Antonio Monari

List of Publications by Year
in descending order

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209 papers	4,392 citations	126858 33 h-index	189801 50 g-index
259 all docs	259 docs citations	259 times ranked	4260 citing authors

#	Article	IF	Citations
1	Toward a Quantitative Assessment of Electronic Transitionsâ€™ Charge-Transfer Character. Journal of Chemical Theory and Computation, 2014, 10, 3896-3905.	2.3	139
2	A new record excited state ³MLCT lifetime for metalorganic iron(<scp>ii</scp>) complexes. Physical Chemistry Chemical Physics, 2016, 18, 12550-12556.	1.3	132
3	An Ironâ€Based Photosensitizer with Extended Excitedâ€State Lifetime: Photophysical and Photovoltaic Properties. European Journal of Inorganic Chemistry, 2015, 2015, 2469-2477.	1.0	124
4	New Insight into the Topology of Excited States through Detachment/Attachment Density Matrices-Based Centroids of Charge. Journal of Chemical Theory and Computation, 2014, 10, 3906-3914.	2.3	121
5	Theoretical Modeling of Large Molecular Systems. Advances in the Local Self Consistent Field Method for Mixed Quantum Mechanics/Molecular Mechanics Calculations. Accounts of Chemical Research, 2013, 46, 596-603.	7.6	104
6	Benzophenone Ultrafast Triplet Population: Revisiting the Kinetic Model by Surface-Hopping Dynamics. Journal of Physical Chemistry Letters, 2016, 7, 622-626.	2.1	89
7	Accurate Estimation of the Standard Binding Free Energy of Netropsin with DNA. Molecules, 2018, 23, 228.	1.7	85
8	NHC-Based Iron Sensitizers for DSSCs. Inorganics, 2018, 6, 63.	1.2	76
9	3,5-Bis(ethynyl)pyridine and 2,6-Bis(ethynyl)pyridine Spanning Two Fe(Cp*)(dppe) Units: Role of the Nitrogen Atom on the Electronic and Magnetic Couplings. Inorganic Chemistry, 2011, 50, 12601-12622.	1.9	69
10	Molecular Basis of SARS-CoV-2 Infection and Rational Design of Potential Antiviral Agents: Modeling and Simulation Approaches. Journal of Proteome Research, 2020, 19, 4291-4315.	1.8	68
11	Lipid Peroxidation in Membranes: The Peroxyl Radical Does Not â€œFloatâ€. Journal of Physical Chemistry Letters, 2014, 5, 1653-1658.	2.1	67
12	Heteroleptic Pyridylâ€Carbene Iron Complexes with Tuneable Electronic Properties. European Journal of Inorganic Chemistry, 2014, 2014, 3747-3753.	1.0	59
13	Probing the reactivity of singlet oxygen with purines. Nucleic Acids Research, 2016, 44, 56-62.	6.5	57
14	A QM/MM study on the spinach plastocyanin: Redox properties and absorption spectra. Computational and Theoretical Chemistry, 2012, 990, 119-125.	1.1	55
15	Spectral properties of polypyridyl ruthenium complexes intercalated in DNA: theoretical insights into the surrounding effects of [Ru(dppz)(bpy)2]2+. Physical Chemistry Chemical Physics, 2012, 14, 12496.	1.3	54
16	Photophysical Properties of Ruthenium(II) Polypyridyl DNA Intercalators: Effects of the Molecular Surroundings Investigated by Theory. Chemistry - A European Journal, 2014, 20, 12901-12909.	1.7	54
17	Theoretical Study of New Ruthenium-Based Dyes for Dye-Sensitized Solar Cells. Journal of Physical Chemistry A, 2011, 115, 3596-3603.	1.1	49
18	Understanding DNA under oxidative stress and sensitization: the role of molecular modeling. Frontiers in Chemistry, 2015, 3, 43.	1.8	48

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19	Resolving the Benzophenone DNA-Photosensitization Mechanism at QM/MM Level. Journal of Physical Chemistry Letters, 2015, 6, 576-580.	2.1	48
