

BII – Structure and Dynamics of Macromolecular Complexes Publication List

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| 1. | Tan ZW, Tee WV, Samsudin F, Guarnera E, Bond PJ, Berezovsky IN. Allosteric perspective on the mutability and druggability of the SARS-CoV-2 Spike protein. bioRxiv |
| 2. | Allen JD, Chawla H, Samsudin F, Zuzic L, Shivgan AT, Watanabe Y, He W, 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. Biochemistry 2021, 60, 27, 2153–2169 |
| 3. | Zuzic L, Samsudin F, Shivgan AT, Raghuvamsi PV, Marzinek JK, Boags A, Pedebos C, Tulsian NK, Warwicker J, MacAry P, Crispin M, Khalid S, Anand GS, Bond PJ. Uncovering cryptic pockets in the SARS-CoV-2 spike glycoprotein. Biorxiv |
| 4. | Raghuvamsi PV, Tulsian NK, Samsudin F, Qian X, Purushotorman K, Yue G, Kozma MM, Hwa WY, Lescar J, Bond PJ, MacAry PA, Anand GS. SARS-CoV-2 S protein: ACE2 interaction reveals novel allosteric targets. Elife 10, e63646 |
| 5. | Petruk G, Puthia M, Petrlova J, Samsudin F, Strömdahl A-C, Cerps S, Uller L, Kjellström S, Bond PJ, Schmidtchen A. SARS-CoV-2 Spike protein binds to bacterial lipopolysaccharide and boosts proinflammatory activity. Journal of Molecular Cell Biology 12 (12), 916-932 |
| 6. | Samsudin F, Gan SKE, Bond PJ. The impact of Gag non-cleavage site mutations on HIV-1 viral fitness from integrative modelling and simulations. Computational and structural biotechnology journal 19, 330-342 |
| 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 10 (11), 1572 |
| 8. | Du D, Neuberger A, Orr MW, Newman CE, Hsu P-C, Samsudin F, Szewczak-Harris A, Ramos LM, Debela M, Khalid S, Storz G, Luisi BF. Interactions of a bacterial RND transporter with a transmembrane small protein in a lipid environment. Structure 28 (6), 625-634. e6 |
| 9. | Szczepaniak J, Holmes P, Rajasekar K, Kaminska R, Samsudin F, Inns PG, Rassam P, Khalid S, Murray SM, Redfield C, Kleanthous C. The lipoprotein Pal stabilises the bacterial outer membrane during constriction by a mobilisation-and-capture mechanism. Nature communications 11 (1), 1-14 |
| 10. | Samsudin F, Yeo JY, Gan SKE, Bond PJ. Not all therapeutic antibody isotypes are equal: the case of IgM versus IgG in Pertuzumab and Trastuzumab. Chemical science 11 (10), 2843-2854 |
| 11. | Huber RG, Carpenter TS, Dube N, Holdbrook DA, Ingólfsson HI, Irvine WA, Marzinek JK, Samsudin F, Allison JR, Khalid S, Bond PJ. Multiscale modeling and simulation approaches to lipid–protein interactions. Lipid-Protein Interactions, 1-30 |
| 12. | Boags AT, Samsudin F, Khalid S. Binding from both sides: TolR and full-length OmpA bind and maintain the local structure of the E. coli cell wall. Structure 27 (4), 713-724. e2 |
| 13. | Samsudin F, Khalid S. Movement of arginine through OprD: the energetics of permeation and the role of lipopolysaccharide in directing arginine to the protein. The Journal of Physical Chemistry B 123 (13), 2824-2832 |
| 14. | Boags A, Samsudin F, Khalid S. Details of hydrophobic entanglement between small molecules and Braun’s lipoprotein within the cavity of the bacterial chaperone LolA. Scientific reports 9 (1), 1-8 |

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| 15. | Khalid S, Piggot TJ, Samsudin F. Atomistic and coarse grain simulations of the cell envelope of Gram-negative bacteria: what have we learned? Accounts of chemical research 52 (1), 180-188 |
| 16. | Chorev DS, Baker LA, Wu D, Beilsten-Edmands V, Rouse SL, Zeev-Ben-Mordehai T, Jiko C, Samsudin F, Gerle C, Khalid S, Stewart AG, Matthews SJ, Grünewald K, Robinson CV. Protein assemblies ejected directly from native membranes yield complexes for mass spectrometry. Science 362 (6416), 829-834 |
| 17. | Housden NG, Rassam P, Lee S, Samsudin F, Kaminska R , Sharp C , Goult JD , Francis M-L , Khalid S, Bayley H, Kleanthous C. Directional porin binding of intrinsically disordered protein sequences promotes colicin epitope display in the bacterial periplasm. Biochemistry 57 (29), 4374-4381 |
| 18. | Punekar AS, Samsudin F, Lloyd AJ, Dowson CG, Scott DJ , Khalid S, Roper DI. The role of the jaw subdomain of peptidoglycan glycosyltransferases for lipid II polymerization. The Cell Surface 2, 54-66 |
| 19. | Hsu PC, Samsudin F, Shearer J, Khalid S. It Is Complicated: Curvature, Diffusion, and Lipid Sorting within the Two Membranes of Escherichia coli. The journal of physical chemistry letters 8 (22), 5513-5518 |
| 20. | Samsudin F, Boags A, Piggot TJ, Khalid S. Braun's lipoprotein facilitates OmpA interaction with the Escherichia coli cell wall. Biophysical journal 113 (7), 1496-1504 |
| 21. | Boags A, Hsu PC, Samsudin F, Bond PJ, Khalid S. Progress in molecular dynamics simulations of Gram-negative bacterial cell envelopes. The journal of physical chemistry letters 8 (11), 2513-2518 |
| 22. | Samsudin S, Ortiz-Suarez ML, Piggot TJ, Bond PJ, Khalid S. OmpA: a flexible clamp for bacterial cell wall attachment. Structure 24 (12), 2227-2235 |
| 23. | Ortiz-Suarez ML, Samsudin F, Piggot TJ, Bond PJ, Khalid S. Full-length OmpA: structure, function, and membrane interactions predicted by molecular dynamics simulations. Biophysical journal 111 (8), 1692-1702 |
| 24. | Samsudin F, Parker JL, Sansom MSP, Newstead S, Fowler PW. Accurate prediction of ligand affinities for a proton-dependent oligopeptide transporter. Cell chemical biology 23 (2), 299-309 |
| 25. | Beale JH, Parker JL, Samsudin F, Barrett AL, Senan A, Bird LE, Scott D, Owens RJ, Sansom MSP, Tucker SJ, Meredith D, Fowler PW, Newstead S. Crystal structures of the extracellular domain from PepT1 and PepT2 provide novel insights into mammalian peptide transport. Structure 23 (10), 1889-1899 |