Electronic Supplementary Material (ESI) for Nanoscale.

Supplementary Information for:

Concentration-dependent binding of CdSe quantum dot on SH3 domain

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Table S1. QD core electrostatic charges. Charges fluctuate among atom types, but the average, maximum and minimum charge for each type are shown.

Atom type	Average Charge	Max. Charge	Min. Charge
Cd	0.53	0.63	0.41
Se	-0.57	-0.53	-0.63

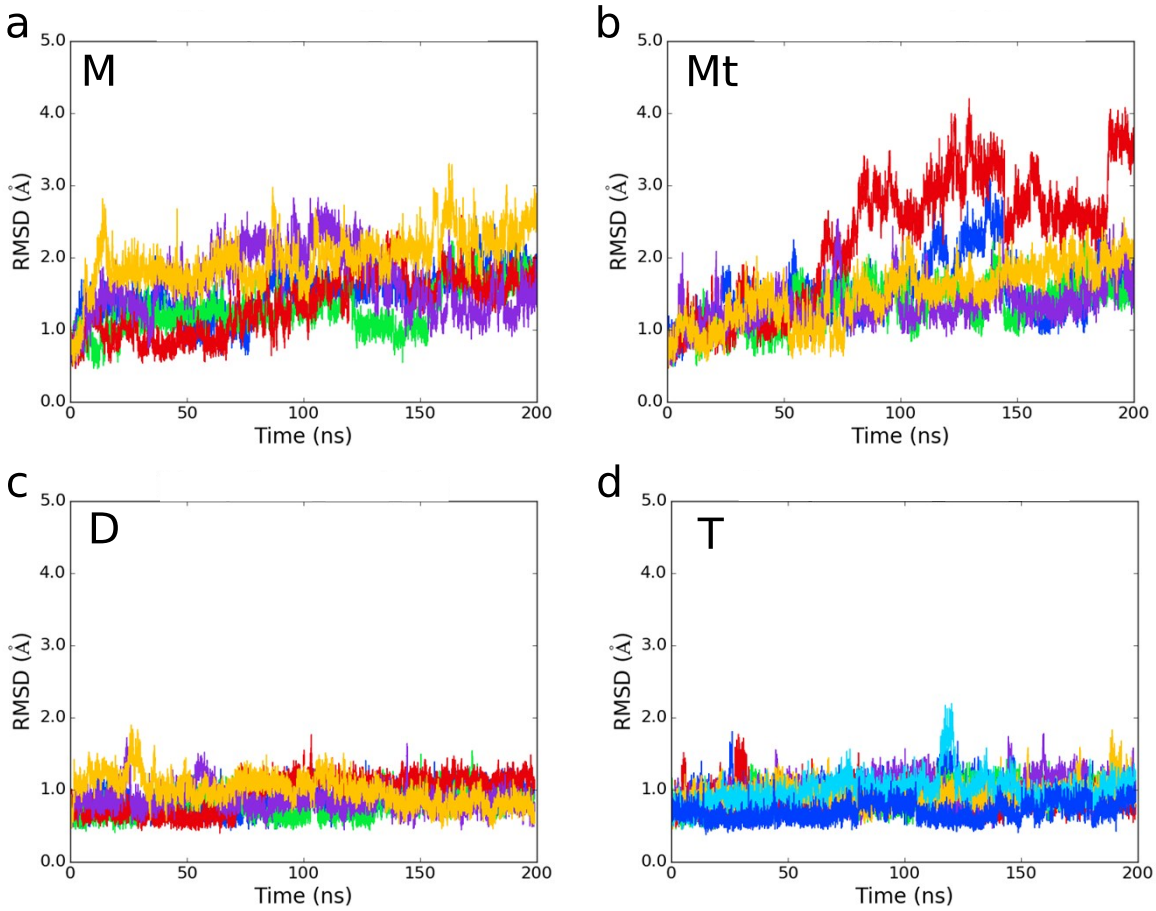

Figure S1. RMSD of SH3 domain in the (a) monomer M, (b) ternary Mt, (c) dimer D, and (d) tetramer T systems. Five trajectories are shown in (a-c); seven trajectories are shown in (d). The largest RMSD trajectory is the red plot in the ternary Mt system. In this trajectory, the QD does not interact with the SH3 domain; rather, the native PRM ligand binds to the PRM active site of the SH3 domain.

