Ol'ha O Brovarets'

List of Publications by Year
in descending order

71	2,284	147566	214527
papers	citations	31 h-index	47 g-index

74	74	74	647
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Can tautomerization of the AÂ·T Watsonâ€“Crick base pairviadouble proton transfer provoke point mutations during DNA replication? A comprehensive QM and QTAIM analysis. Journal of Biomolecular Structure and Dynamics, 2014, 32, 127-154.	2.0	137
2	Intermolecular CHÂ·Â·Â·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
3	Why the tautomerization of the GÂ·C Watsonâ€“Crick base pairviathe DPT does not cause point mutations during DNA replication? QM and QTAIM comprehensive analysis. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1474-1499.	2.0	90
4	The significant role of the intermolecular CHâ‹¯O/N hydrogen bonds in governing the biologically important pairs of the DNA and RNA modified bases: a comprehensive theoretical investigation. Journal of Biomolecular Structure and Dynamics, 2015, 33, 1624-1652.	2.0	80
5	The nature of the transition mismatches with Watsonâ€“Crick architecture: the G*Â·T or GÂ·T* DNA base mispair or both? A QM/QTAIM perspective for the biological problem. Journal of Biomolecular Structure and Dynamics, 2015, 33, 925-945.	2.0	69
6	Can DNA-binding proteins of replisome tautomerize nucleotide bases?Ab initiomodel study. Journal of Biomolecular Structure and Dynamics, 2012, 29, 1101-1109.	2.0	67
7	Tautomeric transition between wobble AÂ·C DNA base mispair and Watsonâ€“Crick-like AÂ·C* mismatch: microstructural mechanism and biological significance. Physical Chemistry Chemical Physics, 2015, 17, 15103-15110.	1.3	64
8	The physicochemical essence of the purineÂ·pyrimidine transition mismatches with Watson-Crick geometry in DNA: AÂ·C*versaA*Â·C. A QM and QTAIM atomistic understanding. Journal of Biomolecular Structure and Dynamics, 2015, 33, 28-55.	2.0	64
9	Is the DPT tautomerization of the long AÂ·G Watsonâ€“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
10	How many tautomerization pathways connect Watsonâ€“Crick-like C*Â·T DNA base mispair and wobble mismatches?. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2297-2315.	2.0	61
11	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
12	Does the tautomeric status of the adenine bases change upon the dissociation of the A*Â·Asyn Topalâ€“Fresco DNA mismatch? A combined QM and QTAIM atomistic insight. Physical Chemistry Chemical Physics, 2014, 16, 3715.	1.3	58
13	DPT tautomerization of the long Aâ^™A* 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
14	Atomistic nature of the DPT tautomerisation of the biologically important CÂ·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
15	New structural hypostases of the AÂ·T and GÂ·C Watsonâ€“Crick DNA base pairs caused by their mutagenic tautomerisation in a wobble manner: a QM/QTAIM prediction. RSC Advances, 2015, 5, 99594-99605.	1.7	55
16	DPT tautomerisation of the wobble guanineÂ·thymine DNA base mispair is not mutagenic: QM and QTAIM arguments. Journal of Biomolecular Structure and Dynamics, 2015, 33, 674-689.	2.0	55
17	Atomistic understanding of the CÂ·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
18	How stable are the mutagenic tautomers of DNA bases?. Biopolymers and Cell, 2010, 26, 72-76.	0.1	53

