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Number of citations: 352

List of publications with primary scientific contributions

1. **D.R. Bell**, G. Domeniconi, C.-C. Yang, L. Zhang, G. Cong. 2020. Dynamics-based peptide-MHC binding optimization by a convolutional variational autoencoder. *In preparo*.
2. **D.R. Bell**, Y. Song, S. Lee, R. Zhou. 2020. An *in silico* mutagenesis study of autoantigen optimization for potential T1D vaccine design. *In preparo*.
3. **D.R. Bell**, J.K. Weber, W. Yin, T. Huynh, W. Duan, R. Zhou. 2020. *In silico* design and validation of high-affinity RNA aptamers targeting epithelial cellular adhesion molecule dimers. PNAS. 117: 8486-8493.
4. R. Ahmed, Z. Omidian, A. Giwa, B. Cornwell, N. Majety, **D.R. Bell**, S. Lee,..., R. Zhou, C. Jie, T. Donner, A.R.A. Hamid. 2019. A Public BCR Present in a Unique Dual-Receptor-Expressing Lymphocyte from Type 1 Diabetes Patients Encodes a Potent T Cell Autoantigen. Cell. 177: 1583-1599.
5. **D.R. Bell***, S.-G. Kang*, T. Huynh, R. Zhou. 2018. Concentration-dependent binding of CdSe quantum dots on the SH3 domain. Nanoscale. 10: 351-358.
6. **D.R. Bell**, S. Y. Cheng, P. Ren. 2017. Capturing RNA Folding Free Energy with Coarse-Grained Molecular Dynamics Simulations. Scientific Reports. 7: 45812.
7. **D.R. Bell***, R. Qi*, Z. Jing*, J. Y. Xiang, C. Mejias, M. J. Schnieders, J. W. Ponder, P. Ren. 2016. Calculating binding free energies of host-guest systems using the AMOEBA polarizable force field. Physical Chemistry Chemical Physics. 18: 30261-30269.
8. J. R. Houser, D. J. Busch, **D.R. Bell**, B. Li, P. Ren, and J. C. Stachowiak. 2016. The Impact of Physiological Crowding on the Diffusivity of Membrane Bound Proteins. Soft Matter 12: 2127-2134.
9. **D.R. Bell**, Z. Xia, and P. Ren. RNA Coarse-Grained Model Theory. Many-body effects and electrostatics in multi-scale computation of biomolecules. Ed. Qian Cui, Markus Meuwly, and Pengyu Ren. Singapore: Pan Stanford Publishing, 2015.

(*Co-first authors)

List of publications with secondary scientific contributions

1. C. Zhang, **D.R. Bell**, M. Harger, P. Ren. 2017. Polarizable Multipole-Based Force Field for Aromatic Molecules and Nucleobases. Journal of Chemical Theory and Computation. 13 (2), 666-678.
2. Z. Xia, **D.R. Bell**, Y. Shi, and P. Ren. 2013. RNA 3D structure prediction by using a coarse-grained model and experimental data. The Journal of Physical Chemistry B 117(11):3135-3144.
3. J.M. Obliosca, S. Y. Cheng, Y.-A. Chen, M. F. Llanos, Y.-L. Liu, D. M. Imphean, **D.R. Bell**, J. T. Petty, P. Ren, H.-C. Yeh. 2017. LNA Thymidine Monomer Enables Differentiation of the Four Single-Nucleotide Variants by Melting Temperature. Journal of the American Chemical Society. 139(20): 7110-7116.

List of publications with majority writing contributions

1. L. Zhang, **D.R. Bell**, B. Luan, and R. Zhou. 2019. Exploring the binding mechanism between human profilin (PFN1) and polyproline-10 through binding mode screening. The Journal of Chemical Physics. 150(1), 015102.
2. D. Ma, X.Y. Meng, **D.R. Bell**, S. Liu, R. Zhou. 2018. Inhibition of CYP2C8 by metallofullerenol Gd@C82(OH)22 through blocking substrate channels and substrate recognition sites. Carbon. 127, 667-675.
3. M. Feng, **D.R. Bell**, R. Zhou. 2017. Propensity of a single-walled carbon nanotube-peptide to mimic a KK10 peptide in an HLA-TCR complex. The Journal of Chemical Physics. 147 (22), 225101.
4. M. Feng, **D.R. Bell**, J. Luo, R. Zhou. 2017. Impact of graphyne on structural and dynamical properties of calmodulin. Physical Chemistry Chemical Physics. 19, 10187-10195.
5. X. Wang, B. Li, **D.R. Bell**, W. Li, R. Zhou. 2017. Hydrogen and methane storage and release by MoS2 nanotubes for energy storage. Journal of Materials Chemistry A. 5(44) 23020-23027.
6. Z. Gu, Y.C. Yang, C. Ge, J.K. Weber, **D.R. Bell**, R. Zhou. 2015. Surface curvature relation to protein adsorption for carbon-based nanomaterials. Scientific Reports. 5, 10886.
7. C. Narth, L. Lagardere, E. Polack, N. Gresh, Q. Wang, **D.R. Bell**, J.A. Rackers, J. W. Ponder, P. Ren, J.-P. Piquemal. 2016. Scalable improvement of SPME multipolar electrostatics in anisotropic polarizable molecular mechanics using a general short-range penetration correction up to quadrupoles. Journal of Computational Chemistry. 37 (5), 494-506.

List of Presentations

1. **D.R. Bell**, S.-G. Kang, R. Zhou. 2018. CdSe quantum dot aggregation-dependent toxicity on the SH3 domain. 256th ACS National Meeting & Exposition, Boston, Massachusetts. Presentation.
2. **D.R. Bell**, Z. Xia, P. Ren. 2015. Weighing energetics against best fit in RNA structure prediction. 249th ACS National Meeting & Exposition, Denver, Colorado. Poster.
3. **D.R. Bell**, P. Selokar, and T. D. Lillian. 2012. Simulation of Plectonemic Supercoil Diffusion Along Extended DNA. Proceedings 56th Annual Meeting, Biophysical Society, San Diego, California. Poster.

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