

Bioinformatics Institute Publications – 2018***(Sorted by: Newest to Oldest)*

NO	PUBLICATION
1.	Tan ZW, Guarnera E, Berezovsky IN. <u>Exploring chromatin hierarchical organization via Markov State Modelling.</u> PLoS Computational Biology, 2018 Dec 31;14(12), doi: 10.1371/journal.pcbi.100668, PMID: 30596637
2.	Ivanov SM, Huber RG, Alibay I, Warwicker J, Bond PJ. <u>Energetic Fingerprinting of Ligand Binding to Paralogous Proteins: The Case of the Apoptotic Pathway.</u> Journal of Chemical Information and Modeling, 2018 Dec 24. doi: 10.1021/acs.jcim.8b00765, PMID: 30582811
3.	Phua SX, Chan KF, Su TTC. <u>Automated submission script to AlloSigMA webserver: a viable approach for allosteric effects scanning.</u> APD Trove 2018, 1:3, doi: 10.30943/2018/20122018
4.	Han AX, Maurer-Stroh S, Russell CA. <u>Individual immune selection pressure has limited impact on seasonal influenza virus evolution.</u> Nature Ecology & Evolution, 2018, Dec 3, doi: 10.1038/s41559-018-0741-x, PMID: 30510176
5.	Romero Romero ML, Yang F, Lin YR, Toth-Petroczy A, Berezovsky IN, Gonçarenc A, Yang W, Wellner A, Kumar-Deshmukh F, Sharon M, Baker D, Varani G, Tawfik DS. <u>Simple yet functional phosphate-loop proteins.</u> Proceedings of the National Academy of Sciences of the United States of America, PNAS, doi: 10.1073/pnas.1812400115
6.	Ghosh M, Wang LC, Huber RG, Gao Y, Morgan LK, Tulsian NK, Bond PJ, Kenney LJ, Anand GS. <u>Engineering an Osmosensor by Pivotal Histidine Positioning within Disordered Helices.</u> Structure, 27, 1-13, Feb 5, doi: 10.1016/j.str.2018.10.012, PMID: 30503779
7.	Berger KA, Pigott DM, Tomlinson F, Godding D, Maurer-Stroh S, Taye B, Sirota FL, Han AX, Lee RTC, Gunalan V, Eisenhaber F, Hay SI, Russell CA. <u>The Geographic Variation of Surveillance and Zoonotic Spillover Potential of Influenza Viruses in Domestic Poultry and Swine.</u> Open Forum Infectious Diseases, Vol. 5, issue 12, 1 Dec 2018, doi: 10.1093/ofid/ofy318

8.	<p>Kannan S, Tan DS, Verma CS. <u>Effects of Single Nucleotide Polymorphisms on the Binding of Afatinib to EGFR: A Potential Patient Stratification Factor Revealed by Modeling Studies.</u> Journal of Chemical Information and Modeling, 2018 Nov 27. doi: 10.1021/acs.jcim.8b00491, PMID: 30481018</p>
9.	<p>Wong A, Chen S, Yang LK, Kanagasundaram Y, Crasta K. <u>Lipid accumulation facilitates mitotic slippage-induced adaptation to anti-mitotic drug treatment.</u> Cell Death Discovery 4, Article no: 109. 2018, doi: 10.1038/s41420-018-0127-5</p>
10.	<p>Wirawan M, Fibriansah G, Marzinek JK, Lim XX, Ng TS, Sim AYL, Zhang Q, Kostyuchenko VA, Shi J, Smith SA, Anand G, Crowe Je JR, Bond PJ, Lok SM. <u>Mechanism of Enhanced Immature Dengue Virus Attachment to Endosomal Membrane Induced by prM Antibody.</u> Cell Death Discovery 4, Article no: 109. 2018, doi: 10.1038/s41420-018-0127-5</p>
11.	<p>Guarnera E, Berezovsky IN. <u>On the perturbation nature of allostery: sites, mutations, and signal modulation.</u> Current Opinion in Structural Biology, Vol. 56, June 2019, Pg 18-27, doi: 10.1016/j.sbi.2018.10.008</p>
12.	<p>Lin YB, Deepak RNVK, Zheng ZXJ, Fan H, Zheng L. <u>A dual substrate-accessing mechanism of a major facilitator superfamily protein facilitates lysophospholipid flipping across the cell membrane.</u> Journal of Biological Chemistry, 2018, October 29, doi: 10.1074/jbc.RA118.005548, PMID: 30373772</p>
13.	<p>Tan ZW, Tee WV, Guarnera E, Booth L, Berezovsky IN. <u>AlloMAPS: allosteric mutation analysis and polymorphism of signaling database.</u> Nucleic Acids Research, 2018, Oct 26, doi:10.1093/nar/gky1028, PMID: 30365033</p>
14.	<p>Narang V, Lu Y, Tan C, Camous XFN, Nyunt SZ, Carre C, Mok EWH, Wong G, Maurer-Stroh S, Abel B, Burdin N, Poidinger M, Tambyah PA, Bosco N, Visan L, Ng TP, Larbi A. <u>Influenza Vaccine-Induced Antibody Responses Are Not Impaired by Frailty in the Community-Dwelling Elderly With Natural Influenza Exposure.</u> Frontiers in Immunology, 24 Oct 2018, Vol. 9, Article 265, doi: 10.3389/fimmu.2018.02465, PMID: 30405641</p>
15.	<p>Chew S, Zeng Y, Khoo D, Hong Yu MY, Ahmed S, Chiam KH. <u>Enrichment and Identification of Neural Stem Cells in Neurospheres using Rigidity-Tunable Gels.</u> Tissue Engineering Part A, 15 Oct 2018, doi: 10.1089/ten.TEA.2018.0221</p>

