

Patrick Trouillas

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

102 papers	3,773 citations	33 h-index	58 g-index
106 ext. papers	4,287 ext. citations	5.4 avg, IF	5.15 L-index

#	Paper	IF	Citations
102	A DFT study of the reactivity of OH groups in quercetin and taxifolin antioxidants: The specificity of the 3-OH site. <i>Food Chemistry</i> , 2006 , 97, 679-688	8.5	267
101	Stabilizing and Modulating Color by Copigmentation: Insights from Theory and Experiment. <i>Chemical Reviews</i> , 2016 , 116, 4937-82	68.1	258
100	Free radical scavenging by natural polyphenols: atom versus electron transfer. <i>Journal of Physical Chemistry A</i> , 2013 , 117, 2082-92	2.8	172
99	FDG-PET improves tumour detection in patients with paraneoplastic neurological syndromes. <i>Brain</i> , 2004 , 127, 2331-8	11.2	170
98	Antioxidant, anti-inflammatory and antiproliferative properties of sixteen water plant extracts used in the Limousin countryside as herbal teas. <i>Food Chemistry</i> , 2003 , 80, 399-407	8.5	153
97	UV/Visible spectra of natural polyphenols: A time-dependent density functional theory study. <i>Food Chemistry</i> , 2012 , 131, 79-89	8.5	144
96	Mechanism of the antioxidant action of silybin and 2,3-dehydrosilybin flavonolignans: a joint experimental and theoretical study. <i>Journal of Physical Chemistry A</i> , 2008 , 112, 1054-63	2.8	135
95	Density functional theory study of the conformational, electronic, and antioxidant properties of natural chalcones. <i>Journal of Physical Chemistry A</i> , 2007 , 111, 1138-45	2.8	124
94	Chalcones: structural requirements for antioxidant, estrogenic and antiproliferative activities. <i>Anticancer Research</i> , 2001 , 21, 3949-56	2.3	119
93	Positioning of antioxidant quercetin and its metabolites in lipid bilayer membranes: implication for their lipid-peroxidation inhibition. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 1309-18	3.4	95
92	Free radical scavenging activities measured by electron spin resonance spectroscopy and B16 cell antiproliferative behaviors of seven plants. <i>Journal of Agricultural and Food Chemistry</i> , 2001 , 49, 3321-7	5.7	87
91	Structure-function relationship for saponin effects on cell cycle arrest and apoptosis in the human 1547 osteosarcoma cells: a molecular modelling approach of natural molecules structurally close to diosgenin. <i>Bioorganic and Medicinal Chemistry</i> , 2005 , 13, 1141-9	3.4	73
90	Castanea sativa Mill. leaves as new sources of natural antioxidant: an electronic spin resonance study. <i>Journal of Agricultural and Food Chemistry</i> , 2005 , 53, 282-8	5.7	68
89	Free radical scavenging properties of guaiacol oligomers: a combined experimental and quantum study of the guaiacyl-moiety role. <i>Journal of Physical Chemistry A</i> , 2009 , 113, 13881-91	2.8	64
88	Antioxidant properties of phenolic Schiff bases: structure-activity relationship and mechanism of action. <i>Journal of Computer-Aided Molecular Design</i> , 2013 , 27, 951-64	4.2	63
87	Flavonolignan 2,3-dehydroderivatives: Preparation, antiradical and cytoprotective activity. <i>Free Radical Biology and Medicine</i> , 2016 , 90, 114-25	7.8	62
86	Crystal-storing histiocytosis with renal Fanconi syndrome: pathological and molecular characteristics compared with classical myeloma-associated Fanconi syndrome. <i>Nephrology Dialysis Transplantation</i> , 2010 , 25, 2982-90	4.3	62

