Russo Nino

List of Publications by Year in Descending Order

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	On the Scavenging Ability of Scutellarein against the OOH Radical in Water and Lipid-like Environments: A Theoretical Study.. *Antioxidants*, **2022**, 11,	7.1	2
430	Beryllium ion coordination in Ammonia, methanol and water solvents. *Journal of Molecular Liquids*, **2022**, 360, 119414	6	0
429	Computational Study Reveals the Role of Water Molecules in the Inhibition Mechanism of LAT1 by 1,2,3-Dithiazoles. *Journal of Chemical Information and Modeling*, **2021**,	6.1	5
428	Quantum Mechanical Predictions of the Antioxidant Capability of Moracin C Isomers. *Frontiers in Chemistry*, **2021**, 9, 666647	5	3
427	Anticancer Activity, DNA Binding, and Photodynamic Properties of a N?C?N-Coordinated Pt(II) Complex. *Inorganic Chemistry*, **2021**, 60, 10350-10360	5.1	5
426	Phenolic matrix effect on aroma formation of terpenes during simulated wine fermentation - Part I: Phenolic acids. *Food Chemistry*, **2021**, 341, 128288	8.5	14
425	Computationally designed p-coumaric acid analogs: searching for neuroprotective antioxidants. *New Journal of Chemistry*, **2021**, 45, 14369-14380	3.6	5
424	The platination mechanism of RNase A by arsenoplatin: insight from the theoretical study. *Inorganic Chemistry Frontiers*, **2021**, 8, 1795-1803	6.8	2
423	Theoretical investigation on bisarylselanylbenzo-2,1,3-selenadiazoles as potential photosensitizers in photodynamic therapy. *Journal of Chemical Physics*, **2021**, 154, 084113	3.9	0
422	Insights into the Catalytic Mechanism of Domains CD1 and CD2 in Histone Deacetylase 6 from Quantum Calculations. *ACS Catalysis*, **2021**, 11, 3084-3093	13.1	3
421	A Boron-Containing Compound Acting on Multiple Targets Against Alzheimer's Disease. Insights from Ab Initio and Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2021**, 61, 3397-3410	6.1	6
420	Photophysical properties of heavy atom containing tetrasulfonyl phthalocyanines as possible photosensitizers in photodynamic therapy. *Journal of Computational Chemistry*, **2021**, 42, 1803-1808	3.5	2
419	Photophysical properties of methyl ketone based multi-responsive electrochromic materials: A theoretical investigation. *Journal of Molecular Liquids*, **2021**, 338, 116576	6	1
418	The Se-S Bond Formation in the Covalent Inhibition Mechanism of SARS-CoV-2 Main Protease by Ebselen-like Inhibitors: A Computational Study. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	3
417	Capsaicin, a Powerful OH-Inactivating Ligand. *Antioxidants*, **2020**, 9,	7.1	5
416	How Lanthanide Ions Affect the Addition-Elimination Step of Methanol Dehydrogenases. *Chemistry - A European Journal*, **2020**, 26, 11334-11339	4.8	9
415	Chalcogen effects on the primary antioxidant activity of chrysin and quercetin. *New Journal of Chemistry*, **2020**, 44, 9073-9082	3.6	11

414	Mechanism of action of the curcumin cis-diammineplatinum(II) complex as a photocytotoxic agent. *Inorganic Chemistry Frontiers*, **2020**, 7, 2759-2769	6.8	3
413	Effect of Copper on the Mitochondrial Carnitine/Acylcarnitine Carrier Via Interaction with Cys136 and Cys155. Possible Implications in Pathophysiology. *Molecules*, **2020**, 25,	4.8	6
412	The Generation of the Oxidant Agent of a Mononuclear Nonheme Fe(II) Biomimetic Complex by Oxidative Decarboxylation. A DFT Investigation. *Molecules*, **2020**, 25,	4.8	1
411	How the Destabilization of a Reaction Intermediate Affects Enzymatic Efficiency: The Case of Human Transketolase. *ACS Catalysis*, **2020**, 10, 2872-2881	13.1	9