20	Interfacial charge separation and photovoltaic efficiency in Fe(<scp>ii</scp>)â€“carbene sensitized solar cells. Physical Chemistry Chemical Physics, 2016, 18, 28069-28081.	1.3	48
21	Improved Treatment of Surrounding Effects: UV/vis Absorption Properties of a Solvated Ru(II) Complex. Journal of Chemical Theory and Computation, 2012, 8, 1536-1541.	2.3	47
22	Theoretical evidence of photo-induced charge transfer from DNA to intercalated ruthenium (II) organometallic complexes. Chemical Physics Letters, 2013, 578, 133-137.	1.2	47
23	Benzophenone and DNA: Evidence for a Double Insertion Mode and Its Spectral Signature. Journal of Physical Chemistry Letters, 2013, 4, 4119-4124.	2.1	42
24	A QM/MM Study of the Absorption Spectrum of Harmane in Water Solution and Interacting with DNA: The Crucial Role of Dynamic Effects. Journal of Physical Chemistry B, 2013, 117, 4973-4980.	1.2	42
25	Circular Dichroism of DNA G-Quadruplexes: Combining Modeling and Spectroscopy To Unravel Complex Structures. Journal of Physical Chemistry B, 2016, 120, 3113-3121.	1.2	42
26	Excited-states of a rhenium carbonyl diimine complex: solvation models, spinâ€“orbit coupling, and vibrational sampling effects. Physical Chemistry Chemical Physics, 2017, 19, 27240-27250.	1.3	40
27	Make it clean, make it safe: A review on virus elimination via adsorption. Chemical Engineering Journal, 2021, 412, 128682.	6.6	40
28	Interaction of Palmatine with DNA: An Environmentally Controlled Phototherapy Drug. Journal of Physical Chemistry B, 2015, 119, 410-419.	1.2	39
29	Thermodynamics of the Interaction between the Spike Protein of Severe Acute Respiratory Syndrome Coronavirus-2 and the Receptor of Human Angiotensin-Converting Enzyme 2. Effects of Possible Ligands. Journal of Physical Chemistry Letters, 2020, 11, 9272-9281.	2.1	39
30	Correlation of bistranded clustered abasic DNA lesion processing with structural and dynamic DNA helix distortion. Nucleic Acids Research, 2016, 44, 8588-8599.	6.5	37
31	Synthesis and Computational Study of a Pyridylcarbene Fe(II) Complex: Unexpected Effects of fac/mer Isomerism in Metal-to-Ligand Triplet Potential Energy Surfaces. Inorganic Chemistry, 2018, 57, 10431-10441.	1.9	37
32	Iron(<scp>ii</scp>) complexes with diazinyl-NHC ligands: impact of Ï€-deficiency of the azine core on photophysical properties. Dalton Transactions, 2019, 48, 10915-10926.	1.6	37
33	Photophysics of chlorin e6: from one- and two-photon absorption to fluorescence and phosphorescence. RSC Advances, 2017, 7, 10992-10999.	1.7	36
34	Ab initio molecular dynamics of thiophene: the interplay of internal conversion and intersystem crossing. Physical Chemistry Chemical Physics, 2017, 19, 25662-25670.	1.3	36
35	Full configuration interaction study of the metal-insulator transition in model systems: LiN linear chains (N=2,4,6,8). Journal of Chemical Physics, 2008, 128, 024701.	1.2	35
36	Impact of the fac/mer Isomerism on the Excited-State Dynamics of Pyridyl-carbene Fe(II) Complexes. Inorganic Chemistry, 2019, 58, 5069-5081.	1.9	35

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37	Molecular Dynamics Insights into Polyamineâ€“DNA Binding Modes: Implications for Crossâ€Link Selectivity. Chemistry - A European Journal, 2017, 23, 12845-12852.	1.7	34
38	From Physical Mixtures to Co-Crystals: How the Coformers Can Modify Solubility and Biological Activity of Carbamazepine. Molecular Pharmaceutics, 2018, 15, 268-278.	2.3	34
