Russo Nino

List of Publications by Citations

431 papers	12,947 citations	54 h-index	90 g-index
446 ext. papers	14,237 ext. citations	4.3 avg, IF	6.66 L-index

#	Paper	IF	Citations
431	The molecular basis of working mechanism of natural polyphenolic antioxidants. *Food Chemistry*, **2011**, 125, 288-306	8.5	717
430	Antioxidant Properties of Phenolic Compounds: H-Atom versus Electron Transfer Mechanism. *Journal of Physical Chemistry A*, **2004**, 108, 4916-4922	2.8	481
429	Iron chelation by the powerful antioxidant flavonoid quercetin. *Journal of Agricultural and Food Chemistry*, **2006**, 54, 6343-51	5.7	320
428	Structure, Conformation, and Electronic Properties of Apigenin, Luteolin, and Taxifolin Antioxidants. A First Principle Theoretical Study. *Journal of Physical Chemistry A*, **2004**, 108, 92-96	2.8	244
427	Food Antioxidants: Chemical Insights at the Molecular Level. *Annual Review of Food Science and Technology*, **2016**, 7, 335-52	14.7	222
426	Antioxidant activity of trans-resveratrol toward hydroxyl and hydroperoxyl radicals: a quantum chemical and computational kinetics study. *Journal of Organic Chemistry*, **2012**, 77, 3868-77	4.2	183
425	A physicochemical examination of the free radical scavenging activity of Trolox: mechanism, kinetics and influence of the environment. *Physical Chemistry Chemical Physics*, **2013**, 15, 4642-50	3.6	154
424	Bond energies and attachments sites of sodium and potassium cations to DNA and RNA nucleic acid bases in the gas phase. *Journal of the American Chemical Society*, **2001**, 123, 10272-9	16.4	144
423	LANL2DZ basis sets recontracted in the framework of density functional theory. *Journal of Chemical Physics*, **2006**, 125, 104107	3.9	136
422	A density functional study of small copper clusters: Cun (n?5). *Journal of Chemical Physics*, **1996**, 105, 9546-9556	3.9	136
421	Density functional computations of the energetic and spectroscopic parameters of quercetin and its radicals in the gas phase and in solvent. *Theoretical Chemistry Accounts*, **2004**, 111, 210-216	1.9	135
420	Theoretical determination of electron affinity and ionization potential of DNA and RNA bases. *Journal of Computational Chemistry*, **2000**, 21, 1243-1250	3.5	126
419	Semiempirical molecular modeling into quercetin reactive site: structural, conformational, and electronic features. *Journal of Agricultural and Food Chemistry*, **2000**, 48, 3232-7	5.7	122
418	Protonation of thymine, cytosine, adenine, and guanine DNA nucleic acid bases: Theoretical investigation into the framework of density functional theory. *Journal of Computational Chemistry*, **1998**, 19, 989-1000	3.5	116
417	Interaction of cysteine with Cu2+ and group IIb (Zn2+, Cd2+, Hg2+) metal cations: a theoretical study. *Journal of Mass Spectrometry*, **2005**, 40, 300-6	2.2	111
416	Gas-phase metal ion (Li+, Na+, Cu+) affinities of glycine and alanine. *Journal of Inorganic Biochemistry*, **2000**, 79, 179-85	4.2	107
415	Theoretical Study of Two-State Reactivity of Transition Metal Cations: The Difficult Case of Iron Ion Interacting with Water, Ammonia, and Methane. *Journal of Physical Chemistry A*, **2004**, 108, 1069-1081	2.8	106

