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D05.2 Statement on the completion of the publication list

Deeping collaboration on novel biomolecular electronics based on "smart" nanomaterials			
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Reviews		
Version	Reviewer	Date
V0.1	IMBG	22/11/2020
V0.2	ZSI	23/11/2020

IMBG publications in scientific journals reffered in Scopus, Web of Science Core Collection in 2017-2020

2017

1.	Molecular modeling and molecular dynamics simulation study of archaeal leucyl-tRNA synthetase in complex with different mischarged tRNA in editing conformation	Journal of Molecular Graphics and Modelling - 2017, V. 76. P. 289-295. http://dx.doi.org/doi:10.1016/j.jmgm.2017.06.022	A.V. Rayevsky, M. Sharifi, M.A. Tukalo	
2.	$d(A)_3d(T)_3$ and $d(G)_3d(C)_3$ B-DNA mini-helixes: the DFT/M06-2x and DFT/B97-D3 comparison of geometrical and energetic characteristics	Journal of Molecular Modeling 23 (10), 289 (2017) DOI: 10.1007/s00894-017-3449-y	L Gorb, TA Zubatiuk, R Zubatyuk, D Hovorun, J Leszczynski	
3.	Enthalpy-entropy compensation: the role of solvation	Eur Biophys J. 2017 May; 46(4):301-308. doi: 10.1007/s00249-016-1182-6. https://www.researchgate.net/publication/309590885_Enthalpy-entropy_compensation_the_role_of_solvation	Dragan AI, Read CM, Crane-Robinson C.	
4.	Izatizon, as an izatin-thiosemicarbazone derivative, has antiviral, anti-tumor actions and no side effects	International Journal of Pharmaceutical Science Invention -2017 -V.6. -Is.5. – P.7-9, *Impact factor 1,695*, Індія. http://www.ijpsi.org/Papers/Vol6(5)/B06050709.pdf	Bolsunova Ol'ha I., Zaika Leonid A., Potopalsky Anatoliy I., Voznyuk Anna V.	
5.	A QM/QTAIM detailed look at the Watson-Crick↔wobble tautomeric transformations of the 2-aminopurine·pyrimidine mispairs	Journal of Biomolecular Structure & Dynamics. – 2017. – DOI: 10.1080/07391102.2017.1331864	Brovarets' O.O., Voiteshenko, I.S, Pérez-Sánchez H.E., & Hovorun D.M.	
6.	A new mechanism of post-transfer editing by aminoacyl-tRNA synthetases: Catalysis of hydrolytic reaction by bacterial-type prolyl-tRNA synthetase	*Journal of Biomolecular Structure and Dynamics.* – 2017. – V. 35, N 3. – P. 669-682. https://doi.org/10.1080/07391102.2016.1155171	Boyarshin K.S., Priss A.E., Rayevskiy A.V., Ilchenko M.M., Dubey I.Ya., Kriklivyi I.A., Yaremchuk A.D., Tukalo M.A.	

7.	Computational Modeling and Molecular Dynamics Simulations of Mammalian Cytoplasmic Tyrosyl-tRNA Synthetase and Its Complexes with Substrates.	*Journal* Biomol Struct Dyn. 2017 , Vol.35, N13, 2772-2788 . *Impact factor 3,123.* PMID: 27615678 DOI: 10.1080/07391102.2016.1235512	Kravchuk VO, Savytskyi OV, Odynets KO, Mykuliak VV, Kornelyuk AI.	
8.	A QM/QTAIM research under the magnifying glass of the DPT tautomerisation of the wobble mispairs involving 2-aminopurine	New Journal of Chemistry 41 (15), 7232-7243 (2017) DOI:10.1039/c7nj00717e	OO Brovarets', IS Voiteshenko, H Pérez-Sánchez, DM Hovorun	
9.	Physico-chemical profiles of the wobble↔ Watson-Crick G*· 2AP (w)↔ G· 2AP (WC) and A· 2AP (w)↔ A*· 2AP (WC) tautomerisations: a QM/QTAIM comprehensive survey.	Physical Chemistry & Chemical Physics: 20 (1), 623-636 (2017) DOI: 10.1039/c7cp05139e	OO Brovarets', IS Voiteshenko, DM Hovorun	
10	Synthesis, spectral characterization of novel Pd(II), Pt(II) □-coordination compounds based on N-allylthioureas. Cytotoxic properties and DNA binding ability	J. of Inorganic Biochemistry. 168, 98–106 (2017). DOI:10.1016/j.jinorgbio.2016.12.004	H.H. Repich, V.V. Orysyk, L.G. Palchykovska, S.I. Orysyk, Yu.L. Zborovskii, O.V. Vasylchenko, O.V. Storozhuk, A.A. Biluk, V.V. Nikulina, L.V. Garmanchuk, V.I. Pekhnyo, M.V. Vovk	
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13	Structure and Function of Enterocyte in Intrauterine Growth Retarded Pig Neonates.	Disease Markers. 2017.vol. 2017, Article ID 5238134, 9 pages, 2017. doi:10.1155/2017/5238134"	K. Ferenc,T. Pilżys, T. Skrzypek, D. Garbicz, M. Marcinkowski, M. Dylewska,P. Gładysz, O. Skorobogatov, Z. Gajewski, E. Grzesiuk, R. Zabielski.	
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