

Ol'ha O Brovarets'

List of Publications by Year in descending order

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71
papers

2,284
citations

147566

31
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47
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74
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74
docs citations

74
times ranked

647
citing authors

#	ARTICLE	IF	CITATIONS
1	Novel horizons of the conformationally-tautomeric transformations of the G \hat{A} -T base pairs: quantum-mechanical investigation. <i>Molecular Physics</i> , 2022, 120, .	0.8	0
2	Novel mechanisms of the conformational transformations of the biologically important G \hat{A} -C nucleobase pairs in Watson \hat{A} -Crick, Hoogsteen and wobble configurations via the mutual rotations of the bases around the intermolecular H-bonds: a QM/QTAIM study. <i>RSC Advances</i> , 2021, 11, 25700-25730.	1.7	2
3	Conformational equilibrium, IR and Raman vibrational spectra of the quercetin molecule in different solvents: A comprehensive quantum-chemical investigation. <i>Chemical Physics Impact</i> , 2021, 3, 100033.	1.7	2
4	Atomistic mechanisms of the tautomerization of the G \hat{A} -C base pairs through the proton transfer: quantum-chemical survey. <i>Journal of Molecular Modeling</i> , 2021, 27, 367.	0.8	0
5	Conformational diversity of the quercetin molecule: a quantum-chemical view. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 2817-2836.	2.0	23
6	Conformational transitions of the quercetin molecule <i>via</i> the rotations of its rings: a comprehensive theoretical study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 2865-2883.	2.0	14
7	A new era of the prototropic tautomerism of the quercetin molecule: A QM/QTAIM computational advances. <i>Journal of Biomolecular Structure and Dynamics</i> , 2020, 38, 4774-4800.	2.0	11
8	A Quantum-Mechanical Looking Behind the Scene of the Classic G \hat{A} -C Nucleobase Pairs Tautomerization. <i>Frontiers in Chemistry</i> , 2020, 8, 574454.	1.8	5
9	Energy of the CH \hat{A} -O H-bonds and others specific contacts in the quercetin molecule: QM/QTAIM approximation formulas. <i>Journal of Molecular Liquids</i> , 2020, 313, 113456.	2.3	3
10	A Hidden Side of the Conformational Mobility of the Quercetin Molecule Caused by the Rotations of the O3H, O5H and O7H Hydroxyl Groups: In Silico Scrupulous Study. <i>Symmetry</i> , 2020, 12, 230.	1.1	6
11	A Never-Ending Conformational Story of the Quercetin Molecule: Quantum-Mechanical Investigation of the O3 \hat{A} -H and O4 \hat{A} -H Hydroxyl Groups Rotations. <i>Applied Sciences (Switzerland)</i> , 2020, 10, 1147.	1.3	7
12	Is high performance computing a requirement for novel drug discovery and how will this impact academic efforts?. <i>Expert Opinion on Drug Discovery</i> , 2020, 15, 981-985.	2.5	17
13	Quantum dancing of the wobble G \hat{A} -T(U/5BrU) nucleobase pairs and its biological roles. <i>Chemical Physics Impact</i> , 2020, 1, 100006.	1.7	2
14	Key microstructural mechanisms of the 2-aminopurine mutagenicity: Results of extensive quantum-chemical research. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 2716-2732.	2.0	10
15	Novel Tautomerisation Mechanisms of the Biologically Important Conformers of the Reverse L \hat{A} -w \hat{A} in, Hoogsteen, and Reverse Hoogsteen G \hat{A} -C* DNA Base Pairs via Proton Transfer: A Quantum-Mechanical Survey. <i>Frontiers in Chemistry</i> , 2019, 7, 597.	1.8	13
16	Novel Conformationally-Tautomeric Properties of the Biologically Important at DNA Base Pairs. <i>Biophysical Journal</i> , 2019, 116, 75a.	0.2	2
17	Intramolecular tautomerization of the quercetin molecule due to the proton transfer: QM computational study. <i>PLoS ONE</i> , 2019, 14, e0224762.	1.1	9
18	Atomistic mechanisms of the double proton transfer in the H-bonded nucleobase pairs: QM/QTAIM computational lessons. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 1880-1907.	2.0	21

