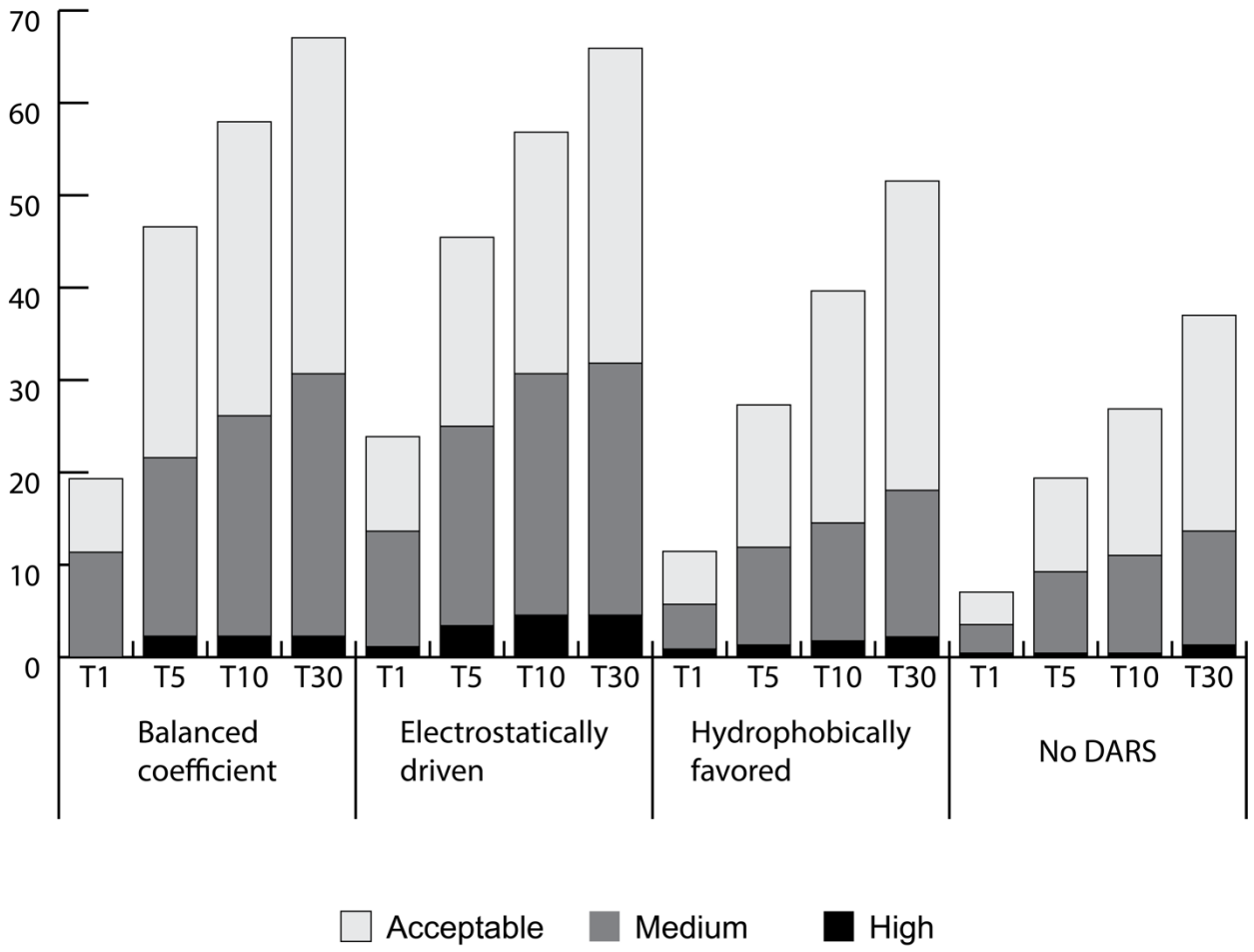

Figure S1. Success rates for enzyme containing complexes using different sets of weight in the scoring function of ClusPro, related to Figure 4A. The four standard sets in the server are the balanced set (00), the electrostatic-favored set (02), the hydrophobicity favored set (04), and the set without the pairwise structure based potential DARS (06).

