Human Brain Project

Heidelberg Institute for Theoretical Studies

HITS

SDA

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Software for simulating macromolecular diffusion

TECHNOLOGY DESCRIPTION

SDA (Simulation of Diffusional Association) is a Brownian dynamics simulation code that can be used to simulate the diffusion of biomacromolecules in aqueous solution. It is particularly useful for studying the effects of electrostatic steering on molecular diffusional association processes. The association of two molecules can be simulated to compute bimolecular diffusional association rate constants under dilute conditions and to predict the structures of diffusional encounter complexes, subject to biochemical constraints. SDA can also be used to simulate concentrated protein solutions and to investigate the diffusional association of proteins with solid surfaces. SDA 7 is available for standalone use and some of the functionality is implemented in the webSDA webserver.

Prediction of bimolecular diffusional association rate constants

Modelling effects of crowding on macromolecular diffusion

AREAS

Computational Biophysics | Macromolecular Diffusion | Protein Engineering

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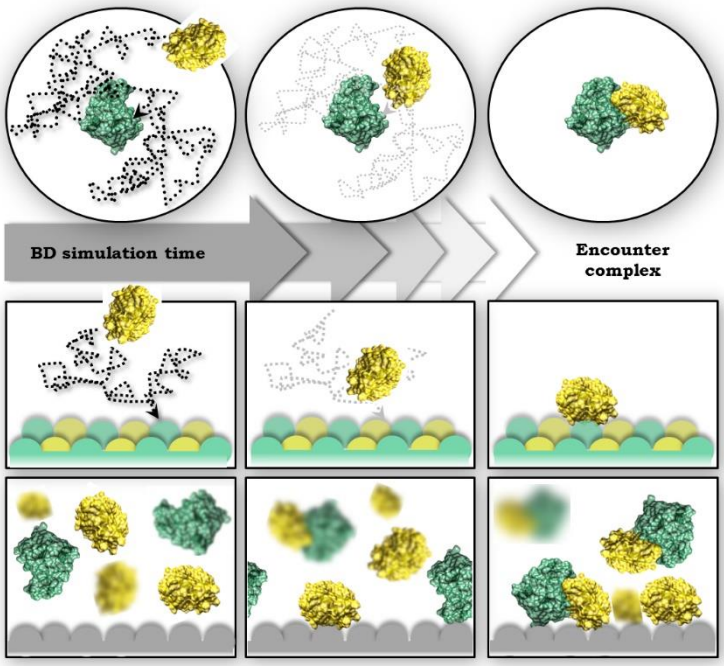
COMPETITIVE ADVANTAGES

- Molecules can be represented by a set of 3D structures
- Association processes between macromolecules and molecular diffusion to surfaces can be simulated
- Includes a simple mean field model for hydrodynamic interactions between proteins
- The ProMetCS force field can be used for protein-gold surface interactions
- Modular structure of the code facilitates implementation of new features
- Simulations can be run in parallel on a shared-memory computer architecture

SDA is a flexible tool to study biomolecular diffusional association processes

APPLICATION & MARKET POTENTIAL

- **Protein science :** SDA has been applied to study protein binding properties in many basic research projects.
- **Protein design and engineering** : SDA can aid the design of point mutations.
- **Systems pharmacology/biology**: SDA can aid the estimation of binding parameters in biochemical kinetic models.
- **Materials science**: SDA has been applied to investigate protein interactions with nanoparticles and solid surfaces.



Bruce et al, (2015) Liquids-Lecture Notes, IAS Series, 28, 259

TECHNOLOGY READINESS LEVEL

1 2 3 4 5 6 7 **8** 9

REFERENCES

- Martinez *et al.* (2015), *J. Comput. Chem.* **36**, 1631.
- Yu *et al.* (2015), *Nucl. Acids Res*. **43**, W220.
- https://mcm.h-its.org/sda
- The simulation methodology in SDA has been continuously developed and applied over the last 25 years; some examples are given at the above URL.

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Tech sheet designed and co-developed by Universidad Politécnica de Madrid