BII – Algorithms & Models of Protein Machinery Publication List

1.	**Su CTT#, Lua WH#, Poh JJ, Ling WL, Yeo JY, Gan SKE (2021).** Molecular insights of nickel binding to therapeutic antibodies as a possible new antibody superantigen. Frontiers in Immunology, 12:676048, doi: 10.3389/fimmu.2021.676048.
2.	**Ling WL, Su CTT, Lua WH, Poh JJ, Ng YL, Wipat A, Gan SKE (2020).** Essentially leading antibody production: An investigation of amino acids, myeloma and natural V-region signal peptides in producing Pertuzumab and Trastuzumab variants. Frontiers in Immunology, 11:604318, doi: 10.3389/fimmu.2020.604318.
3.	**Chan KF#, Su CTT#, Krah A, Phua SX, Bond PJ, Gan SKE (2020).** An alternative HIV-1 nonnucleoside Reverse Transcriptase inhibition mechanism: Targeting the p51 subunit. Molecules, 25:5902; doi:10.3390/molecules25245902.
4.	**Su CTT, Sinha S, Eisenhaber B*, Eisenhaber F* (2020).** Structural modelling of the lumenal domain of human GPAA1, the metallo-peptide synthetase subunit of the transamidase complex, reveals zinc-binding mode and two flaps surrounding the active site. Biology Direct, 15:14, doi: 10.1186/s13062-020-00266-3.
5.	**Yeo JY, Goh GR, Su CTT, Gan SKE (2020).** The Determination of HIV-1 RT Mutation Rate, Its Possible Allosteric Effects, and Its Implications on Drug Resistance. Viruses, 12(3), 297, doi: 10.3390/v12030297
6.	**Su CTT, Koh DWS, Gan SKE (2019).** Reviewing HIV-1 Gag Mutations in Protease Inhibitors Resistance: Insights for Possible Novel Gag Inhibitor Designs. Molecules, 2019, 24(18), 3243; doi: 10.3390/molecules24183243.
7.	**Lua WH#, Su CTT#, Yeo JY, Poh JJ, Ling WL, Phua SX, Gan SKE (2019).** Role of IgE-VH in FcεRIα and superantigen binding in allergy and immunotherapy. Journal of Allergy and Clinical Immunology, 144(2), p514-523.e5, doi: 10.1016/j.jaci.2019.03.028
8.	**Phua SX, Chan KF, Su CTT, Poh JJ, Gan SKE (2019).** Perspective: The promises of a holistic view of proteins—impact on antibody engineering and drug discovery. Bioscience Reports, 39, BSR20181958, doi: 10.1042/BSR20181958
9.	**Phua SX, Chan KF, Su CTT (2018).** Automated submission script to AlloSigMA webserver: a viable approach for allosteric effect scanning. APD Trove, 1(3), doi:10.30943/2018/20122018
10.	**Su CTT#, Lua WH#, Ling WL, Gan SKE (2018).** Allosteric effects between the antibody constant and variable regions: A study of IgA Fc mutations on antigen binding. Antibodies, 7(20), doi:10.3390/antib7020020
11.	**Su CTT (2018).** Allostery advocates in monoclonal antibody engineering towards antigen binding. Biophysical Journal, 114(3), supplement 1, p422a-423a, doi: 10.1016/j.bpj.2017.11.2341
12.	**Chiang RZH, Gan SKE*, Su CTT* (2018).** A computational study for rational HIV-1 nonnucleoside Reverse Transcriptase inhibitor selection and the discovery of novel allosteric pockets for inhibitor design. Bioscience Report, 38, doi: 10.1042/BSR20171113
13.	**Su CTT*, Kwoh CK, Verma CS, Gan SKE*(2017).** Modeling the full-length HIV-1 Gag polyprotein reveals the role of its p6 subunit in viral maturation and the effect of non-cleavage site mutations in protease drug resistance. Journal of Biomolecular Structure and Dynamics, p1-12, doi: 10.1080/07391102.2017.1417160
14.	**Su CTT#, Ling WL#, Lua WH, Poh JJ, Gan SKE (2017).** The role of Antibody Vk Framework 3 region towards Antigen binding: Effects on recombinant production and Protein L binding**.** Scientific Reports, 7:3766.
15.	**Lua WH, Ling WL, Su CTT, Verma CS, Eisenhaber B, Eisenhaber F, Gan SKE (2017).** Discovery of a novel splice variant of Fcar (CD89) unravels sequence segments necessary for efficient secretion: a story of bad signal peptides and good ones that nevertheless do not make it. Cell Cycle, doi: 10.1080/15384101.2017.1281480

16.	**Su CTT, Ling WL, Lua WH, Haw YX, Gan SKE (2016).** Structural analyses of 2015-updated drug-resistant mutations in HIV-1 Protease: An implication of Protease Inhibitor cross-resistance. BMC Bioinformatics, 17(Suppl 19): 500
17.	**Su CTT, Nguyen TD, Zheng J, Kwoh CK (2014).** IFACEwat: the interfacial water-implemented re-ranking algorithm to improve the discrimination of near-native structures for protein rigid docking. BMC Bioinformatics, 15(Suppl 16): S9.
18.	**Su CTT #, Ouyang X#, Zheng J, Kwoh CK (2013).** Structural analysis of the novel influenza A (H7N9) viral Neuraminidase interactions with current approved neuraminidase inhibitors Oseltamivir, Zanamivir, and Peramivir in the presence of mutation R289K. BMC Bioinformatics, 14(Suppl 16): S7.
19.	**Su CTT, Schoenbach C, Kwoh CK (2013).** Molecular docking analysis of 2009-H1N1 and 2004- H5N1 influenza virus HLA-B*4405-restricted HA epitope candidates: Implications for TCR cross recognition and vaccine development. BMC Bioinformatics, 14(Suppl 2): 521.
20.	**Ouyang X, Zhuo S, Su CTT, Ge Z, Li R, Kwoh CK (2012).** CovalentDock: Automated covalent docking with parameterized covalent linkage energy estimation and molecular geometry. J. Comput Chem, 34(4): 326-36
21.	**Handoko SD, Ouyang X, Su CTT, Kwoh CK, Ong YS (2012).** QuickVina: Accelerating AutodockVina using gradient-based heuristics for global optimization. IEEE/ACM Trans. Comput. Biology. Bioinform, 9(5): 1266-1272
22.	**Liu Q, Hoi S, Su CTT, Li ZH, Kwoh CK, Wong L, Li J (2011).** Structural analysis of the hot spots in the binding between H1N1 HA and the 2D1 antibody: do the mutations of the H1N1 from 1918 to 2009 affect much on this binding? Bioinformatics, 27(18): 2529-2536.
23.	**Su CTT, Handoko SD, Schonbach C, Li X, Kwoh CK (2010).** A Possible Mutation that Enables H1N1 Influenza A Virus to Escape Antibody Recognition. IEEE International Conference on Bioinformatics & Biomedicine, Hongkong (2010), doi: 10.1109/BIBM.2010.5706541
24.	**Handoko SD, Su CTT, Kwoh CK, and Ong YS. (2010).** Structural Analysis of (TCR–)HLA/peptideComplexes: An Initial Study. Proceedings of IEEE International Conference on Bioinformatics and Biomedicine Workshops, pp.63-66.
25.	Su CTT, Do AT, Tran LT. (2004). **Building the structural model of mini-Proinsulin.** Proceeding of the Workshop on Computational Biology and Molecular Biology, Ho Chi Minh City, Vietnam, Sep 2004.