BII Early Career Researchers Group - Membrane Biophysics and Drug Delivery Publication List

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

1.	**Jianguo Li, Srinivasaraghavan Kannan, Pietro Aronica, Christopher J. Brown, Anthony W Partridge, Chandra S. Verma.** Molecular descriptors suggest stapling as a strategy for optimizing membrane permeability of cyclic peptides. J. Chem. Phys., Accepted (2022).
2.	**Ting DSJ, Li J, Verma CS, Goh ETL, Nubile M, Mastropasqua L, Said DG, Beuerman RW, Lakshminarayanan R, Mohammed I and Dua HS.** Evaluation of Host Defense Peptide (CaD23)-Antibiotic Interaction and Mechanism of Action: Insights From Experimental and Molecular Dynamics Simulations Studies. Front. Pharmacol. 12:731499 (2021)
3.	**Aronica PGA, Reid LM, Desai N, Li J, Fox SJ, Yadahalli S, Essex JW, Verma CS.** Computational Methods and Tools in Antimicrobial Peptide Research. J. Chem. Inf. Model. 2021, 61, 7, 3172–3196 (2021)
4.	**Kannan S, Aronica PGA, Nguyen TB, Li J, Verma CS.** Computational Design of Macrocyclic Binders of S100B(ββ): Novel Peptide Theranostics. Molecules 26, 721 (2021).
5.	**Kumar A, Mohanram H, Li J, Ferrand H Le, Verma CS, Miserez A.** Disorder–Order Interplay of a Barnacle Cement Protein Triggered by Interactions with Calcium and Carbonate Ions: A Molecular Dynamics Study. Chemistry of Materials, 32, 8845-8859 (2020).
6.	**Li J, Beuerman R, Verma CS.** Dissecting the Molecular Mechanism of Colistin Resistance in mcr-1 Bacteria. Journal of Chemical Information and Modeling, 60, 4975-4984 (2020).
7.	**Li J, Beuerman R, Verma CS**. Mechanism of polyamine induced colistin resistance through electrostatic networks on bacterial outer membranes. BBA-Biomembranes, 1862, 183297 (2020) (corresponding author).
8.	**Zhou L, Chan CY, Stephanie C, Gueguen N, Valérie D, Koh SK, Li J, Gao Y, Deng L, Verma CS, Beuerman R, Chan CY, Milea D, Reynier P.** Increased Protein S-Glutathionylation in Leber's Hereditary Optic Neuropathy (LHON). International Journal of Molecular Sciences, 21, 3027 (2020).
9.	**Li J, Beuerman R, Verma CS.** The effect of molecular shape on oligomerization of hydrophobic drugs: molecular simulations of ciprofloxacin and Nutlin. Journal of Chemical Physics. 148:104902 (2018).
10.	**Li J, Beuerman RW, Verma CS**. Molecular insights into the membrane affinities of model hydrophobes. ACS Omega. 3:2498-2507 (2018).
11.	**Fox SJ, Lakshminarayanan R, Beuerman RW, Li J, Verma CS.** Conformational Transitions of Melittin between Aqueous and Lipid Phases: Comparison of Simulations with Experiments. Journal of Physical Chemistry B. 122:8698-8705 (2018). (corresponding author)
12.	**Chan CY, Soh ACK, Kioh DYQ, Li J, Verma CS, Koh SK, Beuerman RW, Zhou L, Chan ECY.** Reactive Metabolite-induced Protein Glutathionylation: a Potentially Novel Mechanism Underlying Acetaminophen Hepatotoxicity. Mol Cell Proteomics. 17:2034-2050 (2018).
13.	**Koh JJ, Lin S, Bai Y, Sin WWL, Aung TT, Li J, Verma CS, Pervushin K, Beuerman RW, Liu S.** Antimicrobial Activity Profiles of Amphiphilic Xanthone Derivatives are a Function of Their Molecular Oligomerization. BBA-Biomembrane, BBA-Biomembranes, 1860:2281-2298 (2018).
