intDesc-LP ver1.1 User manual

Riken
Center for Computational Science
HPC- and AI-driven Drug Development Platform Division
2023/11/04

Table of Contents

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 install manual: Chapter 2.3)
│  ├ run_test.sh
│  └ data.zip
├ <sample>
│  ├ 3aox_prep0.mol2 (See this manual: chapter 4.1)
│  ├ ligand_select.yaml (See this manual: chapter 4.2)
│  ├ vdw_radius.yaml (See this manual: chapter 4.3)
│  ├ param.yaml (See this manual: chapter 4.4)
│  └ priority.yaml (See this 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 this manual: chapter 4.6)
└ requirements.txt (See install 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. Usage

```
$ python interaction_descriptor.py [function name] ¥
                        [mol2 file] ¥
                        [Interaction target molecule specification file] ¥
                        [van der waals radius definition file] ¥
                        [interaction threshold setting file] ¥
                        [interaction priority file] ¥
                        [prefix of output file name] ¥
                        (--allow_mediate_position numerical value) ¥
                        (--on_14) ¥
                        (--dup) ¥
                        (--no_mediate) ¥
                        (--no_out_total) ¥
                        (--no_out_pml)
```

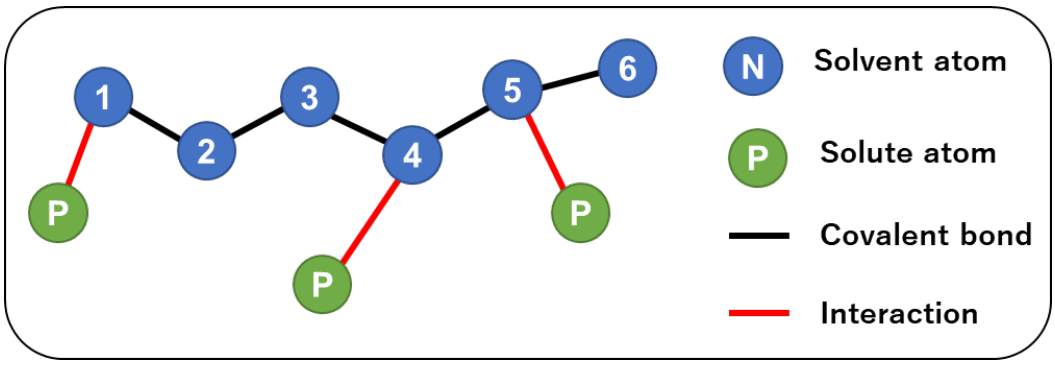
Arguments	Explain
Function name	Specify executive function. Currently, only "**ligand**" can be specified to perform protein-ligand interaction calculations.
mol2 file	See Chapter 3.2.1
Interaction target molecule specification file	See Chapter 3.2.3
van der waals radius definition file	See Chapter 3.2.4
interaction threshold setting file	See Chapter 3.2.5
interaction priority file	See Chapter 3.2.6
refix of output file name	prefix (string without extension) of the output file. (e.g. output)

[option: --allow_mediate_position “value”]

Specify this option to limit the output for solvent-mediated interactions. For solvent-mediated interactions, the output is restricted if the positional relationship between solvent atoms is farther than specified.

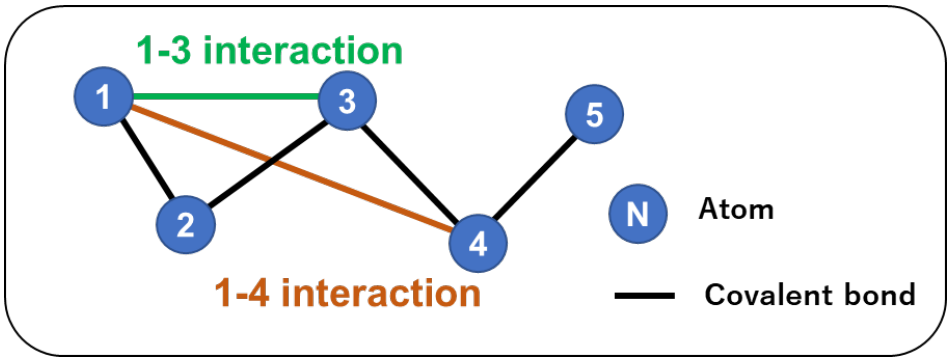
Example: When "--allow_mediate_pos 4" is specified.

In the example in the figure below, "Solute P vs Solvent 1 - Solvent 4 vs Solute P" is detected as a solvent-mediated interaction, but "Solute P vs Solvent 1 - Solvent 5 vs Solute P" is not.



[option: --on_14]

Specify this option if you wish to detect 1-3, 1-4 interactions. Among the interactions detected between atoms connected by covalent bonds, as shown in the figure below, the interactions detected between neighboring atoms through 1~2 atoms will be detected.



[option: --dup]

Specify this option if you want to detect overlapping interactions between the same heavy atoms.

[option: --no_mediate]

Specify this option if you do not want to detect "solvent-mediated interactions.

[option: --no_out_total]

Specify this option if you do not want to output a "total results file”.

[option: --no_out_pml]

Specify this option if you do not want to output a "visualization file”.

3. Example（L_IT009）

Example calculation of intDesc for ALK (protein) and EMH (ligand) (IT009)

3.1 Execution Commands

```
$ python interaction_descriptor.py ligand¥
                          IT009_3aox_ALK_moe_addH_minH_gasteiger_mod.mol2 ¥
                          mol_select.yaml ¥
                          vdw_radius.yaml ¥
                          param.yaml ¥
                          priority.yaml ¥
                          L_IT009
```

3.2

3.2.1 Mol2 file（IT009_3aox_ALK_moe_addH_minH_gasteiger_mod.mol2）

See Section 4.1

```
@<TRIPOS>MOLECULE
3AOX.A
5520 5340 539 0 0
BIOPOLYMER
USER_CHARGES


@<TRIPOS>ATOM
   1 N      -16.8940    35.4790    -2.3240 N.3     1 SER1086  -0.3180 BACKBONE
   2 H1     -16.6844    35.8513    -3.2575 H       1 SER1086   0.1190 BACKBONE
   3 H2     -17.2581    36.2855    -1.8256 H       1 SER1086   0.1190 BACKBONE
   4 CA     -15.5750    35.1060    -1.7420 C.3     1 SER1086   0.1077 BACKBONE
   5 HA     -15.6920    34.9911    -0.6637 H       1 SER1086   0.0579 BACKBONE
……
@<TRIPOS>BOND.
   1    1    2  1   BACKBONE.
   2    1    3  1   BACKBONE.
   3    1    4  1   BACKBONE.
   4    4    5  1   BACKBONE.
   5    4    6  1   BACKBONE.
……
@<TRIPOS>SUBSTRUCTURE.
  1 SER1086    4 RESIDUE 4 A  SER  1.
  2 THR1087   15 RESIDUE 4 A  THR  2.
  3 ILE1088   29 RESIDUE 4 A  ILE  2.
  4 MET1089   48 RESIDUE 4 A  MET  2.
  5 THR1090   65 RESIDUE 4 A  THR  2.
……
```

3.2.2 Interaction target molecule specification file (mol_select.yaml)

See Chapter 4.2

```
ligand:
  name: EMH
solvent_1:
  name: HOH
  chain: A
protein:
  chain: A
```

3.2.3 van der waals radius definition file (vdw_radius.yaml)