39	Recent advances in iron-complexes as drug candidates for cancer therapy: reactivity, mechanism of action and metabolites. Dalton Transactions, 2020, 49, 11451-11466.	1.6	34
40	Role of RNA Guanine Quadruplexes in Favoring the Dimerization of SARS Unique Domain in Coronaviruses. Journal of Physical Chemistry Letters, 2020, 11, 5661-5667.	2.1	33
41	A theoretical study of linear beryllium chains: Full configuration interaction. Journal of Chemical Physics, 2009, 130, 024301.	1.2	32
42	The problem of interoperability: A common data format for quantum chemistry codes. International Journal of Quantum Chemistry, 2007, 107, 2082-2091.	1.0	31
43	Theoretical computation of Betain B30 solvatochromism using aÂPolarizable Continuum Model. Dyes and Pigments, 2014, 100, 24-31.	2.0	31
44	Repair Rate of Clustered Abasic DNA Lesions by Human Endonuclease: Molecular Bases of Sequence Specificity. Journal of Physical Chemistry Letters, 2016, 7, 3760-3765.	2.1	30
45	Assessing One- and Two-Photon Optical Properties of Boron Containing Arenes. Journal of Physical Chemistry C, 2016, 120, 17916-17926.	1.5	30
46	FORTRAN Interface for Code Interoperability in Quantum Chemistry:â€‰ The Q5Cost Library. Journal of Chemical Information and Modeling, 2007, 47, 1271-1277.	2.5	29
47	Dynamics of the excited-state hydrogen transfer in a (dG)Â·(dC) homopolymer: intrinsic photostability of DNA. Chemical Science, 2018, 9, 7902-7911.	3.7	29
48	Novel Molecular-Dynamics-Based Protocols for Phase Space Sampling in Complex Systems. Frontiers in Chemistry, 2018, 6, 495.	1.8	28
49	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.	1.5	27
50	The metal-insulator transition in dimerized HÃ¼ckel chains. Journal of Chemical Physics, 2008, 129, 134104.	1.2	26
51	A priori modeling of chemical reactions on computational grid platforms: Workflows and data models. Chemical Physics, 2012, 398, 192-198.	0.9	26
52	Photoinduced intersystem crossing in DNA oxidative lesions and epigenetic intermediates. Chemical Communications, 2020, 56, 4404-4407.	2.2	25
53	From non-covalent binding to irreversible DNA lesions: nile blue and nile red as photosensitizing agents. Scientific Reports, 2016, 6, 28480.	1.6	24
54	Hydrogen abstraction by photoexcited benzophenone: consequences for DNA photosensitization. Physical Chemistry Chemical Physics, 2016, 18, 7829-7836.	1.3	24

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55	Kohnâ€™s localization in the insulating state: One-dimensional lattices, crystalline versus disordered. Journal of Chemical Physics, 2010, 133, 064703.	1.2	23
56	Fullâ€configurationâ€interaction study of the metalâ€insulator transition in a model system: H_n linear chains n=4, 6,â€¦, 16. International Journal of Quantum Chemistry, 2011, 111, 3416-3423.	1.0	22
57	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. Journal of Computational Chemistry, 2014, 35, 611-621.	1.5	22
58	All-organic chromophores for dye-sensitized solar cells: A theoretical study on aggregation. Dyes and Pigments, 2014, 101, 203-211.	2.0	22
59	Modeling DNA electronic circular dichroism by QM/MM methods and Frenkel Hamiltonian. Theoretical Chemistry Accounts, 2015, 134, 1.	0.5	22
60	Nile blue and Nile red optical properties predicted by TD-DFT and CASPT2 methods: static and dynamic solvent effects. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	22
61	Photophysical Properties of Benzophenone-Based TADF Emitters in Relation to Their Molecular Structure. Journal of Physical Chemistry A, 2022, 126, 473-484.	1.1	22