14.	**Lau QY, Li J, Sani MA, Sinha S, Li Y, Ng FM, Kang C, Bhattacharjya S, Separovic F, Verma CS, Chia CSB.** Elucidating the Bactericidal Mechanism of Action of the Linear Antimicrobial Tetrapeptide BRBR-NH2. BBA-Biomembranes, 1860: 1517-1527 (2018) (co-first author).

15.	**Yadahalli S, Li J, Lane DP, Gosavi S, Verma CS**. Characterizing the conformational landscape of MDM2-binding p53 peptides using Molecular Dynamics simulations. Scientific reports. 7:15600 (2017).
16.	**Li J, Hu Z, Beuerman R, Verma CS.** Molecular Environment Modulates Conformational Differences between Crystal and Solution States of Human β-Defensin 2. Journal of Physical Chemistry B. 121: 2739-2747 (2017)
17.	**Li J, Koh JJ, Liu S, Lakshminarayanan R, Verma CS, Beuerman RW.** Membrane Active Antimicrobial Peptides: Translating Mechanistic Insights to Design. Frontiers in Neuroscience. 11: 73 (2017)
18.	**Chen Y, Li T, Li J, Cheng S, Wang J, Verma C, Zhao Y, Wu C.** Stabilization of Peptides against Proteolysis through Disulfide-Bridged Conjugation with Synthetic Aromatics. Organic & Biomolecular Chemistry. 15: 1921-1929 (2017)
19.	**Lin S, Koh JJ, Aung TT, Lim F, Li J, Zou H, Wang L, Lakshminarayanan R, Verma CS, Wang Y, Tan DT, Cao D, Beuerman RW, Ren L, Liu S.** Symmetrically Substituted Xanthone Amphiphiles Combat Gram-positive Bacterial Resistance with Enhanced Membrane Selectivity. Journal of Medicinal Chemistry, 60: 1362–1378 (2017)
20.	**Fox SJ, Li J, Tan YS, Nguyen MN, Pal A, Ouaray Z, Yadahalli S, Kannan S.** The Multifaceted Roles of Molecular Dynamics Simulations in Drug Discovery. Current Pharmaceutical Design. 22: 3585-3600 (2016)
21.	**Lakshminarayanan R, Tan WX, Aung TT, Goh ET, Muruganantham N, Li J, Chang JY, Dikshit N, Saraswathi P, Lim RR, Kang TS, Balamuralidhar V, Sukumaran B, Verma CS, Sivaraman J, Chaurasia SS, Liu S, Beuerman RW.** Branched Peptide, B2088, Disrupts the Supramolecular Organization of Lipopolysaccharides and Sensitizes the Gram-negative Bacteria. Scientific Reports. 6: 25905 (2016)
22.	**Koh JJ, Zou H, Lin S, Lin H, Soh RT, Lim FH, Koh WL, Li J, Lakshminarayanan R, Verma C, Tan DT, Cao D, Beuerman RW, Liu S.** Nonpeptidic Amphiphilic Xanthone Derivatives: Structure-Activity Relationship and Membrane-Targeting Properties. Journal of Medicinal Chemistry. 59: 171-93 (2015)
23.	**Koh JJ, Lin H, Caroline V, Chew YS, Pang LM, Aung TT, Li J, Lakshminarayanan R, Tan DT, Verma C, Tan AL, Beuerman RW, Liu S.** N-Lipidated Peptide Dimers: Effective Antibacterial Agents against Gram-Negative Pathogens through Lipopolysaccharide Permeabilization. Journal of Medicinal Chemistry, 58: 6533-48 (2015)
24.	**Li J, Liu S, Koh JJ, Zou H, Lakshminarayanan R, Bai Y, Pervushin K, Zhou L, Verma C, Beuerman RW.** A novel fragment based strategy for membrane active antimicrobials against MRSA. BBA-Biomembranes. 1848: 1023-1031 (2015) (This paper was highlighted in ASTAR Research, Vol 13, page 40-41, 2015)