#	ARTICLE	IF	CITATIONS
19	Title is missing!. , 2019, 14, e0224762.		0
20	Title is missing!. , 2019, 14, e0224762.		0
21	Title is missing!. , 2019, 14, e0224762.		0
22	Title is missing!. , 2019, 14, e0224762.		0
23	The A $\hat{\cdot}$ T(rWC)/A $\hat{\cdot}$ T(H)/A $\hat{\cdot}$ T(rH) $\hat{\cdot}$ †" A $\hat{\cdot}$ T*(rwWC)/A $\hat{\cdot}$ T*(wH)/A $\hat{\cdot}$ T*(rwH) mutagenic tautomerization via sequential proton transfer: a QM/QTAIM study. RSC Advances, 2018, 8, 13433-13445.	1.7	14
24	A QM/QTAIM detailed look at the Watson $\hat{\cdot}$ "Crick $\hat{\cdot}$ †" wobble tautomeric transformations of the 2-aminopurine $\hat{\cdot}$ pyrimidine mispairs. Journal of Biomolecular Structure and Dynamics, 2018, 36, 1649-1665.	2.0	18
25	Physico-chemical profiles of the wobble $\hat{\cdot}$ †" Watson $\hat{\cdot}$ "Crick G* $\hat{\cdot}$ 2AP(w) $\hat{\cdot}$ †" G $\hat{\cdot}$ 2AP(WC) and A $\hat{\cdot}$ 2AP(w) $\hat{\cdot}$ †" A* $\hat{\cdot}$ 2AP(WC) tautomerisations: a QM/QTAIM comprehensive survey. Physical Chemistry Chemical Physics, 2018, 20, 623-636.	1.3	19
26	Renaissance of the Tautomeric Hypothesis of the Spontaneous Point Mutations in DNA: New Ideas and Computational Approaches. , 2018, , .		13
27	Unexpected Routes of the Mutagenic Tautomerization of the T Nucleobase in the Classical A $\hat{\cdot}$ T DNA Base Pairs: A QM/QTAIM Comprehensive View. Frontiers in Chemistry, 2018, 6, 532.	1.8	15
28	Novel pathway for mutagenic tautomerization of classical $\hat{\cdot}$ †"DNA DNA base pairs via sequential proton transfer through quasi-orthogonal transition states: A QM/QTAIM investigation. PLoS ONE, 2018, 13, e0199044.	1.1	22
29	Non-dissociative structural transitions of the Watson-Crick and reverse Watson-Crick $\hat{\cdot}$ †"DNA DNA base pairs into the Hoogsteen and reverse Hoogsteen forms. Scientific Reports, 2018, 8, 10371.	1.6	25
30	Surprising Conformers of the Biologically Important A $\hat{\cdot}$ T DNA Base Pairs: QM/QTAIM Proofs. Frontiers in Chemistry, 2018, 6, 8.	1.8	22
31	Unexpected A $\hat{\cdot}$ T(WC) $\hat{\cdot}$ †"A $\hat{\cdot}$ T(rWC)/A $\hat{\cdot}$ T(rH) and A $\hat{\cdot}$ T(H) $\hat{\cdot}$ †"A $\hat{\cdot}$ T(rH)/A $\hat{\cdot}$ T(rWC) conformational transitions between the classical A $\hat{\cdot}$ T DNA base pairs: A QM/QTAIM comprehensive study. International Journal of Quantum Chemistry, 2018, 118, e25674.	1.0	20
32	A QM/QTAIM research under the magnifying glass of the DPT tautomerisation of the wobble mispairs involving 2-aminopurine. New Journal of Chemistry, 2017, 41, 7232-7243.	1.4	30
33	Whether 2-aminopurine induces incorporation errors at the DNA replication? A quantum-mechanical answer on the actual biological issue. Journal of Biomolecular Structure and Dynamics, 2017, 35, 3398-3411.	2.0	23
34	Structural grounds for the 2-aminopurine mutagenicity: a novel insight into the old problem of the replication errors. RSC Advances, 2016, 6, 99546-99557.	1.7	26
35	Whether the amino $\hat{\cdot}$ "imino tautomerism of 2-aminopurine is involved into its mutagenicity? Results of a thorough QM investigation. RSC Advances, 2016, 6, 108255-108264.	1.7	20
36	By how many tautomerisation routes the Watson $\hat{\cdot}$ "Crick-like A $\hat{\cdot}$ C* DNA base mispair is linked with the wobble mismatches? A QM/QTAIM vision from a biological point of view. Structural Chemistry, 2016, 27, 119-131.	1.0	28