62	Ground and Excited State Properties of New Porphyrin Based Dyads: A Combined Theoretical and Experimental Study.. Journal of Physical Chemistry A, 2012, 116, 10736-10744.	1.1	21
63	New dyads using (metallo)porphyrins as ancillary ligands in polypyridine ruthenium complexes. Synthesis and electronic properties. Dalton Transactions, 2012, 41, 12865.	1.6	21
64	Unveiling the nature of post-linear response Z-vector method for time-dependent density functional theory. Journal of Chemical Physics, 2017, 147, 024108.	1.2	21
65	Novel quinoxalinone-based pushâ€“pull chromophores with highly sensitive emission and absorption properties towards small structural modifications. Physical Chemistry Chemical Physics, 2018, 20, 21515-21527.	1.3	21
66	Exploring the Photophysics of Polyfluorinated Phthalocyanine Derivatives as Potential Theranostic Agents. Journal of Physical Chemistry C, 2019, 123, 24417-24425.	1.5	21
67	Toward Luminescent Iron Complexes: Unravelling the Photophysics by Computing Potential Energy Surfaces. ChemPhotoChem, 2019, 3, 666-683.	1.5	21
68	Towards Iron(II) Complexes with Octahedral Geometry: Synthesis, Structure and Photophysical Properties. Molecules, 2020, 25, 5991.	1.7	21
69	Structure and Dynamics of RNA Guanine Quadruplexes in SARS-CoV-2 Genome. Original Strategies against Emerging Viruses. Journal of Physical Chemistry Letters, 2021, 12, 10277-10283.	2.1	21
70	QM/MM modeling of Harmane cation fluorescence spectrum in water solution and interacting with DNA. Computational and Theoretical Chemistry, 2014, 1040-1041, 367-372.	1.1	20
71	Two-photon-absorption DNA sensitization via solvated electron production: unraveling photochemical pathways by molecular modeling and simulation. Physical Chemistry Chemical Physics, 2016, 18, 18598-18606.	1.3	20
72	Triplet photosensitization mechanism of thymine by an oxidized nucleobase: from a dimeric model to DNA environment. Physical Chemistry Chemical Physics, 2018, 20, 25666-25675.	1.3	20

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73	Electron localizability and polarizability in tight-binding graphene nanostructures. Theoretical Chemistry Accounts, 2010, 126, 257-263.	0.5	19
74	DNA Photosensitization by an â€œInsiderâ€• Photophysics and Triplet Energy Transfer of 5â€Methylâ€2â€pyrimidone Deoxyribonucleoside. Chemistry - A European Journal, 2015, 21, 11509-11516.	1.7	19
75	Ibuprofen and ketoprofen potentiate UVA-induced cell death by a photosensitization process. Scientific Reports, 2017, 7, 8885.	1.6	19
76	Hypoxia-Selective Dissociation Mechanism of a Nitroimidazole Nucleoside in a DNA Environment. Journal of Physical Chemistry Letters, 2019, 10, 6750-6754.	2.1	19
77	Molecular Bases of DNA Packaging in Bacteria Revealed by All-Atom Molecular Dynamics Simulations: The Case of Histone-Like Proteins inBorrelia burgdorferi. Journal of Physical Chemistry Letters, 2019, 10, 7200-7207.	2.1	19
78	End states and singletâ€“triplet degeneracy in linear atomic chains. Chemical Physics Letters, 2008, 465, 102-105.	1.2	18
79	Asymptotic analysis of the localization spread and polarizability of 1â€D noninteracting electrons. International Journal of Quantum Chemistry, 2012, 112, 653-664.	1.0	18
80	Strong Ï€-delocalization and substitution effect on electronic properties of dithienylpyrrole-containing bipyridine ligands and corresponding ruthenium complexes. Dalton Transactions, 2012, 41, 4833.	1.6	18