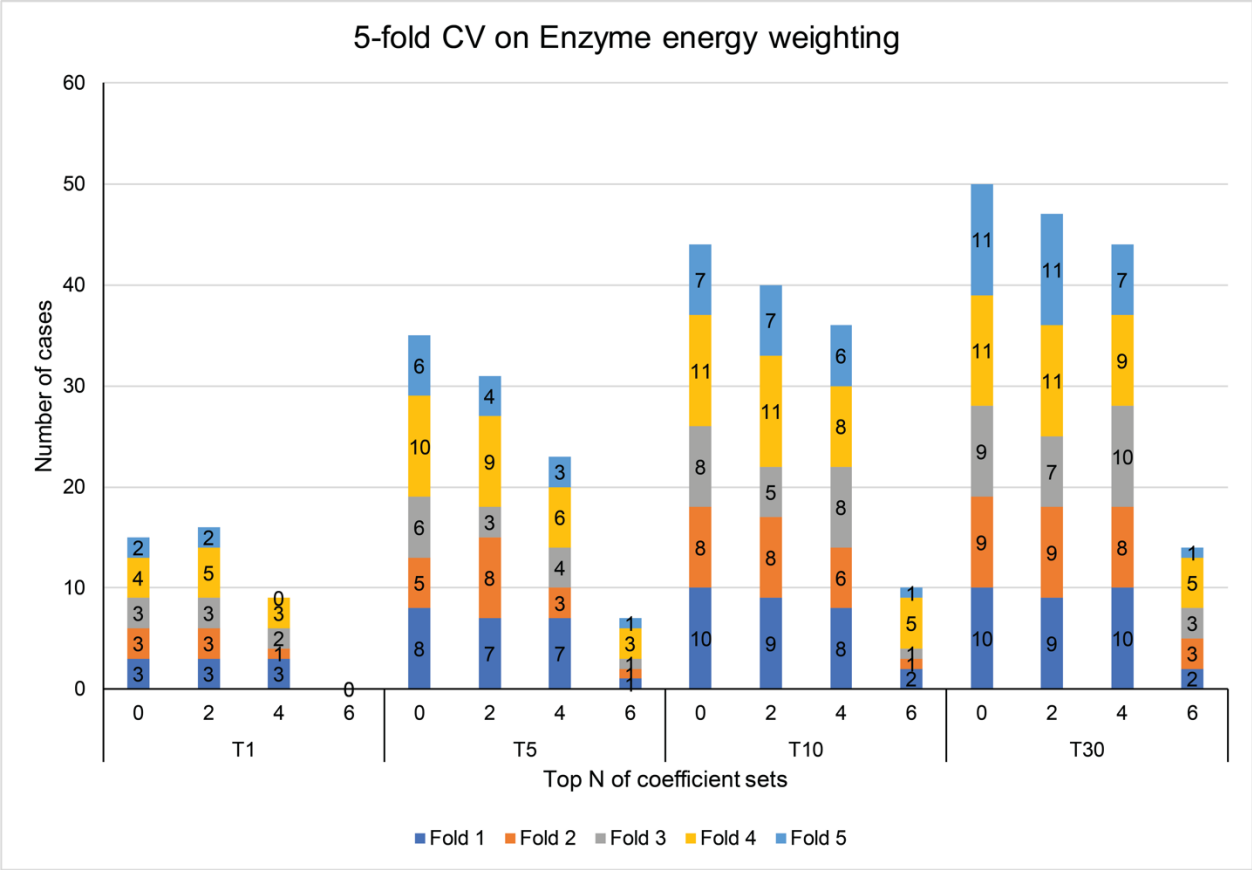

Figure S2. Results of a five-fold cross validation on enzyme-containing BM4 cases using balanced set (00), the electrostatic-favored set (02), the hydrophobicity favored set (04), and the set without the pairwise structure-based potential DARS (06) related to Figure 4A and Figure S1.

