**Supplementary Information**

Contents:

* Supplementary Methods.
* Table S1.
* Figure S1.
* Figure S2.
* Figure S3.

**Supplementary Methods**

Collection of motifs from Protein Data Bank systems with Rosetta

***Protein Data Bank File Collection***

***Protein Data Bank File Preparation***

***Protein-Ligand Motif Collection***

***Protein-Ligand Duplicate Motif Removal***