16.	Poh JJ, Phua SX, Chan KF, Gan SKE. <u>Commentary: Augmented Reality Scientific Phone Apps –making the APD AR Holistic Review app and using existing AR apps for scientific publications.</u> Scientific Phone Apps and Mobile Devices (2018) 4:4, doi:10.30943/2018/28092018
17.	Sinha S, Eisenhaber B, Jensen LJ, Kalbuaji B, Eisenhaber F. <u>Darkness in the Human Gene and Protein Function Space: Widely Modest or Absent Illumination by the Life Science Literature and the Trend for Fewer Protein Function Discoveries Since 2000.</u> Proteomics 2018, Sep 28, doi: 10.1002/pmic.201800093, PMID: 30265449
18.	Kamariah N, Eisenhaber B, Eisenhaber F, Gruber G. <u>Molecular mechanism of the Escherichia coli AhpC in the function of a chaperone under heat-shock conditions.</u> Scientific Reports 8, No. 14151, 2018, doi: 10.1038/s41598-018-32527-7, PMID: 30237544
19.	Wang L, Yan DD, Deepak RNVK, Liu H, Xiao QP, Fan H, Gong WM, Wei ZY, Zhang C. <u>Structures of the Human PGD2 Receptor CRTH2 Reveal Novel Mechanisms for Ligand Recognition.</u> Molecular Cell, 2018, doi: 10.1016/j.molcel.2018.08.009
20.	Sharma KK, Marzinek JK, Tantirimudalige SN, Bond PJ, Wohland T. <u>Single-molecule studies of flavivirus envelope dynamics: Experiment and computation.</u> Progress in Biophysics and Molecular Biology, 2018, Sep 14, doi: 10.1016/j.pbiomolbio.2018.09.001, PMID: 30223001
21.	Krishna Deepak RNV, Abdullah A, Talwar P, Fan H, Ravanan P. <u>Identification of FDA-approved drugs as novel allosteric inhibitors of human executioner caspases.</u> Proteins: Structure, Function and Bioinformatics, 2018 Sep 8. doi: 10.1002/prot.25601, PMID: 30194780
22.	Krah A, Bond PJ. <u>Single mutations in the ε subunit from thermophilic Bacillus PS3 generate a high binding affinity site for ATP.</u> PeerJ 2018, Sep 5, doi: 10.7717/peerj.5505, PMID: 30202650
23.	Sivalingam J, Kenanov D, Ng WH, Lee SS, Phan TT, Maurer-Stroh S, Kon OL. <u>Integrated Multimodal Evaluation of Genotoxicity in ZFN-Modified Primary Human Cells.</u> Book Chapter : Methods in Molecular Biology: Zinc Finger Proteins, 2018;1867:141-164. doi: 10.1007/978-1-4939-8799-3_11, PMID: 30155821