See Chapter 4.3

Use intDesc-LP_ver1.1/sample/vdw_radius.yaml when performing calculations.

```
# Van Der Waals radius definition file
# Version for the second half of FY2022
#
# Van Der Waals Radius of the elements
# # FORMAT RULE
# # - [Element symbol]:[Van der Waals radius]
# # - Enter [Van der Waals radius] in "Å".
H: 1.2
C: 1.7
N: 1.55
O: 1.52
F: 1.47
S: 1.8
Cl: 1.75
Br: 1.85
I: 1.98
Fe: 2.44
Zn: 2.39
Ca: 2.62
Mg: 2.51
Ni: 2.40
P: 1.80
Na: 2.27
K: 2.75
```

3.2.4 interaction threshold setting file (param.yaml)

See Chapter 4.4

Use intDesc-LP_ver1.1/sample/param.yaml when performing calculations.

```
# Interaction threshold setting file
# Version for the second half of FY2022
# interaction_type dist(Ang) angle1(deg) angle2_min(deg) angle2_max(deg)
HB_OH_(N,O): 3.2 60.0 60.0 180.0

# interaction_type dist(Ang) angle1(deg) angle2(deg) angle3(deg)
HB_OH_OH: 3.2 60.0 90.0 60.0

# interaction_type dist(Ang) angle1(deg) angle1_N4(deg) angle2_min(deg)
angle2_max(deg)
HB_NH_(N,O): 3.2 60.0 90.0 60.0 180.0

# interaction_type dist(Ang) angle1(deg) angle1_N4(deg) angle2(deg)
angle3(deg)
HB_NH_OH: 3.2 60.0 90.0 90.0 60.0

# interaction_type dist(Ang)
(Met)_(X): 0.2
```

3.2.5 interaction priority file (priority.yaml)

See Chapter 4.5

Use intDesc-LP_ver1.1/sample/priority.yaml when performing calculations.

```
# Interaction priority specification file
# Version for the second half of FY2022
# Label: Score
OMulPol: 3

CH_PI: 4
CH_N: 2
C_N_vdw: 0
CH_O: 2
C_O_vdw: 0
CH_S: 2
C_S_vdw: 0

S_PI: 4
S_N: 2
S_N_vdW: 0
S_O: 2
S_O_vdW: 0
S_S: 2
SH_S: 1
S_S_vdW: 0
……
```

3.3 Output Files

All output files begin with prefix (L_IT009).

3.3.1 Raw list file (L_IT009_raw_list.txt)

See Chapter 5.1

```
R data/L_IT009/IT009_3aox_ALK_moe_addH_minH_gasteiger_mod.mol2
L EMH
S1 HOH

K L-Pro
I1-2 CH_N 4.1389 4.8789 3.0775 4.4810 5.4621 109.8123 164.7869
LC1 EMH 901 N25 4748 N.pl3
LN1 EMH 901 C29 4749 C.3 1
LN1 EMH 901 C30 4755 C.3 1
LN1 EMH 901 C10 4709 C.ar 1
PC2 LEU 1122 CD2 584 C.3
PN2 LEU 1122 HD21 585 H 1
……
```

3.3.2 Interaction Count list file（L_IT009_interaction_count_list.csv）

See Chapter 5.2

```
L#CH_F#Pro,0
L#CH_F#S1,0
L#CH_F#S1#CH_F#Pro,0
L#CH_F#S1#CH_Hal_Br#Pro,0
L#CH_F#S1#CH_Hal_Cl#Pro,0
L#CH_F#S1#CH_Hal_I#Pro,0
L#CH_F#S1#CH_N#Pro,0
L#CH_F#S1#CH_O#Pro,0
L#CH_F#S1#CH_PI#Pro,0
L#CH_F#S1#CH_S#Pro,0
L#CH_F#S1#Ca_X#Pro,0
L#CH_F#S1#Cl_X#Pro,0
L#CH_F#S1#Dipo#Pro,0
L#CH_F#S1#Elec_NH_N#Pro,0
L#CH_F#S1#Elec_NH_O#Pro,0
L#CH_F#S1#Elec_OH_N#Pro,0
L#CH_F#S1#Elec_OH_O#Pro,0
……
```

3.3.3 One-hot list file（L_IT009_one_hot_list.csv）

See Chapter 5.3

```
LP_HB_NH_O,LP_Elec_NH_N,LP_CH_O,LP_CH_N,LP_CH_PI,LP_Dipo,LP_vdW,LS1_Elec_OH_N,LS1_CH_O,LS1_vdW,S1P_HB_OH_O,S1P
_HB_NH_O,S1P_Elec_NH_O,S1P_CH_O,S1P_vdW,dist,interaction_label,molcular_type,chain,residue,residue_number,atom
_name,atom_number,atom_type,partner_molcular_type,partner_chain,partner_residue,par
tner_residue_number,partner_atom_name,partner_atom_number,partner_atom_type
0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,3.6407,CH_PI,ligand,A,EMH,901,C2,4736,C.ar,protein,A,LEU,1256,CD1,2518,C.3
0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,3.8550,CH_PI,ligand,A,EMH,901,N9,4737,N.pl3,protein,A,LEU,1256,CD2,2522,C.3
0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,3.8959,vdW,ligand,A,EMH,901,N9,4737,N.pl3,protein,A,EDO,802,C1,4783,C.3
……
```

3.3.4 Interaction Sum list file（L_IT009_interaction_sum_list.csv）

See Chapter 5.4

```
0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,3.8550,CH_PI,ligand,A,EMH,901,N9,4737,N.pl3,protein,A,LEU,1256,CD2,2522,C.3
0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,3.8959,vdW,ligand,A,EMH,901,N9,4737,N.pl3,protein,A,EDO,802,C1,4783,C.3
1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,2.7433,HB_NH_O,ligand,A,EMH,901,N9,4737,N.pl3,protein,A,EDO,802,O2,4791,O.3
0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,4.1059,CH_PI,ligand,A,EMH,901,C14,4739,C.ar,protein,A,LEU,1122,CD1,580,C.3
0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,4.2350,CH_PI,ligand,A,EMH,901,C14,4739,C.ar,protein,A,GLY,1202,CA,1656,C.3
0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,3.6976,Dipo,ligand,A,EMH,901,C16,4740,C.2,protein,A,MET,1199,O,1625,O.2
0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,3.6976,Dipo,ligand,A,EMH,901,O20,4741,O.2,protein,A,MET,1199,C,1624,C.2
0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,3.6112,CH_O,ligand,A,EMH,901,O20,4741,O.2,protein,A,ALA,1148,CB,797,C.3
……
```

3.3.5 pml file（L_IT009.pml）

See Chapter 5.5

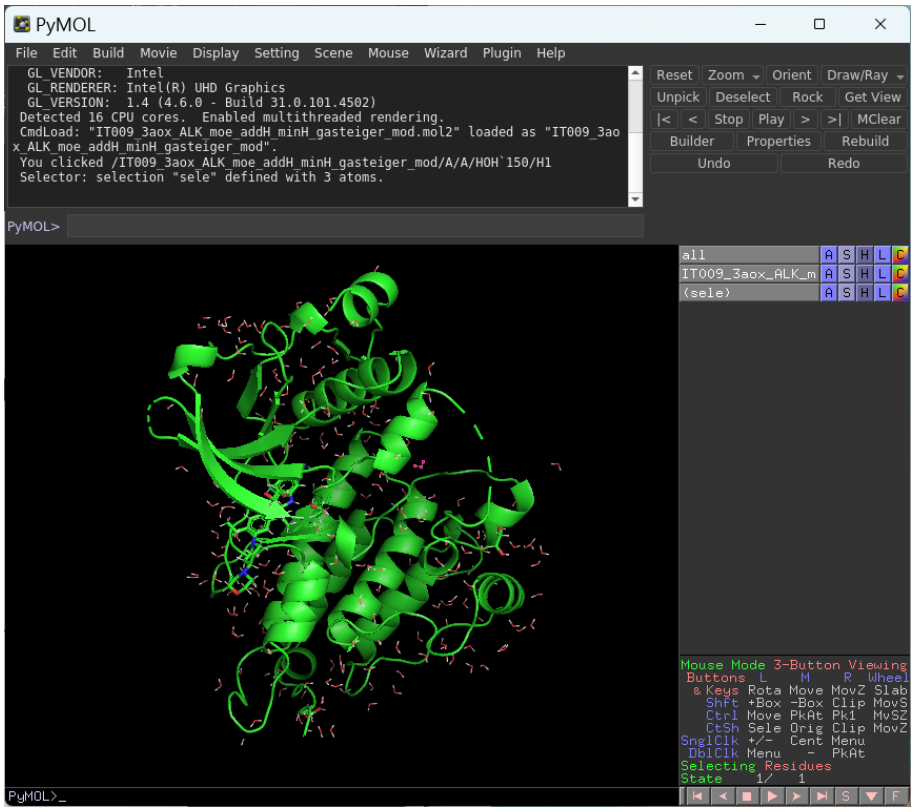
This file is used to display the interactions detected by intDesc-LP using the molecular graphics program PyMOL.

