BII – Multiscale Simulation, Modelling and Design Publications

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

1.	**Kaur H, Jakob RP, Marzinek JK, Green R, Imai Y, Bolla JR, Agustoni E, Robinson CV, Bond PJ, Maier T, Hiller S.** The antibiotic darobactin mimics a β-strand to inhibit outer membrane insertase. Nature 2021, doi: 10.1038/s41586-021-03455-w
2.	**Raghuvamsi PV, Tulsian NK, Samsudin F, Qian X, Purushotorman K, Yue G, Kozma MM, Hwa WY, Lescar J, Bond PJ, MacAry PA, Anan GS.** SARS-CoV-2 S protein:ACE2 interaction reveals novel allosteric targets. Elife, 2021 Feb 8;10:e63646. doi: 10.7554/eLife.63646, PMID: 33554856, doi: 10.7554/eLife.63646
3.	**Fibriansah G, Lim EXY, Marzinek JK, Ng TS, Tan JL, Huber RG, Lim XN, Chew VSY, Kostyuchenko VA, Shi J, Anand GS, Bond PJ, Crowe JE Jr, Lok SM.** Antibody affinity versus dengue morphology influences neutralization. PLOS Pathogens, 2021, 17(2): e1009331. PMID: 33621239, doi: 10.1371/journal.ppat.1009331
4.	**Samsudin F, Gan SKE, Bond PJ.** (2020) The impact of Gag non-cleavage site mutations on HIV-1 viral fitness from integrative modelling and simulations. Comput Struct Biotechnol J. 2020 Dec 23;19:330-342. doi: 10.1016/j.csbj.2020.12.022. eCollection 2021.
5.	**Chan KF, Su TTC, Krah A, Phua SX, Yeo YJ, Ling WL, Bond PJ, Gan SKE.** (2020) An Alternative HIV-1 Non-Nucleoside Reverse Transcriptase Inhibition Mechanism: Targeting the p51 Subunit. Molecules, 2020, Vol: 25, Pg: 5902, doi: 10.3390/molecules25245902
6.	**Petruk G, Puthia M, Petrlova J, Samsudin F, Strömdahl AC, Cerps S, Uller L, Kjellström S, Bond PJ, Schmidtchen A.** (2020) SARS-CoV-2 Spike protein binds to bacterial lipopolysaccharide and boosts proinflammatory activity. J Mol Cell Biol. 2020 Dec 9:mjaa067. doi: 10.1093/jmcb/mjaa067. Online ahead of print.
7.	**Petruk G, Petrlova J, Samsudin F, Giudice RD, Bond PJ, Schmidtchen A.** Concentration- and pH-dependent oligomerization of the thrombin-derived C-terminal peptide TCP-25. Biomolecules 2020, 10(11), 1572; doi: 10.3390/biom10111572
8.	**Krah A, van der Hoeven B, Mestrom L, Tonin F, Knobel KCC, Bond PJ, McMillan DGG.** (2020) A second shell residue modulates a conserved ATP-binding site with radically different affinities for ATP. Biochimica et Biophysica Acta (BBA), Vol 1865, Issue 1, Jan 2021, doi: 10.1016/j.bbagen.2020.129766
9.	**Faulkner M, Szabó I, Weetman SL, Sicard F, Huber RG, Bond PJ, Rosta E, Liu LN.** (2020) Molecular simulations unravel the molecular principles that mediate selective permeability of carboxysome shell protein. Scientific Reports, 10, Article 17501, 2020, doi: 10.1038/s41598-020-74536-5
10.	**Zuzic L, Marzinek JK, Warwicker J, Bond PJ.** (2020) A Benzene-Mapping approach for uncovering cryptic pockets in membrane-bound proteins. bioRxiv, 5 Apr 2020, doi: 10.1101/2020.04.04.025163
11.	**Shearer J, Marzinek JK, Bond PJ, Khalid S.** (2020) Molecular dynamics simulations of bacterial outer membrane lipid extraction: Adequate sampling? J Chem Phys. 2020 Jul 28;153(4):044122. doi: 10.1063/5.0017734. PMID: 32752683