414	Spectroscopic properties of porphyrin-like photosensitizers: insights from theory. *Journal of Physical Chemistry B*, **2006**, 110, 2398-404	3.4	104
413	Radical scavenging ability of gallic acid toward OH and OOH radicals. Reaction mechanism and rate constants from the density functional theory. *Journal of Physical Chemistry B*, **2014**, 118, 10380-9	3.4	101
412	On the hydrolysis mechanism of the second-generation anticancer drug carboplatin. *Chemistry - A European Journal*, **2007**, 13, 10108-16	4.8	101
411	Gas and liquid phase acidity of natural antioxidants. *Journal of Agricultural and Food Chemistry*, **2006**, 54, 3078-85	5.7	100
410	Interaction of Li+, Na+, and K+ with the Proline Amino Acid. Complexation Modes, Potential Energy Profiles, and Metal Ion Affinities. *Journal of Physical Chemistry B*, **2003**, 107, 2588-2594	3.4	98
409	Structural and electronic characterization of the complexes obtained by the interaction between bare and hydrated first-row transition-metal ions (Mn(2+), Fe(2+), Co(2+), Ni(2+), Cu(2+), Zn(2+)) and glycine. *Journal of Physical Chemistry B*, **2006**, 110, 24666-73	3.4	97
408	Lithium Affinity for DNA and RNA Nucleobases. The Role of Theoretical Information in the Elucidation of the Mass Spectrometry Data. *Journal of Physical Chemistry B*, **2001**, 105, 4735-4741	3.4	95
407	Structures and electronic absorption spectra of a recently synthesised class of photodynamic therapy agents. *Chemistry - A European Journal*, **2006**, 12, 6797-803	4.8	94
406	The second-generation anticancer drug Nedaplatin: a theoretical investigation on the hydrolysis mechanism. *Journal of Physical Chemistry B*, **2009**, 113, 14473-9	3.4	90
405	Reaction of SC+(1D,3D) with H2O, NH3, and CH4: a density functional study. *Journal of the American Chemical Society*, **2001**, 123, 2588-96	16.4	90
404	Pyranoanthocyanins: a theoretical investigation on their antioxidant activity. *Journal of Agricultural and Food Chemistry*, **2010**, 58, 8862-71	5.7	89
403	Theoretical study of ammonia and methane activation by first-row transition metal cations M(+) (M = Ti, V, Cr). *Journal of the American Chemical Society*, **2002**, 124, 1471-80	16.4	89
402	Density-Functional Approach to Hardness Evaluation and Its Use in the Study of the Maximum Hardness Principle. *Journal of the American Chemical Society*, **1998**, 120, 9053-9058	16.4	87
401	OsB2 and RuB2, ultra-incompressible, hard materials: First-principles electronic structure calculations. *Chemical Physics Letters*, **2006**, 425, 311-314	2.5	86
400	Detailed Investigation of the OH Radical Quenching by Natural Antioxidant Caffeic Acid Studied by Quantum Mechanical Models. *Journal of Chemical Theory and Computation*, **2011**, 7, 4218-33	6.4	85
399	The inactivation of lipid peroxide radical by quercetin. A theoretical insight. *Physical Chemistry Chemical Physics*, **2010**, 12, 7662-70	3.6	83
398	About the Mulliken electronegativity in DFT. *Theoretical Chemistry Accounts*, **2005**, 114, 38-45	1.9	81
397	Absorption spectra of first-row transition metal complexes of bacteriochlorins: a theoretical analysis. *Journal of Physical Chemistry B*, **2005**, 109, 12214-21	3.4	74