3.3.5.1 Visualization with PyMOL

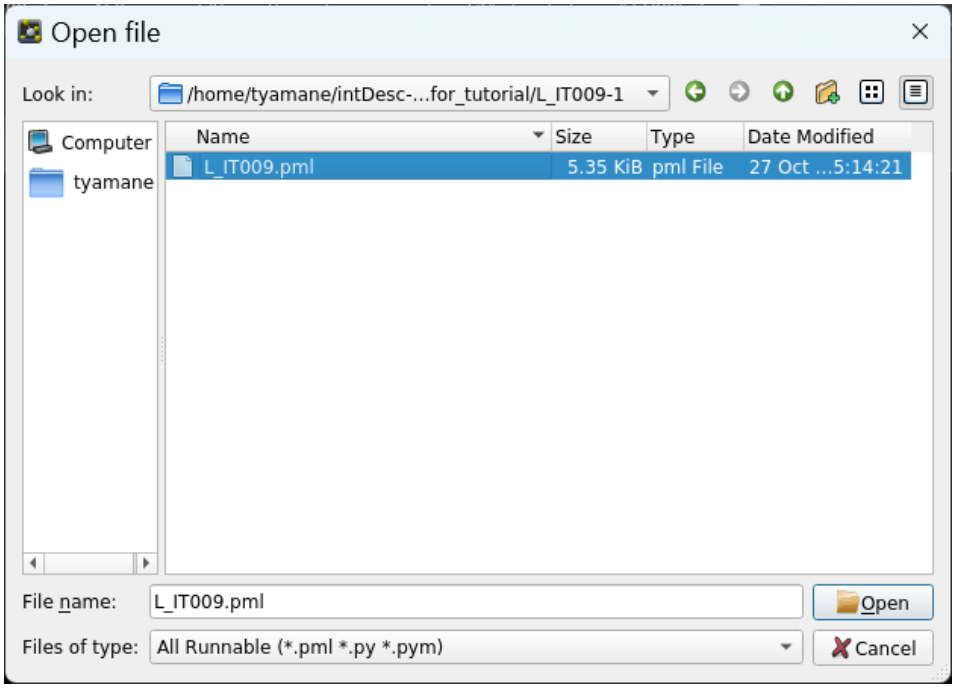
The output pml file (L_IT009.pml) is used for visualization. (See Chapter 5.5)

The process of visualization with PyMOL is as followsa:

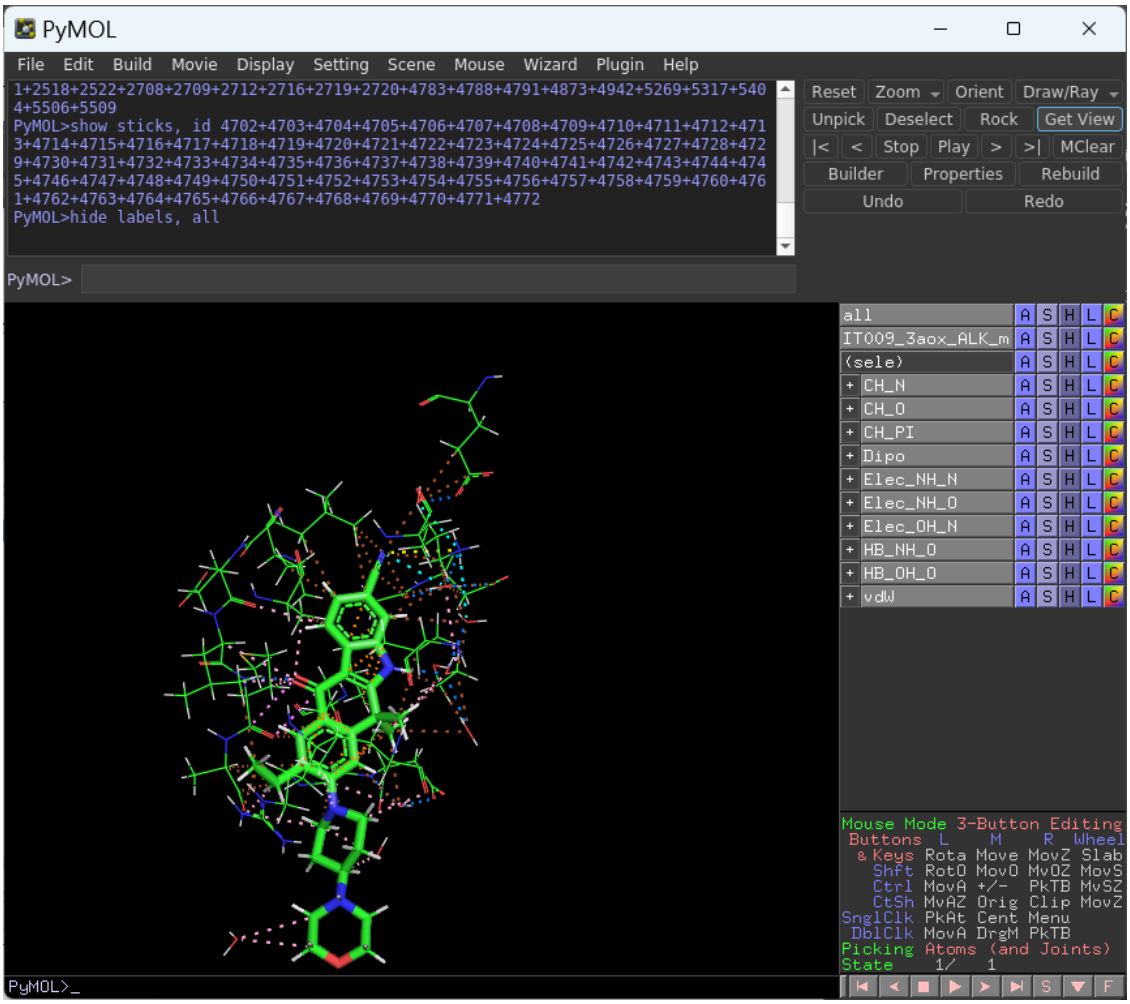
1. Display mol2 file (IT009_3aox_ALK_moe_addH_minH_gasteiger_mod.mol2) in PyMOL



2. Select "L_IT009.pml" from “File > RunScript” and click "Open



3. The interaction descriptor to be analyzed is displayed.



4. Input files

4.1 Structural file

Load a file in Mol2 format (reference: https://zhanggroup.org//DockRMSD/mol2.pdf) as a structure file.

This program refers to the following sections in the file.

Section	Necessity	Remarks
ATOM	○	—
BOND	○	—
SUBSTRUCTURE	—	Information in this section is required when using Chain IDs in the Interacting Molecule Designation File.