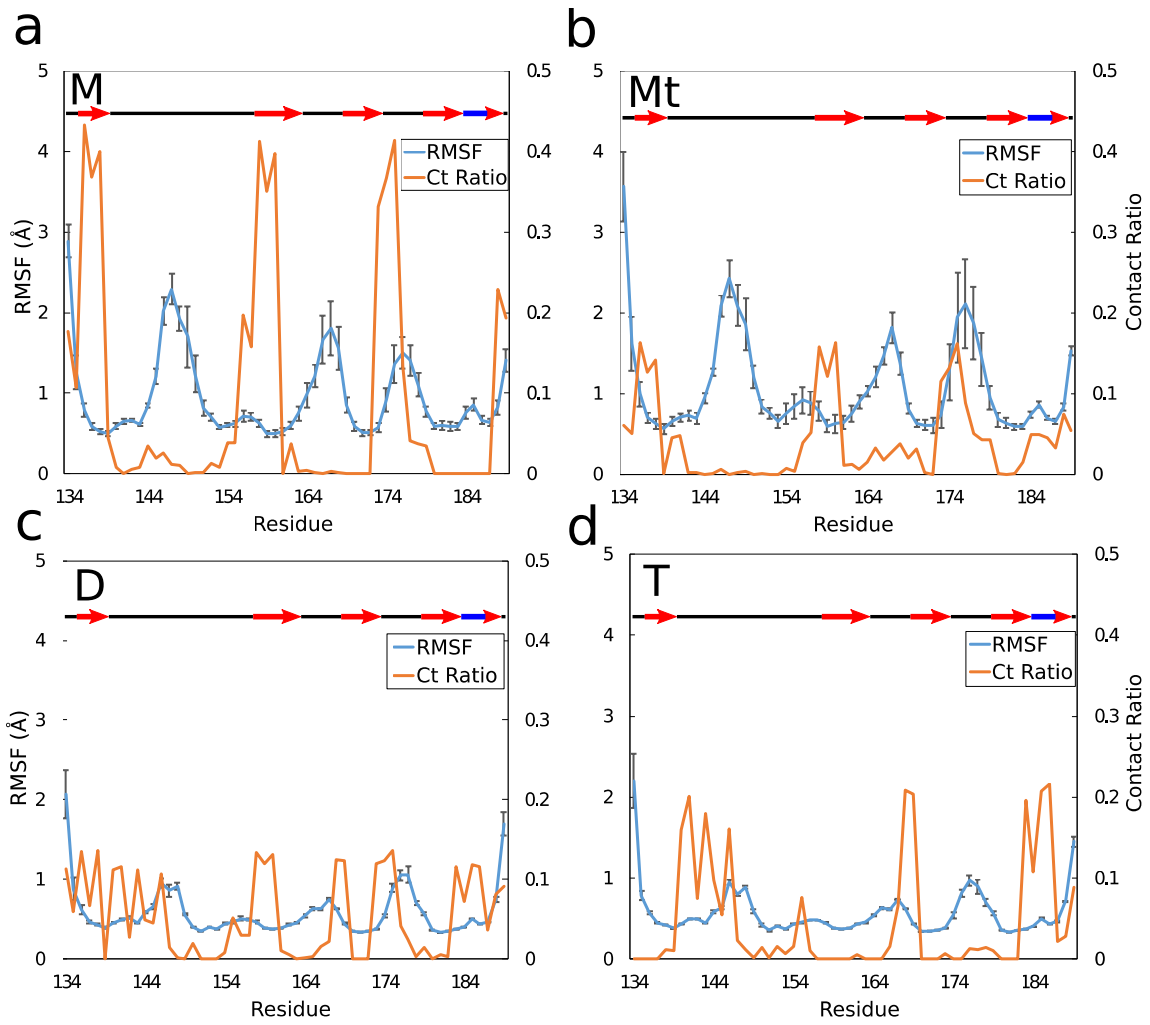

Figure S2. RMSF (blue) of SH3 domain in the (a) monomer M, (b) ternary Mt, (c) dimer D, and (d) tetramer T systems. Contact ratio (orange) included for reference. Error bars shown on RMSF plots are standard error.

