## Supporting Information for:

## GroScore: Accurate Scoring of Protein-Protein Binding Poses using Explicit-Solvent Free-Energy Calculations

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**Figure S1.** Work profiles for all unbinding processes of the best-scoring pose (excluding poses with strand ends buried inside the binding partner or enlaced strands) of CAPRI targets T29-T40.



**Figure S2.** Work profiles for all unbinding processes of the best-scoring pose (excluding poses with strand ends buried inside the binding partner or enlaced strands) of CAPRI targets T41-T97.



**Figure S3.** Scatterplots of the calculated Gscore free-energy scores against the Interface-RMSDs (I-RMSD) of the docked poses with respect to the experimentally determined structures for CAPRI targets T29-T40. Approximate 1D and 2D distributions of values were computed using Kernel Density Estimation.



**Figure S4.** Scatterplots of the calculated Gscore free-energy scores against the Interface-RMSDs (I-RMSD) of the docked poses with respect to the experimentally determined structures for CAPRI targets T41-T97. Approximate 1D and 2D distributions of values were computed using Kernel Density Estimation.



**Figure S5.** Progression of percentages of structures with different qualities, i.e. acceptable (\*), medium (\*\*) and high (\*\*\*) quality, in the simulated fraction for different targets.