396	A combined theoretical and experimental study on the oxidation of fulvic acid by the sulfate radical anion. *Photochemical and Photobiological Sciences*, **2009**, 8, 992-7	4.2	72
395	A molecular simulation study on gas diffusion in a dense poly(ether‐ether‐ketone) membrane. *Polymer*, **2001**, 42, 521-533	3.9	71
394	Proton Affinity and Protonation Sites of Aniline. Energetic Behavior and Density Functional Reactivity Indices. *Journal of Physical Chemistry A*, **2000**, 104, 4017-4021	2.8	70
393	Neutral and acidic hydrolysis reactions of the third generation anticancer drug oxaliplatin. *Journal of Physical Chemistry B*, **2009**, 113, 831-8	3.4	69
392	A comparative study of the catalytic mechanisms of the zinc and cadmium containing carbonic anhydrase. *Journal of the American Chemical Society*, **2005**, 127, 4242-53	16.4	69
391	Fukui Indices from Perturbed Kohn‐Sham Orbitals and Regional Softness from Mayer Atomic Valences. *Journal of Physical Chemistry A*, **2001**, 105, 1959-1967	2.8	69
390	Gas-phase chemistry of actinides ions: new insights into the reaction of UO+ and UO2+ with water. *Journal of the American Chemical Society*, **2007**, 129, 4229-39	16.4	67
389	Gas-Phase Absolute Ca2+ and Mg2+ Affinity for Nucleic Acid Bases. A Theoretical Determination. *Journal of Physical Chemistry A*, **2003**, 107, 11533-11538	2.8	64
388	Mechanism of nitrate reduction by Desulfovibrio desulfuricans nitrate reductase--a theoretical investigation. *Chemistry - A European Journal*, **2006**, 12, 2532-41	4.8	63
387	Topological Analysis of the Reaction of Mn+ (7S,5S) with H2O, NH3, and CH4 Molecules. *Journal of Physical Chemistry A*, **2003**, 107, 4862-4868	2.8	62
386	Potential energy surfaces for the gas-phase interaction between alpha-alanine and alkali metal Ions (Li+, Na+, K+). A density functional study. *Inorganic Chemistry*, **2001**, 40, 6439-43	5.1	62
385	Antioxidant properties of several coumarin‐chalcone hybrids from theoretical insights. *RSC Advances*, **2015**, 5, 565-575	3.7	61
384	Theoretical and experimental investigation on the oxidation of gallic acid by sulfate radical anions. *Journal of Physical Chemistry A*, **2008**, 112, 1188-94	2.8	60
383	On the hardness evaluation in solvent for neutral and charged systems. *Journal of the American Chemical Society*, **2002**, 124, 1494-9	16.4	60
382	Structural and Electronic Characterization of Antioxidants from Marine Organisms. *Theoretical Chemistry Accounts*, **2006**, 115, 361-369	1.9	59
381	Peptide hydrolysis by the binuclear zinc enzyme aminopeptidase from Aeromonas proteolytica: a density functional theory study. *Journal of Physical Chemistry B*, **2008**, 112, 2494-500	3.4	58
380	Spin‐Orbit Charge Recombination Intersystem Crossing in Phenothiazine‐Anthracene Compact Dyads: Effect of Molecular Conformation on Electronic Coupling, Electronic Transitions, and Electron Spin Polarizations of the Triplet States. *Journal of Physical Chemistry C*, **2018**, 122, 27850-27865	3.8	56
379	Which one among Zn(II), Co(II), Mn(II), and Fe(II) is the most efficient ion for the methionine aminopeptidase catalyzed reaction?. *Journal of the American Chemical Society*, **2007**, 129, 7776-84	16.4	55

378	Density functional approach to the structures and EPR parameters of open shell systems. The case of fluorovinyl radicals. *Chemical Physics Letters*, **1993**, 212, 5-11	2.5	54
377	Enzymatic Flexibility and Reaction Rate: A QM/MM Study of HIV-1 Protease. *ACS Catalysis*, **2015**, 5, 5617-5626	9.1	53
376	On the applicability of the HSAB principle through the use of improved computational schemes for chemical hardness evaluation. *Journal of Computational Chemistry*, **2004**, 25, 994-1003	3.5	53
375	Atomic Radii Scale and Related Size Properties from Density Functional Electronegativity Formulation. *Journal of Physical Chemistry A*, **2003**, 107, 5461-5465	2.8	53
374	Human insulin-degrading enzyme working mechanism. *Journal of the American Chemical Society*, **2009**, 131, 14804-11	16.4	52
373	On the inhibitor effects of bergamot juice flavonoids binding to the 3-hydroxy-3-methylglutaryl-CoA reductase (HMGR) enzyme. *Journal of Agricultural and Food Chemistry*, **2010**, 58, 10768-73	5.7	51
372	Understanding zinc(II) chelation with quercetin and luteolin: a combined NMR and theoretical study. *Journal of Physical Chemistry B*, **2015**, 119, 83-95	3.4	50
371	General trends in the molecular physics of azabiphenyls. *Molecular Physics*, **1983**, 49, 599-619	1.7	50
370	Gas-phase reactions of the bare Th2+ and U2+ ions with small alkanes, CH4, C2H6, and C3H8: experimental and theoretical study of elementary organoactinide chemistry. *Journal of the American Chemical Society*, **2011**, 133, 1955-70	16.4	49
369	V3: Structure and vibrations from density functional theory, Franck□Condon factors, and the pulsed-field ionization zero-electron-kinetic energy spectrum. *Journal of Chemical Physics*, **2001**, 114, 4036-4044	3.9	49
368	Newly developed basis sets for density functional calculations. *Journal of Computational Chemistry*, **2005**, 26, 175-84	3.5	48
367	First-principle time-dependent study of magnesium-containing porphyrin-like compounds potentially useful for their application in photodynamic therapy. *Journal of Physical Chemistry B*, **2008**, 112, 4123-30	3.4	47
366	Density functional study of the antioxidant activity of some recently synthesized resveratrol analogues. *Food Chemistry*, **2013**, 141, 2017-24	8.5	46
365	Catalytic mechanism of the arylsulfatase promiscuous enzyme from Pseudomonas aeruginosa. *Chemistry - A European Journal*, **2013**, 19, 2185-92	4.8	46
364	Which one among the Pt-containing anticancer drugs more easily forms monoadducts with G and A DNA bases? A comparative study among oxaliplatin, nedaplatin, and carboplatin. *Inorganic Chemistry*, **2011**, 50, 6965-71	5.1	46
363	A Computational Study (TDDFT and RICC2) of the Electronic Spectra of Pyranoanthocyanins in the Gas Phase and Solution. *Journal of Chemical Theory and Computation*, **2011**, 7, 1073-81	6.4	46
362	Gas-phase theoretical prediction of the metal affinity of copper(I) ion for DNA and RNA bases. *Journal of Mass Spectrometry*, **2003**, 38, 265-70	2.2	46
361	Theoretical Determination of Electronic Spectra and Intersystem Spin-Orbit Coupling: The Case of Isoindole-BODIPY Dyes. *Journal of Chemical Theory and Computation*, **2014**, 10, 4006-13	6.4	45