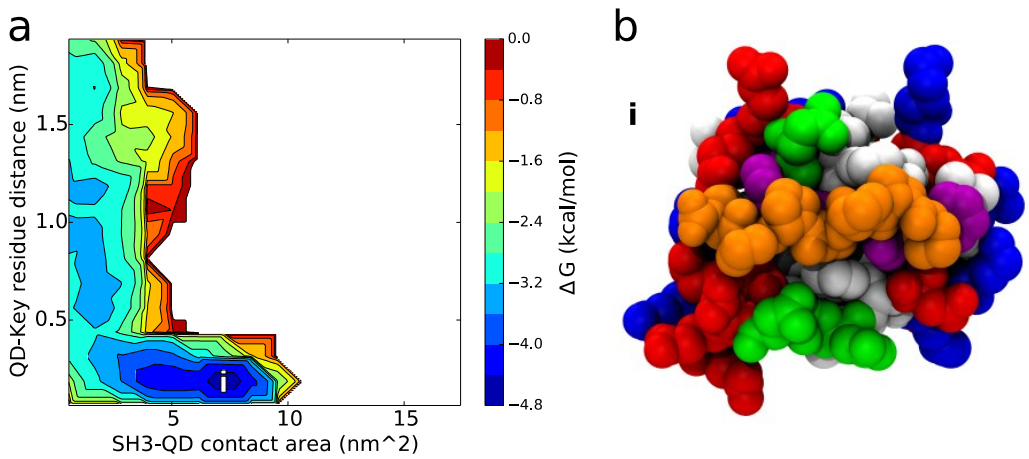

Figure S3. (a) PRM-SH3 binding free energy surface. (b) Main binding well (i) structure. PRM is shown in orange over the binding site residues (purple).