410	Iodine substituted phosphorus corrole complexes as possible photosensitizers in photodynamic therapy: Insights from theory. *Journal of Computational Chemistry*, **2020**, 41, 1395-1401	3.5	8
409	The Antioxidant Capability of Higenamine: Insights from Theory. *Antioxidants*, **2020**, 9,	7.1	11
408	Attosecond dynamics simulations of glycine irradiated by particle: Comment on "A never-ending story in the sky: The secrets of chemical evolution" by C. Puzzarini and V. Barone. *Physics of Life Reviews*, **2020**, 32, 114-116	2.1	2
407	Rationalization of the Superior Anticancer Activity of Phenanthriplatin: An In-Depth Computational Exploration. *Chemistry - A European Journal*, **2020**, 26, 259-268	4.8	8
406	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
405	The Effects of the Metal Ion Substitution into the Active Site of Metalloenzymes: A Theoretical Insight on Some Selected Cases. *Catalysts*, **2020**, 10, 1038	4	10
404	On the Catalytic Activity of the Engineered Coiled-Coil Heptamer Mimicking the Hydrolase Enzymes: Insights from a Computational Study. *International Journal of Molecular Sciences*, **2020**, 21,	6.3	4
403	Breaking the barrier: an osmium photosensitizer with unprecedented hypoxic phototoxicity for real world photodynamic therapy. *Chemical Science*, **2020**, 11, 9784-9806	9.4	34
402	Sequestering Ability of a Synthetic Chelating Agent towards Copper(II) and Iron(III): A Detailed Theoretical and Experimental Analysis. *Chemistry - an Asian Journal*, **2020**, 15, 3266-3274	4.5	2
401	Os(II) Oligothienyl Complexes as a Hypoxia-Active Photosensitizer Class for Photodynamic Therapy. *Inorganic Chemistry*, **2020**, 59, 16341-16360	5.1	19
400	Hydration of Aromatic Nitriles Catalyzed by Mn-OH Complexes: A Rationalization from Quantum Chemical Investigations. *Organometallics*, **2020**, 39, 3352-3361	3.8	3
399	Theoretical exploration of the photophysical properties of two-component Ru-porphyrin dyes as promising assemblies for a combined antitumor effect. *Dalton Transactions*, **2020**, 49, 12653-12661	4.3	2
398	Computational Mechanistic Insights on the NO Oxidation Reaction Catalyzed by Non-Heme Biomimetic Cr-N-Tetramethylated Cyclam Complexes. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	2
397	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. *Angewandte Chemie - International Edition*, **2019**, 58, 3976-3980	16.4	17

396	Theoretical exploration of the reduction reaction of monofunctional phenanthriplatin Pt(IV) prodrugs. *Inorganica Chimica Acta*, **2019**, 495, 118951	2.7	0
395	Rational Design of Modified Oxobacteriochlorins as Potential Photodynamic Therapy Photosensitizers. *International Journal of Molecular Sciences*, **2019**, 20,	6.3	5
394	Structures, binding energies and temperature effects in (left[{{text{Mg}}left({{text{NH}}}_{3} } right)_{n = 1 - 10} } right]^{2 + }) clusters. *Theoretical Chemistry Accounts*, **2019**, 138, 1	1.9	8
393	How Metal Coordination in the Ca-, Ce-, and Eu-Containing Methanol Dehydrogenase Enzymes Can Influence the Catalysis: A Theoretical Point of View. *Challenges and Advances in Computational Chemistry and Physics*, **2019**, 487-501	0.7	3
392	Antitumor Platinium(IV) Prodrugs: A Systematic Computational Exploration of Their Reduction Mechanism by l-Ascorbic Acid. *Inorganic Chemistry*, **2019**, 58, 3851-3860	5.1	13
391	Structures, binding energies, temperature effects, infrared spectroscopy of [Mg(NH)] clusters from DFT and MP2 investigations. *Journal of Computational Chemistry*, **2019**, 40, 1707-1717	3.5	11
390	Elusive Intermediates in the Breakdown Reactivity Patterns of Prodrug Platinum(IV) Complexes. *Journal of the American Society for Mass Spectrometry*, **2019**, 30, 1881-1894	3.5	6
