

### Supplementary Table 1.

**List of sequence and protein structure databases implemented in the ENDscript server.** Sequence databases are used by ENDscript to detect proteins homologous to the PDB query (PDBAA is the default). Protein structure and internal databases are employed to speed-up the ENDscript process and to gather additional information compiled in the resulting data and files. All these databases are automatically updated on a weekly basis.

| Database name                      | Description   | Source                             |
|------------------------------------|---|------------------------------------|
| <i>Sequence databases</i>          |   |                                    |
| ARATH                              | Complete proteome from <i>Arabidopsis thaliana</i>        | UniProtKB/Swiss-Prot               |
| BOVIN                              | Complete proteome from <i>Bos taurus</i>                  | UniProtKB/Swiss-Prot               |
| CAEEL                              | Complete proteome from <i>Caenorhabditis elegans</i>      | UniProtKB/Swiss-Prot               |
| CANFA                              | Complete proteome from <i>Canis familiaris</i>            | UniProtKB/Swiss-Prot               |
| CHICK                              | Complete proteome from <i>Gallus gallus</i>               | UniProtKB/Swiss-Prot               |
| DANRE                              | Complete proteome from <i>Danio rerio</i>                 | UniProtKB/Swiss-Prot               |
| DROME                              | Complete proteome from <i>Drosophila melanogaster</i>     | UniProtKB/Swiss-Prot               |
| HUMAN                              | Complete proteome from <i>Homo sapiens</i>                | UniProtKB/Swiss-Prot               |
| MOUSE                              | Complete proteome from <i>Mus musculus</i>                | UniProtKB/Swiss-Prot               |
| <u>PDBAA</u>                       | Sequences derived from PDB protein structures             | NCBI/RCSB PDB                      |
| PDBAA50                            | Clustering of PDB protein chains at 50% sequence identity | Maintained by the ENDscript server |
| PDBAA70                            | Clustering of PDB protein chains at 70% sequence identity | Maintained by the ENDscript server |
| PDBAA90                            | Clustering of PDB protein chains at 90% sequence identity | Maintained by the ENDscript server |
| PDBAA95                            | Clustering of PDB protein chains at 95% sequence identity | Maintained by the ENDscript server |
| PIG                                | Complete proteome from <i>Sus scrofa</i>                  | UniProtKB/Swiss-Prot               |
| RAT                                | Complete proteome from <i>Rattus norvegicus</i>           | UniProtKB/Swiss-Prot               |
| SWISSPROT                          | Non-redundant, manually annotated and reviewed            | UniProtKB/Swiss-Prot               |
| TREMBL                             | Automatically annotated and not reviewed                  | UniProtKB/TrEMBL                   |
| YEAST                              | Complete proteome from <i>Saccharomyces cerevisiae</i>    | UniProtKB/Swiss-Prot               |
| <i>Protein structure databases</i> |   |                                    |
| PDB                                | PDB coordinate files                                      | RCSB PDB                           |
| PDB/BIOUNIT                        | PDB biological assembly coordinate files                  | RCSB PDB                           |
| <i>Internal databases</i>          |   |                                    |
| END_SPDB_DB                        | PDB coordinate files processed by the program SPDB        | Maintained by the ENDscript server |
| END_DSSP_DB                        | PDB coordinate files processed by the program DSSP        | Maintained by the ENDscript server |

23. Martin, J. and Lavery, R. (2012) Arbitrary protein-protein docking targets biologically relevant interfaces. BMC biophysics, 5, 7.
24. Ritchie, D.W. and Venkatraman, V. (2010) Ultra-fast FFT protein docking on graphics processors. Bioinformatics (Oxford, England), 26, 2398-2405.