4.2 Interaction target molecule specification file

File defining the molecular structure to be calculated（.yaml)。

Since the program does not automatically detect molecular structures, it is necessary to explicitly specify the molecular structure in the structure file, such as protein, ligand, solvent, etc.

```
# Format)
[Molecular type name]:
  [item]: [value]

# Example)
solvent:
  name: HOH
ligand:
  name: EMH
protein:
  chain: A
```

Molecular type nam※1	Target molecule
protein_[N]	protein
ligand_[N]	ligand
solvent_[N]	solvent

※1 Multiple molecular type names may be listed by number.

・unnumbered：protein

・numbered：protein_[N] (N=1,2,…n)

Item	Subject	Necessity	Remarks
num	Residue number	○	“num” cannot be specified at the same time as “name”.
name	Residue name	○	“name” cannot be specified at the same time as “num”.
chain	Chain ID		When specifying more than one, NUM and NAME cannot be specified.
type	backbone / sidechain		Main chain: atoms that are "C, N, CA, O, H, HA Side chain: Atoms other than "C, N, CA, O, H, HA

The format for each item is as follows

Items	Format	Examples	sample description
Residue number	num: A	Specify residue number 100	num: 100
Residue number(s)	num: [A, B]	Specify residue numbers 100, 101	num: [100, 101]
Residue number (range)	num: A:B	Specify residue numbers 100 to 110	num: 100:110
residue name	name: A	Specify residue name Gly	name: GLY
Residue name(s)	name: [A, B]	Specify residue name Gly, Arg	name: [GLY, ARG]
Chain ID	chain: A	Specify Chain H	chain: H
Chain ID(s)	chain: [A, B]	Specify Chain H, L	chain: [H, L]
Main chaine	type: main	-	-
Side chaine	type: side	-	-

[Example: When specifying multiple chains]

	Items			
target molecule	residue name	residue number	Chain	Main/side chain
protein			A, B	
ligand	EMH			
solvent	HOH		A	

```
solvent:
  name: HOH
  chaih: A
ligand:
  name: EMH
protein:
  chain: [A, B]
```

[Example: Define multiple ligands.]

	Items			
target molecule	residue name	residue number	Chain	Main/side chain
protein			A	
ligand	XXX, YYY			
solvent	HOH			

```
solvent:
  name: HOH
ligand:
  name: [XXX, YYY]
protein:
  chain: [A, B]
```

4.3 van der waals radius definition file

van der waals A file (.yaml) to set the radius.

```
# Format)
[chemical symbol]: [van der waals radius (Å)]

# Sample description)
H: 1.2
C: 1.7
N: 1.55
O: 1.52
…
```

Target atoms: "H, C, N, O, F, S, Cl, Br, I, Fe, Zn, Ca, Mg, Ni, P, Na, K".

4.4 interaction threshold setting file

A file (.yaml) that sets the thresholds to be used for interaction determination.

```
# Format)
[interaction label]: [threshold]

# sample description)
…
CH_F: 1.0 3.05 180.0 137.15
NH_F: 1.0 2.99 180.0 145
SH_F: 1.0 3.3 180.0 145
…
```

[Interaction threshold table definition]

interaction specification string	interaction name	threshold							
HB_NH_(N,O)	Hydrogen bond 1	dist	angle1	angle1_N4	angle2_min	angle2_max	–	–	–
HB_NH_OH	Hydrogen bond 1	dist	angle1	angle1_N4	angle2	angle3	–	–	–
HB_OH_(N,O)	Hydrogen bond 2	dist	angle1	angle2_min	angle2_max	–	–	–	–
HB_OH_OH	Hydrogen bond 2	dist	angle1	angle2	angle3	–	–	–	–
CH_N	CH_N interaction	buffer	dist1	dist2	angle1	angle2	–	–	–
CH_O	CH_O interaction	buffer	dist1	angle1	–	–	–	–	–
SH_N	SH_N interaction	buffer	angle1	–	–	–	–	–	–
SH_O	SH_O interaction	buffer	angle1	–	–	–	–	–	–
Elec_(NH,OH)_(N,O)	electrostatic interaction	dist	buffer	angle1	angle1_N4	angle2_min	angle2_max	–	–
Elec_(N, O)H_OH	electrostatic interaction	dist	buffer	angle1	angle1_N4	angle2	angle3	–	–
vdW	van_der_waals interaction	buffer	diff	dist1	dist2	dist3	–	–	–
PI_PI	π-π stacking interaction	buffer	angle1	angle1	–	–	–	–	–
Dipo	dipole-dipole interaction	buffer	angle1	angle2	angle3	charge	hydro	–	–
OMulPol	orthogonal multipole interaction	buffer	angle1_min	angle1_max	angle2	angle3	charge	–	–
CH_PI	CH-π interaction	buffer	coef	dist1	dist2	angle1	angle2	–	–
NH_PI	NH-π interaction	buffer	coef	dist1	dist2	angle1	angle2	–	–
OH_PI	OH-π interaction	buffer	coef	dist1	dist2	angle1	angle2	–	–
SH_PI	SH-π interaction	buffer	coef	dist1	dist2	angle1	angle2	–	–
Hal_(X)_N	Halogen Interaction I	buffer	angle	–	–	–	–	–	–
Hal_(X)_O	Halogen Interaction I	buffer	angle	–	–	–	–	–	–
Hal_(X)_S	Halogen Interaction I	buffer	angle	–	–	–	–	–	–
CH_F	CH-F interaction	buffer	dist1	angle1	angle2	–	–	–	–
NH_F	NH-F interaction	buffer	dist1	angle1	angle2	–	–	–	–
OH_F	OH-F interaction	buffer	dist1	angle1	angle2	dist2	–	–	–
SH_F	SH-F interaction	buffer	dist1	angle1	angle2	–	–	–	–
CH_Hal_(X)	CH-Hal interaction	buffer	angle1	angle2	angle3	angle4	–	–	–
NH_Hal_(X)	NH-Hal interaction	buffer	angle1	angle2	angle3	angle4	–	–	–
OH_Hal_(X)	OH-Hal interaction	buffer	angle1	angle2	angle3	angle4	–	–	–
SH_Hal_(X)	SH-Hal interaction	buffer	angle1	angle2	angle3	angle4	–	–	–
Hal_PI_(X)	Haloge n-π interaction	buffer	coef	angle1	dihedral	–	–	–	–
CH_S	CH-S interaction	buffer	dist1	dist2	angle1	angle2	–	–	–
OH_S	OH-S interaction	buffer	angle1	–	–	–	–	–	–
SH_S	SH-S interaction	buffer	angle1	–	–	–	–	–	–
NH_S	NH-S interaction	buffer	dist1	dist2	angle1_min	angle1_max	angle2_min	angle2_max	–
S_O	S-O interaction	buffer	–	–	–	–	–	–	–
S_N	S-N interaction	buffer	–	–	–	–	–	–	–
S_PI	S-π interaction	buffer	coef	angle1	angle2	dihedral	–	–	–
S_S	S-S interaction	buffer	angle1	–	–	–	–	–	–
S_F	S-F interaction	buffer	angle1	–	–	–	–	–	–
(Met)_(X)	Interactions between metals and heavy atoms	dist	–	–	–	–	–	–	–
(Ion)_(X)	Interactions between ions and heavy atoms	buffer	–	–	–	–	–	–	–

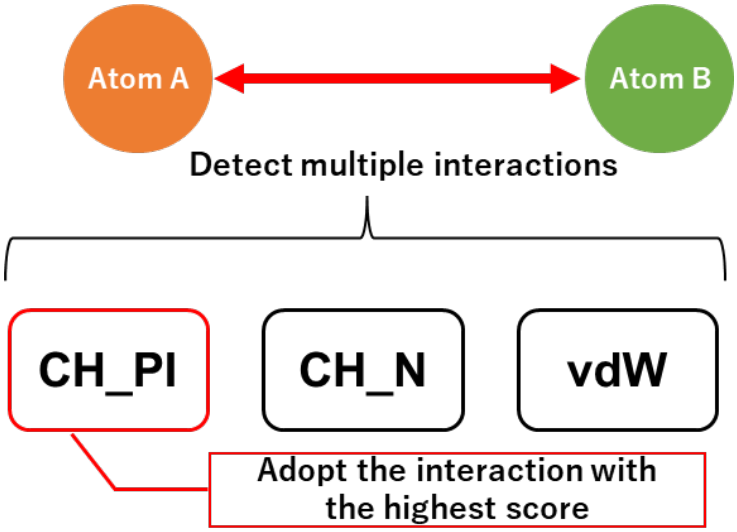
4.5 interaction priority file

A file (.yaml) that sets the priority of the interaction.