360	Catalytic activity of a Eclass zinc and cadmium containing carbonic anhydrase. Compared work mechanisms. *Physical Chemistry Chemical Physics*, **2011**, 13, 3468-77	3.6	45
359	Methane CHI Bond Activation by Gas-Phase Th+ and U+: Reaction Mechanisms and Bonding Analysis. *Organometallics*, **2009**, 28, 3716-3726	3.8	45
358	Spectrophotometric study of the copigmentation of malvidin 3-O-glucoside with p-coumaric, vanillic and syringic acids. *Food Chemistry*, **2013**, 141, 3614-20	8.5	44
357	A comparative study of the antioxidant power of flavonoid catechin and its planar analogue. *Journal of Agricultural and Food Chemistry*, **2007**, 55, 7944-9	5.7	44
356	Spin-Orbit Charge-Transfer Intersystem Crossing (ISC) in Compact Electron Donor-Acceptor Dyads: ISC Mechanism and Application as Novel and Potent Photodynamic Therapy Reagents. *Chemistry - A European Journal*, **2020**, 26, 1091-1102	4.8	44
355	Reaction mechanism of molybdoenzyme formate dehydrogenase. *Chemistry - A European Journal*, **2008**, 14, 8674-81	4.8	43
354	Insertion Reaction of Mn+ Bare Metal Cation into the NHI and CHI Bonds of Ammonia and Methane. *Journal of Physical Chemistry A*, **2002**, 106, 8937-8944	2.8	43
353	Halogen atom effect on the photophysical properties of substituted aza-BODIPY derivatives. *Physical Chemistry Chemical Physics*, **2017**, 19, 2530-2536	3.6	42
352	The catalytic mechanism of protein phosphatase 5 established by DFT calculations. *Chemistry - A European Journal*, **2013**, 19, 14081-9	4.8	42
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348	The role of glutathione in cadmium ion detoxification: coordination modes and binding properties--a density functional study. *Journal of Inorganic Biochemistry*, **2009**, 103, 50-7	4.2	40
347	On the Potential Use of Squaraine Derivatives as Photosensitizers in Photodynamic Therapy: A TDDFT and RICC2 Survey. *Journal of Chemical Theory and Computation*, **2009**, 5, 1849-57	6.4	40
346	The preferred reaction path for the oxidation of methanol by PQQ-containing methanol dehydrogenase: addition-elimination versus hydride-transfer mechanism. *Chemistry - A European Journal*, **2007**, 13, 2109-17	4.8	40
345	Model potential for As and LCGTO MP LSD calculation of geometry, electronic structure and photoelectron spectra for As2 and As4. *Chemical Physics Letters*, **1987**, 142, 169-174	2.5	40
344	Homogeneous Gold Catalysis: Hydration of 1,2-Diphenylacetylene with Methanol in Aqueous Media. A Theoretical Viewpoint. *Organometallics*, **2012**, 31, 3074-3080	3.8	39
343	Correlation between Energy, Polarizability, and Hardness Profiles in the Isomerization Reaction of HNO and ClNO. *Journal of Physical Chemistry A*, **2001**, 105, 442-450	2.8	39