389	Oenin/Syringic Acid Copigmentation: Insights From a Theoretical Study. *Frontiers in Chemistry*, **2019** , 7, 579	5	6
388	Photophysical Exploration of Dual-Approach Pt-BODIPY Conjugates: Theoretical Insights. *Inorganic Chemistry*, **2019**, 58, 9882-9889	5.1	10
387	A study on the physicochemical properties and cytotoxic activity of p-sulfocalix[4]arene-nedaplatin complex. *Journal of Physics: Conference Series*, **2019**, 1310, 012011	0.3	6
386	Insight on the chelation of aluminum(III) and iron(III) by curcumin in aqueous solution. *Journal of Molecular Liquids*, **2019**, 296, 111805	6	19
385	The Catalytic Mechanism of Human Transketolase. *ChemPhysChem*, **2019**, 20, 2881-2886	3.2	10
384	The role of the halogen bond in iodothyronine deiodinase: Dependence on chalcogen substitution in naphthyl-based mimetics. *Journal of Computational Chemistry*, **2019**, 40, 944-951	3.5	10
383	The Onset of Dehydrogenation in Solid Ammonia Borane: An Ab Initio Metadynamics Study. *Angewandte Chemie*, **2019**, 131, 4016-4020	3.6	7
382	Why hydroxy-proline improves the catalytic power of the peptidoglycan N-deacetylase enzyme: insight from theory. *Physical Chemistry Chemical Physics*, **2019**, 21, 23338-23345	3.6	9
381	Theoretical insight into joint photodynamic action of a gold(i) complex and a BODIPY chromophore for singlet oxygen generation. *Physical Chemistry Chemical Physics*, **2019**, 21, 3446-3452	3.6	5
380	Computational Investigation of the Influence of Halogen Atoms on the Photophysical Properties of Tetraphenylporphyrin and Its Zinc(II) Complexes. *Journal of Physical Chemistry A*, **2018**, 122, 2809-2815	2.8	11
379	Chemical Insights into the Antioxidant Mechanisms of Alkylseleno and Alkyltelluro Phenols: Periodic Relatives Behaving Differently. *Chemistry - A European Journal*, **2018**, 24, 8686-8691	4.8	9

378	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
377	Investigation of the host-guest complexation between 4-sulfocalix[4]arene and nedaplatin for potential use in drug delivery. *Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy* , **2018**, 193, 528-536	4.4	30
376	Excitation energies, singlet-triplet energy gaps, spin-orbit matrix elements and heavy atom effects in BOIMPYs as possible photosensitizers for photodynamic therapy: a computational investigation. *Physical Chemistry Chemical Physics*, **2018**, 20, 2656-2661	3.6	15
375	Theoretical Insights into the Switching Off/On of O Photosensitization in Chemicontrolled Photodynamic Therapy. *Chemistry - A European Journal*, **2018**, 24, 3512-3519	4.8	10
374	Insights from Computations on the Mechanism of Reduction by Ascorbic Acid of Pt Prodrugs with Asplatin and Its Chlorido and Bromido Analogues as Model Systems. *Chemistry - A European Journal*, **2018**, 24, 9572-9580	4.8	10
373	Anion-π weak interactions in a heteroaromatic calixarene receptor. A theoretical investigation. *Inorganica Chimica Acta*, **2018**, 470, 379-384	2.7	10
372	BODIPY for photodynamic therapy applications: computational study of the effect of bromine substitution on O photosensitization. *Journal of Molecular Modeling*, **2018**, 24, 183	2	8
371	Oenin and Quercetin Copigmentation: Highlights From Density Functional Theory. *Frontiers in Chemistry*, **2018**, 6, 245	5	10
370	QM Cluster or QM/MM in Computational Enzymology: The Test Case of LigW-Decarboxylase. *Frontiers in Chemistry*, **2018**, 6, 249	5	10
369	Antioxidant properties and free radical scavenging mechanisms of cyclocurcumin. *New Journal of Chemistry*, **2018**, 42, 12698-12705	3.6	8
