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Dockground: Benchmarks, Docoys, Templates, and other knowledge resources for DOCKING

RRID:SCR_007412 Type: Tool

Proper Citation

Dockground: Benchmarks, Docoys, Templates, and other knowledge resources for DOCKING (RRID:SCR_007412)

Resource Information

URL: http://dockground.bioinformatics.ku.edu/

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Description: Data sets, tools and computational techniques for modeling of protein interactions, including docking benchmarks, docking decoys and docking templates. Adequate computational techniques for modeling of protein interactions are important because of the growing number of known protein 3D structures, particularly in the context of structural genomics. The first release of the DOCKGROUND resource (Douguet et al., Bioinformatics 2006: 22:2612-2618) implemented a comprehensive database of cocrystallized (bound) protein-protein complexes in a relational database of annotated structures. Additional releases added features to the set of bound structures, such as regularly updated downloadable datasets: automatically generated nonredundant set, built according to most common criteria, and a manually curated set that includes only biological nonobligate complexes along with a number of additional useful characteristics. Also included are unbound (experimental and simulated) protein-protein complexes. Complexes from the bound dataset are used to identify crystallized unbound analogs. If such analogs do not exist, the unbound structures are simulated by rotamer library optimization. Thus, the database contains comprehensive sets of complexes suitable for large scale benchmarking of docking algorithms. Advanced methodologies for simulating unbound conformations are being explored for the next release. The Dockground project is developed by the Vakser lab at the Center for Bioinformatics at the University of Kansas. Parts of Dockground were codeveloped by Dominique Douguet from the Center of Structural Biochemistry (INSERM U554 - CNRS UMR5048), Montpellier, France.

Synonyms: Dockground, Dockground: Benchmarks Docoys Templates other knowledge resources for DOCKING, Dockground: Benchmarks Docoys Templates and other knowledge resources for DOCKING

Resource Type: data set, data or information resource

Defining Citation: PMID:17803215, PMID:16928732

Keywords: protein 3d structure, protein interaction, protein interface, protein model, structural genomics, co-crystallized, protein complex, protein recognition, protein modeling, structure prediction, protein-protein complex, benchmark

Funding: NIH ; NIGMS R01 GM074255; NIGMS R01 GM61889

Resource Name: Dockground: Benchmarks, Docoys, Templates, and other knowledge resources for DOCKING

Resource ID: SCR_007412

Alternate IDs: nif-0000-02757

Record Creation Time: 20220129T080241+0000

Record Last Update: 20250428T053327+0000

Ratings and Alerts

No rating or validation information has been found for Dockground: Benchmarks, Docoys, Templates, and other knowledge resources for DOCKING.

No alerts have been found for Dockground: Benchmarks, Docoys, Templates, and other knowledge resources for DOCKING.

Data and Source Information

Source: <u>SciCrunch Registry</u>

Usage and Citation Metrics

We found 8 mentions in open access literature.

Listed below are recent publications. The full list is available at <u>dkNET</u>.

Pozzati G, et al. (2022) Scoring of protein-protein docking models utilizing predicted interface

residues. Proteins, 90(7), 1493.

Vakser IA, et al. (2014) Protein-protein docking: from interaction to interactome. Biophysical journal, 107(8), 1785.

Negroni J, et al. (2014) Assessing the applicability of template-based protein docking in the twilight zone. Structure (London, England : 1993), 22(9), 1356.

Sinha R, et al. (2012) Protein docking by the interface structure similarity: how much structure is needed? PloS one, 7(2), e31349.

Ruvinsky AM, et al. (2011) Side-chain conformational changes upon Protein-Protein Association. Journal of molecular biology, 408(2), 356.

Liu S, et al. (2011) DECK: Distance and environment-dependent, coarse-grained, knowledgebased potentials for protein-protein docking. BMC bioinformatics, 12, 280.

Li L, et al. (2011) ASPDock: protein-protein docking algorithm using atomic solvation parameters model. BMC bioinformatics, 12, 36.

Ruvinsky AM, et al. (2008) Chasing funnels on protein-protein energy landscapes at different resolutions. Biophysical journal, 95(5), 2150.