When multiple interactions are determined between the same heavy atoms, the interaction with the highest score among the priorities set in this file is assigned.

```
# Format)
[interaction label]: [priority]

# sample description)
CH_PI: 3
CH_N: 2
C_N_vdw: 0
…
```



4.6 Molecule Definition File

File to define water molecule names (.txt)

・Lines beginning with "#" are recognized as comment lines.

・Define the name of the water molecule on each line.

```
# Definition of water molecule name
# List the names recognized by Pymol
HOH
TIP
```

5. Output files

5.1 Raw list file

File with output detailing detected interactions.

```
R 3aox_prep0.mol2  ……(1) input structure file name
L EMH              ……(2) Selected ligands
S HOH              ……(3) Selected Solvents
                                                    (4)Details section
K L-Pro
I1-2 CH_N 4.1389 4.8789 3.0769 4.4810 5.4621 109.8123 164.8236
LC1 EMH 901 N25 4767 N.pl3
LN1 EMH 901 C29 4768 C.3 1
LN1 EMH 901 C30 4770 C.3 1
LN1 EMH 901 C10 4746 C.ar 1
PC2 LEU 1122 CD2 581 C.3
PN2 LEU 1122 CG 579 C.3 1
PN2 LEU 1122 HD22 591 H 1
PN2 LEU 1122 HD21 590 H 1
PN2 LEU 1122 HD23 592 H 1

K L-Pro
I1-2 CH_O 3.5377 3.9295 2.6266 4.7151 95.6216 143.6507
LC1 EMH 901 C4 4741 C.ar
LN1 EMH 901 C6 4743 C.ar ar
LN1 EMH 901 C2 4759 C.ar ar
LN1 EMH 901 H4 4777 H 1
PC2 GLU 1197 O 1613 O.2
PN2 GLU 1197 C 1612 C.2 2
```

[(4) Detailes section]

<table>
<tr><th>item</th><th>Description.</th><th>Format</th></tr>
<tr><td>K</td><td>Labels according to atomic pairs of detected interactions
<table>
<tr><th>label</th><th>Interaction pair</th></tr>
<tr><td>L-Pro</td><td>Ligand - Protein</td></tr>
<tr><td>L-S[N]</td><td>Ligand - Solvent</td></tr>
<tr><td>L-S[N]-Pro</td><td>Ligand - Solvent - Protein</td></tr>
</table></td><td>K [label]</td></tr>
<tr><td>I1-2</td><td>Interaction labels between the first and second atoms and geometrical information of the criteria※1</td><td>I1-2 [interaction label] [distance, angle etc]…</td></tr>
<tr><td>I3-4</td><td>Interaction labels between the third and fourth atoms and geometrical information of the criteria</td><td>I3-4 [interaction label] [distance, angle etc]…</td></tr>
<tr><td>LC1</td><td>The first atom involved in the interaction (ligand atom)</td><td>LC1 [residue name] [residue number] [atom name] [atom number] [atom_type]</td></tr>
<tr><td>PC2</td><td>The second atom involved in the interaction (protein atom)</td><td>PC2[residue name] [residue number] [atom name] [atom number] [atom_type]</td></tr>
<tr><td>SC2</td><td>The second atom involved in the interaction (solvent atom)</td><td>SC2[residue name] [residue number] [atom name] [atom number] [atom_type]</td></tr>
<tr><td>SC3</td><td>The third atom involved in the interaction (solvent atom)</td><td>SC3 [residue name] [residue number] [atom name] [atom number] [atom_type]</td></tr>
<tr><td>PC4</td><td>The fourth atom involved in the interaction (protein atom)</td><td>PC4 [residue name] [residue number] [atom name] [atom number] [atom_type]</td></tr>
<tr><td>LN*</td><td>The atom that interacts with LC* through covalent bonds.</td><td>LN* [residue name] [residue number] [atom name] [atom number] [atom_type] [bond type with LC*]</td></tr>
<tr><td>PN*</td><td>The atom that interacts with PC* through covalent bonds.</td><td>PN* [residue name] [residue number] [atom name] [atom number] [atom_type] [bond type with PC*]</td></tr>
<tr><td>SN*</td><td>The atom that interacts with SC* through covalent bonds.</td><td>SN* [residue name] [residue number] [atom name] [atom number] [atom_type] [bond type with SC*]</td></tr>
</table>

※1 See [I line details] for information displayed in each interaction.

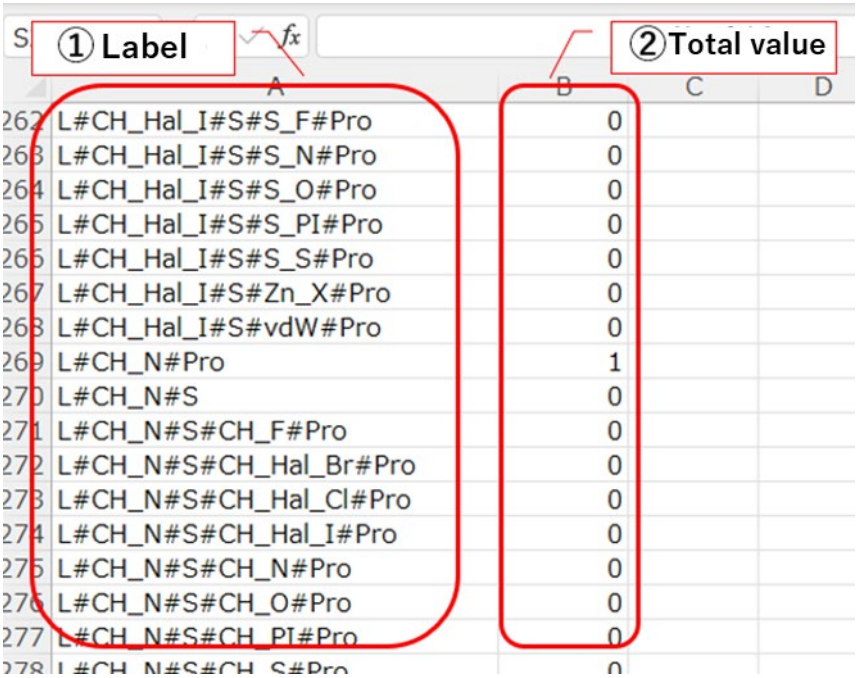
[I line details]

