Supplementary Material

Computational investigation of proton transfer, pKa shifts and pH-optimum of protein-DNA and protein-RNA complexes

Yunhui Peng and Emil Alexov*

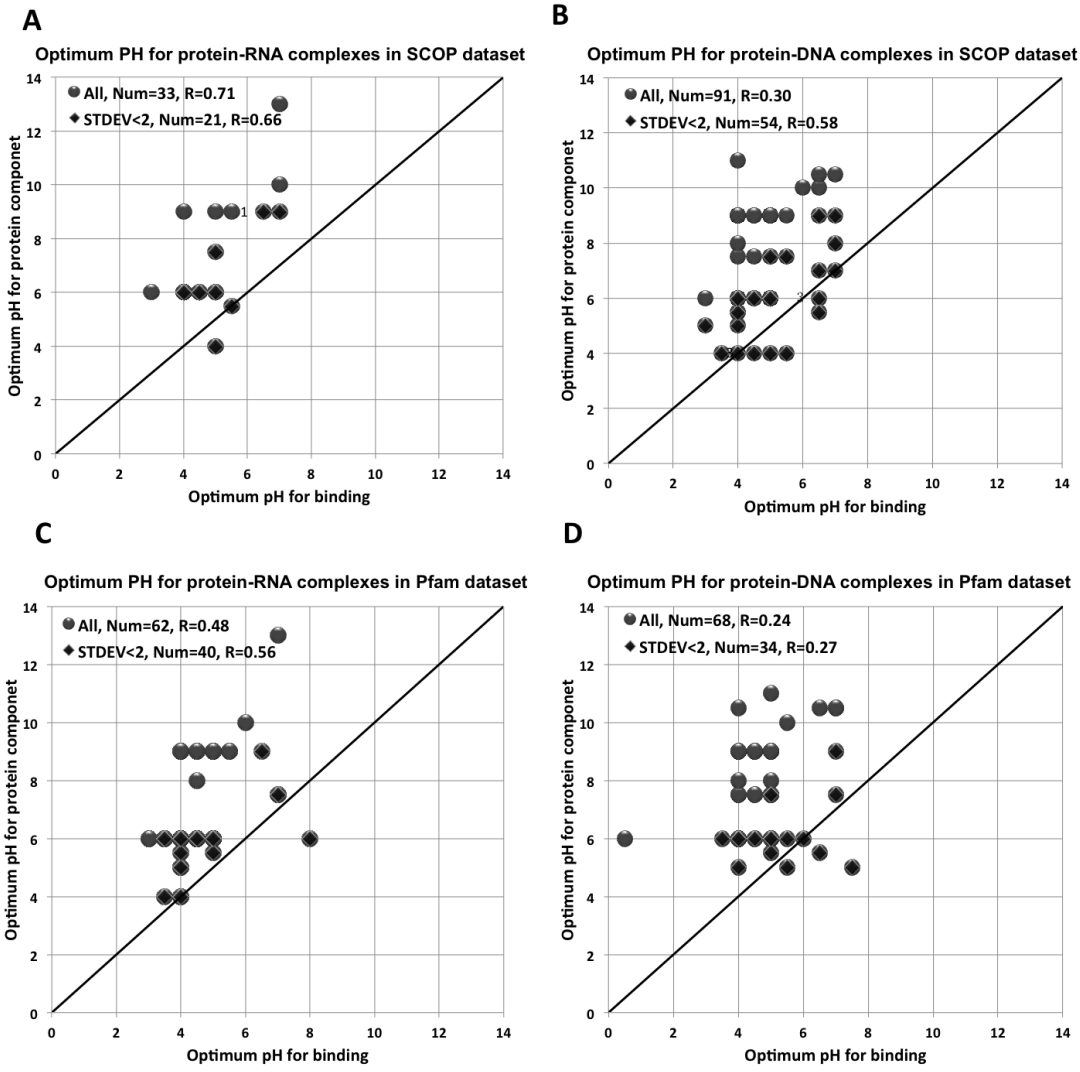

Figure 1: Correlation plot of pH-optimum of binding and stability of the corresponding binding protein. The pH-optimum is taken at the middle of the "flat" pH interval where the binding and folding free energies are almost pH independent. Pearson product-moment correlation coefficient is calculated for all cases and also for cases in which outliers are excluded (standard deviation > 2 pH units). Due to the resolution of the protocol, each dot in the graphs represents multiple cases.

