

### **DB3:**

A database of protein-protein complexes consisting of 1879 co-crystallized interacting native structures (each containing two chains) with resolution better than 2 Å, and no missing backbone atoms; The database was assembled using the 'Build Database' option from Dockground [1] and used before in [2,3]. Hydrogen atoms were geometrically fixed to all structures using REDUCE [4], version. 2 [5].

### **References:**

1. Protein models: the grand challenge of protein docking.  
Anishchenko I. et al.  
Proteins Struct. Funct. Bioinforma, 2014, 82, 278–287.
2. SARAMAint: The Complementarity Plot for Protein-Protein Interface  
Sankar Basu, Dhananjay Bhattacharyya, and Bjorn Wallner\*  
Journal of Bioinformatics and Intelligent Control, 2014, 3:309-314.
3. Finding correct protein-protein docking models using ProQDock.  
Sankar Basu, Bjorn Wallner\*  
Bioinformatics. 2016, 32 (12): i262-i270.  
doi: 10.1093/bioinformatics/btw257
4. Asparagine and glutamine: using hydrogen atom contacts in the choice of sidechain amide orientation, Word, et al., 1999, J. Mol. Biol. **285**, 1735-1747.
5. <http://kinemage.biochem.duke.edu/downloads/software/reduce/reduce.2.21.mod040509dcr.linux.RH9>