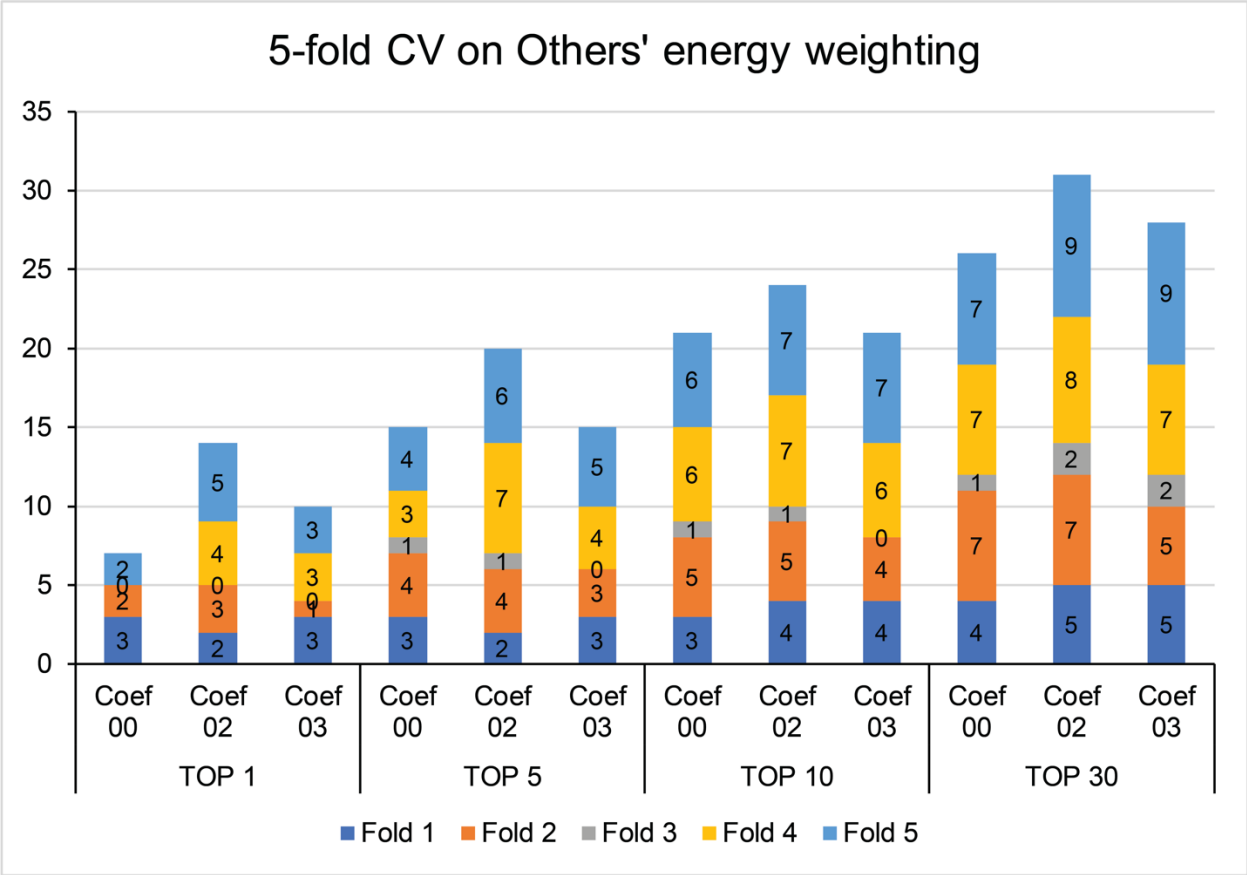

Figure S3. Results of a five-fold cross validation on others-containing BM4 cases using balanced set (00), the electrostatic-favored set (02), and others' mode (03) related to Figure 4B.

