

Curriculum Vitae

Lin Li

Department of Physics and Astronomy,
Clemson University
SC, United States, 29631
Email: lli5@g.clemson.edu
Phone: 1-636-364-8518

Education and work experience:

- **Research Associate (Biophysics)**, Clemson University, 2013-now
Advisor: Prof. Emil Alexov
 - **Postdoct (Biophysics)**, Clemson University, 2011-2013
Advisor: Prof. Emil Alexov
 - **Ph.D. (Biophysics)**, Huazhong University of Science and Technology, 2005-2011
Advisor: Prof. Yi Xiao
 - **B.S. (Applied Physics)**, Huazhong University of Science and Technology, 2001-2005
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Research experience:

DelPhi Development

DelPhi is a widely used Poisson Boltzmann Equation solver. I have developed a Gaussian smooth method to DelPhi software, which is used to model the inhomogeneous dielectric properties of macromolecules. This method has been proved to be more accurate than the traditional 2-dielectric constant methods.

MEMPOT

A Membrane Potential (MEMPOT) tool is developed and implemented into DelPhi program. Using this MEMPOT tool, one can easily calculate the electrostatic potential distribution across the membrane.

ASPDock

I have developed a docking algorithm (ASPDock) to calculate binding free energy of protein complexes, which improves the accuracy of prediction effectively. Comparisons with other state-of-the-art docking algorithms showed that ASP score indeed gives higher success rate than the pure shape complementarity score of FTDock.

SRM

I also developed a Softly Restricting Method (SRM), which utilizes the unreliable binding site information to enhance success rate of docking. It only reduces hit count

number and success rate slightly if the predicted information is completely wrong. However, when the predicted information is correct or partially correct, SRM increases the hit count number and success rate significantly.

CAPRI

Using ASPDock and Softly Restricting Method, my team has participated in two rounds of Critical Assessment of PRediction of Interactions (CAPRI). We got high-quality hits for T40 and T41 and the best LRMSD were 2.35 Å and 1.41 Å, respectively.

Teaching experience:

2013-2015 Fall: Computational Physics (PHYS-3150)

Selected Awards:

2001-2002: HUST Scholarship

2002-2003: National Scholarship by Chinese Government

Skills and Software

<u>Programming language</u>	: Fortran/C/C++/Bash/Matlab
<u>Molecular Simulations</u>	: DelPhi/Tinker /NAMD
<u>Protein-protein docking</u>	: ASPDock/SRM/FTDock/ZDOCK/GRAMM
<u>Graphic</u>	: Chimera/PyMOL/Photoshop/Flash
<u>Homology Modeling</u>	: SWISS-MODEL/I-TASSER

Publications and Poster Presentations

Publications:

1. Lin Wang, Lin Li, and Emil Alexov. *pKa Predictions for Proteins, RNAs and DNAs with the Gaussian Dielectric Function Using DelPhiPKa*. *Proteins: Structure, Function, and Bioinformatics* (2015).
2. Lin Li, Lin Wang, Emil Alexov, *On the energy components governing molecular recognition in the framework of continuum approaches*, *Frontiers in Molecular Biosciences* 2 (2015): 5.
3. Tugba G. Kucukkal, Marharyta Petukh, Lin Li, and Emil Alexov, *Structural and physico-chemical effects of disease and non-disease nsSNPs on proteins*, *Current opinion in structural biology* 32 (2015): 18-24.
4. Lin Li, Chuan Li, Emil Alexov, *On the Modeling of Polar Component of Solvation Energy Using Smooth Gaussian-Based Dielectric Function*, *Journal of Theoretical and Computational Chemistry*, 2014.
5. Roberta P. Dias[§], Lin Li[§], Thereza A. Soares and Emil Alexov, *Modeling the Electrostatic Potential of Asymmetric Lipopolysaccharide Membranes: The*