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19	DPT tautomerisation of the GÂ·A_{syn}and A*Â·G*_{syn}DNA mismatches: a QM/QTAIM combined atomistic investigation. Physical Chemistry Chemical Physics, 2014, 16, 9074-9085.	1.3	49
20	The physico-chemical mechanism of the tautomerisation via the DPT of the long Hypâˆ—Â·Hyp Watsonâ€“Crick base pair containing rare tautomer: A QM and QTAIM detailed look. Chemical Physics Letters, 2013, 578, 126-132.	1.2	48
21	A novel conception for spontaneous transversions caused by homo-pyrimidine DNA mismatches: a QM/QTAIM highlight. Physical Chemistry Chemical Physics, 2015, 17, 21381-21388.	1.3	46
22	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 ETQq0 0 0 rgBT /Overlock 10 Tf 50	0.7	46
23	The physico-chemical â€œanatomyâ€•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
24	Novel physico-chemical mechanism of the mutagenic tautomerisation of the Watsonâ€“Crick-like AÂ·G and CÂ·T DNA base mispairs: a quantum-chemical picture. RSC Advances, 2015, 5, 66318-66333.	1.7	43
25	Proton tunneling in the Aâˆ™T Watson-Crick DNA base pair: myth or reality?. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2716-2720.	2.0	43
26	How does the long GÂ·G* Watsonâ€“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
27	Is there adequate ionization mechanism of the spontaneous transitions? Quantum-chemical investigation. Biopolymers and Cell, 2010, 26, 398-405.	0.1	41
28	Wobbleâ†”Watson-Crick tautomeric transitions in the homo-purine DNA mismatches: a key to the intimate mechanisms of the spontaneous transversions. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2710-2715.	2.0	39
29	Does the GÂ·G[*]_{syn}DNA mismatch containing canonical and rare tautomers of the guanine tautomerise through the DPT? A QM/QTAIM microstructural study. Molecular Physics, 2014, 112, 3033-3046.	0.8	38
30	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
31	Structural, energetic and tautomeric properties of the TÂ·Tâˆ—/Tâˆ—Â·T DNA mismatch involving mutagenic tautomer of thymine: A QM and QTAIM insight. Chemical Physics Letters, 2014, 592, 247-255.	1.2	37
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	By how many tautomerisation routes the Watsonâ€“Crick-like AÂ·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
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	Non-dissociative structural transitions of the Watson-Crick and reverse Watson-Crick ĐÂ·Đ¢ DNA base pairs into the Hoogsteen and reverse Hoogsteen forms. Scientific Reports, 2018, 8, 10371.	1.6	25
36	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

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37	Conformational diversity of the quercetin molecule: a quantum-chemical view. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2817-2836.	2.0	23
38	Novel pathway for mutagenic tautomerization of classical Ðâ˜™Ð¢ DNA base pairs via sequential proton transfer through quasi-orthogonal transition states: A QM/QTAIM investigation. PLoS ONE, 2018, 13, e0199044.	1.1	22
39	Surprising Conformers of the Biologically Important AÂ·T DNA Base Pairs: QM/QTAIM Proofs. Frontiers in Chemistry, 2018, 6, 8.	1.8	22
40	Atomistic mechanisms of the double proton transfer in the H-bonded nucleobase pairs: QM/QTAIM computational lessons. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1880-1907.	2.0	21
41	Whether the aminoâ€“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
42	Unexpected AÂ·T(WC)â†”AÂ·T(rWC)/AÂ·T(rH) and AÂ·T(H)â†”AÂ·T(rH)/AÂ·T(rWC) conformational transitions between the classical AÂ·T DNA base pairs: A QM/QTAIM comprehensive study. International Journal of Quantum Chemistry, 2018, 118, e25674.	1.0	20
43	A QM/QTAIM microstructural analysis of the tautomerisationviathe DPT of the hypoxanthineÂ·adenine nucleobase pair. Molecular Physics, 2014, 112, 2005-2016.	0.8	19
44	Physico-chemical profiles of the wobble â†” Watsonâ€“Crick G*Â·2AP(w) â†” GÂ·2AP(WC) and AÂ·2AP(w) â†” A*Â·2AP(WC) tautomerisations: a QM/QTAIM comprehensive survey. Physical Chemistry Chemical Physics, 2018, 20, 623-636.	1.3	19
45	A QM/QTAIM detailed look at the Watsonâ€“Crickâ†”wobble tautomeric transformations of the 2-aminopurineÂ·pyrimidine mispairs. Journal of Biomolecular Structure and Dynamics, 2018, 36, 1649-1665.	2.0	18
46	Is high performance computing a requirement for novel drug discovery and how will this impact academic efforts?. Expert Opinion on Drug Discovery, 2020, 15, 981-985.	2.5	17
47	Unexpected Routes of the Mutagenic Tautomerization of the T Nucleobase in the Classical AÂ·T DNA Base Pairs: A QM/QTAIM Comprehensive View. Frontiers in Chemistry, 2018, 6, 532.	1.8	15
48	The AÂ·T(rWC)/AÂ·T(H)/AÂ·T(rH) â†” AÂ·T*(rwWC)/AÂ·T*(wH)/AÂ·T*(rwH) mutagenic tautomerization via sequential proton transfer: a QM/QTAIM study. RSC Advances, 2018, 8, 13433-13445.	1.7	14
49	Conformational transitions of the quercetin molecule via the rotations of its rings: a comprehensive theoretical study. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2865-2883.	2.0	14
50	Renaissance of the Tautomeric Hypothesis of the Spontaneous Point Mutations in DNA: New Ideas and Computational Approaches. , 2018, , .		13
51	Novel Tautomerisation Mechanisms of the Biologically Important Conformers of the Reverse LÃ¶wdin, Hoogsteen, and Reverse Hoogsteen G*Â·C* DNA Base Pairs via Proton Transfer: A Quantum-Mechanical Survey. Frontiers in Chemistry, 2019, 7, 597.	1.8	13
52	A new era of the prototropic tautomerism of the quercetin molecule: A QM/QTAIM computational advances. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4774-4800.	2.0	11
53	Key microstructural mechanisms of the 2-aminopurine mutagenicity: Results of extensive quantum-chemical research. Journal of Biomolecular Structure and Dynamics, 2019, 37, 2716-2732.	2.0	10
54	Intramolecular tautomerization of the quercetin molecule due to the proton transfer: QM computational study. PLoS ONE, 2019, 14, e0224762.	1.1	9

