

## **BII – Physics and Evolution of Biological Macromolecules**

*\*\*(Publications sorted: Newest – Oldest)*

1.	<b>Yin M, Goncarenco A, Berezovsky IN.</b> <a href="#">Deriving and Using Descriptors of Elementary Functions in Rational Protein Design.</a> <i>Frontiers in Bioinformatics</i> , 13 Apr 21, doi: 10.3389/fbinf.2021.657529
2.	<b>Guarnera E, Tan ZW, Berezovsky IN.</b> <a href="#">Three-dimensional Chromatin Ensemble Reconstruction via Stochastic Embedding.</a> <i>Structure</i> 2021
3.	<b>Tee WV, Guarnera E, Berezovsky IN.</b> Disorder driven allosteric control of protein activity. <i>Current Research in Structural Biology</i> , Volume 2, 2020, Pages 191-203
4.	<b>Tan ZW, Guarnera E, Tee WV, Berezovsky IN.</b> (2020) <a href="#">AlloSigMA 2: paving the way to designing allosteric effectors and to exploring allosteric effects of mutations.</a> <i>Nucleic Acids Res.</i> 2020 May 11. pii: gkaa338. doi: 10.1093/nar/gkaa338.
5.	<b>Guarnera E, Berezovsky IN.</b> (2020) <a href="#">Allosteric drugs and mutations: chances, challenges, and necessity.</a> <i>Curr. Opin. Struct. Biol.</i> 62, 149-157.
6.	<b>Tee WV, Guarnera E, Berezovsky IN.</b> (2019). <a href="#">On the Allosteric Effect of nsSNPs and the Emerging Importance of Allosteric Polymorphism.</a> <i>Journal of Molecular Biology</i> , Vol. 431, Issue 19, 6 Sept 2019, Pg 3933-3942, doi: 10.1016/j.jmb.2019.07.012, PMID: 31306666
7.	<b>Berezovsky IN.</b> (2019). <a href="#">Towards descriptor of elementary functions for protein design.</a> <i>Current Opinion in Structural Biology</i> , 2019, Vol 58, Pg 159-165. doi: 10.1016/j.sbi.2019.06.010
8.	<b>Guarnera E, Berezovsky IN.</b> (2019). <a href="#">Towards comprehensive allosteric control over protein activity.</a> <i>Structure</i> 27, 866-879.
9.	<b>Wodak SJ, Paci E, Dokholyan NV, Berezovsky IN, Horovitz A, Li J, Hilser VJ, Bahar I, Karanicolas J, Stock G, Hamm P, Stote RH, Eberhardt J, Chebaro Y, Dejaegere A, Cecchini M, Changeux JP, Bolhuis PG, Vreede J, Faccioli P, Orioli S, Ravasio R, Yan L, Brito C, Wyart M, Gkeka P, Rivalta I, Palermo G, McCammon JA, Panecka-Hofman J, Wade RC, Di Pizio A, Niv MY, Nussinov R, Tsai CJ, Jang H, Padhorny D, Kozakov D, McLeish T.</b> (2019). <a href="#">Allostery in its many disguises: from theory to applications.</a> <i>Structure</i> 27, 566-578.
10.	<b>Guarnera E, Berezovsky IN.</b> (2019). <a href="#">On the perturbation nature of allostery: sites, mutations, and signal modulation.</a> <i>Curr. Opin. Struct. Biol.</i> 56, 18-27.
11.	<b>Tan ZW, Tee WV, Guarnera E, Booth L, Berezovsky IN.</b> (2019). <a href="#">AlloMAPS: Allosteric mutation analysis and polymorphism of signaling database.</a> <i>Nucl. Acids. Res.</i> 47, D265-D270.
12.	<b>Romero Romero ML, Yang F, Lin YR, Toth-Petroczy A, Berezovsky IN, Goncarenco A, Yang W, Wellner A, Kumar-Deshmukh F, Sharon M, Baker D, Varani G, Tawfik DS.</b> (2018). <a href="#">Simple yet functional Phosphate-loop proteins.</a> <i>Proc. Nat. Acad. Sci. USA</i> 115, E11943-E11950.
13.	<b>Tan ZW, Guarnera E, Berezovsky IN.</b> (2018). <a href="#">Exploring chromatin hierarchical organization via Markov State Modelling.</a> <i>PLoS Comp Biol</i> 14, e1006228.
14.	<b>Tee WV, Guarnera E, Berezovsky IN.</b> (2018). <a href="#">Reversing allosteric communication: from detecting allosteric sites to inducing and tuning targeted allosteric response.</a> <i>PLoS Comp</i>