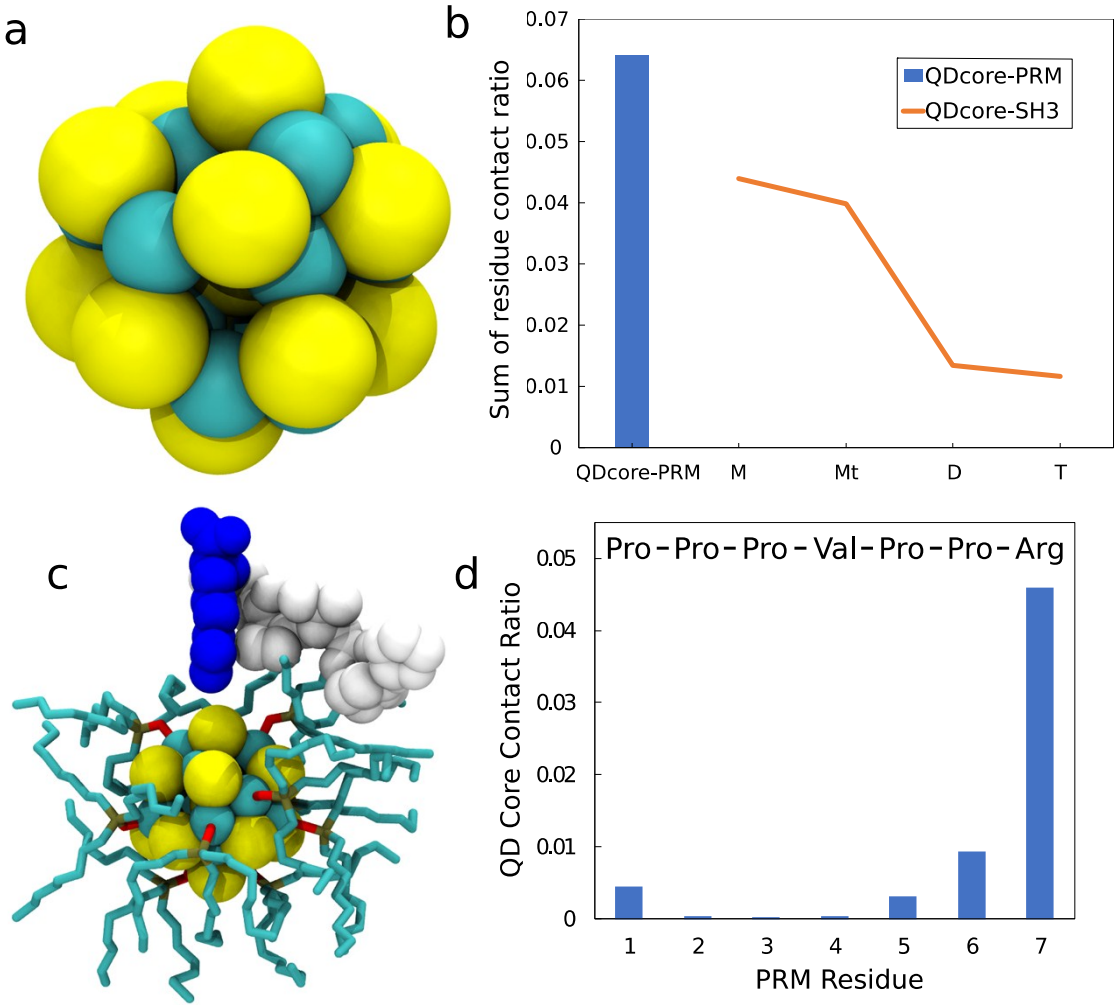

Figure S4. $(CdSe)_{13}$ QD core analysis. (a) Bare $(CdSe)_{13}$ QD core. (b) Sum of QD core-residue contact ratios with PRM (blue) and SH3 systems (orange line). Note that with higher QD concentration, QD core makes fewer contacts with SH3 domain, indicating the QD core is being sequestered. (c) PRM contacting the QD core through a favorable electrostatics interaction: the positively charged arginine of PRM (blue) is interacting a partially negatively charged selenium atom on the surface of the QD core. (d) QD core contact ratios across PRM residues. This plot clearly shows the preference for the positively charged arginine residue of PRM to contact the QDcore.

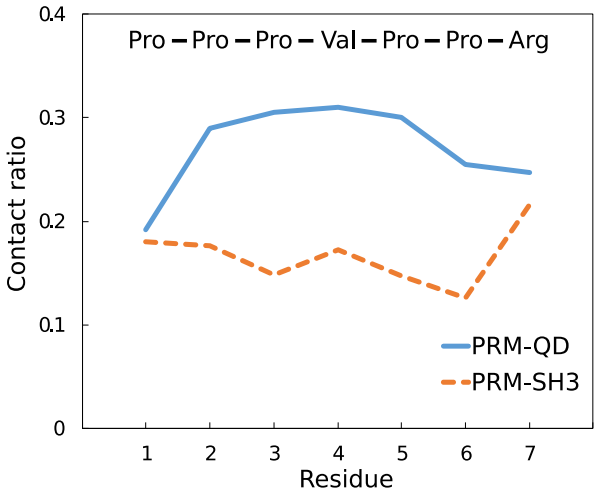

Figure S5. PRM-QD (blue solid) and PRM-SH3 (orange dashed) contact ratio for the ternary Mt system. The PRM sequence is given at the top. PRM-QD contact ratio includes contacts with the QD core and TOPO coating molecules.