85	Benchmarking of Force Fields for Molecule-Membrane Interactions. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4143-51	6.4	61
84	Highlights on Anthocyanin Pigmentation and Copigmentation: A Matter of Flavonoid π -Stacking Complexation To Be Described by DFT-D. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 2034-43	6.4	58
83	Phospholipids and cholesterol: Inducers of cancer multidrug resistance and therapeutic targets. <i>Drug Resistance Updates</i> , 2020 , 49, 100670	23.2	58
82	A theoretical study of the conformational behavior and electronic structure of taxifolin correlated with the free radical-scavenging activity. <i>Food Chemistry</i> , 2004 , 88, 571-582	8.5	56
81	New aspects of the antioxidant properties of phenolic acids: a combined theoretical and experimental approach. <i>Physical Chemistry Chemical Physics</i> , 2009 , 11, 7659-68	3.6	55
80	Synergism of antioxidant action of vitamins E, C and quercetin is related to formation of molecular associations in biomembranes. <i>Chemical Communications</i> , 2015 , 51, 7713-6	5.8	50
79	Unravelling the immunopathological mechanisms of heavy chain deposition disease with implications for clinical management. <i>Kidney International</i> , 2017 , 91, 423-434	9.9	49
78	Synthesis, molecular structure, computational study and in vitro anticancer activity of dinuclear thiolato-bridged pentamethylcyclopentadienyl Rh(III) and Ir(III) complexes. <i>Dalton Transactions</i> , 2013 , 42, 15457-63	4.3	48
77	Tuning color variation in grape anthocyanins at the molecular scale. <i>Food Chemistry</i> , 2013 , 141, 4349-57	8.5	44
76	Electrochemical investigation of flavonolignans and study of their interactions with DNA in the presence of Cu(II). <i>Bioelectrochemistry</i> , 2011 , 82, 117-24	5.6	44
75	Base-catalyzed oxidation of silybin and isosilybin into 2,3-dehydro derivatives. <i>Tetrahedron Letters</i> , 2013 , 54, 315-317	2	40
74	Application of recent double-hybrid density functionals to low-lying singlet-singlet excitation energies of large organic compounds. <i>Journal of Chemical Physics</i> , 2013 , 139, 164104	3.9	38
73	Theoretical investigation of the formation of a new series of antioxidant depsides from the radiolysis of flavonoid compounds. <i>Radiation Research</i> , 2007 , 168, 243-52	3.1	38
72	A new antioxidant from wild nutmeg. <i>Food Chemistry</i> , 2010 , 118, 489-496	8.5	37
71	Ursolic acid triggers calcium-dependent apoptosis in human Daudi cells. <i>Anti-Cancer Drugs</i> , 2000 , 11, 737-45	2.4	36
70	Reactivity of flavonoids with 1-hydroxyethyl radical: a gamma-radiolysis study. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2004 , 1670, 28-39	4	34
69	In silico pharmacology: Drug membrane partitioning and crossing. <i>Pharmacological Research</i> , 2016 , 111, 471-486	10.2	33
68	Large-artery stroke in a young patient with Crohn's disease. Role of vitamin B6 deficiency-induced hyperhomocysteinemia. <i>Journal of the Neurological Sciences</i> , 2004 , 221, 113-5	3.2	29

