

Refereed Journals

1. Anandakrishnan, R., Zhang, Z., Donovan-Maiye, R., Zuckerman, D. M. Biophysical comparison of ATP synthesis mechanisms shows a kinetic advantage for the rotary process. *Proceedings of the National Academy of Sciences*, Sep. 2016; 201608533+.
URL <http://dx.doi.org/10.1073/pnas.1608533113>
2. Anandakrishnan, R., Drozdetski, A., Walker, R. C., Onufriev, A. V. Speed of conformational change: Comparing explicit and implicit solvent molecular dynamics simulations. *Biophysical Journal*, Mar. 2015; **108** (5), 1153–1164.
URL <http://dx.doi.org/10.1016/j.bpj.2014.12.047>
3. Lin, H., Chen, W., Anandakrishnan, R., Plewczynski, D. Application of machine learning method in genomics and proteomics. *Scientific World Journal* 2015, 914780+.
URL <https://www.hindawi.com/journals/tswj/2015/914780/>
4. Izadi, S., Anandakrishnan, R., Onufriev, A. V. Building water models: A different approach. *J. Phys. Chem. Lett.*, Nov. 2014; **5** (21), 3863–3871.
URL <http://dx.doi.org/10.1021/jz501780a>
5. Anandakrishnan, R., Baker, C., Izadi, S., Onufriev, A. V. Point charges optimally placed to represent the multipole expansion of charge distributions. *PLoS ONE*, Jul. 2013; **8** (7), e67715+.
URL <http://dx.doi.org/10.1371/journal.pone.0067715>
6. Anandakrishnan, R., Aguilar, B., Onufriev, A. V. H++ 3.0: automating pK prediction and the preparation of biomolecular structures for atomistic molecular modeling and simulations. *Nucleic acids research*, Jul. 2012; **40** (Web Server issue), W537–W541.
URL <http://dx.doi.org/10.1093/nar/gks375>
7. Anandakrishnan, R. A partition function approximation using elementary symmetric functions. *PLoS ONE*, Dec. 2012; **7** (12), e51352+.
URL <http://dx.doi.org/10.1371/journal.pone.0051352>
8. Anandakrishnan, R., Daga, M., Onufriev, A. V. An $n \log n$ generalized born approximation. *Journal of Chemical Theory and Computation*, Mar. 2011; **7** (3), 544–559.
URL <http://dx.doi.org/10.1021/ct100390b>

9. Warren, A. S., Anandakrishnan, R., Zhang, L. Functional bias in molecular evolution rate of arabidopsis thaliana. *BMC Evolutionary Biology*, 2010; **10**, 125+.
URL <http://bmcevolbiol.biomedcentral.com/articles/10.1186/1471-2148-10-125>
10. Anandakrishnan, R., Scogland, T. R. W., Fenley, A. T., Gordon, J. C., Feng, W.-c., Onufriev, A. V. Accelerating electrostatic surface potential calculation with multi-scale approximation on graphics processing units. *Journal of Molecular Graphics and Modelling*, Jun. 2010; **28** (8), 904–910.
URL <http://dx.doi.org/10.1016/j.jmgm.2010.04.001>
11. Aguilar, B., Anandakrishnan, R., Ruscio, J. Z., Onufriev, A. V. Statistics and physical origins of pK and ionization state changes upon Protein-Ligand binding. *Biophysical Journal*, Mar. 2010; **98** (5), 872–880.
URL <http://dx.doi.org/10.1016/j.bpj.2009.11.016>
12. Anandakrishnan, R., Onufriev, A. V. An $n \log n$ approximation based on the natural organization of biomolecules for speeding up the computation of long range interactions. *Journal of computational chemistry*, Mar. 2010; **31** (4), 691–706.
URL <http://dx.doi.org/10.1002/jcc.21357>
13. Anandakrishnan, R., Onufriev, A. Analysis of basic clustering algorithms for numerical estimation of statistical averages in biomolecules. *Journal of Computational Biology*, Mar. 2008; **15** (2), 165–184.
URL <http://dx.doi.org/10.1089/cmb.2007.0144>