intDesc-LP ver1.1 Install manual.

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1.   Package Summary of intDesc-LP_ver1.1

The intDesc-LP program archive (intDesc-LP_ver1.1.zip) contains the following files.

```
<intDesc-LP_ver1.1>
├ <install_test> (See this manual: Chapter 2.3)
│  ├ run_test.sh
│  └ data.zip
├ <sample>
│  ├ 3aox_prep0.mol2 (See user manual: chapter 4.1)
│  ├ ligand_select.yaml (See user manual: chapter 4.2)
│  ├ vdw_radius.yaml (See user manual: chapter 4.3)
│  ├ param.yaml (See user manual: chapter 4.4)
│  └ priority.yaml (See user manual: chapter 4.5)
├ interaction.py (Subscript)*
├ interaction_descriptor.py (Main script)*
├ mol2.py (Subscript)*
├ my_math.py (Subscript)*
├ group.yaml** (System file)*
├ water_definition.txt  (See user manual: chapter 4.6)
└ requirements.txt (See this manual: Chapter 2.1)
```

* These files are not edited by the user.

** group.yaml is a system file that lists each interaction and its group. It is mainly referred to when outputting files, especially the group names in the "Interaction Sum list file".

1.1 Definition of interactions handled by intDesc-LP

See supplements to the following papers currently submitted.

Ohta, M. et al., "intDesc: Software for comprehensive and precise identification, visualization, and enumeration of ligand-protein interactions" (Submitted)

2. Install

2.1 Environment required for intDesc-LP

It works with the following software:

- python 3 series （3.8.5) [1]
- python Libraries
  - numpy (1.12.4) [1]
  - networkx (2.6.3) [1]
  - pyyaml (6.0) [1]
  - biopandas (0.2.9) [1]
  - mdanalysis (0.20.1) [1]

1 Version at the time of development

The included "requirements.txt" file can be used to install the necessary libraries.

The execution command is as follows:

```
pip install -r requirements.txt
```

*Use the "pip3" command according to your environment.

2.2 Installation Method

Extract "intDesc-LP_ver1.1.zip" to any directory.

The archive expansion commands are as follows:

```
unzip intDesc-LP_ver1.1.zip
```

2.3 Installation Test

Use "install_test" in the program to test the reproducibility of output results.

Implementation Procedure

1. go to the "install_test" directory
2. Execute the following command.

```
bash run_test.sh
```

When the command is executed, the test is started. After the test is completed, each output file is checked for reproducibility. If reproducibility is confirmed, "OK" is output as shown below.

```
L_IT009.pml: OK
L_IT009_dup.pml: OK
L_IT009_dup_interaction_count_list.csv: OK
L_IT009_dup_interaction_sum_list.csv: OK
L_IT009_dup_on14.pml: OK
L_IT009_dup_on14_interaction_count_list.csv: OK
…
```

If reproducibility is not acceptable, "FAILED" will be output as shown below.

```
L_IT019.csv: OK
L_IT019.pml: OK
L_IT019.txt: FAILED
md5sum: WARNING: 1 computed checksum did NOT match
```