368	Theoretical determination of the aquation reaction mechanism of cyclometalated benzimidazole Ru(II) and Ir(III) anticancer complexes. *Inorganica Chimica Acta*, **2018**, 470, 325-330	2.7	2
367	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
366	Photophysical Properties of Nitrated and Halogenated Phosphorus Tritolylcorrole Complexes: Insights from Theory. *Molecules*, **2018**, 23,	4.8	4
365	On the Inhibition Mechanism of Glutathione Transferase P1 by Piperlongumine. Insight From Theory. *Frontiers in Chemistry*, **2018**, 6, 606	5	13
364	Can BODIPY Dimers Act as Photosensitizers in Photodynamic Therapy? A Theoretical Prediction. *Frontiers in Physics*, **2018**, 6,	3.9	8
363	Antioxidant Properties of the Vam3 Derivative of Resveratrol. *Molecules*, **2018**, 23,	4.8	4
362	On the Electrochromic Properties of Borepins: A Computational Prediction. *ACS Omega*, **2018**, 3, 9556-9563	3.9	1
361	Structural characterization of aluminium(III) and iron(III) complexes of coumarinic acid in aqueous solutions from combined experimental and theoretical investigations. *New Journal of Chemistry*, **2018**, 42, 11006-11012	3.6	10

360	Complexation behaviour of caffeic, ferulic and p-coumaric acids towards aluminium cations: a combined experimental and theoretical approach. *New Journal of Chemistry*, **2017**, 41, 5182-5190	3.6	29
359	How Can Methanol Dehydrogenase from Methylacidiphilum fumariolicum Work with the Alien Ce Ion in the Active Center? A Theoretical Study. *Chemistry - A European Journal*, **2017**, 23, 8652-8657	4.8	29
358	Experimental and Theoretical Investigation on the Catalytic Generation of Environmentally Persistent Free Radicals from Benzene. *Journal of Physical Chemistry C*, **2017**, 121, 9381-9393	3.8	24
357	Hydrolysis in Acidic Environment and Degradation of Satraplatin: A Joint Experimental and Theoretical Investigation. *Inorganic Chemistry*, **2017**, 56, 6013-6026	5.1	8
356	Direct and cluster-assisted dehydrogenation of methane by Nb and Ta: a theoretical investigation. *Physical Chemistry Chemical Physics*, **2017**, 19, 16178-16188	3.6	5
355	The ability of a zinc pyrrolidine complex to catalyze the synthesis of cyclic carbonates from carbon dioxide and epoxides: a mechanistic theoretical investigation. *Dalton Transactions*, **2017**, 46, 9030-9035	4.3	14
354	Photophysical Properties of S, Se and Te-Substituted Deoxyguanosines: Insight into Their Ability To Act as Chemotherapeutic Agents. *Journal of Chemical Information and Modeling*, **2017**, 57, 234-242	6.1	22
353	The role of metal substitution in the promiscuity of natural and artificial carbonic anhydrases. *Coordination Chemistry Reviews*, **2017**, 345, 73-85	23.2	8
352	Explicit Water Molecules Play a Key Role in the Mechanism of Rhodium-Substituted Human Carbonic Anhydrase. *ChemCatChem*, **2017**, 9, 1047-1053	5.2	10
351	The role of arsenic in the hydrolysis and DNA metalation processes in an arsenous acid-platinum(ii) anticancer complex. *Physical Chemistry Chemical Physics*, **2017**, 19, 1328-1334	3.6	8
350	Halogen atom effect on the photophysical properties of substituted aza-BODIPY derivatives. *Physical Chemistry Chemical Physics*, **2017**, 19, 2530-2536	3.6	42
349	Reaction Mechanism of Low-Spin Iron(III)- and Cobalt(III)-Containing Nitrile Hydratases: A Quantum Mechanics Investigation. *Inorganic Chemistry*, **2017**, 56, 13390-13400	5.1	16
348	Bodipy-squaraine triads: Preparation and study of the intramolecular energy transfer, charge separation and intersystem crossing. *Dyes and Pigments*, **2017**, 147, 560-572	4.6	8
347	Theoretical investigation of the action mechanisms of N,N-di-alkylated diarylamine antioxidants. *Theoretical Chemistry Accounts*, **2017**, 136, 1	1.9	2