81	A FCI benchmark on beryllium dimer: The lowest singlet and triplet states. Chemical Physics Letters, 2013, 568-569, 49-54.	1.2	18
82	Deciphering the photosensitization mechanisms of hypericin towards biological membranes. Physical Chemistry Chemical Physics, 2017, 19, 23187-23193.	1.3	18
83	Ultrafast Spectroscopy of Fe(II) Complexes Designed for Solarâ€Energy Conversion: Current Status and Open Questions. ChemPhysChem, 2022, 23, .	1.0	18
84	A Davidson technique for the computation of dispersion constants: Full CI results for Be and LiH. Chemical Physics, 2004, 306, 153-161.	0.9	17
85	Conformational polymorphism or structural invariance in DNA photoinduced lesions: implications for repair rates. Nucleic Acids Research, 2017, 45, 3654-3662.	6.5	17
86	Intersystem Crossing as a Key Component of the Nonadiabatic Relaxation Dynamics of Bithiophene and Terthiophene. Journal of Chemical Theory and Computation, 2018, 14, 4530-4540.	2.3	17
87	The three Endonuclease III variants of Deinococcus radiodurans possess distinct and complementary DNA repair activities. DNA Repair, 2019, 78, 45-59.	1.3	17
88	Optical properties of photodynamic therapy drugs in different environments: the paradigmatic case of temoporfin. Physical Chemistry Chemical Physics, 2020, 22, 16956-16964.	1.3	17
89	In silico drug discovery of IKK-Î² inhibitors from 2-amino-3-cyano-4-alkyl-6-(2-hydroxyphenyl) pyridine derivatives based on QSAR, docking, molecular dynamics and drug-likeness evaluation studies. Journal of Biomolecular Structure and Dynamics, 2022, 40, 886-902.	2.0	17
90	Competing ultrafast photoinduced electron transfer and intersystem crossing of [Re(CO)$$_3$$(Dmp)(His124)(Trp122)]$$^+$$ in Pseudomonas aeruginosa azurin: a nonadiabatic dynamics study. Theoretical Chemistry Accounts, 2020, 139, 65.	0.5	17

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91	Restoring the size consistency of multireference configuration interactions through class dressings: Applications to ground and excited states. Journal of Chemical Physics, 2008, 129, 064112.	1.2	16
92	Stability of the Guanine Endoperoxide Intermediate: A Computational Challenge for Density Functional Theory. Journal of Physical Chemistry A, 2014, 118, 11612-11619.	1.1	16
93	UVâ€“vis absorption spectrum of a novel Ru(II) complex intercalated in DNA: [Ru(2,2â€²-bipy)(dppz)(2,2â€²-ArPy)]+. Journal of Molecular Modeling, 2014, 20, 2082.	0.8	16
94	2,5-Dithienylpyrrole (DTP) as a donor component in DTPâ€“Ïâ€“A organic sensitizers: photophysical and photovoltaic properties. RSC Advances, 2015, 5, 4041-4050.	1.7	16
95	Fluorene-imidazole dyes excited states from first-principles calculationsâ€”Topological insights. Theoretical Chemistry Accounts, 2016, 135, 1.	0.5	16
96	Probing optical properties of thiophene derivatives for two-photon absorption. Theoretical Chemistry Accounts, 2017, 136, 1.	0.5	16
97	Resolving the Singlet Excited State Manifold of Benzophenone by First-Principles Simulations and Ultrafast Spectroscopy. Journal of Chemical Theory and Computation, 2018, 14, 2570-2585.	2.3	16
98	Steady-State Linear and Non-linear Optical Spectroscopy of Organic Chromophores and Bio-macromolecules. Frontiers in Chemistry, 2018, 6, 86.	1.8	16
99	Computational Modeling of Exciton Localization in Self-Assembled Perylene Helices: Effects of Thermal Motion and Aggregate Size. Journal of Physical Chemistry C, 2019, 123, 6427-6437.	1.5	16
