BII – Function and Structure of RNA Group Publications

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

1.	**De Falco L, Silva NM, Huber RG, Martins IC.** The Pseudo-Circular Genomes of Flaviviruses: Structures, Mechanisms, and Functions of Circularization**.** Cells 2021, 10(3), 642. doi: 10.3390/cells10030642
2.	**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
3.	**Mayrhofer JE, Enzler F, Feichtner A, Röck R, Fleischmann J, Raffeiner A, Tschaikner P, Ogris E, Huber RG, Hartl M, Schneider R, Troppmair J, Torres-Quesada O, Stefan E.** Mutation-oriented profiling of autoinhibitory kinase conformations predicts RAF inhibitor efficacies**.** Proceedings of the National Academy of Sciences of the United States of America (PNAS), Nov 23;202012150. doi: 10.1073/pnas.2012150117, PMID: 33229534
4.	**Faulkner M, Szabó I, Weetman SL, Sicard F, Huber RG, Bond PJ, Rosta E, Liu LN.** 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
5.	**Marzinek JK, Huber RG, Bond PJ. (2020)** Multiscale modeling and simulation of viruses. Current Opinion in Structural Biology 61 (2020) 146-152. IF: 7.179
6.	**Tan LK, Wong WY, Yang HT, Huber RG, Bond PJ, Ng LC, Maurer-Stroh S, Hapuarachchige CH. (2020).** Flavivirus Cross-Reactivity to Dengue Nonstructural Protein 1 Antigen Detection Assays. Diagnostics 10 (2020) 11. IF: 2.489
7.	**Krah A, Huber RG, Zachariae U, Bond PJ. (2020).** On the ion coupling mechanism of the MATE transporter ClbM. BBA Biomembranes 1862 (2020) 183137. IF: 3.790
8.	**Köck EM, Bernard J, Podewitz M, Dinu DF, Huber RG, Liedl KR, Grothe H, Bertel E, Schlögl R, Loerting T. (2020)** Alpha carbonic acid revisited: Carbonic acid monomethyl ester as a solid and its conformational isomerism in the gas phase. Chemistry – A European Journal 26 (2020) 285-305 2. IF: 5.160
9.	**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 Appl Fluoresc. 2019 Sep 26. doi: 10.1088/2050-6120/ab481f. [Epub ahead of print]
10.	**Röck R, Mayrhofer JE, Torres-Quesada O, Enzler F, Raffeiner A, Raffeiner P, Feichtner A, Huber RG, Koide S, Taylor SS, Troppmair J, Stefan E.** (2019). BRAF inhibitors promote intermediate BRAF(V600E) conformations and binary interactions with activated RAS. Sci Adv. 2019 Aug 14;5(8):eaav8463. doi: 10.1126/sciadv.aav8463. eCollection 2019 Aug.
11.	**Holdbrook DA, Huber RG, Marzinek JK, Stubbusch A, Schmidtchen A, Bond PJ.** (2019). Multiscale modeling of innate immune receptors: Endotoxin recognition and regulation by host defense peptides. Pharmacol Res. 2019 Sep;147:104372. doi:

	10.1016/j.phrs.2019.104372. Epub 2019 Jul 24.
12.	**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 Mol Biol. 2019;2003:1-30. doi: 10.1007/978-1-4939-9512-7_1.
13.	**Kamariah N, Huber RG, Nartey W, Bhushan S, Bond PJ, Grüber G.** (2019). Structure and subunit arrangement of Mycobacterial F1FO ATP synthase and novel features of the unique mycobacterial subunit δ. J Struct Biol. 2019 Aug 1;207(2):199-208. doi: 10.1016/j.jsb.2019.05.008. Epub 2019 May 24.
14.	**Cai S , Lukamto DH , Toh JKC , Huber RG , Bond PJ , Jee JE , Lim TC , Liu P , Chen L , Qu QV , Lee SS , Lee SG .** (2019). Directing GDNF-Mediated Neuronal Signaling with Proactively Programmable Cell-Surface Saccharide-Free Glycosaminoglycan Mimetics. Chemical Communications 55 (2019) 1259-1262.