67	A Blue-Light-Emitting BODIPY Probe for Lipid Membranes. <i>Langmuir</i> , 2016 , 32, 3495-505	4	28
66	Local low dose curcumin treatment improves functional recovery and remyelination in a rat model of sciatic nerve crush through inhibition of oxidative stress. <i>Neuropharmacology</i> , 2018 , 139, 98-116	5.5	28
65	The 4-O-methyl metabolites of catecholamines in man: chromatographic identification of 3-hydroxy,4-methoxyphenylacetic acid (homo-iso-vanillic acid) in cerebrospinal fluid. <i>Journal of Neurochemistry</i> , 1972 , 19, 81-6	6	26
64	Elucidation of antioxidant properties of wood bark derived saturated diarylheptanoids: a comprehensive (DFT-supported) understanding. <i>Phytochemistry</i> , 2014 , 103, 178-187	4	25
63	Synthesis, characterisation and in vitro anticancer activity of hexanuclear thiolato-bridged arene ruthenium metalla-prisms. <i>Chemistry - A European Journal</i> , 2013 , 19, 3198-203	4.8	25
62	Radiolysis of quercetin in methanol solution: observation of depside formation. <i>Journal of Agricultural and Food Chemistry</i> , 2002 , 50, 4827-33	5.7	25
61	Interaction of wine anthocyanin derivatives with lipid bilayer membranes. <i>Computational and Theoretical Chemistry</i> , 2016 , 1077, 80-86	2	24
60	Redox properties of individual quercetin moieties. <i>Free Radical Biology and Medicine</i> , 2019 , 143, 240-251	7.8	24
59	Photoprotective capacities of lichen metabolites: a joint theoretical and experimental study. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2012 , 111, 17-26	6.7	24
58	Influence of a flavan-3-ol substituent on the affinity of anthocyanins (pigments) toward vinylcatechin dimers and proanthocyanidins (copigments). <i>Journal of Physical Chemistry B</i> , 2012 , 116, 14089-99	3.4	24
57	Optical properties of wine pigments: theoretical guidelines with new methodological perspectives. <i>Tetrahedron</i> , 2015 , 71, 3079-3088	2.4	23
56	Radiolysis of kaempferol in water/methanol mixtures. Evaluation of antioxidant activity of kaempferol and products formed. <i>Journal of Agricultural and Food Chemistry</i> , 2003 , 51, 1270-7	5.7	23
55	Computational approaches in cancer multidrug resistance research: Identification of potential biomarkers, drug targets and drug-target interactions. <i>Drug Resistance Updates</i> , 2020 , 48, 100662	23.2	22
54	Stereochemistry and conformation of skyllamycin, a non-ribosomally synthesized peptide from <i>Streptomyces</i> sp. Acta 2897. <i>Chemistry - A European Journal</i> , 2014 , 20, 4948-55	4.8	21
53	Antioxidant, metal-binding and DNA-damaging properties of flavonolignans: a joint experimental and computational highlight based on 7-O-galloylsilybin. <i>Chemico-Biological Interactions</i> , 2013 , 205, 173-80	5	21
52	Impact of lipid composition and photosensitizer hydrophobicity on the efficiency of light-triggered liposomal release. <i>Physical Chemistry Chemical Physics</i> , 2017 , 19, 11460-11473	3.6	20
51	Quercetin-imprinted chromatographic sorbents revisited: optimization of synthesis and rebinding protocols for application to natural resources. <i>Journal of Chromatography A</i> , 2014 , 1364, 128-39	4.5	20
50	Lipid bilayer membrane affinity rationalizes inhibition of lipid peroxidation by a natural lignan antioxidant. <i>Journal of Physical Chemistry B</i> , 2013 , 117, 5043-9	3.4	20