Interaction name	Interaction label	Item 1.	Item 2.	Item 3.	Item 4.	Item 5.	Item 6.	Item 7.	Item 8.	Item 9.	Item 10.
Hydrogen bond 1	HB_NH_N	distance(d)	angle(θ1)	angle(θ2)	–	–	–	–	–	–	–
Hydrogen bond 1	HB_NH_O	distance(d)	angle(θ1)	angle(θ2)	–	–	–	–	–	–	–
Hydrogen bond 1	HB_NH_O	distance(d)	angle(θ1)	angle(θ2)	angle(θ3)	–	–	–	–	–	–
Hydrogen bond 2	HB_OH_N	distance(d)	angle(θ1)	angle(θ2)	–	–	–	–	–	–	–
Hydrogen bond 2	HB_OH_O	distance(d)	angle(θ1)	angle(θ2)	–	–	–	–	–	–	–
Hydrogen bond 2	HB_OH_O	distance(d)	angle(θ1)	angle(θ2)	angle(θ3)	–	–	–	–	–	–
CH_N interaction	CH_N	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	angle(θ2)	–	–	–
CH_N interaction	CH_N	distance(d1)	distance(d2)	distance(d3)	distance(d4)	angle(θ1)	angle(θ2)	–	–	–	–
CH_O interaction	CH_O	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
CH_O interaction	CH_O	distance(d1)	distance(d2)	distance(d3)	distance(d4)	angle(θ1)	–	–	–	–	–
SH_N interaction	SH_N	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
SH_N interaction	SH_N	distance(d1)	distance(d2)	distance(d3)	distance(d4)	angle(θ1)	–	–	–	–	–
SH_O interaction	SH_O	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
SH_O interaction	SH_O	distance(d1)	distance(d2)	distance(d3)	distance(d4)	angle(θ1)	–	–	–	–	–
Electrostatic interaction	Elec_NH_N	distance(d)	angle(θ1)	angle(θ2)	–	–	–	–	–	–	–
Electrostatic interaction	Elec_NH_O	distance(d)	angle(θ1)	angle(θ2)	–	–	–	–	–	–	–
Electrostatic interaction	Elec_NH_O	distance(d)	angle(θ1)	angle(θ2)	angle(θ3)	–	–	–	–	–	–
Electrostatic interaction	Elec_OH_N	distance(d)	angle(θ1)	angle(θ2)	–	–	–	–	–	–	–
Electrostatic interaction	Elec_OH_O	distance(d)	angle(θ1)	angle(θ2)	–	–	–	–	–	–	–
Electrostatic interaction	Elec_OH_O	distance(d)	angle(θ1)	angle(θ2)	angle(θ3)	–	–	–	–	–	–
Van Del Waals interaction	vdW	distance(d1)	distance(dNearest)	distance(diffVDW)	–	–	–	–	–	–	–
π-π stacking interaction	PI_PI	distance(d)	angle(θ1)	angle(θ2)	–	–	–	–	–	–	–
Dipole-dipole interaction	Dipo	distance(d1)	distance(d2)	angle(θ1)	angle(θ2)	angle(θ3)	charge(atom1)	charge(atom4)	–	–	–
Dipole-dipole interaction	Dipo	distance(d1)	distance(d2)	angle(θ1)	angle(θ2)	angle(θ3)	charge(atom2)	charge(atom3)	–	–	–
Orthogonal multipole interaction	OMulPol	distance(d1)	distance(d2)	angle(θ1)	angle(θ2)	angle(θ3)	charge difference(e1)	charge difference(e2)	–	–	–
CH-π interaction	CH_PI	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	distance(dNrm)	angle(θ1)	angle(θ2)	–	–
NH-π interaction	NH_PI	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	distance(dNrm)	angle(θ1)	angle(θ2)	–	–
OH-π interaction	OH_PI	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	distance(dNrm)	angle(θ1)	angle(θ2)	–	–
SH-π interaction	SH_PI	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	distance(dNrm)	angle(θ1)	angle(θ2)	–	–
Halogen Interaction I	Hal_Cl_N	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	–	–	–	–	–	–
Halogen Interaction I	Hal_Cl_N	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
Halogen Interaction I	Hal_Cl_O	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	–	–	–	–	–	–
Halogen Interaction I	Hal_Cl_O	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
Halogen Interaction I	Hal_Cl_S	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	–	–	–	–	–	–
Halogen Interaction I	Hal_Cl_S	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
Halogen Interaction I	Hal_Br_N	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	–	–	–	–	–	–
Halogen Interaction I	Hal_Br_N	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
Halogen Interaction I	Hal_Br_O	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	–	–	–	–	–	–
Halogen Interaction I	Hal_Br_O	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
Halogen Interaction I	Hal_Br_S	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	–	–	–	–	–	–
Halogen Interaction I	Hal_Br_S	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
Halogen Interaction I	Hal_I_N	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	–	–	–	–	–	–
Halogen Interaction I	Hal_I_N	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
Halogen Interaction I	Hal_I_O	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	–	–	–	–	–	–
Halogen Interaction I	Hal_I_O	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
Halogen Interaction I	Hal_I_S	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	–	–	–	–	–	–
Halogen Interaction I	Hal_I_S	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–

Interaction name	Interaction label	Item 1.	Item 2.	Item 3.	Item 4.	Item 5.	Item 6.	Item 7.	Item 8.	Item 9.	Item 10.
NH-F interaction	NH_F	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	–	–	–	–	–
OH-F interaction	OH_F	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	–	–	–	–	–
SH-F interaction	SH_F	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	–	–	–	–	–
CH-F interaction	CH_F	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	–	–	–	–	–
CH-Hal interaction	CH_Hal_Cl	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	angle(θ3)	angle(θ4)	–	–	–
CH-Hal interaction	CH_Hal_Br	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	angle(θ3)	angle(θ4)	–	–	–
CH-Hal interaction	CH_Hal_I	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	angle(θ3)	angle(θ4)	–	–	–
OH-Hal interaction	OH_Hal_Cl	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	angle(θ3)	angle(θ4)	–	–	–
OH-Hal interaction	OH_Hal_Br	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	angle(θ3)	angle(θ4)	–	–	–
OH-Hal interaction	OH_Hal_I	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	angle(θ3)	angle(θ4)	–	–	–
NH-Hal interaction	NH_Hal_Cl	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	angle(θ3)	angle(θ4)	–	–	–
NH-Hal interaction	NH_Hal_Br	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	angle(θ3)	angle(θ4)	–	–	–
NH-Hal interaction	NH_Hal_I	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	angle(θ3)	angle(θ4)	–	–	–
SH-Hal interaction	SH_Hal_Cl	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	angle(θ3)	angle(θ4)	–	–	–
SH-Hal interaction	SH_Hal_Br	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	angle(θ3)	angle(θ4)	–	–	–
SH-Hal interaction	SH_Hal_I	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	angle(θ2)	angle(θ3)	angle(θ4)	–	–	–
Halogen-π interaction	Hal_PI_Cl	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(dNrm)	distance(d5)	distance(d6)	angle(θ1)	Dihedral angle(τ1)	–
Halogen-π interaction	Hal_PI_Br	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(dNrm)	distance(d5)	distance(d6)	angle(θ1)	Dihedral angle(τ1)	–
Halogen-π interaction	Hal_PI_I	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(dNrm)	distance(d5)	distance(d6)	angle(θ1)	Dihedral angle(τ1)	–
CH-S interaction	CH_S	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	angle(θ2)	–	–	–
CH-S interaction	CH_S	distance(d1)	distance(d2)	distance(d3)	distance(d4)	angle(θ1)	angle(θ2)	–	–	–	–
OH-S interaction	OH_S	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
OH-S interaction	OH_S	distance(d1)	distance(d2)	distance(d3)	distance(d4)	angle(θ1)	–	–	–	–	–
SH-S interaction	SH_S	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
SH-S interaction	SH_S	distance(d1)	distance(d2)	distance(d3)	distance(d4)	angle(θ1)	–	–	–	–	–
NH-S interaction	NH-S	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
NH-S interaction	NH-S	distance(d1)	distance(d2)	distance(d3)	distance(d4)	angle(θ1)	–	–	–	–	–
S-O interaction	S_O	distance(d1)	distance(d2)	distance(d3)	distance(d4)	–	–	–	–	–	–
S-O interaction	S_O	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	–	–	–	–	–
S-F interaction	S_F	distance(d1)	distance(d2)	distance(d3)	distance(d4)	angle(θ1)	–	–	–	–	–
S-F interaction	S_F	distance(d1)	distance(d2)	distance(d3)	angle(θ1)	–	–	–	–	–	–
S-N interaction	S_N	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	–	–	–	–	–
S-π interaction	S_PI	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	distance(dNrm)	angle(θ1)	–	–	–
S-π interaction	S_PI	distance(d1)	distance(d2)	distance(d4)	distance(d5)	distance(dNrm)	distance(d6)	distance(d7)	angle(θ2)	Dihedral angle(τ1)	–
S-S interaction	S_S	distance(d1)	distance(d2)	distance(d3)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–
S-S interaction	S_S	distance(d1)	distance(d2)	distance(d4)	distance(d5)	angle(θ1)	–	–	–	–	–
S-S interaction	S_S	distance(d1)	distance(d2)	distance(d3)	distance(d4)	angle(θ1)	–	–	–	–	–
Interactions between metals and heavy atoms	Fe_X (X=Atoms other than hydrogen)	distance(d1)	distance(d2)	distance(d3)	–	–	–	–	–	–	–
Interactions between metals and heavy atoms	Zn_X (X=Atoms other than hydrogen)	distance(d1)	distance(d2)	distance(d3)	–	–	–	–	–	–	–
Interactions between metals and heavy atoms	Ca_X (X=Atoms other than hydrogen)	distance(d1)	distance(d2)	distance(d3)	–	–	–	–	–	–	–
Interactions between metals and heavy atoms	Mg_X (X=Atoms other than hydrogen)	distance(d1)	distance(d2)	distance(d3)	–	–	–	–	–	–	–
Interactions between metals and heavy atoms	Ni_X (X=Atoms other than hydrogen)	distance(d1)	distance(d2)	distance(d3)	–	–	–	–	–	–	–
Interactions between ions and heavy atoms	Na_X (X=Atoms other than hydrogen)	distance(d)	–	–	–	–	–	–	–	–	–
Interactions between ions and heavy atoms	K_X (X=Atoms other than hydrogen)	distance(d)	–	–	–	–	–	–	–	–	–
Interactions between ions and heavy atoms	Cl_X (X=Atoms other than hydrogen)	distance(d)	–	–	–	–	–	–	–	–	–