346	Trimethylphosphate and Dimethylphosphate Hydrolysis by Binuclear Cd , Mn , and Zn -Fe Promiscuous Organophosphate-Degrading Enzyme: Reaction Mechanisms. *Chemistry - A European Journal*, **2017**, 23, 13742-13753	4.8	6
345	Density Functional Determination of the Energetics of the Formation of trans-Stilbene Catalyzed by Sulfenate Anions. *ChemCatChem*, **2017**, 9, 278-281	5.2	7
344	Time-Dependent Density Functional Computations of the Spectrochemical Properties of Dithiolodithiole and Thiophene Electrochromic Systems. *Materials*, **2017**, 10,	3.5	2
343	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

342	Mechanistic Explanation of the Weak Carbonic Anhydrase's Esterase Activity. *Molecules*, **2017**, 22,	4.8	3
341	Theoretical Exploration of Type I/Type II Dual Photoreactivity of Promising Ru(II) Dyads for PDT Approach. *Inorganic Chemistry*, **2016**, 55, 11185-11192	5.1	40
340	A DFT investigation of a bulky biomimetic model catalyzing the 5'-outer ring deiodination of thyroxine. *Journal of Molecular Modeling*, **2016**, 22, 287	2	2
339	Computational Insight on CO2 Fixation to Produce Styrene Carbonate Assisted by a Single-Center Aluminum(III) Catalyst and Quaternary Ammonium Salts. *ChemCatChem*, **2016**, 8, 1167-1175	5.2	17
338	Investigation of the Inertness to Hydrolysis of Platinum(IV) Prodrugs. *Inorganic Chemistry*, **2016**, 55, 1580-6	5.1	24
337	Food Antioxidants: Chemical Insights at the Molecular Level. *Annual Review of Food Science and Technology*, **2016**, 7, 335-52	14.7	222
336	Photophysical properties prediction of selenium- and tellurium-substituted thymidine as potential UVA chemotherapeutic agents. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	28
335	22π-Electrons [1.1.1.1.1] pentaphyrin as a new photosensitizing agent for water disinfection: experimental and theoretical characterization. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	10
334	Coumarin-Chalcone Hybrids as Peroxyl Radical Scavengers: Kinetics and Mechanisms. *Journal of Chemical Information and Modeling*, **2016**, 56, 662-70	6.1	32
333	A deeper insight on the radical scavenger activity of two simple coumarins toward OOH radical. *Computational and Theoretical Chemistry*, **2016**, 1077, 133-138	2	8
332	Soybean aglycones antioxidant activity. A theoretical investigation. *Computational and Theoretical Chemistry*, **2016**, 1077, 119-124	2	8
331	Antioxidant properties comparative study of natural hydroxycinnamic acids and structurally modified derivatives: Computational insights. *Computational and Theoretical Chemistry*, **2016**, 1077, 39-47	2	34
330	Can Expanded Bacteriochlorins Act as Photosensitizers in Photodynamic Therapy? Good News from Density Functional Theory Computations. *Molecules*, **2016**, 21, 288	4.8	29
329	Synergistic Effects of Metals in a Promising Ru(II) -Pt(II) Assembly for a Combined Anticancer Approach: Theoretical Exploration of the Photophysical Properties. *Chemistry - A European Journal*, **2016**, 22, 9162-8	4.8	23
328	Electro-optical Properties of Neutral and Radical Ion Thienosquaraines. *Chemistry - A European Journal*, **2016**, 22, 10179-86	4.8	22
327	PDT-correlated photophysical properties of thienopyrrole BODIPY derivatives. Theoretical insights. *Dyes and Pigments*, **2016**, 130, 9-15	4.6	37
326	Mechanistic investigation of trimethylamine-N-oxide reduction catalysed by biomimetic molybdenum enzyme models. *Physical Chemistry Chemical Physics*, **2016**, 18, 8428-36	3.6	3
325	TDDFT investigation on methylviologen, 3,7-diazabenzophosphole, and helical helquat electrochromic systems. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	7