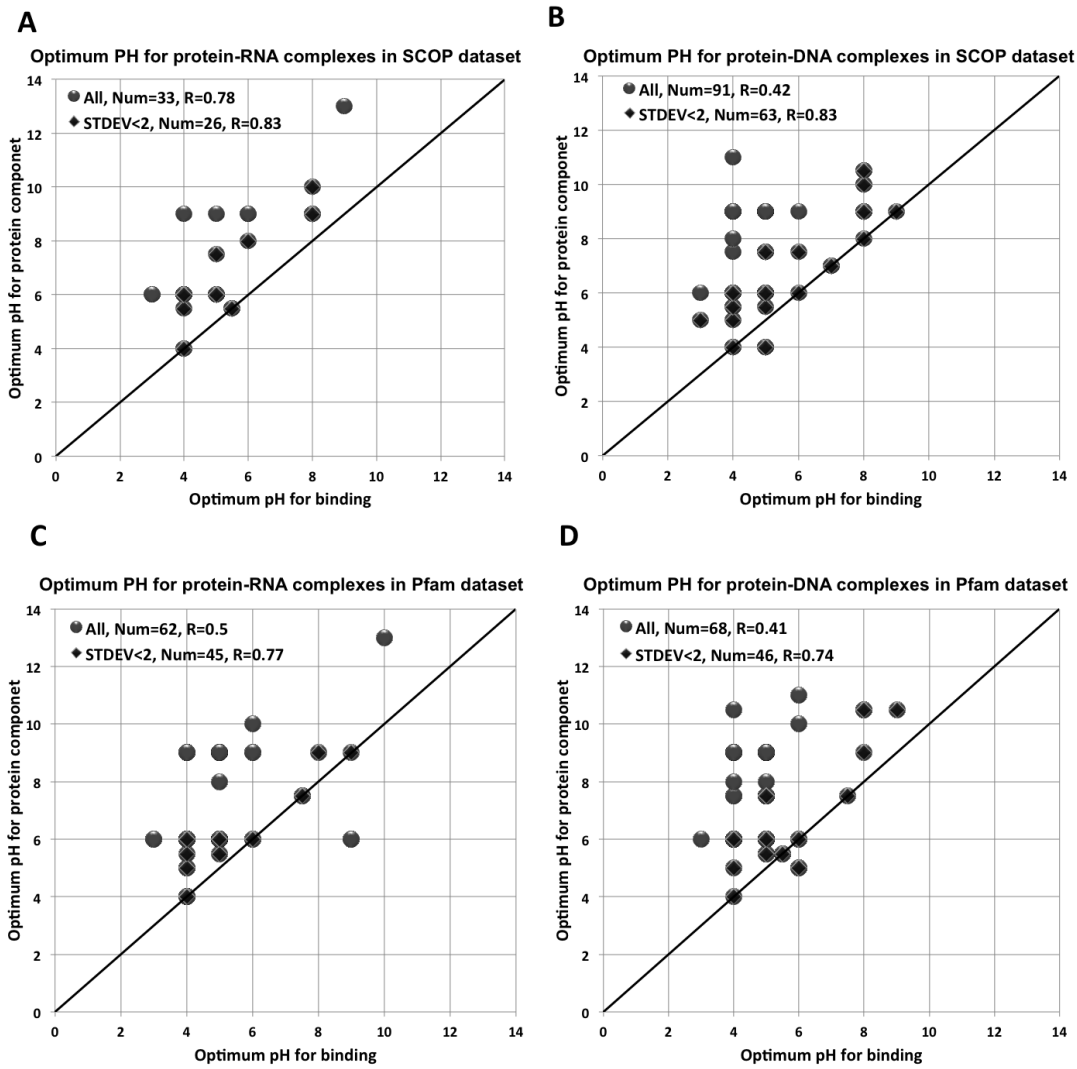

Figure 2: Correlation plot of pH-optimum of binding and stability of the corresponding binding protein. The pH-optimum of the binding is taken at the middle of the "flat" pH region where the binding is almost pH independent. The pH-optimum of the corresponding binding protein folding is taken to be within the "flat" pH region – however, the closest value to the pH-optimum of the binding value is selected. Pearson product-moment correlation coefficient is calculated for all cases and also for cases in which outliers are excluded (standard deviation > 2 pH units). Due to the resolution of the protocol, each dot in the graphs represents multiple cases.