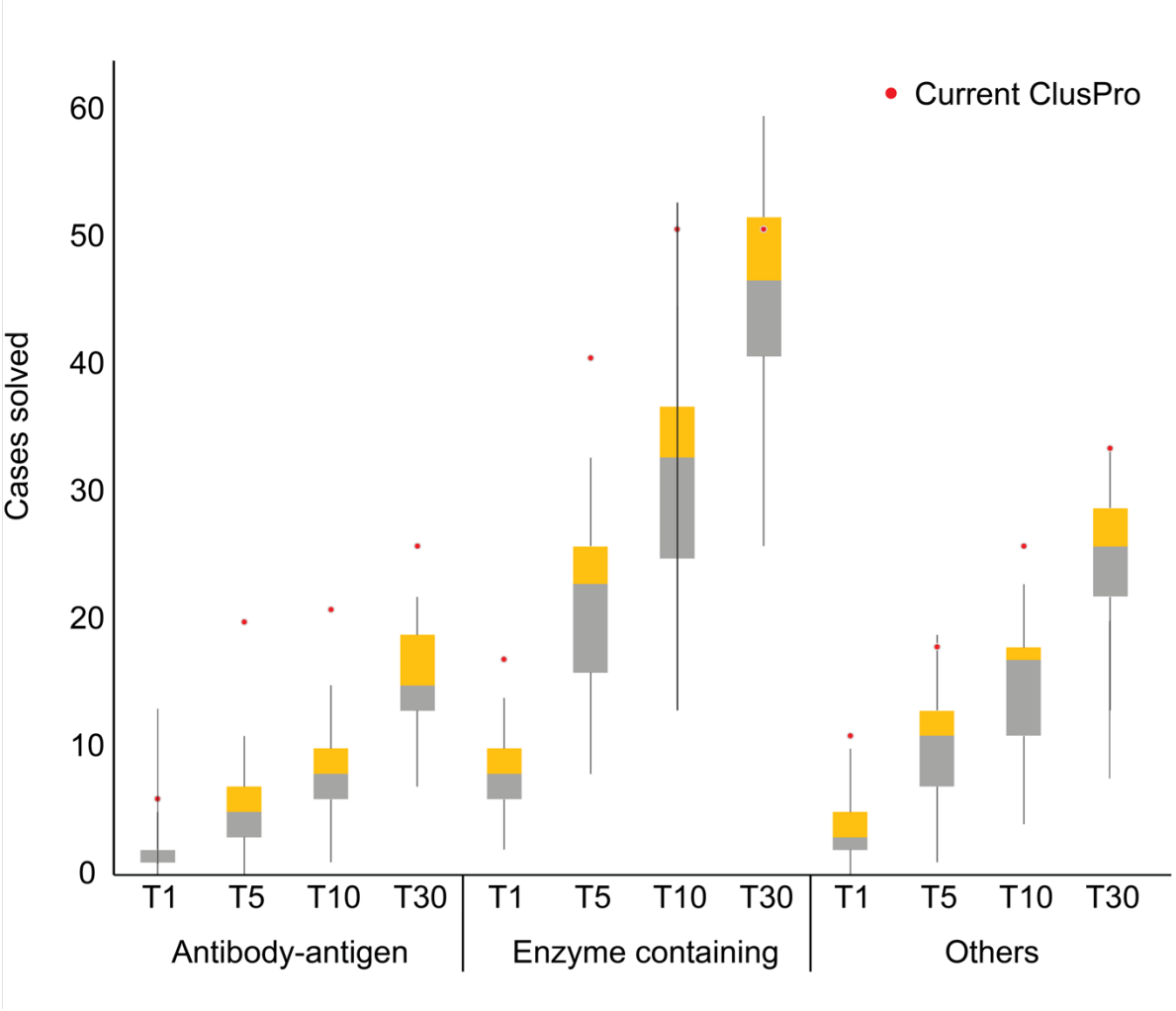

Figure S4. Comparing the performance of ClusPro with the currently implemented weight coefficients to the performance range with the 105 different coefficient sets. Related to Figure 4C.