49	p-Hydroxyphenyl-pyranoanthocyanins: An Experimental and Theoretical Investigation of Their Acid-Base Properties and Molecular Interactions. <i>International Journal of Molecular Sciences</i> , 2016 , 17,	6.3	19
48	Novel flavonolignan hybrid antioxidants: From enzymatic preparation to molecular rationalization. <i>European Journal of Medicinal Chemistry</i> , 2017 , 127, 263-274	6.8	18
47	Can cerebrovascular reactivity be assessed by dynamic susceptibility contrast-enhanced MRI?. <i>Neuroradiology</i> , 1998 , 40, 1-5	3.2	18
46	Redox reactions obtained by gamma irradiation of quercetin methanol solution are similar to in vivo metabolism. <i>Radiation Research</i> , 2003 , 159, 218-27	3.1	17
45	H-atom acceptor capacity of free radicals used in antioxidant measurements. <i>International Journal of Quantum Chemistry</i> , 2011 , 111, 1131-1142	2.1	16
44	Antioxidant-Inspired Drug Discovery: Antitumor Metabolite Is Formed in Situ from a Hydroxycinnamic Acid Derivative upon Free-Radical Scavenging. <i>Journal of Medicinal Chemistry</i> , 2019 , 62, 1657-1668	8.3	16
43	Oxidation of protein tyrosine or methionine residues: From the amino acid to the peptide. <i>Journal of Physics: Conference Series</i> , 2011 , 261, 012003	0.3	15
42	Radiodermatitis prevention with sucralfate in breast cancer: fundamental and clinical studies. <i>Supportive Care in Cancer</i> , 2011 , 19, 57-65	3.9	15
41	Discovery of the first non-planar flavonoid that can strongly inhibit xanthine oxidase: protoapigenone 1?-O-propargyl ether. <i>Tetrahedron Letters</i> , 2013 , 54, 6529-6532	2	14
40	Lignin Modification Supported by DFT-Based Theoretical Study as a Way to Produce Competitive Natural Antioxidants. <i>Molecules</i> , 2019 , 24,	4.8	13
39	Synthesis and conformation of a novel fluorescein-Zn-porphyrin dyad and intramolecular energy transfer. <i>New Journal of Chemistry</i> , 2016 , 40, 3843-3856	3.6	13
38	Regio- and stereocontrolled synthesis of oligostilbenoids: theoretical highlights at the supramolecular level. <i>Journal of Natural Products</i> , 2013 , 76, 538-46	4.9	13
37	Toward understanding the protein oxidation processes: DH addition on tyrosine, phenylalanine, or methionine?. <i>International Journal of Quantum Chemistry</i> , 2011 , 111, 1143-1151	2.1	13
36	Atomistic Picture of Fluorescent Probes with Hydrocarbon Tails in Lipid Bilayer Membranes: An Investigation of Selective Affinities and Fluorescent Anisotropies in Different Environmental Phases. <i>Langmuir</i> , 2018 , 34, 9072-9084	4	12
35	Mechanisms of transformation of the antioxidant kaempferol into depsides. Gamma-radiolysis study in methanol and ethanol. <i>Radiation Research</i> , 2003 , 160, 355-65	3.1	12
34	Flavonolignans As a Novel Class of Sodium Pump Inhibitors. <i>Frontiers in Physiology</i> , 2016 , 7, 115	4.6	12
33	Multidrug resistance-associated protein 4 (MRP4) controls ganciclovir intracellular accumulation and contributes to ganciclovir-induced neutropenia in renal transplant patients. <i>Pharmacological Research</i> , 2016 , 111, 501-508	10.2	12
32	Structural patterns of the human ABCC4/MRP4 exporter in lipid bilayers rationalize clinically observed polymorphisms. <i>Pharmacological Research</i> , 2018 , 133, 318-327	10.2	11

