REINDEER Software

Protein-Ligand Feature Generator

REINDEER is a software for generating a feature vector for a protein-ligand complex.

REINDEER SOFTWARE
{PROTEIN-LIGAND FEATURE GENERATOR}

Clicking here for more information

Cautions

Implemented Methods

Cautions

1- Provided protein-ligand complex should have hydrogen atoms.

2- File formarts for protein and ligand are *.pdb* and *.mol2*. In the case of ECIF, instead of *.mol2*, *.sdf* file should be provided.

3- All protein-ligand complexes should be provided as the below example:

```
./test
├── 1a1e
│   ├── 1a1e_ligand.mol2
│   ├── 1a1e_ligand.sdf
│   └── 1a1e_protein.pdb
├── 1a28
│   ├── 1a28_ligand.mol2
│   ├── 1a28_ligand.sdf
│   └── 1a28_protein.pdb
├── 1a30
    ├── 1a30_ligand.mol2
    ├── 1a30_ligand.sdf
    └── 1a30_protein.pdb
```

Implemented Methods

Current version of REINDEER provides four feature generation methods:

1- Occurrence of Interatomic Contact (OIC) - Ref

2- Distance-Weighted Interatomic Contact (DWIC) - Ref

3- Extended Connectivity Interaction Feature (ECIF) - Ref

4- Multi-Shell Occurrence of Interatomic Contact (MS-OIC) - Ref

Enter the path of the folder of structures:

../test/

Enter number of CPU core for parallelization:

REINDEER only needs these inputs. For help click on exclamation mark.

-1

Enter a name path for saving generated features:

./feature_vector

Push the button for your desired feature vector:

Generate OIC

By clicking on each botton, feature generation procedure will be started.

Generate DWIC

Generate ECIF

Generate MS-OIC

Generate MS-OIC

After finishing a procedure, this message will be appeared

Generated features are save into ./feature_vector_ms_oic.csv