100	Photophysical Investigation of Iron(II) Complexes Bearing Bidentate Annulated Isomeric Pyridine-NHC Ligands. Journal of Physical Chemistry C, 2020, 124, 18379-18389.	1.5	16
101	Trans-to-cis photoisomerization of cyclocurcumin in different environments rationalized by computational photochemistry. Physical Chemistry Chemical Physics, 2020, 22, 4749-4757.	1.3	16
102	The Effect of the Basis-Set Superposition Error on the Calculation of Dispersion Interactions:â€‰ A Test Study on the Neon Dimer. Journal of Chemical Theory and Computation, 2007, 3, 477-485.	2.3	15
103	Full-configuration-interaction study of the metal-insulator transition in model systems: Peierls dimerization in Hn rings and chains. Journal of Chemical Physics, 2013, 138, 074315.	1.2	15
104	Photophysics of Acetophenone Interacting with <scp>DNA</scp>: Why the Road to Photosensitization is Open. Photochemistry and Photobiology, 2015, 91, 323-330.	1.3	15
105	Simulating the Electronic Circular Dichroism Spectra of Photoreversible Peptide Conformations. Journal of Chemical Theory and Computation, 2017, 13, 3290-3296.	2.3	15
106	Evaluation of temoporfin affinity to Î²-cyclodextrins assuming self-aggregation. Journal of Photochemistry and Photobiology A: Chemistry, 2018, 367, 13-21.	2.0	15
107	Ultrafast dynamics in polycyclic aromatic hydrocarbons: the key case of conical intersections at higher excited states and their role in the photophysics of phenanthrene monomer. Physical Chemistry Chemical Physics, 2019, 21, 16981-16988.	1.3	15
108	Targeting G-quadruplexes with Organic Dyes: Chelerythrineâ€“DNA Binding Elucidated by Combining Molecular Modeling and Optical Spectroscopy. Antioxidants, 2019, 8, 472.	2.2	15

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109	Full configuration-interaction study of the metal-insulator transition in model systems. Journal of Physics: Conference Series, 2008, 117, 012005.	0.3	14
110	Effects of mutations on the absorption spectra of copper proteins: a QM/MM study. Theoretical Chemistry Accounts, 2012, 131, 1.	0.5	14
111	Photophysical Properties of Novel Two-Photon Absorbing Dyes: Assessing Their Possible Use for Singlet Oxygen Generation. Journal of Physical Chemistry C, 2018, 122, 16315-16324.	1.5	14
112	Induced Night Vision by Singlet-Oxygen-Mediated Activation of Rhodopsin. Journal of Physical Chemistry Letters, 2019, 10, 7133-7140.	2.1	14
113	Photophysical properties of bichromophoric Fe(II) complexes bearing an aromatic electron acceptor. Theoretical Chemistry Accounts, 2019, 138, 1.	0.5	14
114	Triggering Tautomerization of Curcumin by Confinement into Liposomes. ChemPhotoChem, 2019, 3, 1034-1041.	1.5	14
115	First-principles characterization of the singlet excited state manifold in DNA/RNA nucleobases. Physical Chemistry Chemical Physics, 2020, 22, 15496-15508.	1.3	14
116	Halochromic luminescent quinoxalinones as a basis for pH-sensing in organic and aqueous solutions. Dyes and Pigments, 2021, 186, 108958.	2.0	14
117	Full Configuration-Interaction Study on the Tetrahedral Li4 Cluster. Journal of Chemical Theory and Computation, 2008, 4, 404-413.	2.3	13
118	A theoretical study of BeN linear chains: Variational and perturbative approaches. Journal of Chemical Physics, 2009, 131, 034309.	1.2	13
119	Determination of spin Hamiltonians from projected single reference configuration interaction calculations. I. Spin 1/2 systems. Journal of Chemical Physics, 2010, 133, 044106.	1.2	13
