Supporting Information

Molecular basis for the increased affinity of an RNA recognition motif with re-engineered specificity: A molecular dynamics and enhanced sampling simulations study.


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**S1 Text. Are similar types of motion sampled similarly across different MD simulations?** Principal component (PC) analysis can reveal the dominant modes of motion in a simulation, by identifying eigenvectors of the so-called covariance matrix [1, 2]. Comparing PC projections provide a metric of similarity between the dominant modes of motion across independent MD simulations [1, 2]. This has been done here, using the cpptraj module[3] of Amber 16 [4], to assess whether the same types of motion are sampled similarly across individual MD trajectories of the pre-miR20b and Rbfox•pre-miR20b systems. First, to ensure that the eigenvectors obtained from each simulation match, we calculated the covariance matrix for non-hydrogen atoms using all the trajectories combined. Each frame was RMS-fit to the overall average coordinates in order to remove global rotational and translational motions. Next, the projection along the eigenvectors of each coordinate frame from the first simulation trajectory was calculated; this was then repeated for the second simulation trajectory and so on. Finally, at each frame $t$, a histogram for each simulation of the PC projection values for a given PC is constructed. Figure S1 shows the overlap of histograms of the PC projections for the three most dominant modes of motion. Since the histograms are very similar in all the cases, these results suggest that the same types of motion are sampled in all independent simulations.

**References**