Package ‘fibos’

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Title Occlusion Surface Using the Occluded Surface and Fibonacci Occluded Surface

Version 1.2.3

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Description The Occluded Surface (OS) algorithm is a widely used approach for analyzing atomic packing in biomolecules as described by Pattabiraman N, Ward KB, Fleming PJ (1995) <doi:10.1002/jmr.300080603>. Here, we introduce 'fibos', an 'R' and 'Python' package that extends the 'OS'' methodology, as presented in Soares HHM, Romanelli JPR, Fleming PJ, da Silveira CH (2024) <doi:10.1101/2024.11.01.621530>.

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Imports fs, dplyr, readr, stringr, tidyr, reticulate, glue

NeedsCompilation yes

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Contents

`fibos_config` *Install the 'Python' 'fibos' Module*

Description

This function creates a 'Python' virtual environment and installs the 'Python' module 'fibos' required for the full functionality of this package. It handles different system configurations and ensures that the correct compiler paths are set.

Usage

```
fibos_config()
```

Value

Invisible NULL. Called for its side effects.

Note

This function will install external software (a 'Python' package) on your system. Administrator/sudo privileges might be required on some systems.

Examples

```
# Set up the 'Python' environment and install the required module
fibos_config()
```

`occluded_surface` *Occluded Surface (OS)*

Description

The 'Occluded Surface (OS)' algorithm is a widely used approach for analyzing atomic packing in biomolecules. Here, we introduce 'FIBOS', an 'R' and 'Python' package that extends the 'OS' methodology with enhancements. The homonymous function 'occluded_surface' calculates 'OS' per atom.

Usage

```
occluded_surface(pdb, method = "FIBOS")
```

Arguments

`pdb`	4-digit PDB id (will fetch it from the RCSB repository) or the path to a PDB local file.
`method`	Method to be used: 'OS' (classic) or 'FIBOS'(default).The classic 'OS' covers the surface radially with one of the axes as a reference when allocating the dots. In 'FIBOS', Fibonacci spirals were used to allocate the dots, which is known to produce lower axial anisotropy as well as more evenly spaced points on a sphere.

Details

'Occluded Surface (OS)' (Pattabiraman et al. 1995) method distributes dots (representing patches of area) across the atom surfaces. Each dot has a normal that extends until it reaches either a van der Waals surface of a neighboring atom (the dot is considered occluded) or covers a distance greater than the diameter of a water molecule (the dot is considered non-occluded and disregarded). Thus, with the summed areas of dots and the lengths of normals, it is possible to compose robust metrics capable of inferring the average packing density of atoms, residues, proteins, as well as any other group of biomolecules.

For more details, see (Fleming et al, 2000) and (Soares, et al, 2024)

Value

A table containing:

`ATOM` the atomic contacts for each atom.

`NUMBER OF POINTS` the number of dots (patches of area) on atomic surface.

`AREA` the summed areas of dots.

`RAYLENGTH` the average lengths of normals normalized by 2.8 Å (water diameter). So, raylen is a value between 0 and 1. A raylen close to 1 indicates worse packaging.

`DISTANCE` the average distances of contacts in (Å).

Author(s)

Herson Soares, Joao Romanelli, Patrick Fleming, Carlos Silveira.

References

Fleming PJ, Richards FM (2000). "Protein packing: Dependence on protein size, secondary structure and amino acid composition." `doi:10.1006/jmbi.2000.3750`

Pattabiraman N, Ward KB, Fleming PJ (1995). "Occluded molecular surface: Analysis of protein packing." `doi:10.1002/jmr.300080603`

Soares HHM, Romanelli JPR, Fleming PJ, da Silveira CH (2024). "bioRxiv, 2024.11.01.621530." `doi:10.1101/2024.11.01.621530`

See Also

`osp()`

Examples

```
library(fibos)

#Configure the environment
fibos_config()

# Calculate FIBOS per atom and create .srf files in fibos_files folder
pdb_fibos <- occluded_surface("1ptx", method = "FIBOS")

# Calculate OSP metric per residue from .srf file in fibos_files folder
pdb_osp <- osp(fs::path("fibos_files","prot_1ptx.srf"))
```

`osp` *Occluded Surface Packing (OSP)*

Description

Implements the 'occluded surface' packing density metric (OSP) averaged by residue, as described in (Fleming and Richards 2000).

Usage

```
osp(file)
```

Arguments

`file`	a SRF File (.srf) generated by 'occluded_surface' in fibos_files folder.

Value

A table containing:

`Resnum` residue id.

`Resname` residue name.

`OS` the summed areas of dots in residue.

`` `os*[1-raylen]` `` 'OS' areas weighted by (1-raylen). Raylen is the average lengths of normals normalized by 2.8 Å (water diameter). So, raylen is a value between 0 and 1. A raylen close to 1 indicates worse packaging, and the 'OS' will be reduced.

`OSP` average occluded surface packing value (OSP) by residue.

Author(s)

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References

Fleming PJ, Richards FM (2000). "Protein packing: Dependence on protein size, secondary structure and amino acid composition." `doi:10.1006/jmbi.2000.3750`

Pattabiraman N, Ward KB, Fleming PJ (1995). "Occluded molecular surface: Analysis of protein packing." `doi:10.1002/jmr.300080603`

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See Also

`occluded_surface()`

Examples

```
library(fibos)

#Configure the Environment
fibos_config()

# Calculate FIBOS per atom and create .srf files in fibos_files folder
pdb_fibos <- occluded_surface("1ptx", method = "FIBOS")
# Calculate OSP metric per residue from .srf file in fibos_files folder
pdb_osp <- osp(fs::path("fibos_files","prot_1ptx.srf"))
```

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