12.	**Shivgan AT, Marzinek JK, Huber RG, Krah A, Henchman RH, Matsudaira P, Verma CS, Bond PJ.** (2020) Extending the Martini coarse-grained forcefield to N-glycans. Journal of Chemical Information and Modeling, 23 Jul 2020, 60(8):3864-3883, DOI: 10.1021/acs.jcim.0c00495 PMID: 32702979
13.	**Krah A, Marzinek JK, Bond PJ.** (2020) Characterizing the Hydration Properties of Proton Binding Sites in the ATP Synthase c-Rings of Bacillus Species. J Phys Chem B. 2020 Aug 20;124(33):7176-7183. doi: 10.1021/acs.jpcb.0c03896. Epub 2020 Aug 7. PMID: 32687713
14.	**Krah A, Huber RG, McMillan DGG, Bond PJ.** (2020) The Molecular Basis for Purine Binding Selectivity in the Bacterial ATP Synthase ϵ Subunit. Chembiochem. 2020 Nov 16;21(22):3249-3254. doi: 10.1002/cbic.202000291. Epub 2020 Aug 4. PMID: 32608105
15.	**Huber RG, Marzinek JK, Boon PLS, Yue W, Bond PJ.** (2020) Computational modelling of flavivirus dynamics: The ins and outs. Methods. 2020 Jun 8:S1046-2023(19)30326-3. doi: 10.1016/j.ymeth.2020.06.004. PMID: 32526282
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17.	**Samsudin F, Yeo JY, Gan SK, Bond PJ**. (2020) Not all therapeutic antibody isotypes are equal: the case of IgM versus IgG in Pertuzumab and Trastuzumab. Chem Sci. 2020 Feb 12;11(10):2843-2854. doi: 10.1039/c9sc04722k. eCollection 2020 Mar 14. PMID: 32206268
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19.	**Petrlova J, Petruk G, Huber RG, McBurnie EW, van der Plas MJA, Bond PJ, Puthia M, Schmidtchen A** (2020). Thrombin-derived C-terminal fragments aggregate and scavenge bacteria and their proinflammatory products. Journal of Biological Chemistry, 2020 Mar 13;295(11):3417-3430. doi: 10.1074/jbc.RA120.012741
20.	**Marzinek JK, Huber RG, Bond PJ** (2020). Multiscale modelling and simulation of viruses. Current Opinion in Structural Biology 2020, 61:146-152, doi: 10.1016/j.sbi.2019.12.019
21.	**Tan LK, Wong WY, Yang HT, Huber RG, Bond PJ, Ng LC, Maurer-Stroh S, Hapuarachchi HC.** (2019). Flavivirus Cross-Reactivity to Dengue Nonstructural Protein 1 Antigen Detection Assays. Diagnostics, Vol 10, Issue 1, doi: 10.3390/diagnostics10010011
22.	**Krah A, Huber RG, Zachariae U, Bond PJ.** (2019). On the ion coupling mechanism of the MATE transporter ClbM. BBA - Biomembranes, Vol. 1862, Issue 2, 1 Feb 2020, doi: 10.1016/j.bbamem.2019.183137
23.	**Kamariah N, Huber RG, Nartey W, Bhushan S, Bond PJ, Gruber G.** (2019). The structural basis for membrane assembly of immunoreceptor signalling complexes. Journal of Molecular Modeling, 2019 Aug 27;25(9):277. doi: 10.1007/s00894-019-4165-6
24.	**Kamariah N, Huber RG, Nartey W, Bhushan S, Bond PJ, Gruber G** (2019). Structure and subunit arrangement of Mycobacterial F1FO ATP synthase and novel features of the unique mycobacterial subunit ? Journal of Structural Biology, Vol. 207, Issue 2, 1 Aug 2019, Pg 199-208, doi: 10.1016/j.jsb.2019.05.00

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26.	**Huber RG, Carpenter TS, Dube N, Holdbrook DA, Ingólfsson HI, Irvine WA, Marzinek JK, Samsudin F, Allison JR, Khalid S, Bond PJ.** (2019). Multiscale Modeling and Simulation Approaches to Lipid-Protein Interactions. Methods in Molecular Biology 2019, Vol. 2003, Pg 1-30. doi: 10.1007/978-1-4939-9512-7_1
27.	**Holdbrook D, Huber RG, Marzinek JK, Stubbusch AS, Bond PJ.** (2019). Multiscale modeling of innate immune receptors: Endotoxin recognition and regulation by host defense peptides. Pharmacological Research 2019 Jul 24;147:104372. doi: 10.1016/j.phrs.2019.104372
28.	**Kubankova M, Chambers J, Huber RG, Bond PJ, Marciniak S, Kuimova M.** (2019). Linker length affects photostability of protein-targeted sensor of cellular microviscosity. Methods and Applications in Fluorescence, 2019 Sep 26. doi: 10.1088/2050-6120/ab481f
29.	**Lim XN, Shan C, Marzinek JK, Dong H, Ng TS, Ooi JSG, Fibriansah G, Wang J, Verma CS, Bond PJ, Shi PY, Lok SM.** (2019). Molecular basis of dengue virus serotype 2 morphological switch from 29°C to 37°C. PLOS Pathogens, Sep 2019, Vol. 15, Issue 9, doi 10.1371/journal.ppat.1007996
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33.	**Sharma KK, Lim XX, Tantirimudalige SN, Gupta A, Marzinek JK, Holdbrook D, Lim XYE, Bond PJ, Anand GS, Wohland T.** (2019). Infectivity of Dengue Virus Serotypes 1 and 2 Is Correlated with E-Protein Intrinsic Dynamics but Not to Envelope Conformations. Structure. 2019 Jan 2. pii: S0969-2126(18)30462-3. doi: 10.1016/j.str.2018.12.006.
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