324	Structure and properties of a copper-mediated nucleobase pair from density functional theory investigation. *Inorganica Chimica Acta*, **2016**, 452, 194-198	2.7	1
323	Can fused thiophene□pyrrole-containing rings act as possible new electrochromic dyes? A computational prediction. *Theoretical Chemistry Accounts*, **2016**, 135, 1	1.9	7
322	Catalytic role of dinuclear □acetylide gold(I) complexes in the hydroamination of terminal alkynes: theoretical insights. *Journal of Chemical Theory and Computation*, **2015**, 11, 581-90	6.4	16
321	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
320	New insights in the catalytic mechanism of tyrosine ammonia-lyase given by QM/MM and QM cluster models. *Archives of Biochemistry and Biophysics*, **2015**, 582, 107-15	4.1	19
319	Mass Spectrometric and Computational Investigation of the Protonated Carnosine-Carboplatin Complex Fragmentation. *Inorganic Chemistry*, **2015**, 54, 7885-97	5.1	3
318	Collision-induced dissociation products of the protonated dipeptide carnosine: structural elucidation, fragmentation pathways and potential energy surface analysis. *Physical Chemistry Chemical Physics*, **2015**, 17, 12673-82	3.6	5
317	Photophysical properties of free and metallated meso-substituted tetrabenzotriazaporphyrin from density functional theory investigation. *Dyes and Pigments*, **2015**, 120, 335-339	4.6	36
316	Theoretical investigation on the restoring step of the carbonic anhydrase catalytic cycle for natural and promiscuous substrates. *Archives of Biochemistry and Biophysics*, **2015**, 582, 101-6	4.1	6
315	DFT Investigation of the Mechanism of Action of Organoiridium(III) Complexes As Anticancer Agents. *Inorganic Chemistry*, **2015**, 54, 10801-10	5.1	23
314	Direct Hydrogenation of Carbon Dioxide by an Artificial Reductase Obtained by Substituting Rhodium for Zinc in the Carbonic Anhydrase Catalytic Center. A Mechanistic Study. *ACS Catalysis*, **2015**, 5, 5397-5409	13.1	19
313	Enzymatic Flexibility and Reaction Rate: A QM/MM Study of HIV-1 Protease. *ACS Catalysis*, **2015**, 5, 5617-5626	13.1	53
312	The heavy atom effect on Zn(ii) phthalocyanine derivatives: a theoretical exploration of the photophysical properties. *Physical Chemistry Chemical Physics*, **2015**, 17, 23595-601	3.6	41
311	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
310	Antioxidant properties of several coumarin□chalcone hybrids from theoretical insights. *RSC Advances*, **2015**, 5, 565-575	3.7	61
309	Fragmentation pathways analysis for the gas phase dissociation of protonated carnosine-oxaliplatin complexes. *Dalton Transactions*, **2015**, 44, 4455-67	4.3	5
308	Computational Investigation on the Mechanism of Amide Bond Formation by using Phosphine-Based Redox Catalysis. *ChemCatChem*, **2015**, 7, 2309-2312	5.2	4
307	Triesterase and promiscuous diesterase activities of a di-Co(II)-containing organophosphate degrading enzyme reaction mechanisms. *Chemistry - A European Journal*, **2015**, 21, 3736-45	4.8	16

306	Mechanism of thyroxine deiodination by naphthyl-based iodothyronine deiodinase mimics and the halogen bonding role: a DFT investigation. *Chemistry - A European Journal*, **2015**, 21, 8554-60	4.8	7
305	The working mechanism of the β-carbonic anhydrase degrading carbonyl sulphide (COSase): a theoretical study. *Physical Chemistry Chemical Physics*, **2015**, 17, 14843-8	3.6	13
304	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
303	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
302	Ab initio calculations on the (1)O2 quenching mechanism by trans-resveratrol. *Physical Chemistry Chemical Physics*, **2014**, 16, 12773-81	3.6	11