15.	**Huber RG, Lim XN, Ng WC, Sim A, Poh HX, Shen Y, Lim SY, Sundstrom AKB, Sun XY, Aw JG, Too HK, Boey PH, Wilm A, Chawla T, Choy MJ, Jiang L, Sessions PF, Loh XJ, Alonso S, Hibberd M, Nagarajan N, Ooi EE, Bond PJ, Sessions OM, Wan Y.** (2019). Structure Mapping of Dengue and Zika Viruses Reveals New Functional Long-Range Interactions. Nature Communications 10 1408.
16.	**Ivanov S, Huber RG, Alibay I, Warwicker J, Bond PJ.** (2019). Energetic Fingerprinting of Ligand Binding to Paralogous Proteins: The Case of the Apoptotic Pathway. Journal of Chemical Information and Modeling 59 245-261.
17.	**Ghosh M, Wang LC, Huber RG, Gau YF, Morgan LK, Bond PJ, Kenney LJ, Anand GS.** (2018). Engineering an Osmosensor by Pivotal Histidine Positioning Within Disordered Helices. Structure 27 302-314.
18.	**Lim TC, Cai ST, Huber RG, Bond PJ, Xian PSC, Khou SL, Gao SJ, Lee SS, Lee SG.** (2018). Facile Saccharide-free Mimetics that Recapitulate the Key Features of Glycosaminoglycan Sulfation Patterns. Chemical Science 9 7940-7947.
19.	**Marzinek JK, Bag N, Huber RG, Holdbrook DA, Wohland T, Verma CS, Bond PJ.** (2018). A funneled conformational landscape governs flavivirus fusion peptide interaction with lipid membranes. Journal of Chemical Theory and Computation 14 3920-3932.
20.	**Boon PLS, Saw WG, Lim XX, Raghuvamsi PV, Huber RG, Marzinek JK, Holdbrook DA, Anand GS, Gruber G, Bond PJ.** (2018). Partial Intrinsic disorder governs the dengue capsid protein conformational ensemble. ACS Chemical Biology 13 1621-1630.
21.	**Huber RG, Berglund NA, Kargas V, Marzinek JK, Holdbrook DA, Piggot TJ, Schmidtchen A, Bond PJ.** (2018). A thermodynamic funnel drives bacterial lipyploysaccharide transfer in the TLR4 pathway. Structure 26 1151-1161.
22.	**Chambers JE, Kubankova M, Huber RG, Lopez-Duarte I, Avezov E, Bond PJ, Marciniak SJ, Kuimova MK.** (2018). An Optical Technique for Mapping Microviscosity Dynamics in Cellular Organelles. ACS Nano 10.1021/acsnano.9b00177.
23.	**Ivanov SM, Cawley A, Huber RG, Bond PJ, Warwicker J.** (2017). Protein-protein interactions in paralogues: Electrostatics modulates specificity on a conserved steric scaffold. PLoS one 12 e0185928.

24.	**Holdbrook DA, Burmann BM, Huber RG, Petoukhov MV, Svergun DI, Hiller S, Bond PJ.** (2017). A Spring-Loaded Mechanism Governs the Clamp-like Dynamics of the Skp Chaperone. Structure 25 1079-1088.
25.	**Petrlova J, Hansen FC, van der Plas MJA, Huber RG, Mörgelin M, Malmsten M, Bond PJ, Schmidtchen A.** (2017). Aggregation of thrombin-derived C-terminal fragments – a novel host defense mechanism. Proceedings of the National Academy of Sciences of the USA 114 E4213-E4222.
26.	**Kam YW, Lee YPC, Teo TH, Howland SW, Amrun SN, Lum FM, See P, Kng QR, Huber RG, Xu MH, Tan HL, Choo A, Maurer-Stroh S, Ginhoux F, Fink K, Wang CI, Ng LFP, Rénia L.** (2017). Cross-reactive dengue human monoclonal antibody prevents severe pathologies and death from Zica virus infections. JCI Insight 2 e92428.