5.2 Interaction Count list file

A file that outputs the number of interactions detected.



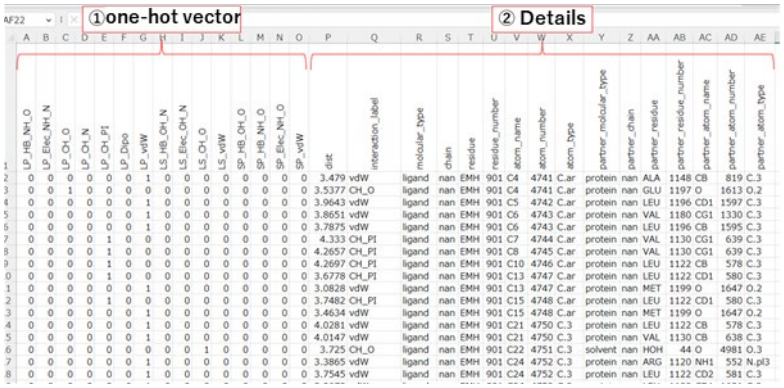
【①Label】

①Label	Interaction pair
L#[interaction label]#Pro	ligand - protein
L#[interaction label]#S[N]	ligand - solvent
L#[interaction label]#S[N]#[interaction label]#Pro	ligand - solvent – protein
Pro#[interaction label]#S[N]	protein - solvent

5.3 One-hot list file

A file in which the detected interactions are output as one hot vector.

This file is only output by the Ligand-Protein Interaction Descriptor Calculator.



【① one-hot vector】

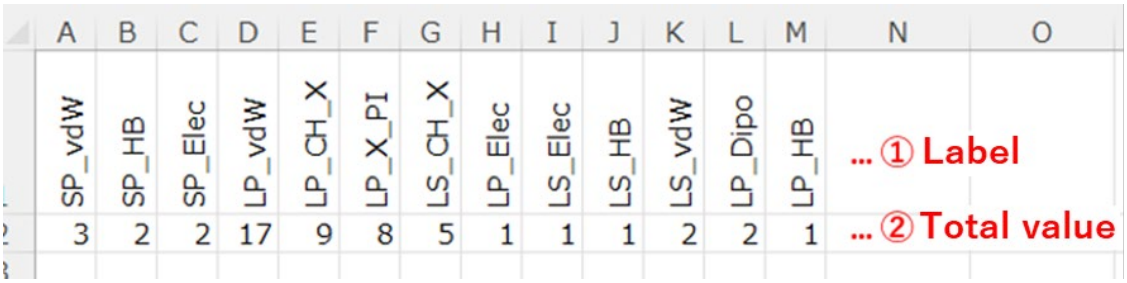
ラベル書式	相互作用ペア
LP_[interaction label]	Ligand – Protein
LS[N]_[interaction label]	Ligand – Solvent
S[N]P_[interaction label]	Solvent – Protein

【② Details】

項目	説明
dist	Interatomic distance of interacting pairs
interaction_label	interaction label
molcular_type	Molecular type of interaction pair (ligand, solvent)
chain	Chain ID of interaction pair (ligand, solvent)
residue	Residue name of interaction pair (ligand, solvent)
residue_number	Residue number of interaction pair (ligand, solvent)
atom_name	Atomic name of interaction pair (ligand, solvent)
atom_number	Atomic number of interaction pair (ligand, solvent)
atom_type	atom_type of interaction pair (ligand, solvent)
partner_molcular_type	Molecular type of interacting pair (protein, water)
partner_chain	Chain ID of interaction pair (protein, water)
partner_residue	Residue name of interaction pair (protein, water)
partner_residue_number	Residue number of interaction pair (protein, water)
partner_atom_name	Atomic name of interacting pair (protein, water)
partner_atom_number	Atomic number of interacting pair (protein, water)
partner_atom_type	atom_type of interaction pair (protein, water)

5.4 Interaction Sum list file

A file containing Interaction tabulation results by group of detected interactions.



【① Label】

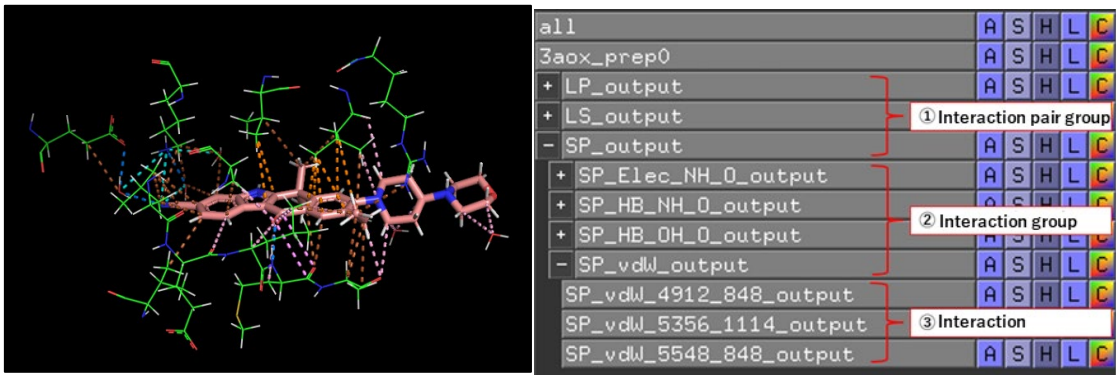
ラベル	相互作用ペア
LP_[group name]	Ligand – Protein
LS[N]_[group name]	Ligand – Solvent
S[N]P_[group name]	Solvent – Protein