	Biol 14, e1006228.
15.	<b>Kurochkin IV, Guarnera E, Berezovsky IN.</b> (2018). <a href="#">Insulin-Degrading enzyme in the fight against Alzheimer's Disease.</a> Trends in Pharm Sci 39, 49-58.
16.	<b>Guarnera E, Tan ZW, Zheng Z, Berezovsky IN.</b> (2017). <a href="#">AlloSigMA: Allosteric signalling and mutation analysis server.</a> Bioinformatics 33, 3996-3998.
17.	<b>Berezovsky IN, Guarnera E, Zheng Z.</b> (2017). <a href="#">Basic units of protein structure, folding, and function.</a> Prog Bioph & Mol Biol 128, 85-99.
18.	<b>Berezovsky IN, Guarnera E, Zheng Z, Eisenhaber B, Eisenhaber F.</b> (2017). <a href="#">Protein function machinery: from basic structural units to modulation of activity.</a> Curr. Opin. Struct. Biol. 42, 67-74.
19.	<b>Berezovsky IN, Bastolla U.</b> (2017). <a href="#">Proteins: bridging theory and experiment.</a> Curr. Opin. Struct. Biol. 42, viii-x.
20.	<b>Kurochkin IV, Guarnera E, Wong JH, Eisenhaber F, Berezovsky IN.</b> (2017). <a href="#">Towards allosterically increased catalytic activity of insulin degrading enzyme (IDE) against amyloid peptides.</a> Biochemistry 56, 228-239.
21.	<b>Eisenhaber B, Kuchibhatla D, Sherman W, Sirota FL, Berezovsky IN, Wong WC, Eisenhaber F.</b> (2016). <a href="#">The recipes for protein sequence-based function prediction and its implementation in ANNOTATOR software environment.</a> Methods in Molecular Biology (Data Mining Techniques for the Life Sciences, Eds. O. Carugo and F. Eisenhaber) 1415, 477-506, Springer, New York.
22.	<b>Guarnera E, Berezovsky IN.</b> (2016). <a href="#">Allosteric sites: remote control in regulation of protein activity.</a> Curr. Opin. Struct. Biol. 37, 1-8.
23.	<b>Guarnera E, Berezovsky IN.</b> (2016). <a href="#">Structure-based statistical mechanical model accounts for the causality and energetics of allosteric communication.</a> PLoS Comp Biol 12, e1004678.
24.	<b>Zheng Z, Goncarenco A, Berezovsky IN.</b> (2016). <a href="#">Nucleotide binding database NBDB – a collection of sequence motifs with specific protein-ligand interactions.</a> Nucl. Acids. Res. 44, D301-D304.
25.	<b>Berezovsky IN, Zheng Z, Kurotani A, Tokmakov AA, Kurochkin IV.</b> (2015). <a href="#">Organization of the multiaminoacyl-tRNA synthetase complex and the co-translational protein folding.</a> Protein Science 24, 1475-1485.
26.	<b>Goncarenco A, Berezovsky IN.</b> (2015). <a href="#">Protein function from its emergence to diversity in contemporary proteins.</a> Physical Biology 12, 045002.
27.	<b>Goncarenco A, Berezovsky IN.</b> (2014). <a href="#">The fundamental tradeoff in genomes and proteomes of prokaryotes established by the genetic code, codon entropy, and physics of nucleic acids and proteins.</a> Biology Direct 9, 29.
28.	<b>Goncarenco A, Ma BG, Berezovsky IN.</b> (2014). <a href="#">Molecular mechanisms of adaptation emerging from the physics and evolution of nucleic acids and proteins.</a> Nucl. Acids. Res. 42, 2879-2892.
29.	<b>Goncarenco A, Mitternacht S, Yong T, Eisenhaber B, Eisenhaber F, Berezovsky IN.</b> (2013). <a href="#">SPACER: Server for Predicting Allosteric Communication and Effects of Regulation.</a> Nucl. Acids. Res. 41, W266-W272.