120	To what extent are the photophysical properties of quinoxaline- and quinoxalinone-based chromophores predictable?. Dyes and Pigments, 2019, 170, 107580.	2.0	13
121	Structure of the 5â€² untranslated region in SARS-CoV-2 genome and its specific recognition by innate immune systemviathe human oligoadenylate synthase 1. Chemical Communications, 2022, 58, 2176-2179.	2.2	13
122	Electronic Bistability in Linear Beryllium Chains. Journal of Physical Chemistry A, 2009, 113, 5240-5245.	1.1	12
123	Beryllium chains interacting with Graphene Nanoislands: From anti-ferromagnetic to ferromagnetic ground state. Chemical Physics Letters, 2010, 496, 306-309.	1.2	12
124	QM/MM calculation of absorption spectra of complex systems: The case of human serum albumin. Computational and Theoretical Chemistry, 2014, 1040-1041, 360-366.	1.1	12
125	Probing halogenâ€“halogen interactions in solution. Physical Chemistry Chemical Physics, 2017, 19, 32443-32450.	1.3	12
126	Cooperative Effects of Cytosine Methylation on DNA Structure and Dynamics. Journal of Physical Chemistry B, 2019, 123, 7365-7371.	1.2	12

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127	transâ€“cis Photoisomerization of a biomimetic cyclocurcumin analogue rationalized by molecular modelling. Physical Chemistry Chemical Physics, 2021, 23, 12842-12849.	1.3	12
128	Synthesis and Photoswitching Properties of Bioinspired Dissymmetric Î³-Pyrone, an Analogue of Cyclocurcumin. Journal of Organic Chemistry, 2021, 86, 8112-8126.	1.7	12
129	Theoretical Study of Be_NLinear Chains: Optimized Geometries and Harmonic Frequencies. Journal of Chemical Theory and Computation, 2009, 5, 1266-1273.	2.3	11
130	Coupled-Cluster study of â€˜no-pairâ€™ bonding in the tetrahedral Cu4 cluster. Chemical Physics Letters, 2011, 503, 215-219.	1.2	11
131	Human DNA Telomeres in Presence of Oxidative Lesions: The Crucial Role of Electrostatic Interactions on the Stability of Guanine Quadruplexes. Antioxidants, 2019, 8, 337.	2.2	11
132	Recognition of a tandem lesion by DNA bacterial formamidopyrimidine glycosylases explored combining molecular dynamics and machine learning. Computational and Structural Biotechnology Journal, 2021, 19, 2861-2869.	1.9	11
133	Forever Young: Structural Stability of Telomeric Guanine Quadruplexes in the Presence of Oxidative DNA Lesions**. Chemistry - A European Journal, 2021, 27, 8865-8874.	1.7	11
134	Common Format for Quantum Chemistry Interoperability: Q5Cost Format and Library. Lecture Notes in Computer Science, 2008, , 1094-1107.	1.0	11
135	Microscopic interactions between ivermectin and key human and viral proteins involved in SARS-CoV-2 infection. Physical Chemistry Chemical Physics, 2021, 23, 22957-22971.	1.3	11
136	Donâ€™t help them to bury the light. The interplay between intersystem crossing and hydrogen transfer in photoexcited curcumin revealed by surface-hopping dynamics. Physical Chemistry Chemical Physics, 2021, 23, 24757-24764.	1.3	11
137	Autophagy and evasion of the immune system by SARS-CoV-2. Structural features of the non-structural protein 6 from wild type and Omicron viral strains interacting with a model lipid bilayer. Chemical Science, 2022, 13, 6098-6105.	3.7	11
138	Thermodynamics of DNA: sensitizer recognition. Characterizing binding motifs with all-atom simulations. Physical Chemistry Chemical Physics, 2016, 18, 33180-33186.	1.3	10