27.	**Bernard J, Köck EM, Huber RG, Liedl KR, Call L, Schlögl R, Grothe H, Loerting T.** (2017). Carbonic acid monoethyl ester as a pure solid and its conformational isomerism in the gas phase. RSC Advances 7 22222-22233.
28.	**Chang HH, Grad YH, Camerini D, Huber RG, Bond PJ, Maruer-Stroh S, Lipsitch M.** (2017). Designing serological diagnostics based on evolutionarily divergent immunogenic regions in the Zika virus genome. Bulletin of the World Health Organization.
29.	**Schauperl M, Czodrowski P, Fuchs JE, Huber RG, Waldner BJ, Podewitz M, Kramer C, Liedl KR.** (2017). Binding Pose Flip Explained via Enthalpic and Entropic Contributions. Journal of Chemical Information and Modeling 57 345-354.
30.	**Huber RG, Marzinek JK, Holdbrook D, Bond PJ.** (2016). Multiscale Molecular Dynamics Simulation Approaches to the Structure and Dynamics of Viruses. Progress in Biophysics and Molecular Biology In press. DOI: 10.1016/j.pbiomolbio.2016.09.010.
31.	**Ivanov SM, Huber RG, Warwicker J, Bond PJ.** (2016). Energetics and Dynamics Across the Bcl-2-family-dependent Apoptosis Pathway Reveal Distinct Evolutionary Determinants of Specificity and Affinity. Structure 24 2024-2033.
32.	**Lea-Smith D, Ortiz-Suarez M, Lenn T, Nurnberg D, Bears L, Davey M, Cotton C, Mastroianni G, Bombelli P, Ungerer P, Stevens T, Smith A, Huber RG, Bond PJ, Mullineaux C, Howe C, Parolini L.** (2016). Hydrocarbons are essential for optimal cell size, division and growth of cyanobacteria. Plant Physiology 172 1928-1940.
33.	**Huber RG, Kulemzina I, Ang K, Chavda AP, Suranthran S, Teh JT, Kenanov D, Liu GW, Rancati G, Szmyd R, Kaldis P, Bond PJ, Ivanov D.** (2016). Imparining Cohesin Smc1/3 Head Engagement Compensates for the Lack of Eco1 Function. Structure 24. 1991-1999.
34.	**Maurer-Stroh S, Mak T, Ng Y, Phuah S, Huber RG, Marzinek JK, Holdbrook DA, Lee RT, Cui L, Lin RT.** (2016). South-east Asian Zika Strain Linked to Cluster of Cases in Singapore, August 2016. Eurosurveillance 21 30347.
35.	**Kulemzina I, Ang K, Zhao XD, Teh JT, Verma V, Suranthran S, Chavda AP, Huber RG, Eisenhaber B, Eisenhaber F, Yan J, Ivanov D.** (2016). A Reversible Association between Smc Coiled Coils Is Regulated by Lysine Acetylation and is Required for Cohesin Association with the DNA. Molecular Cell 63 1044-1054.
36.	**Holdbrook DA, Huber RG, Marzinek JK, Bond PJ, Khaled SJ.** (2016). Dynamics of

	crowded vesicles: local and global responses to membrane composition. PLoS ONE 11 e0156963.
37.	**Marzinek JK, Holdbrook DA, Huber RG, Verma CS, Bond PJ.** (2016). Dengue Viral Membrane Coaxed into Shape by Molecular Simulations. Structure 24 1410-1420.
38.	**Marzinek JK, Lakshminarayanan R, Goh E, Huber RG, Panzade S, Verma CS, Bond PJ.** (2016). Characterizing the Conformational Landscape of Flavivirus Fusion Peptides via Simulation and Experiment. Scientific Reports 6 19160.
39.	**Scherl M, Müller T, Kreutz CR, Huber RG, Zass E, Liedl KR, Kräutler.** (2016). Chlorophyll Catabolites in Fall Leaves of the Wych Elm Tree Present a Novel Glycosylation Motif. Chemistry - A European Journal 22 9498–9503.