24.	Lim TC, Cai ST, Huber RG, Bond PJ, Chia XSP, Khou SL, Gao SJ, Lee SS, Lee SG. <u>Facile saccharide-free mimetics that recapitulate key features of glycosaminoglycan sulfation patterns.</u> Chemical Science, 2018, 9, 7940-7947, doi: 10.1039/C8SC02303D
25.	Fox SJ, Lakshminarayanan R, Beuerman RW, Li JG, Verma CS. <u>Conformational Transitions of Melittin between Aqueous and Lipid Phases: Comparison of Simulations with Experiments.</u> The Journal of Physical Chemistry B, 2018, doi: 10.1021/acs.jpcb.8b06781
26.	Chan S, Tan YS, Wu KX, Cheung C, Loke D. <u>Ultra-High Signal Detection of Human Embryonic Stem Cells Driven by Two-Dimensional Materials.</u> ACS Applied Bio Materials, 2018, 1, Pg 210-215, doi: 10.1021/acsabm.8b00085.
27.	Yip AK, Nguyen AT, Rizwan M, Wong ST, Chiam KH, Yim EKF. <u>Anisotropic traction stresses and focal adhesion polarization mediates topography-induced cell elongation.</u> Biomaterials, Vol. 181, October 2018, Pg 103-112, doi: 10.1016/j.biomaterials.2018.07.057, PMID: 30081301
28.	Ng YXR, Wong YS, Yeo YJ, Koh LZC, Wilson C, Gan SKE. <u>The Associations between Dietary Practices and Dietary Quality, Biological Health Indicators, Perceived Stress, Religiosity, Culture, and Gender in Multi-Cultural Singapore.</u> Journal of Ethnic Foods, 2018, doi: 10.1016/j.jef.2018.07.003
29.	Song TL, Nairismagi ML, Laurensia Y, Lim JQ, Tan J, Li ZM, Pang WL, Kizhakeyil A, Wijaya GC, Huang DC, Nagarajan S, Chia BK, Cheah D, Liu YH, Zhang F, Rao HL, Tang T, Wong EK, Bei JX, Iqbal J, Grigoropoulos NF, Ng SB, Chng WJ, Teh BT, Tan SY, Verma NK, Fan H, Lim ST, Ong CK. <u>Oncogenic activation of STAT3 pathway drives PD-L1 expression in natural killer/T cell lymphoma.</u> Blood 2018 Jul 27, doi: 10.1182/blood-2018-01-829424, Pubmed: 30054295
30.	Lim JYV, Du WN, Chen YZ, Fan H. <u>A benchmarking study on virtual ligand screening against homology models of human GPCRs.</u> Proteins: Structure, Function, and Bioinformatics, 2018 Jul 27, doi: 10.1002/prot.25533, Pubmed: 30051928
31.	Zhao H, Li H, Maurer-Stroh S, Guo Y, Deng Q, Cheng L. <u>Supervised Segmentation of Un-annotated Retinal Fundus Images by Synthesis.</u> IEEE Transactions on Medical Imaging, 2018 Jul 24. doi: 10.1109/TMI.2018.2854886, PMID: 30047872

32.	<p>Harel T, Quek DQY, Wong BH, Cazenave-Gassiot A, Wenk MR, Fan H, Berger I, Shmueli D, Shaag A, Silver DL, Elpeleg O, Edvardson S. <u>Homozygous mutation in MFSD2A, encoding a lysolipid transporter for docosahexanoic acid, is associated with microcephaly and hypomyelination.</u> Neurogenetics 2018 Jul 24. doi: 10.1007/s10048-018-0556-6, Pubmed: 30043326</p>
33.	<p>Slikker JR, De Souza Lima TA, Archella D, De Silva JB Junior, Barton-Maclaren T, Bo L, Buvinich D, Chaudhry Q, Chuan P, Deluyker H, Domselaar G, Freitas M, Hardy B, Eicher HG, Kee K, Liao CD, Loo LH, Okuda H, Orisakwe OE, Patri A, Sactitono C, Chi L, Silva P, Sistare F, Thakkar S, Tong W, Valdez ML, Whelan M, Zhao-Wong A. <u>Emerging technologies for food and drug safety.</u> Regulatory Toxicology and Pharmacology, Vol. 98, Oct 2018, Pg 115-128, doi: 10.1016/j.yrtph.2018.07.013, Pubmed: 30048704</p>
34.	<p>Saravanan , Holdbrook DA, Petrlova J, Singh S, Berglund N, Choong YK, Kjellstrom S, Bond PJ, Malmsten M, Schmidtchen A. <u>Structural basis for endotoxin neutralisation and anti-inflammatory activity of thrombin-derived C-terminal peptides.</u> Nature Communications, 2018 Jul 17;9(1):2762. doi: 10.1038/s41467-018-05242-0, PMID: 30018388</p>
35.	<p>Chan CYJ, Soh CKA, Kioh YQD, Li JG, Verma CS, Koh SK, Beuerman RW, Zhou L, Chan YCE. <u>Reactive Metabolite-induced Protein Glutathionylation: a Potentially Novel Mechanism Underlying Acetaminophen Hepatotoxicity.</u> Molecular & Cellular Proteomics, 2018, Jul 13, doi: 10.1074/mcp.RA118.000875, PMID: 30006487</p>
36.	<p>Ramesh K, Lama D, Tan KW, Nguyen VS, Chew FT, Verma CS, Mok YK. <u>Homologous Lympho-Epithelial Kazal-type Inhibitor Domains Delay Blood Coagulation by Inhibiting Factor X and XI with Differential Specificity.</u> Structure, 26, Pg 1178-1186, Sept 4, 2018, doi: 10.1016/j.str.2018.05.018, PMID: 30017565</p>

