**Figure S1.** Protein-protein interaction scoring matrices: (A) sidechain-sidechain van-der Waals scoring matrix; (B) sidechain-backbone van-der Waals scoring matrix; (C) sidechain-sidechain special-bond scoring matrix; (D) sidechain-backbone special-bond scoring matrix. The sidechain-sidechain scoring matrices are symmetric and sidechain-backbone scoring matrices are nonsymmetric. For sidechain-sidechain van-der Waals scoring matrix, the scores are high (yellow blocks) when large-aliphatic residues (i.e. Val, Leu, Ile, and Met) interact to large-aliphatic residues or aromatic residues (i.e. Phe, Tyr, and Trp) interact to aromatic residue. In contrast, the scores are low (orange blocks) when nonpolar residues interact to polar residues. The top 2 highest scores are 3.0 (Met. interacting to Met) and 2.9 (Trp interacting to Trp). For sidechain-sidechain special-bond scoring matrix, the scores are high when an interacting residues (i.e. Cys to Cys) form a disulfide bond or basic residues (i.e. Arg, Lys, and His) interact to acidic residues (Asp and Glu). The scoring values are zero if nonpolar residues interact to other residues.
Figure S2. The relationship between Z-values of the 3D-partner server and the sequence identity on the data set NR-563. The 3D-partner can yield 4,206 protein-protein interaction candidates by setting three criteria, including the sequence identity is more than 15%, CR exceeds 50%, and E-value is lower than 0.05. Among these 4,206 candidates, 226 (CR > 80% and sequence identity > 25%) and 3,980 candidates were recoded in the positive (blue) and negative (red) sets, respectively.