| **No.** | **Script** | **Purpose** |
| --- | --- | --- |
| 01 | chain\_data.py | make the table for chain list |
| 02 | compare\_foldx\_ppcheck.py | compare FoldX and PPCheck results |
| 03 | compare\_naccess.py | cross-check interface, RBI and pRBI residues with NACCESS records and remove buried residues |
| 04 | consurf\_data.py | to cross-check cs results with other residues |
| 05 | consurfdata\_inter.py | convert Consurf data into table with aa, score and count columns |
| 06 | consurfdata\_rbi.py | convert Consurf data into table with aa, score and count columns for tRBIs and pRBIs |
| 07 | create\_pdb\_list.py | creates a list of PDB ids from a file |
| 08 | final\_consurf.py | convert Consurf data into table with aa, score and count columns |
| 09 | final\_foldx.py | to get hotspot propensities |
| 10 | final\_intaa.py | convert INTAA data into table with aa, score and count columns |
| 11 | find\_interface\_res.py | identify all interface residues interacting within a 5 angstrom cut-off radius + assigns interaction types based on the amino acids and specific atoms involved (PIC-based) |
| 12 | find\_rbi.py | additional filters over interface residues to identify RBIs and pRBIs |
| 13 | find\_rbi\_no\_hydrogen\_filter.py | RBI criteria, without hydrogen filter |
| 14 | foldx\_data.py | to cross-check FoldX hs results with other residues |
| 15 | foldxdata.py | trbi-prbi hs propensities |
| 16 | foldx\_data\_inter.py | convert FoldX data into table with aa, score and count columns for interface residues |
| 17 | get\_all\_interface\_pdb\_names.py | to get names of all PDBs with interface residues |
| 18 | get\_all\_rbi\_names.py | to get a list of all PDBs with RBIs |
| 19 | ic\_data.py | crosscheck IC data with other residues |
| 20 | intaa\_data.py | to crosscheck INTAA results with other residues |
| 21 | intaa\_inter.py | convert INTAA data into table with aa pair, score and count columns |
| 22 | intaa\_rbi.py | convert INTAA data into table with aa pair, score and count columns |
| 23 | interface\_aa\_freq.py | generate interface\_aa\_count.csv |
| 24 | interface\_interaction\_pairs.py | find a.a. pairs at the interface |
| 25 | interface\_int\_freq.py | generates interface\_int\_type.csv |
| 26 | kruskal\_wilcoxon.py | code for the Kruskal-Wallis and Wilcoxon tests |
| 27 | networkx.py | run NetworkX for network analysis |
| 28 | nox.py | parse NOXClass output |
| 29 | num\_rbi.py | count number of pRBIs per RBI |
| 30 | plot.R | some figures for the project |
| 31 | plot\_deg\_dis.R | plot degree distributions |
| 32 | ppcheck\_data.py | compile PPCheck data |
| 33 | rbi\_aa\_freq.py | generates nofilter\_trbi\_aa\_prop.csv and nofilter\_prbi\_aa\_prop.csv |
| 34 | rbi\_interface.py | check if RBI file's and interface file's PDB IDs match, and copy to new folder if they do |
| 35 | rbi\_int\_freq.py | generates nofilter\_rbi\_int\_type.csv |
| 36 | run\_rbi.py | run find\_rbi\_no\_hydrogen\_filter.py |