31	cis-trans Isomerization of silybins A and B. <i>Beilstein Journal of Organic Chemistry</i> , 2014 , 10, 1047-1063	2.5	11
30	Stacked polyphenolic dimers: A case study using dispersion-corrected methods. <i>Chemical Physics Letters</i> , 2013 , 578, 120-125	2.5	11
29	Dimerisation process of silybin-type flavonolignans: insights from theory. <i>ChemPhysChem</i> , 2011 , 12, 1135-1142	3.4	11
28	Chemoenzymatic Preparation and Biophysical Properties of Sulfated Quercetin Metabolites. <i>International Journal of Molecular Sciences</i> , 2017 , 18,	6.3	10
27	Mechanism of one-electron oxidation of metformin in aqueous solution. <i>Physical Chemistry Chemical Physics</i> , 2013 , 15, 9871-8	3.6	10
26	Combining (Non)linear Optical and Fluorescence Analysis of DiD To Enhance Lipid Phase Recognition. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 5350-5359	6.4	10
25	Oligostilbenoids from the heartwood of <i>N. Heimii</i> : role of non-covalent association in their biogenesis. <i>Chemistry - an Asian Journal</i> , 2015 , 10, 198-211	4.5	9
24	Dimerization of quercetin, Diels-Alder vs. radical-coupling approach: a joint thermodynamics, kinetics, and topological study. <i>Journal of Molecular Modeling</i> , 2016 , 22, 190	2	9
23	Lipocarbazole, an efficient lipid peroxidation inhibitor anchored in the membrane. <i>Bioorganic and Medicinal Chemistry</i> , 2015 , 23, 4866-4870	3.4	8
22	Binding Modes and Selectivity of Ruthenium Complexes to Human Telomeric DNA G-Quadruplexes. <i>Chemistry - A European Journal</i> , 2018 , 24, 15577-15588	4.8	7
21	Reactivities of MeO-substituted PBN-type nitrones. <i>New Journal of Chemistry</i> , 2019 , 43, 15754-15762	3.6	6
20	Radiolytic transformation of 2,2',4,4'-tetrahydroxychalcone. <i>Radiation Research</i> , 2006 , 165, 730-40	3.1	6
19	Single nucleotide polymorphisms of ABCC2 modulate renal secretion of endogenous organic anions. <i>Biochemical Pharmacology</i> , 2017 , 140, 124-138	6	5
18	Nitrone-Trolox conjugate as an inhibitor of lipid oxidation: Towards synergistic antioxidant effects. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2019 , 1861, 1489-1501	3.8	5
17	Conformational investigation of antibiotic proximicin by X-ray structure analysis and quantum studies suggest a stretched conformation of this type of peptide. <i>Bioorganic and Medicinal Chemistry</i> , 2013 , 21, 3582-9	3.4	5
16	Electrical and Optical Properties of Ion Implanted C60. <i>Fullerenes, Nanotubes, and Carbon Nanostructures</i> , 1996 , 4, 1299-1315		5
15	Tuning Optical Properties of Chalcone Derivatives: A Computational Study. <i>Journal of Physical Chemistry A</i> , 2019 , 123, 194-201	2.8	5
14	MRP4 is responsible for the efflux transport of mycophenolic acid and glucuronide (MPAG) from hepatocytes to blood. <i>Xenobiotica</i> , 2021 , 51, 105-114	2	5

13	Acylglucuronide in alkaline conditions: migration vs. hydrolysis. <i>Journal of Molecular Modeling</i> , 2013 , 19, 2423-32	2	4
12	Reactivity of chalcones with 1-hydroxymethyl radicals. <i>Radiation Research</i> , 2006 , 166, 928-41	3.1	4
11	The Physical Chemistry of Polyphenols 2016 , 1-35		4
10	Deciphering the Peculiar Behavior of Elapachone in Lipid Monolayers and Bilayers. <i>Langmuir</i> , 2019 , 35, 14603-14615	4	3
9	One-pot and catalyst-free amidation of ester: a matter of non-bonding interactions. <i>Tetrahedron Letters</i> , 2011 , 52, 6796-6799	2	3
8	-Substituted β -Phenyl--butyl Nitrones: Spin-Trapping, Redox and Neuroprotective Properties. <i>ACS Omega</i> , 2020 , 5, 30989-30999	3.9	3
7	Oxidative Stress Evaluation in Ischemia Reperfusion Models: Characteristics, Limits and Perspectives. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	3
6	Unraveling the performance of dispersion-corrected functionals for the accurate description of weakly bound natural polyphenols. <i>Journal of Molecular Modeling</i> , 2015 , 21, 291	2	2
5	Tunable optical properties of silymarin flavonolignans. <i>Journal of Photochemistry and Photobiology A: Chemistry</i> , 2016 , 328, 154-162	4.7	1
4	Exploring the Use of the Suzuki Coupling Reaction in the Synthesis of 4?-Alkyl-2?-hydroxyacetophenones. <i>Synlett</i> , 2014 , 25, 564-568	2.2	1
3	Structure and Dynamics of Dioleoyl-Phosphatidylcholine Bilayers under the Influence of Quercetin and Rutin. <i>Langmuir</i> , 2020 , 36, 11776-11786	4	1
2	Lipid bilayer position and orientation of novel carprofens, modulators of β -secretase in Alzheimer's disease. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018 , 1860, 2224-2233	3.8	0
1	Synthesis and Studies of New Fluorescein-Porphyrin Dyads: A Theoretical and Experimental Approach. <i>ChemistrySelect</i> , 2018 , 3, 10959-10970	1.8	