37.	<p>Georgilis A, Klotz S, Hanley CJ, Herranz N, Weirich B, Morancho B, Leote AC, D'Artista L, Gallage S, Seehawer M, Carroll T, Dharmalingam G, Wee KB, Mellone M, Pombo J, Heide D, Guccione E, Arribas J, Barbosa-Morais NL, Heikenwalder M, Thomas GJ, Zender L, Gil J. <u>PTBP1-Mediated Alternative Splicing Regulates the Inflammatory Secretome and the Pro-tumorigenic Effects of Senescent Cells</u>. Cancer Cell, Vol. 34, Issue 1, Pg 85-102, 9 July 2018, doi: 10.1016/j.ccr.2018.06.007, PMID: 29990503</p>
38.	<p>Ng SB, Kanagasundaram Y, Fan H, Arumugam P, Eisenhaber B, Eisenhaber F. <u>The 160K Natural Organism Library, a unique resource for natural products research</u>. Nature Biotechnology, Vol. 36, No. 7, July 2018, Pg 570-573, doi: 10.1038/nbt.4187, PMID: 29979661</p>
39.	<p>Singh V, Deepak RNV, Sengupta B, Joshi AS, Fan H, Sen P, Thakur AK. <u>Calmidazolium Chloride and Its Complex with Serum Albumin Prevent Huntingtin Exon1 Aggregation</u>. Molecular Pharmaceutics, 2018, Aug 6, 15 (8), pp 3356–3368, doi:10.1021/acs.molpharmaceut.8b00380</p>
40.	<p>Liu BH, Jobichen C, Chia CS, Chan THM, Tang JP, Chung TXY, Li J, Poulsen A, Hung AW, Koh-Stenta XY, Tan YS, Verma CS, Tan HK, Wu CS, Li F, Hill J, Joy J, Yang H, Chai L, Sivaraman K, Tenen DG. <u>Targeting cancer addiction for SALL4 by shifting its transcriptome with a pharmacologic peptide</u>. Proceedings of the National Academy of Sciences of the United States of America (PNAS), July 24, 2018, Vol. 115, no. 30, Pg E7119-E7128, doi: 10.1073/pnas.1801253115</p>
41.	<p>Maurer-Stroh S, Zhao H, Li HQ, Cheng L. <u>Synthesizing retinal and neuronal images with generative adversarial nets</u>. Medical Image Analysis, 2018 Jul 4;49:14-26. doi: 10.1016/j.media.2018.07.001</p>
42.	<p>Lackenby A, Besselaar TG, Daniels RS, Fry A, Gregory V, Gubareva LV, Huang W, Hurt AC, Leang SK, Lee RTC, Lo J, Lollis L, Maurer-Stroh S, Odagiri T, Pereyaslov D, Takashita E, Wang D, Zhang W, Meijer A. <u>Global update on the susceptibility of human influenza viruses to neuraminidase inhibitors and status of novel antivirals</u>. Antiviral Research 2018 Jul 3;157:38-46. doi: 10.1016/j.antiviral.2018.07.001, PMID: 29981793</p>
43.	<p>Ooi CP, Gan SKE, Ko E. BME361 Advanced Experimental Biomedical Laboratory Proficiency. Book Chapter : Singapore University of Social Sciences, Educational Technology & Production, ISBN: 9789814787338</p>