25.	**Koh JJ, Lin S, Aung TT, Lim F, Zou H, Bai Y, Li J, Lin H, Pang LM, Koh WL, Salleh SM, Lakshminarayanan R, Zhou L, Qiu S, Pervushin K, Verma CS, Tan DT, Cao D, Liu S, Beuerman RW.** Amino Acid Modified Xanthone Derivatives: Novel, Highly Promising Membrane-Active Antimicrobials for Multidrug-Resistant Gram-Positive Bacterial Infections. Journal of Medicinal Chemistry. 58: 739-752 (2015)
26.	**Lakshminarayanan R, Liu S, Li J, Nandhakumar M, Aung TT, Goh E, Chang JY, Saraswathi P, Tang C, Safie SR, Lin LY, Riezman H, Lei Z, Verma CS, Beuerman RW.** Synthetic Multivalent Antifungal Peptides Effective against Fungi. Plos One. 9: e87730 (2014)
27.	**Zou H, Koh JJ, Li J, Qiu S, Aung TT, Lin H, Lakshminarayanan R, Dai X, Tang C, Lim FH, Zhou L, Tan AL, Verma C, Tan DT, Chan HS, Saraswathi P, Cao D, Liu S, Beuerman RW.** Design and Synthesis of Amphiphilic Xanthone Based Membrane Targeting Antimicrobials with Improved Membrane Selectivity. Journal of medicinal chemistry. 56: 2359−2373 (2013)
28.	**Li J, Liu S, Lakshminarayanan R, Bai Y, Pervushin K, Verma CS, Beuerman RW.** Molecular simulations suggest how a branched antimicrobial peptide perturbs a bacterial membrane and enhances permeability. BBA-Biomembranes. 1828: 1112-1121 (2013).

29.	**Li J, Lakshminarayanan R, Bai Y, Liu S, Zhou L, Verma CS, Pervushin K, Beuerman RW.** Molecular dynamics simulations of a branched antimicrobial peptide: Effects of different force fields. Journal of Chemical Physics. 137: 215101 (2012) (corresponding author).
30.	**Koh JJ, Qiu S, Zou H, Lakshminarayanan R, Li J, Zhou X, Tang C, Saraswathi P, Verma CS, Tan DT, Tan AL, Liu S, Beuerman RW.** Rapid Bactericidal Action of Alpha-mangostin against MRSA as an Outcome of Membrane Targeting. BBA-Biomembranes. 1828: 834-844 (2012).
31.	**Bai Y, Liu S, Li J, Lakshminarayanan R, Sarawathi P, Tang C, Ho D, Verma CS, Beuerman RW, Pervushin K.** Progressive structuring of a branched antimicrobial peptide on the path to the inner membrane target. Journal of Biological Chemistry. 287:26606-17 (2012).
32.	**Shah D, Li J, Shaikh AR, Rajagopalan R.** Arginine-Aromatic Interactions and Their Effects on Arginine-Induced Solubilization of Aromatic Solutes and Suppression of Protein Aggregation. Biotechnology Progress. 28: 223-231. (2012)
33.	**Li J, Garg M, Shah D, Rajagopalan R.** Solubilization of aromatic and hydrophobic moieties by arginine in aqueous solutions. Journal of Chemical Physics. 133: 054902.(2010) (This paper was also selected into Virtual Journal of Biological physics research, 2010, 15)
34.	**Li J, Rajagopalan R, Jiang J.** Polymer-Induced Phase Separation and Crystallization in IgG Solutions. Journal of Chemical Physics. 128: 205105. (2008) (This paper was also selected into Virtual Journal of Biological physics research, 2008, 15)
35.	**Li J, Rajagopalan R, Jiang J.** Role of Solvent in Protein Phase Behavior: Influence of Temperature-Dependent Potential. Journal of Chemical Physics. 128: 235104. (2008) (This paper was also selected into Virtual Journal of Biological physics research, 2008, 16)