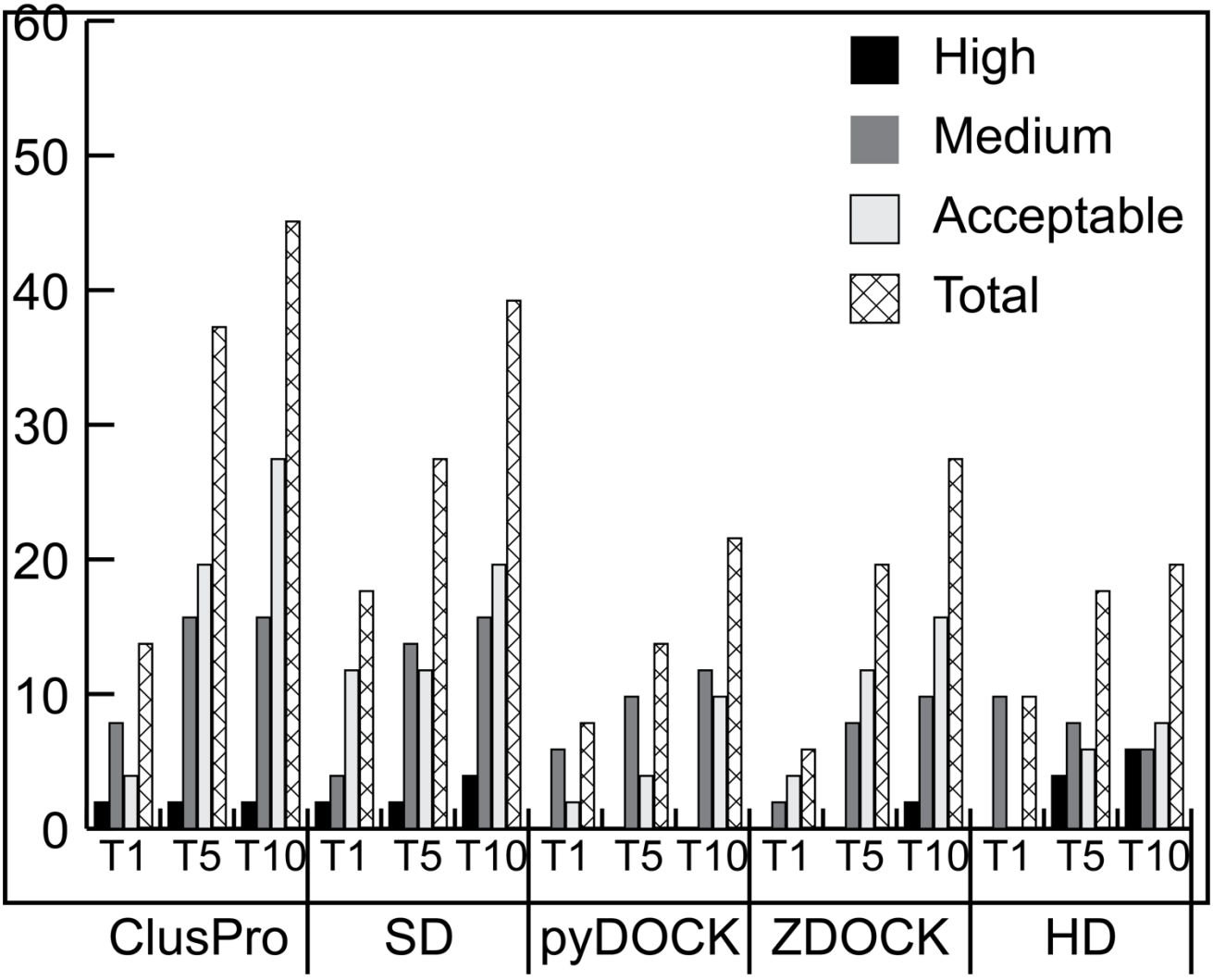

Figure S5. Comparing the success rate of ClusPro to those of four other servers. The results shown are based on docking 51 of the 55 complexes added to version 4 of the Protein Docking Benchmark (BM4) to form version 5 (BM5, see Vreven et al., 2015). The targets 1EXB, 4GXU, 4FQI, and 4GAM were removed due to problems with alignment or masking. Results for SwarmDock (SD), pyDOCK, and HADDOCK (HD) are from the original publication (Vreven et al., 2015). Running ClusPro we used the antibody mode and automated masking for antibody-antigen complexes, the electrostatically driven coefficient (02) set for enzymes, and the others mode with the three different weight sets (parameters 03) for “other” type targets. Note that the performance of SwarmDock has been subsequently improved as shown in Figure 5.