40.	**von Grafenstein S, Wallnoefer HG, Kirchmair J, Fuchs JE, Huber RG, Schmidtke M, Sauerbrei A, Rollinger JM, Liedl KR.** (2015). Interface dynamics explain assembly dependency of influenza neuraminidase catalytic activity. Journal of Biomolecular Structure and Dynamics 33 104-120.
41.	**Pummer BG, Budke C, Augustin-Bauditz S, Niedermeier D, Felgitsch L, Kampf CJ, Huber RG, Liedl KR, Loerting T, Moschen T.** (2015). Ice nucleation by water-soluble macromolecules. Atmospheric Chemistry and Physics 15 4077-4091.
42.	**Huber RG, Eibl C, Fuchs JE.** (2015). Intrinsic flexibility of NLRP pyrin domains is a key factor in their conformational dynamics, fold stability, and dimerization. Protein Science 24 2015 174-181.
43.	**Fuchs JE, Waldner BJ, Huber RG, von Grafenstein S, Kramer C, Liedl KR.** (2015). Independent Metrics for Protein Backbone and Side-Chain Flexibility: Time Scales and Effects of Ligand Binding. Journal of Chemical Theory and Computation 11 2015 851-860.
44.	**Huber RG, Fan H, Bond PJ.** (2015). The Structural Basis for Activation and Inhibition of ZAP-70 Kinase Domain. PLoS Computational Biology 11 2015 e1004560.
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46.	**Schauperl M, Fuchs JE, Waldner BJ, Huber RG, Kramer C, Liedl KR.** (2015). Characterizing Protease Specificity: How Many Substrates Do We Need? PloS one 10 e0142658.
47.	**Waldner BJ, Fuchs JE, Huber RG, von Grafenstein S, Schauperl M, Kramer C, Liedl KR.** (2015). Quantitative Correlation of Conformational Binding Enthalpy with Substrate Specificity of Serine Proteases. The Journal of Physical Chemistry B 120 299-308.
48.	**Faustino AF, Guerra GM, Huber RG, Hollmann A, Bond PJ, Castanho MARB, Da Poian AT, Almeida FCL, Santos NC, Martins I.** (2015). Conformational changes governing dengue virus capsid protein function and its inhibition by pep14 23.Protein Science 24 126-127.
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51.	**Faustino AF, Guerra GM, Huber RG, Hollmann A, Domingues MM, Barbosa GM, Enguita FJ, Bond PJ, Castanho MARB, Da Poial AT.** (2014). Understanding dengue virus capsid protein disordered N-terminus and pep14-23-based inhibition. ACS Chemical Biology 10 517-526.
52.	**Bernard J, Huber RG, Liedl KR, Grothe H, Loerting T.** (2013). Matrix Isolation Studies of Carbonic Acid: The Vapor Phase above the ß-Polymorph. Journal of the American Chemical Society 135 7732-7737.
53.	**Fuchs JE, von Grafenstein S, Huber RG, Margreiter MA, Spitzer GM, Wallnoefer HG, Liedl KR.** (2013). Cleavage entropy as quantitative measure of protease specificity. PLOS Computational Biology 9 e1003007.
54.	**Bachmann VA, Riml A, Huber RG, Baillie GS, Liedl KR, Valovka T, Stefan E.** (2013). Reciprocal regulation of PKA and Rac signaling. Proceedings of the National Academy of Sciences of the USA 110 8531-8536.
55.	**Huber RG, Fuchs JE, von Grafenstein S, Laner M, Wallnoefer HG, Abdelkader N, Kroemer RT, Liedl KR.** (2013). Entropy from state probabilities: hydration entropy of cations. The Journal of Physical Chemistry B 117 6466-6472.
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58.	**Fuchs JE, Huber RG, von Grafenstein S, Wallnoefer HG, Spitzer GM, Fuchs D, Liedl KR.** (2012). Dynamic regulation of phenylalanine hydroxylase by simulated redox manipulation. PloS one 7 2012 e53005.
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