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37	Tautomeric transition between wobble A $\hat{\cdot}$ C DNA base mispair and Watson $\hat{\cdot}$ Crick-like A $\hat{\cdot}$ C* mismatch: microstructural mechanism and biological significance. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 15103-15110.	1.3	64
38	Novel physico-chemical mechanism of the mutagenic tautomerisation of the Watson $\hat{\cdot}$ Crick-like A $\hat{\cdot}$ G and C $\hat{\cdot}$ T DNA base mispairs: a quantum-chemical picture. <i>RSC Advances</i> , 2015, 5, 66318-66333.	1.7	43
39	Wobble $\hat{\cdot}$ Watson-Crick tautomeric transitions in the homo-purine DNA mismatches: a key to the intimate mechanisms of the spontaneous transversions. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 2710-2715.	2.0	39
40	A novel conception for spontaneous transversions caused by homo-pyrimidine DNA mismatches: a QM/QTAIM highlight. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 21381-21388.	1.3	46
41	How many tautomerization pathways connect Watson $\hat{\cdot}$ Crick-like G* $\hat{\cdot}$ T DNA base mispair and wobble mismatches?. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 2297-2315.	2.0	61
42	New structural hypostases of the A $\hat{\cdot}$ T and G $\hat{\cdot}$ C Watson $\hat{\cdot}$ Crick DNA base pairs caused by their mutagenic tautomerisation in a wobble manner: a QM/QTAIM prediction. <i>RSC Advances</i> , 2015, 5, 99594-99605.	1.7	55
43	Proton tunneling in the A $\hat{\cdot}$ T Watson-Crick DNA base pair: myth or reality?. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 2716-2720.	2.0	43
44	The significant role of the intermolecular CH $\hat{\cdot}$ O/N hydrogen bonds in governing the biologically important pairs of the DNA and RNA modified bases: a comprehensive theoretical investigation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 1624-1652.	2.0	80
45	DPT tautomerisation of the wobble guanine $\hat{\cdot}$ thymine DNA base mispair is not mutagenic: QM and QTAIM arguments. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 674-689.	2.0	55
46	The physicochemical essence of the purine $\hat{\cdot}$ pyrimidine transition mismatches with Watson-Crick geometry in DNA: A $\hat{\cdot}$ C* <i>versus</i> A* $\hat{\cdot}$ C. A QM and QTAIM atomistic understanding. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 28-55.	2.0	64
47	The nature of the transition mismatches with Watson $\hat{\cdot}$ Crick architecture: the G* $\hat{\cdot}$ T or G $\hat{\cdot}$ T* DNA base mispair or both? A QM/QTAIM perspective for the biological problem. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 925-945.	2.0	69
48	How Do Long Improper Purine-Purine Pairs of DNA Bases Adapt The Enzymatically Competent Conformation? Structural Mechanism And Its Quantum-Mechanical Grounds. <i>Ukrainian Journal of Physics</i> , 2015, 60, 748-756.	0.1	6
49	Can tautomerization of the A $\hat{\cdot}$ T Watson $\hat{\cdot}$ Crick base pair <i>via</i> double proton transfer provoke point mutations during DNA replication? A comprehensive QM and QTAIM analysis. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014, 32, 127-154.	2.0	137
50	Why the tautomerization of the G $\hat{\cdot}$ C Watson $\hat{\cdot}$ Crick base pair <i>via</i> the DPT does not cause point mutations during DNA replication? QM and QTAIM comprehensive analysis. <i>Journal of Biomolecular Structure and Dynamics</i> , 2014, 32, 1474-1499.	2.0	90
51	Structural, energetic and tautomeric properties of the T $\hat{\cdot}$ T $\hat{\cdot}$ —/T $\hat{\cdot}$ — $\hat{\cdot}$ T DNA mismatch involving mutagenic tautomer of thymine: A QM and QTAIM insight. <i>Chemical Physics Letters</i> , 2014, 592, 247-255.	1.2	37
52	A QM/QTAIM microstructural analysis of the tautomerisation <i>via</i> the DPT of the hypoxanthine $\hat{\cdot}$ adenine nucleobase pair. <i>Molecular Physics</i> , 2014, 112, 2005-2016.	0.8	19
53	Does the tautomeric status of the adenine bases change upon the dissociation of the A* $\hat{\cdot}$ Asyn Topal $\hat{\cdot}$ Fresco DNA mismatch? A combined QM and QTAIM atomistic insight. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 3715.	1.3	58
54	Does the G $\hat{\cdot}$ G [*] <i>syn</i> DNA mismatch containing canonical and rare tautomers of the guanine tautomerise through the DPT? A QM/QTAIM microstructural study. <i>Molecular Physics</i> , 2014, 112, 3033-3046.	0.8	38

