Resource Summary Report

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Adaptive Poisson-Boltzmann Solver

RRID:SCR_008387
Type: Tool

Proper Citation

Adaptive Poisson-Boltzmann Solver (RRID:SCR_008387)

Resource Information

URL: http://www.poissonboltzmann.org/apbs/

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Description: APBS is a software package for modeling biomolecular solvation through solution of the Poisson-Boltzmann equation (PBE), one of the most popular continuum models for describing electrostatic interactions between molecular solutes in salty, aqueous media. APBS was designed to efficiently evaluate electrostatic properties for such simulations for a wide range of length scales to enable the investigation of molecules with tens to millions of atoms. It also provides implicit solvent models of nonpolar solvation which accurately account for both repulsive and attractive solute-solvent interactions. APBS uses FEtk (the Finite Element ToolKit) to solve the Poisson-Boltzmann equation numerically. FEtk is a portable collection of finite element modeling class libraries written in an object-oriented version of C. It is designed to solve general coupled systems of nonlinear partial differential equations using adaptive finite element methods, inexact Newton methods, and algebraic multilevel methods.

Abbreviations: APBS

Resource Type: software resource

Keywords: software package, modeling, biomolecular, electrostatic, molecular, dynamics, binding energy, equilibrium, protein, ligand, solvation, kinetics, simulation, finite element

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Resource Name: Adaptive Poisson-Boltzmann Solver

Resource ID: SCR_008387

Alternate IDs: nif-0000-30035

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Record Last Update: 20250519T203543+0000

Ratings and Alerts

No rating or validation information has been found for Adaptive Poisson-Boltzmann Solver.

No alerts have been found for Adaptive Poisson-Boltzmann Solver.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 49 mentions in open access literature.

Listed below are recent publications. The full list is available at FDI Lab - SciCrunch.org.

Mahana Y, et al. (2024) Structural evidence for protein-protein interaction between the non-canonical methyl-CpG-binding domain of SETDB proteins and C11orf46. Structure (London, England : 1993), 32(3), 304.

Cairo LV, et al. (2024) Stress-dependent condensate formation regulated by the ubiquitin-related modifier Urm1. Cell, 187(17), 4656.

Deák G, et al. (2022) Missense Variants Reveal Functional Insights Into the Human ARID Family of Gene Regulators. Journal of molecular biology, 434(9), 167529.

Zhao R, et al. (2022) Inhibition of histone H3-H4 chaperone pathways rescues C. elegans sterility by H2B loss. PLoS genetics, 18(6), e1010223.

de la Morena-Barrio ME, et al. (2022) Two SERPINC1 variants affecting N-glycosylation of Asn224 cause severe thrombophilia not detected by functional assays. Blood, 140(2), 140.

Jiang X, et al. (2022) DYF-5/MAK-dependent phosphorylation promotes ciliary tubulin unloading. Proceedings of the National Academy of Sciences of the United States of America, 119(34), e2207134119.

Strong LM, et al. (2021) Structural basis for membrane recruitment of ATG16L1 by WIPI2 in autophagy. eLife, 10.

Bründl M, et al. (2021) Simulating PIP2-Induced Gating Transitions in Kir6.2 Channels. Frontiers in molecular biosciences, 8, 711975.

Didychuk AL, et al. (2021) A pentameric protein ring with novel architecture is required for herpesviral packaging. eLife, 10.

Kieuvongngam V, et al. (2020) Structural basis of substrate recognition by a polypeptide processing and secretion transporter. eLife, 9.

Gebala M, et al. (2019) Ion counting demonstrates a high electrostatic field generated by the nucleosome. eLife, 8.

Heidari A, et al. (2018) Electrostatic Variation of Haemagglutinin as a Hallmark of the Evolution of Avian Influenza Viruses. Scientific reports, 8(1), 1929.

Khazina E, et al. (2018) Human LINE-1 retrotransposition requires a metastable coiled coil and a positively charged N-terminus in L1ORF1p. eLife, 7.

Lin DH, et al. (2018) Structural and functional analysis of mRNA export regulation by the nuclear pore complex. Nature communications, 9(1), 2319.

Guo YR, et al. (2017) Structure-based membrane dome mechanism for Piezo mechanosensitivity. eLife, 6.

Ou X, et al. (2017) Ion- and water-binding sites inside an occluded hourglass pore of a trimeric intracellular cation (TRIC) channel. BMC biology, 15(1), 31.

Maharana J, et al. (2017) NOD1CARD Might Be Using Multiple Interfaces for RIP2-Mediated CARD-CARD Interaction: Insights from Molecular Dynamics Simulation. PloS one, 12(1), e0170232.

Vargas AA, et al. (2017) On Biophysical Properties and Sensitivity to Gap Junction Blockers of Connexin 39 Hemichannels Expressed in HeLa Cells. Frontiers in physiology, 8, 38.

Hardianto A, et al. (2017) Exploration of charge states of balanol analogues acting as ATP-competitive inhibitors in kinases. BMC bioinformatics, 18(Suppl 16), 572.

Monroe N, et al. (2017) Structural basis of protein translocation by the Vps4-Vta1 AAA ATPase. eLife, 6.