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55	A Never-Ending Conformational Story of the Quercetin Molecule: Quantum-Mechanical Investigation of the O3â€²H and O4â€²H Hydroxyl Groups Rotations. Applied Sciences (Switzerland), 2020, 10, 1147.	1.3	7
56	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. Symmetry, 2020, 12, 230.	1.1	6
57	How Do Long Improper Purine-Purine Pairs of DNA Bases Adapt The Enzymatycally Competent Conformation? Structural Mechanism And Its Quantum-Mechanical Grounds. Ukrainian Journal of Physics, 2015, 60, 748-756.	0.1	6
58	A Quantum-Mechanical Looking Behind the Scene of the Classic GÂ·C Nucleobase Pairs Tautomerization. Frontiers in Chemistry, 2020, 8, 574454.	1.8	5
59	Energy of the CHâ‹¯O H-bonds and others specific contacts in the quercetin molecule: QM/QTAIM approximation formulas. Journal of Molecular Liquids, 2020, 313, 113456.	2.3	3
60	Novel Conformationally-Tautomeric Properties of the Biologically Important at DNA Base Pairs. Biophysical Journal, 2019, 116, 75a.	0.2	2
61	Novel mechanisms of the conformational transformations of the biologically important GÂ·C nucleobase pairs in Watsonâ€“Crick, Hoogsteen and wobble configurations via the mutual rotations of the bases around the intermolecular H-bonds: a QM/QTAIM study. RSC Advances, 2021, 11, 25700-25730.	1.7	2
62	Where Quantum Biochemistry Meets Structural Bioinformatics: Excited Conformationally-Tautomeric States of the Classical AÂ·T DNA Base Pair. , 0, , .		2
63	Conformational equilibrium, IR and Raman vibrational spectra of the quercetin molecule in different solvents: A comprehensive quantum-chemical investigation. Chemical Physics Impact, 2021, 3, 100033.	1.7	2
64	Quantum dancing of the wobble Gâ€¢T(U/5BrU) nucleobase pairs and its biological roles. Chemical Physics Impact, 2020, 1, 100006.	1.7	2
65	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
66	Atomistic mechanisms of the tautomerization of the GÂ·C base pairs through the proton transfer: quantum-chemical survey. Journal of Molecular Modeling, 2021, 27, 367.	0.8	0
67	Novel horizons of the conformationally-tautomeric transformations of the GÂ·T base pairs: quantum-mechanical investigation. Molecular Physics, 2022, 120, .	0.8	0
68	Title is missing!. , 2019, 14, e0224762.		0
69	Title is missing!. , 2019, 14, e0224762.		0
70	Title is missing!. , 2019, 14, e0224762.		0
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