Supplementary materials

Figure S1. Root mean square fluctuation (RMSF) of the backbone of DPP4 during 100-ns MD simulation.

Figure S2. A representation of the interactions and contacts over time. The top panel shows the total number of specific contacts DPP4 makes with EGCG over the simulation. The bottom panel shows which residues interact with EGCG in each trajectory frame.

Figure S3. Normalized stacked bar chart representation of interactions and contacts over the course of the MD simulation trajectory.
Figure S2

Figure S3