group	target interaction
HB	HB_OH_O
	HB_NH_O
	HB_OH_N
	HB_NH_N
Elec	Elec_OH_O
	Elec_NH_O
	Elec_OH_N
	Elec_NH_N
CH_X	CH_O
	CH_N
	CH_S
	CH_F
	CH_Hal_Cl
	CH_Hal_Br
	CH_Hal_I
OH_X	OH_S
	OH_F
	OH_Hal_Cl
	OH_Hal_Br
	OH_Hal_I
NH_X	NH_S
	NH_F
	NH_Hal_Cl
	NH_Hal_Br
	NH_Hal_I
SH_X	SH_O
	SH_N
	SH_S
	SH_F
	SH_Hal_Cl
	SH_Hal_Br
	SH_Hal_I
X_PI	CH_PI
	NH_PI
	OH_PI
	SH_PI
	S_PI
	Hal_PI_Cl
	Hal_PI_Br
	Hal_PI_I
Hal_X	Hal_Cl_O
	Hal_Cl_N
	Hal_Cl_S
	Hal_Br_O
	Hal_Br_N
	Hal_Br_S
	Hal_I_O
	Hal_I_N
	Hal_I_S
S_X	S_O
	S_N
	S_S
	S_F
OMulPol	OMulPol
PI_PI	PI_PI
Dipo	Dipo
Metal_X	Fe_X
	Zn_X
	Ca_X
	Mg_X
	Ni_X
Ion_X	Na_X
	K_X
	Cl_X
vdW	vdW

5.5 pml file

File to visualize the detected interactions in PyMol.

After starting PyMol and loading the structure file and then the pml file, the interactions are visualized. Only residues containing interaction atoms are displayed, and each interaction is indicated by a distance object. The distance objects are grouped by interaction pair and interaction.



【①Interaction pair group】

Interaction pair group	Interaction pair
LP_[suffix]	Ligand - Protein
LS[N] _[suffix]	Ligand - Solvent
S[N]P_[suffix]	Protein - Solvent

【②Interaction group】

Format：[Interaction pair label]_[Interaction label]_[suffix]

【③ Interaction（distance object)】

Format：[Interaction pair label]_[Interaction label]_[atomic serial number]_[atomic serial number]_[suffix]

Interaction label	Color
HB_NH_N	marine
HB_NH_O	marine
HB_OH_N	marine
HB_OH_O	marine
CH_N	pink
CH_O	pink
SH_N	marine
SH_O	marine
Elec_NH_N	cyan
Elec_NH_O	cyan
Elec_OH_N	cyan
Elec_OH_O	cyan
vdW	brown
PI_PI	warmpink
Dipo	violet
OMulPol	yelloworange
CH_PI	orange
NH_PI	tv_orange
OH_PI	brightorange
SH_PI	tv_orange
Hal_Cl_N	violetpurple
Hal_Cl_O	violetpurple
Hal_Cl_S	violetpurple
Hal_Br_N	violetpurple
Hal_Br_O	violetpurple
Hal_Br_S	violetpurple
Hal_I_N	violetpurple
Hal_I_O	violetpurple
Hal_I_S	violetpurple
NH_F	palegreen
OH_F	palegreen
SH_F	palegreen
CH_F	palegreen
CH_Hal_Cl	splitpea
CH_Hal_Br	splitpea
CH_Hal_I	splitpea
NH_Hal_Cl	splitpea
NH_Hal_Bl	splitpea
NH_Hal_I	splitpea
OH_Hal_Cl	splitpea
OH_Hal_Br	splitpea
OH_Hal_I	splitpea
SH_Hal_Cl	splitpea
SH_Hal_Br	splitpea
SH_Hal_I	splitpea
Hal_PI_Cl	deeppurple
Hal_PI_Br	deeppurple
Hal_PI_I	deeppurple
CH_S	sand
OH_S	chocolate
SH_S	chocolate
NH_S	sand
S_O	Splitpea
S_N	Splitpea
S_PI	lightorange
S_S	sand
S_F	sand
Fe_X	purple
Zn_X	purple
Ca_X	purple
Mg_X	purple
Ni_X	purple
Na_X	lightteal
K_X	lightteal
Cl_X	lightteal

6. Interaction list

Interaction label	Interaction
HB_OH_O	Hydrogen bond（OH-O）
HB_NH_O	Hydrogen bond（NH-O）
HB_OH_N	Hydrogen bond（OH-N）
HB_NH_N	Hydrogen bond（NH-N）
Elec_OH_O	Electrostatic interaction（OH-O）
Elec_NH_O	Electrostatic interaction（NH-O）
Elec_OH_N	Electrostatic interaction（OH-N）
Elec_NH_N	Electrostatic interaction（NH-N）
CH_O	CH-O interaction
CH_N	CH-N interaction
CH_S	CH-S interaction
CH_F	CH-F interaction
CH_Hal_Cl	CH-Halogen Interaction（CH-Cl）
CH_Hal_Br	CH-Halogen Interaction（CH-Br）
CH_Hal_I	CH-Halogen Interaction（CH-I）
OH_S	OH-S interaction
OH_F	OH-F interaction
OH_Hal_Cl	OH-Halogen interaction（OH-Cl）
OH_Hal_Br	OH-Halogen interaction（OH-Br）
OH_Hal_I	OH-Halogen interaction（OH-I）
NH_S	NH-S Interaction
NH_F	NH-F Interaction
NH_Hal_Cl	NH-Halogen interaction（NH-Cl）
NH_Hal_Br	NH-Halogen interaction（NH-Br）
NH_Hal_I	NH-Halogen interaction（NH-I）
SH_O	SH-O interaction
SH_N	SH-N interaction
SH_S	SH-S interaction
SH_F	SH-F interaction
SH_Hal_Cl	SH-Halogen interaction（SH-Cl）
SH_Hal_Br	SH-Halogen interaction（SH-Br）
SH_Hal_I	SH-Halogen interaction（SH-I）
CH_PI	CH-PI interaction
NH_PI	NH-PI interaction
OH_PI	OH-PI interaction
SH_PI	SH-PI interaction
S_PI	S-PI interaction
Hal_PI_Cl	Halogen-π interaction（CH-PI）
Hal_PI_Br	Halogen-π interaction（CH-PI）
Hal_PI_I	Halogen-π interaction（CH-PI）
Hal_Cl_O	Halogen interaction（Cl-O）
Hal_Cl_N	Halogen interaction（Cl-N）
Hal_Cl_S	Halogen interaction（Cl-S）
Hal_Br_O	Halogen interaction（Br_O）
Hal_Br_N	Halogen interaction（Br_N）
Hal_Br_S	Halogen interaction（Br_S）
Hal_I_O	Halogen interaction（I_O）
Hal_I_N	Halogen interaction（I_N）
Hal_I_S	Halogen interaction（I_S）
S_O	S-O interaction
S_N	S-N interaction
S_S	S-S interaction
S_F	S-F interaction
OMulPol	Orthogonal multipole interactions
PI_PI	π - π stacking interaction
Dipo	Dipole - Dipole Interaction
Fe_X	metal interaction (Fe-X)
Zn_X	metal interaction (Zn-X)
Ca_X	metal interaction (Ca-X)
Mg_X	metal interaction (Mg-X)
Ni_X	metal interaction (Ni-X)
Na_X	ionic interaction (Na-X)
K_X	ionic interaction (K-X)
Cl_X	ionic interaction (Cl-X)
vdW	van der waals interaction