342	Protonation of glycine and alanine: proton affinities, intrinsic basicities and proton transfer path. *Computational and Theoretical Chemistry*, **1998**, 430, 41-49		38
341	Hydration of ionic species studied by the reference interaction site model with a repulsive bridge correction. *Journal of Computational Chemistry*, **2008**, 29, 2406-15	3.5	38
340	Gas-phase interaction between DNA and RNA bases and copper (II) ion: A density functional study. *International Journal of Quantum Chemistry*, **2004**, 98, 347-354	2.1	38
339	The mutual influence of non-covalent interactions in pi-electron deficient cavities: the case of anion recognition by tetraoxacalix[2]arene[2]triazine. *Chemical Communications*, **2010**, 46, 5894-6	5.8	37
338	The degradation pathways in chloride medium of the third generation anticancer drug oxaliplatin. *Journal of Physical Chemistry B*, **2008**, 112, 10765-8	3.4	37
337	PDT-correlated photophysical properties of thienopyrrole BODIPY derivatives. Theoretical insights. *Dyes and Pigments*, **2016**, 130, 9-15	4.6	37
336	Photophysical properties of free and metallated meso-substituted tetrabenzotriazaporphyrin from density functional theory investigation. *Dyes and Pigments*, **2015**, 120, 335-339	4.6	36
335	Density functional predictions of antioxidant activity and UV spectral features of nasutin A, isonasutin, ellagic acid, and one of its possible derivatives. *Journal of Agricultural and Food Chemistry*, **2013**, 61, 9650-7	5.7	36
334	On the Pt(+) and Rh(+) Catalytic Activity in the Nitrous Oxide Reduction by Carbon Monoxide. *Journal of Chemical Theory and Computation*, **2008**, 4, 1886-90	6.4	36
333	The role of quantum chemistry in the elucidation of the elementary mechanisms of catalytic processes: from atoms, to surfaces, to enzymes. *Theoretical Chemistry Accounts*, **2007**, 117, 765-779	1.9	36
332	Interaction of Cu(+) and Cu(2+) ions with alpha-alanine. A density functional study. *Journal of Mass Spectrometry*, **2002**, 37, 786-91	2.2	36
331	Interaction of CO with PdAu(111) and PdAu(100) Bimetallic Surfaces: A Theoretical Cluster Model Study. *Journal of Physical Chemistry C*, **2008**, 112, 6073-6081	3.8	35
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329	Ab-initio mechanistic studies of radical reactions. Directive effects in the addition of methyl radical to unsymmetrical fluoroethenes. *Journal of the Chemical Society Perkin Transactions II*, **1986**, 1517-1524		35
328	Antioxidant properties comparative study of natural hydroxycinnamic acids and structurally modified derivatives: Computational insights. *Computational and Theoretical Chemistry*, **2016**, 1077, 39-47	2	34
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326	Metal Atom Effect on the Photophysical Properties of Mg(II), Zn(II), Cd(II), and Pd(II) Tetraphenylporphyrin Complexes Proposed as Possible Drugs in Photodynamic Therapy. *Molecules*, **2017**, 22,	4.8	34
325	Theoretical study of silver-ion-mediated base pairs: the case of C-Ag-C and C-Ag-A systems. *Journal of Physical Chemistry A*, **2015**, 119, 5153-7	2.8	34