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55	Is the DPT tautomerization of the long A ⁺ G Watson-Crick DNA base mispair a source of the adenine and guanine mutagenic tautomers? A QM and QTAIM response to the biologically important question. Journal of Computational Chemistry, 2014, 35, 451-466.	1.5	63
56	DPT tautomerisation of the G ⁺ A _{syn} and A ⁺ G _{syn} DNA mismatches: a QM/QTAIM combined atomistic investigation. Physical Chemistry Chemical Physics, 2014, 16, 9074-9085.	1.3	49
57	How does the long G ⁺ C* Watson-Crick DNA base mispair comprising keto and enol tautomers of the guanine tautomerise? The results of a QM/QTAIM investigation. Physical Chemistry Chemical Physics, 2014, 16, 15886-15899.	1.3	42
58	Intermolecular CH ⁺ ...O/N H-bonds in the biologically important pairs of natural nucleobases: a thorough quantum-chemical study. Journal of Biomolecular Structure and Dynamics, 2014, 32, 993-1022.	2.0	122
59	Atomistic understanding of the C ⁺ T mismatched DNA base pair tautomerization via the DPT: QM and QTAIM computational approaches. Journal of Computational Chemistry, 2013, 34, 2577-2590.	1.5	53
60	Atomistic nature of the DPT tautomerisation of the biologically important C ⁺ C* DNA base mispair containing amino and imino tautomers of cytosine: a QM and QTAIM approach. Physical Chemistry Chemical Physics, 2013, 15, 20091.	1.3	55
61	Parameterization of the hydration free energy computations for organic solutes in the framework of the implicit solvent model with the nonuniform dielectric function. Computational and Theoretical Chemistry, 2013, 1009, 50-54.	1.1	0
62	The physico-chemical "anatomy" of the tautomerization through the DPT of the biologically important pairs of hypoxanthine with DNA bases: QM and QTAIM perspectives. Journal of Molecular Modeling, 2013, 19, 4119-4137.	0.8	45
63	Prototropic tautomerism and basic molecular principles of hypoxanthine mutagenicity: an exhaustive quantum-chemical analysis. Journal of Biomolecular Structure and Dynamics, 2013, 31, 913-936.	2.0	58
64	The physico-chemical mechanism of the tautomerisation via the DPT of the long Hyp ⁺ -Hyp Watson-Crick base pair containing rare tautomer: A QM and QTAIM detailed look. Chemical Physics Letters, 2013, 578, 126-132.	1.2	48
65	DPT tautomerization of the long A ⁺ TMA* Watson-Crick base pair formed by the amino and imino tautomers of adenine: combined QM and QTAIM investigation. Journal of Molecular Modeling, 2013, 19, 4223-4237.	0.8	57
66	Can DNA-binding proteins of replisome tautomerize nucleotide bases? Ab initio model study. Journal of Biomolecular Structure and Dynamics, 2012, 29, 1101-1109.	2.0	67
67	IR Vibrational spectra of H-bonded complexes of adenine, 2-aminopurine and 2-aminopurine+ with cytosine and thymine: Quantum-chemical study. Optics and Spectroscopy (English Translation of) Tj ETQq1 1 0.784314 rgBT45 Overlo	0.784314	45
68	How stable are the mutagenic tautomers of DNA bases?. Biopolymers and Cell, 2010, 26, 72-76.	0.1	53
69	Stability of mutagenic tautomers of uracil and its halogen derivatives: the results of quantum-mechanical investigation. Biopolymers and Cell, 2010, 26, 295-298.	0.1	38
70	Is there adequate ionization mechanism of the spontaneous transitions? Quantum-chemical investigation. Biopolymers and Cell, 2010, 26, 398-405.	0.1	41
71	Where Quantum Biochemistry Meets Structural Bioinformatics: Excited Conformationally-Tautomeric States of the Classical A ⁺ T DNA Base Pair. , 0, , .		2