistry*, **2021**, 76, 105635	8.9	1
9	Assessing protein-ligand binding modes with computational tools: the case of PDE4B. *Journal of Computer-Aided Molecular Design*, **2017**, 31, 563-575	4.2	0
8	Role of ionic liquids on the selectivity and the rate of organic reactions: A computational approach. *Journal of Molecular Graphics and Modelling*, **2019**, 88, 309-317	2.8	0
7	A DFT approach to discriminate the antagonist and partial agonist activity of ligands binding to the NMDA receptor. *Molecular Physics*, **2018**, 116, 323-337	1.7	0
6	Prediction of the 1H NMR spectra of epoxy-fused cyclopentane derivatives by calculations of chemical shifts and spin–spin coupling constants. *Molecular Physics*, **2013**, 111, 3147-3155	1.7	0
5	Origins of the photoinitiation capacity of aromatic thiols as photoinitiators: a computational study. *Physical Chemistry Chemical Physics*, **2021**, 23, 24377-24385	3.6	0
4	Computational Study of Photo-oxidative Degradation Mechanisms of Boron-Containing Oligothiophenes. *Journal of Physical Chemistry A*, **2020**, 124, 1390-1398	2.8	
3	A study on the structures of the substituted (aminomethyl)lithium and (thiomethyl)lithium compounds. *Journal of Molecular Modeling*, **2002**, 8, 156-67	2	
2	Solvent Effect on Vibrational Frequencies of Substituted Acetaldehydes **1993**, 135-139		
1	Shell-like Features and Charge Localization in Protonated Helium Clusters: a Density Functional Study. *Progress in Theoretical Chemistry and Physics*, **2000**, 103-122	0.6	