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323	Density functional study of ammonia activation by late first-row transition metal cations. *Inorganic Chemistry*, **2004**, 43, 4944-52	5.1	34
322	Theoretical calculations of glycine and alanine gas-phase acidities. *Journal of the American Society for Mass Spectrometry*, **1999**, 10, 318-22	3.5	34
321	Breaking the barrier: an osmium photosensitizer with unprecedented hypoxic phototoxicity for real world photodynamic therapy. *Chemical Science*, **2020**, 11, 9784-9806	9.4	34
320	Insights into the coordination mode of quercetin with the Al(III) ion from a combined experimental and theoretical study. *Dalton Transactions*, **2014**, 43, 7269-74	4.3	33
319	Hydration of gas-phase ytterbium ion complexes studied by experiment and theory. *Theoretical Chemistry Accounts*, **2011**, 129, 575-592	1.9	33
318	A proposal for mitochondrial processing peptidase catalytic mechanism. *Journal of the American Chemical Society*, **2011**, 133, 17824-31	16.4	33
317	Conformational behaviour of isomeric bithienyls. An ab initio study. *Journal of the Chemical Society Perkin Transactions II*, **1986**, 907		33
316	B,N-Codoped graphene as catalyst for the oxygen reduction reaction: Insights from periodic and cluster DFT calculations. *Journal of Computational Chemistry*, **2018**, 39, 637-647	3.5	32
315	Coumarin-Chalcone Hybrids as Peroxyl Radical Scavengers: Kinetics and Mechanisms. *Journal of Chemical Information and Modeling*, **2016**, 56, 662-70	6.1	32
314	Atomistic details of the Catalytic Mechanism of Fe(III)-Zn(II) Purple Acid Phosphatase. *Journal of Chemical Theory and Computation*, **2010**, 6, 2424-33	6.4	32
313	Mechanistic investigation of the hydrogenation of O(2) by a transfer hydrogenation catalyst. *Journal of the American Chemical Society*, **2010**, 132, 4178-90	16.4	32
312	A quasilinear RISM approach for the computation of solvation free energy of ionic species. *Chemical Physics Letters*, **2006**, 418, 485-489	2.5	32
311	On the interaction between manganese cation (Mn2+) and the nucleic acid bases (T, U, C, A, G) in the gas phase. *International Journal of Quantum Chemistry*, **2002**, 90, 903-909	2.1	32
310	Oxidation of Ethylbenzene to Acetophenone with N-Doped Graphene: Insight from Theory. *Journal of Physical Chemistry C*, **2014**, 118, 12275-12284	3.8	31
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308	DFT spin□orbit coupling between singlet and triplet excited states: A case of psoralen compounds. *Chemical Physics Letters*, **2010**, 490, 90-96	2.5	31
307	On the origin of the different performance of iron and manganese monocations in catalyzing the nitrous oxide reduction by carbon oxide. *Inorganic Chemistry*, **2007**, 46, 7489-93	5.1	31

306	Chemisorption of atomic and molecular oxygen on the (100) surface of silicon; a theoretical study. *Surface Science*, **1985**, 162, 230-238	1.8	31
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303	Evidence for the formation of a Mo-H intermediate in the catalytic cycle of formate dehydrogenase. *Inorganic Chemistry*, **2012**, 51, 8331-9	5.1	30
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301	Mechanistic aspects of the reaction of Th+ and Th2+ with water in the gas phase. *Inorganic Chemistry*, **2008**, 47, 2083-8	5.1	30
300	Methane activation by chromium oxide cations in the gas phase: a theoretical study. *Journal of Computational Chemistry*, **2006**, 27, 174-87	3.5	30
299	Experimental and theoretical approach to the electronic structure and the molecular conformation of azabiphenyls. Assymetric bipyridines. *Chemical Physics*, **1985**, 96, 435-445	2.3	30
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296	Photophysical properties of NIR-emitting fluorescence probes: insights from TD-DFT. *Physical Chemistry Chemical Physics*, **2013**, 15, 10019-27	3.6	29
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294	On the copper(II) ion coordination by prion protein HGGGW pentapeptide model. *Journal of Physical Chemistry B*, **2007**, 111, 635-40	3.4	29
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290	Can Expanded Bacteriochlorins Act as Photosensitizers in Photodynamic Therapy? Good News from Density Functional Theory Computations. *Molecules*, **2016**, 21, 288	4.8	29
289	Photophysical properties prediction of selenium- and tellurium-substituted thymidine as potential UVA chemotherapeutic agents. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	28

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286	Establishing the catalytic mechanism of human pancreatic □amylase with QM/MM methods. *Journal of Chemical Theory and Computation*, **2015**, 11, 2508-16	6.4	27
285	Bisanthracene bis(dicarboxylic imide)s as potential photosensitizers in photodynamic therapy: a theoretical investigation. *Journal of Chemical Information and Modeling*, **2013**, 53, 2334-40	6.1	27
284	The performance of density functional based methods in the description of selected biological systems and processes. *Physical Chemistry Chemical Physics*, **2012**, 14, 14943-53	3.6	27
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281	Charge transport in poly-imidazole membranes: a fresh appraisal of the Grotthuss mechanism. *Physical Chemistry Chemical Physics*, **2012**, 14, 10910-8	3.6	26
280	Gas-phase reactions of uranate ions, UO(2)(-), UO(3)(-), UO(4)(-), and UO(4)H(-), with methanol: a convergence of experiment and theory. *Inorganic Chemistry*, **2010**, 49, 3836-50	5.1	26
279	Methionine ligand selectively promotes monofunctional adducts between trans-EE platinum anticancer drug and guanine DNA base. *Chemical Communications*, **2011**, 47, 887-9	5.8	26
278	One-electron spin-orbit contribution by effective nuclear charges. *Journal of Computational Chemistry*, **2009**, 30, 832-9	3.5	26
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