44.	Latty SL, Sakai J, Hopkins L, Verstak B, Paramo T, Berglund NA, Cammarota E, Cicuta P, Gay NJ, Bond PJ, Klenerman D, Bryant CE. <u>Activation of Toll-like receptors nucleates assembly of the MyDDosome signaling hub.</u> eLife, 2018 Jan 24;7. pii: e31377. doi: 10.7554/eLife.31377, PMID: 29368691
45.	Kuznetsov VA, Bondarenko V, Wongsurawat T, Yenamandra SP, Jenjaroenpun P. Towards Predictive R-loop Computational Biology: Genome-Scale Prediction of R-loops Reveals Their association with Complex Promoter Structures, G-Quadruplexes and Transcriptionally Active Enhancers. Nuclei Acids Research, 2018 Jun 26. doi: 10.1093/nar/gky554
46.	Koon YL, Zhang SJ, Rahmat B, Koh CG, Chiam KH. <u>Enhanced Delta-Notch Lateral Inhibition Model Incorporating Intracellular Notch Heterogeneity and Tension-Dependent Rate of Delta-Notch Binding that Reproduces Sprouting Angiogenesis Patterns.</u> Scientific Reports 8, No. 9519, 2018, doi: 10.1038/s41598-018-27645-1, PMID: 29934586
47.	Do DV, Strauss B, Cukuroglu E, Macaulay I, Wee KB, Hu TX, Igor RLM, Lee C, Harrison A, Butler R, Dietmann S, Jernej U, Marioni J, Smith CWJ, Göke J, Surani MA. <u>SRSF3 maintains transcriptome integrity in oocytes by regulation of alternative splicing and transposable elements.</u> Cell Discovery 4, Article no: 33 (2018), doi: 10.1038/s41421-018-0032-3
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50.	Su CT, Lua WH, Ling WL, Gan SK. <u>Allosteric Effects between the Antibody Constant and Variable Regions: A Study of IgA Fc Mutations on Antigen Binding.</u> Antibodies 2018, 7(2), 20, doi: 10.3390/antib7020020

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52.	Holdbrook DA, Singh S, Choong YK, Petrlova J, Malmsten M, Bond PJ, Verma NK, Schmidtchen A, Saravanan R. <u>Influence of pH on the activity of thrombin-derived antimicrobial peptides</u> . Biochimica et Biophysica Acta (BBA) - Biomembranes, 2018 Jun 6, doi: 10.1016/j.bbamem.2018.06.002, PMID: 29885294
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54.	Ooi CP, Gan SKE, Ang LP. <u>BME261 Experimental Biomedical Laboratory Skills, Study Guide</u> . Book Chapter : Singapore University of Social Sciences, Educational Technology & Production, ISBN: 9789814787338
55.	Wong YH, Kumar A, Liew CW, Tharakaraman K, Srinivasaraghavan K, Sasisekharan R, Verma CS, Lescar J. <u>Molecular basis for dengue virus broad cross-neutralization by humanized monoclonal antibody 513</u> . Scientific Reports 8, Article no: 8449, (2018), doi: 10.1038/s41598-018-26800-y, PMID: 29855525
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57.	Verma A, Lin F, Tan YC, Hidayat MN, Jobichen C, Fan H, Sivaraman J. <u>Biophysical studies and modelling indicate the binding preference of TAZ WW domain for LATS1 PPxY motif</u> . Biochemical and Biophysical Research Communications, Vol. 502, Issue 3, 20 Jul 2018, Pg 307-312, PMID: 29787761, doi: 10.1016/j.bbrc.2018.05.127

58.	Yeow J, Tan KW, Holdbrook DA, Chong ZS, Marzinek JK, Bond PJ, Chng SS. <u>The architecture of the OmpC-MlaA complex sheds light on the maintenance of outer membrane lipid asymmetry in Escherichia coli.</u> The Journal of Biological Chemistry, 2018 Jul 20;293(29):11325-11340. doi: 10.1074/jbc.RA118.002441, PMID: 29848551
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62.	Sirota FL, Goh F, Low KN, Yang LK, Crasta SC, Eisenhaber B, Eisenhaber F, Kanagasundaram Y, Ng SB. <u>Isolation and Identification of an Anthracimycin Analogue from Nocardiopsis kunsanensis, a Halophile from a Saltern, by Genomic Mining Strategy.</u> Journal of Genomics, Vol. 6, 2018, Pg 63-73, doi:10.7150/jgen.24368
63.	Koh JJ, Lin SM, Bai Y, Sin WLW, Aung TT, Li JG, Verma CS, Pervushin K, Beuerman RW, Liu SP. <u>Antimicrobial activity profiles of Amphiphilic Xanthone derivatives are a function of their molecular Oligomerization.</u> Biochimica et Biophysica Acta (BBA) - Biomembranes, 2018, doi: 10.1016/j.bbamem.2018.05.006, PMID: 29782818

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73.	Aronica P, Fox S, Verma CS. Comparison of Charge Derivation Methods Applied to Amino Acid Parametrization. ACS Omega 2018, 3, Pg 4664-4673, doi: 10.1021/acsomega.8b00438
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