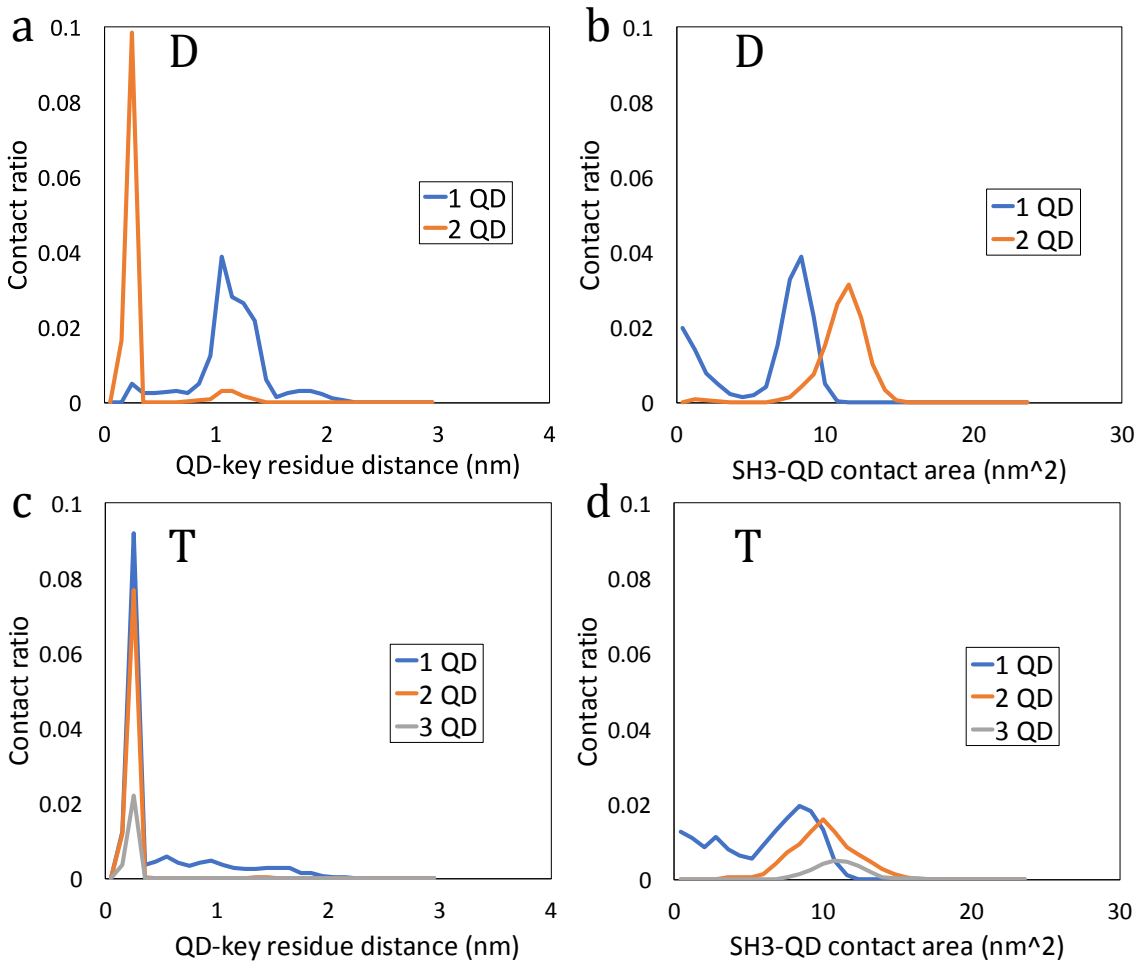

Figure S6. Contact ratio of QD dimer(a-b) and tetramer(c-d) binding SH3 differentiated by number of QDs contacting SH3. (a) Dimer contact ratio as a function of minimum distance to PRM binding site. (b) Dimer contact ratio as a function of QD-SH3 contact area. For dimer system, either 1 or 2 QDs can bind. (c) Tetramer contact ratio as a function of minimum distance to PRM binding site. (d) Tetramer contact ratio as a function of QD-SH3 contact area. The tetramer system adopts a tetrahedral configuration, so 1,2, or 3 QDs can bind at one time.