301	Electronic spectra and intersystem spin-orbit coupling in 1,2- and 1,3-squaraines. *Journal of Computational Chemistry*, **2014**, 35, 2107-13	3.5	30
300	Insight into the promiscuous activity of human carbonic anhydrase against the cyanic acid substrate from a combined QM and QM/MM investigation. *Physical Chemistry Chemical Physics*, **2014**, 16, 16671-6	3.6	17
299	Promiscuous ability of human carbonic anhydrase: QM and QM/MM investigation of carbon dioxide and carbodiimide hydration. *Inorganic Chemistry*, **2014**, 53, 3488-93	5.1	24
298	Oxidation of Ethylbenzene to Acetophenone with N-Doped Graphene: Insight from Theory. *Journal of Physical Chemistry C*, **2014**, 118, 12275-12284	3.8	31
297	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
296	The Role of Chelating Phosphine Rhodium Complexes in Dehydrocoupling Reactions of Amine-Boranes: A Theoretical Investigation Attempting To Rationalize the Observed Behaviors. *ACS Catalysis*, **2014**, 4, 1104-1113	13.1	18
295	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
294	Hydrogen release from dialkylamine-boranes promoted by Mg and Ca complexes: a DFT analysis of the reaction mechanism. *Chemistry - A European Journal*, **2014**, 20, 5967-76	4.8	20
293	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
292	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
291	Density functional study of the antioxidant activity of some recently synthesized resveratrol analogues. *Food Chemistry*, **2013**, 141, 2017-24	8.5	46
290	Theoretical investigation of the absorption spectra and singlet-triplet energy gap of positively charged tetraphenylporphyrins as potential photodynamic therapy photosensitizers. *Canadian Journal of Chemistry*, **2013**, 91, 902-906	0.9	20
289	A DFT study of the applicability of the charge balance model in two-metal enzymes: The case of cAMP-dependent protein kinase. *Chemical Physics Letters*, **2013**, 571, 66-70	2.5	7

288	Photophysical origin of the reduced photodynamic therapy activity of temocene compared to Foscan : insights from theory. *Physical Chemistry Chemical Physics*, **2013**, 15, 16167-71	3.6	34
287	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
286	Hydrophilic annulated dinuclear zinc(II) phthalocyanine as Type II photosensitizers for PDT: a combined experimental and (TD)-DFT investigation. *Journal of Porphyrins and Phthalocyanines*, **2013**, 17, 980-988	1.8	8
285	What occurs by replacing Mn2+ with Co2+ in human arginase I: first-principles computational analysis. *Inorganic Chemistry*, **2013**, 52, 655-9	5.1	18
284	A micro-environmental study of the Zn(+2)-A -16 structural properties. *Biophysical Chemistry*, **2013**, 182, 86-93	3.5	4
283	Photophysical properties of NIR-emitting fluorescence probes: insights from TD-DFT. *Physical Chemistry Chemical Physics*, **2013**, 15, 10019-27	3.6	29
282	EH3 (E = N, P, As) and H2 activation with N-heterocyclic silylene and germylene homologues. *Chemistry - A European Journal*, **2013**, 19, 7835-46	4.8	25
281	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
280	Catalytic mechanism of the arylsulfatase promiscuous enzyme from Pseudomonas aeruginosa. *Chemistry - A European Journal*, **2013**, 19, 2185-92	4.8	46
279	The catalytic mechanism of protein phosphatase 5 established by DFT calculations. *Chemistry - A European Journal*, **2013**, 19, 14081-9	4.8	42
278	Theoretical and experimental investigation on the near-infrared and UV is spectral regions of a newly synthesized triarylamine electrochromic system. *Highlights in Theoretical Chemistry*, **2013**, 351-359		
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