

BII – Multiscale Simulation, Modelling and Design Publications

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

1.	Tan ZW, Tee WV, Samsudin F, Guarnera E, Bond PJ, Berezovsky IN. (2022). Allosteric perspective on the mutability and druggability of the SARS-CoV-2 Spike protein. <i>Structure</i> . In press.
2.	Chawla H, Jossi SE, Faustini SE, Samsudin F, Allen JD, Watanabe Y, Newby ML, Marcial-Juárez E, Lamerton RE, McLellan JS, Bond PJ, Richter AG, Cunningham AF, Crispin M. (2022). Glycosylation and Serological Reactivity of an Expression-enhanced SARS-CoV-2 Viral Spike Mimetic. <i>J Mol Biol.</i> 434:167332.
3.	Tram NDT, Selvarajan V, Boags A, Mukherjee D, Marzinek JK, Cheng B, Jiang ZC, Goh P, Koh JJ, Teo JWP, Bond PJ, Ee PLR. Manipulating turn residues on de novo designed β-hairpin peptides for selectivity against drug-resistant bacteria. <i>Acta Biomater.</i> 2021 Sep 8:S1742-7061(21)00592-4. doi: 10.1016/j.actbio.2021.09.004, PMID: 34506975.
4.	Tan S, Kermasson L, Hilcenko C, Kargas V, Traynor D, Boukerrou AZ, Escudero-Urquijo N, Faille A, Bertrand A, Rossmann M, Goyenechea B, Jin L, Moreil J, Alibeu O, Beaupain B, Bôle-Feysot C, Fumagalli S, Kaltenbach S, Martignoles JA, Masson C, Nitschké P, Parisot M, Pouliet A, Radford-Weiss I, Tores F, de Villartay JP, Zarhrate M, Koh AL, Phua KB, Reversade B, Bond PJ, Bellanné-Chantelot C, Callebaut I, Delhommeau F, Donadieu J, Warren AJ, Revy P. Somatic genetic rescue of a germline ribosome assembly defect. <i>Nature Communications</i> 2021 Aug 19;12(1):5044. doi: 10.1038/s41467-021-24999-5. PMID: 34413298
5.	Allen JD, Chawla H, Samsudin F, Zuzic L, Shivgan AT, Watanabe Y, He WT, Callaghan S, Song G, Yong P, Brouwer PJM, Song Y, Cai Y, Duyvesteyn HME, Malinauskas T, Kint J, Pino P, Wurm MJ, Frank M, Chen B, Stuart DI, Sanders RW, Andrabi R, Burton DR, Li S, Bond PJ, Crispin M. Site-Specific Steric Control of SARS-CoV-2 Spike Glycosylation. <i>Biochemistry.</i> 2021 Jul 13;60(27):2153-2169. doi: 10.1021/acs.biochem.1c00279. Epub 2021 Jul 2. PMID: 34213308
6.	Holdbrook DA, Marzinek JK, Boncel S, Boags A, Tan YS, Huber RG, Verma CS, Bond PJ. The nanotube express: Delivering a stapled peptide to the cell surface. <i>Journal of Colloid and Interface Science</i> , 2021, PMID: 34280765, doi: 10.1016/j.jcis.2021.07.023
7.	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. <i>Nature</i> 2021, doi: 10.1038/s41586-021-03455-w
8.	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. <i>Elife</i> , 2021 Feb 8;10:e63646. doi: 10.7554/eLife.63646, PMID: 33554856, doi: 10.7554/eLife.63646
9.	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. <i>PLOS Pathogens</i> , 2021, 17(2): e1009331. PMID: 33621239, doi: 10.1371/journal.ppat.1009331
10.	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. <i>Comput Struct Biotechnol J.</i> 2020 Dec 23;19:330-342. doi: 10.1016/j.csbj.2020.12.022. eCollection 2021.

11.	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. <i>Molecules</i> , 2020, Vol: 25, Pg: 5902, doi: 10.3390/molecules25245902
12.	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. <i>J Mol Cell Biol.</i> 2020 Dec 9:mjaa067. doi: 10.1093/jmcb/mjaa067. Online ahead of print.
13.	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. <i>Biomolecules</i> 2020, 10(11), 1572; doi: 10.3390/biom10111572
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15.	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. <i>Scientific Reports</i> , 10, Article 17501, 2020, doi: 10.1038/s41598-020-74536-5
16.	Zuzic L, Marzinek JK, Warwicker J, Bond PJ. (2020) A Benzene-Mapping approach for uncovering cryptic pockets in membrane-bound proteins. <i>bioRxiv</i> , 5 Apr 2020, doi: 10.1101/2020.04.04.025163
17.	Shearer J, Marzinek JK, Bond PJ, Khalid S. (2020) Molecular dynamics simulations of bacterial outer membrane lipid extraction: Adequate sampling? <i>J Chem Phys.</i> 2020 Jul 28;153(4):044122. doi: 10.1063/5.0017734. PMID: 32752683
18.	Shivgan AT, Marzinek JK, Huber RG, Krah A, Henschman RH, Matsudaira P, Verma CS, Bond PJ. (2020) Extending the Martini coarse-grained forcefield to N-glycans. <i>Journal of Chemical Information and Modeling</i> , 23 Jul 2020, 60(8):3864-3883, DOI: 10.1021/acs.jcim.0c00495 PMID: 32702979
19.	Krah A, Marzinek JK, Bond PJ. (2020) Characterizing the Hydration Properties of Proton Binding Sites in the ATP Synthase c-Rings of Bacillus Species. <i>J Phys Chem B.</i> 2020 Aug 20;124(33):7176-7183. doi: 10.1021/acs.jpcc.0c03896. Epub 2020 Aug 7. PMID: 32687713
20.	Krah A, Huber RG, McMillan DGG, Bond PJ. (2020) The Molecular Basis for Purine Binding Selectivity in the Bacterial ATP Synthase ϵ Subunit. <i>Chembiochem.</i> 2020 Nov 16;21(22):3249-3254. doi: 10.1002/cbic.202000291. Epub 2020 Aug 4. PMID: 32608105
21.	Huber RG, Marzinek JK, Boon PLS, Yue W, Bond PJ. (2020) Computational modelling of flavivirus dynamics: The ins and outs. <i>Methods.</i> 2020 Jun 8:S1046-2023(19)30326-3. doi: 10.1016/j.ymeth.2020.06.004. PMID: 32526282
22.	Kamariah N, Huber RG, Bond PJ, Müller V, Grüber G. (2020) 3D reconstruction and flexibility of the hybrid engine Acetobacterium woodii F-ATP synthase. <i>Biochem Biophys Res Commun.</i> 2020 Jun 25;527(2):518-524. doi: 10.1016/j.bbrc.2020.04.026. Epub 2020 May 15. PMID: 32423799

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24.	Krah A, Huber RG, Bond PJ. (2020) How Ligand Binding Affects the Dynamical Transition Temperature in Proteins. Chemphyschem. 2020 Mar 3. doi: 10.1002/cphc.201901221. [Epub ahead of print] PMID: 32128947
25.	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
26.	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
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35.	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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