139	The effect of solvent relaxation in the ultrafast time-resolved spectroscopy of solvated benzophenone. Photochemical and Photobiological Sciences, 2018, 17, 323-331.	1.6	10
140	Ionization and fragmentation of uracil upon microhydration. Physical Chemistry Chemical Physics, 2019, 21, 4810-4821.	1.3	10
141	Probing interaction of a trilysine peptide with DNA underlying formation of guanineâ€“lysine cross-links: insights from molecular dynamics. Physical Chemistry Chemical Physics, 2019, 21, 23418-23424.	1.3	10
142	Impact of the Nucleosome Histone Core on the Structure and Dynamics of DNA-Containing Pyrimidineâ€“Pyrimidone (6â€“4) Photoproduct. Journal of Chemical Theory and Computation, 2020, 16, 5972-5981.	2.3	10
143	Interaction of Iron II Complexes with B-DNA. Insights from Molecular Modeling, Spectroscopy, and Cellular Biology. Frontiers in Chemistry, 2015, 3, 67.	1.8	9
144	Absorption Spectroscopy and Photophysics of a Re^Iâ€dppz Probe for DNAâ€Mediated Charge Transport. Chemistry - A European Journal, 2018, 24, 14425-14435.	1.7	9

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145	Theoretical study of the excited state properties of luminescent phospholes. Dyes and Pigments, 2019, 164, 363-371.	2.0	9
146	Experimental and theoretical studies on thymine photodimerization mediated by oxidatively generated DNA lesions and epigenetic intermediates. Physical Chemistry Chemical Physics, 2020, 22, 25661-25668.	1.3	9
147	Chargeâ€Transfer versus Chargeâ€Separated Triplet Excited States of [Re^I(dmp)(CO)₃(His124)(Trp122)]⁺ in Water and in Modified Pseudomonas aeruginosa Azurin Protein. Chemistry - A European Journal, 2019, 25, 2519-2526.	1.7	8
148	Ironâ€™s Wake: The Performance of Quantum Mechanical-Derived Versus General-Purpose Force Fields Tested on a Luminescent Iron Complex. Molecules, 2020, 25, 3084.	1.7	8
149	Structural and morphological changes of breast cancer cells induced by iron(<scp>ii</scp>) complexes. Nanoscale, 2022, 14, 2735-2749.	2.8	8
150	Structural and functional characterization of DdrC, a novel DNA damage-induced nucleoid associated protein involved in DNA compaction. Nucleic Acids Research, 2022, 50, 7680-7696.	6.5	8
151	An enlarged basis Full-CI calculation of C7 dispersion coefficients for the LiHâ€“LiH homodimer. Chemical Physics Letters, 2003, 382, 393-398.	1.2	7
152	Blue satellites on He lines due to He-He collisions. Astronomy and Astrophysics, 2013, 559, A70.	2.1	7
153	Novel Ru-based sunlight harvesters bearing dithienylpyrrolo (DTP)-bipyridine ligands: Synthesis, characterization and photovoltaic properties. Dyes and Pigments, 2014, 101, 318-328.	2.0	7
154	Editorial: Radiation-induced and oxidative DNA damages. Frontiers in Chemistry, 2015, 3, 54.	1.8	7
155	Photophysics of the Singlet Oxygen Sensor Green Chromophore: Self-Production of ¹O₂ Explained by Molecular Modeling. Journal of Physical Chemistry B, 2017, 121, 7586-7592.	1.2	7
156	The Electronic Structure of Graphene Nanoislands: A CAS-SCF and NEVPT2 Study. Advances in Condensed Matter Physics, 2018, 2018, 1-14.	0.4	7
157	Competition between the Photothermal Effect and Emission in Potential Phototherapy Agents. Journal of Physical Chemistry B, 2021, 125, 8733-8741.	1.2	7
158	Bidentate Pyridylâ€NHC Ligands: Synthesis, Ground and Excited State Properties of Their Iron(II) Complexes and the Role of the fac/mer Isomerism. European Journal of Inorganic Chemistry, 2022, 2022, .	1.0	7
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