- MEMPOT Algorithm Implemented in DelPhi***, Journal of computational chemistry (2014). ([§] contributed equally)
6. Praveen Nedumpully-Govindan, **Lin Li**, Emil G Alexov, Mark A Blenner, Feng Ding, **Structural and energetic determinants of tyrosylprotein sulfotransferase sulfation specificity**, Bioinformatics, 2014
 7. **Lin Li**, Chuan Li, Zhe Zhang, Emil Alexov, **On the Dielectric "Constant" of Proteins: Smooth Dielectric Function for Macromolecular Modeling and Its Implementation in DelPhi**, J Chem Theory Comput. 2013 Apr 9;9(4):2126-2136.
 8. **Lin Li**, Yanzhao Huang, and Yi Xiao, **How to Use Not-Always-Reliable Binding Site Information in Protein-Protein Docking Prediction**, PloS one 8.10 (2013)
 9. Chuan Li, **Lin Li**, Marharyta Petukh, Emil Alexov, **Progress in developing Poisson-Boltzmann equation solvers**, Molecular Based Mathematical Biology. Volume 1, Pages 42-62
 10. Chuan Li, Marharyta Petukh, **Lin Li**, Emil Alexov, **Continuous development of schemes for parallel computing of the electrostatics in biological systems: Implementation in DelPhi**, J Comput Chem. 2013 Jun 4. doi: 10.1002/jcc.23340. [Epub ahead of print] PMID: 23733490
 11. Huang, Yangyu, Shiyong Liu, Dachuan Guo, **Lin Li**, and Yi Xiao. **A novel protocol for three-dimensional structure prediction of RNA-protein complexes**, Scientific reports 3 (2013).
 12. **Lin Li**, Li C, Sarkar S, Zhang J, Witham S, Zhang Z, Wang L, Smith N, Petukh M, Alexov E.* **DelPhi: a comprehensive suite for DelPhi software and associated resources**, BMC Biophys, (2012) May14;4(1):9.
 13. Smith N, Campbell B, **Li L**, Li C, Alexov E., **Protein Nano-Object Integrator (ProNOI) for generating atomic style objects for molecular modeling**, BMC Struct Biol. 2012 Dec 5;12:31. doi:10.1186/1472-6807-12-31.
 14. Chuan Li, **Lin Li**, Marharyta Petukh and Emil Alexov; **Progress in developing Poisson-Boltzmann equation solvers**, Molecular Based Mathematical Biology. Volume 1, Pages 42-62.
 15. Petukh M, Zhenirovskyy M, Li C, **Li L**, Wang L, Alexov E, **Predicting nonspecific ion binding using Delphi**, Biophys J. 2012 Jun 20, 102(12)
 16. Chuan Li, **Lin Li**, Jie Zhang, Alexov E.*, **Highly efficient and exact method for parallelization of grid-based algorithms and its implementation in DelPhi**, J Comput Chem. (2012)
 17. Lin Wang, Shawn Witham, Zhe Zhang, **Lin Li**, Michael Hodsdon and Emil Alexov*, **In silico investigation of pH-dependence of prolactin and human growth hormone binding to human prolactin receptor**, Comm. Comp. Phys., (2013), 13, 207-222
 18. Nicholas Smith, Subhra Sarkar, Shawn Witham, Jie Zhang, **Lin Li**, Chuan Li and Emil Alexov*, **DelPhi Web Server v2: Incorporating atomic-style geometrical figures into the computational protocol**, Bioinformatics (2012), 28(12):1655-7.
 19. **Lin Li**, Dachuan Guo, Yangyu Huang, Shiyong Liu, Yi Xiao*, **ASPDock: protein-protein docking algorithm using atomic solvation parameters model**, BMC Bioinformatics, 2011, 12(1): 36.
 20. Changjun Chen, **Lin Li** and Yi Xiao*, **Identification of key residues in proteins by using their physical characters**. Physical Review E. 2006, 73(4): 41926.

21. Changjun Chen, **Lin Li** and Yi Xiao*, *All-Atom Contact Potential Approach to Protein Thermostability Analysis*, *Biopolymers*, 2007, 85(1): 28.

Presentations

1. **Lin Li**, Emil Alexov, *Electrostatic interactions play important roles in kinesin proceeding on microtubule*, Mathematical Biosciences Institute workshop: Multiple Faces of Biomolecular Electrostatics, October 12-16, 2015, Columbus, OH, US.
2. (invited talk) **Lin Li**, Chuan Li, Emil Alexov, *Smooth dielectric function for modeling electrostatics in biological macromolecules*, 246th ACS National Meeting, September 8-12, 2013, Indianapolis, IN, US.
3. (invited talk) **Lin Li**, Chuan Li and Emil Alexov, *Implementing smooth dielectric function to pKa predictions and other applications*, Protein Electrostatics Meeting: July 8-12, 2013, Telluride Science Research Center, Telluride, CO, US.
4. **Lin Li**, Chuan Li, and Emil Alexov, *Modeling proteins and small molecules with inhomogeneous dielectric function: Implementation in DelPhi*, Biophysical Society 57th Annual Meeting: February 2-6, 2013, Philadelphia, PA, US.
5. **Lin Li**, Chuan Li, Zhe Zhang, Emil Alexov, *Modeling bio-molecules with Gaussian smooth dielectric function*. Clemson Bioseminar, January 29, 2013, Clemson University, Clemson, SC, US.
6. **Lin Li**, Lin Wang, Chuan Li, and Emil Alexov, *The effect of non-uniform protein dielectric constant on the electrostatic energy calculations*, 244th ACS National Meeting, August 19-23, 2012, Philadelphia, PA, US.
7. **Lin Li**, *Protein-protein interactions and docking algorithms*, Clemson Bio-seminar, September 9 2011, Clemson University, Clemson, SC, US.
8. **Lin Li**, Ying Chen and Yi Xiao, *Using ASP model in a docking algorithm (Presentation)*, (HUST) Physics Department Seminar, January 12-13, 2009, Wuhan, China.

Posters:

1. **Lin Li**, Lin Wang and Emil Alexov, *Predicting structured water molecules by combined energy calculations and geometrical considerations*, Symposium for Introduction to Research in Physics and Astronomy (SIRPA), BellSouth Auditorium, Clemson, SC, August 22, 2011
2. **Lin Li**, Dachuan Guo, Shiyong Liu and Yi Xiao, *Protein-Protein Docking Algorithm Using ASP Model (Poster)*, Fourth CAPRI Evaluation Meeting, December 9-11,

2009, Barcelona, Spain.

3. **Lin Li**, Dachuan Guo and Yi Xiao, ***Computation of interactions between cannabinoid receptors and G-proteins (Poster)***, the 11th Chinese Conference on Biophysics, Guilin (China), July 12-16, 2009