

Supporting Information

Size-Dependent Impact of CNT on Dynamical Properties of Calmodulin

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Radius of Gyration (R_g) of CaM

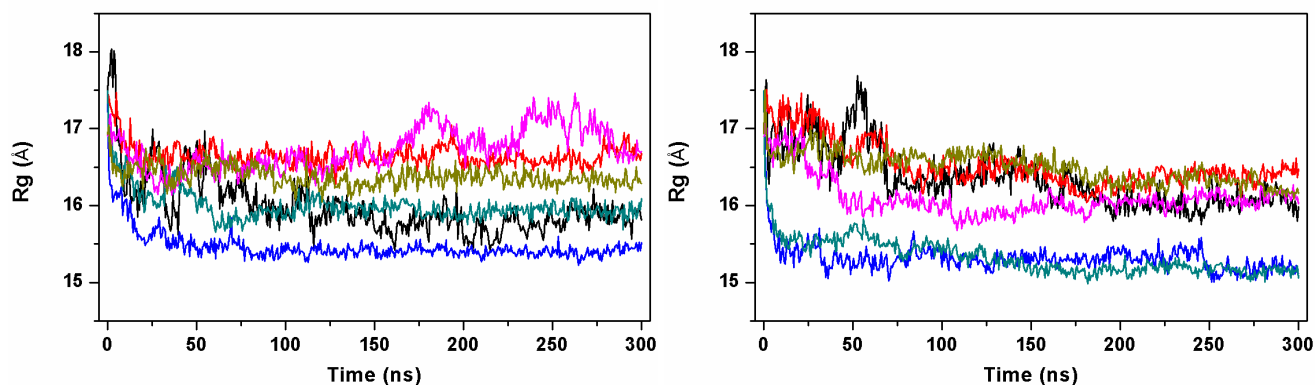


Figure S1. The radius of gyration (R_g) for Holo-CaM (left) and for Apo-CaM (right) in six systems: CaM (black), CaM/M13 (red), CaM/CNT(4,4) (blue), CaM/CNT(5,5) (green), CaM/CNT(6,6) (magenta) and CaM/CNT(7,7) (olive).

The average number of contact heavy atoms of CaM

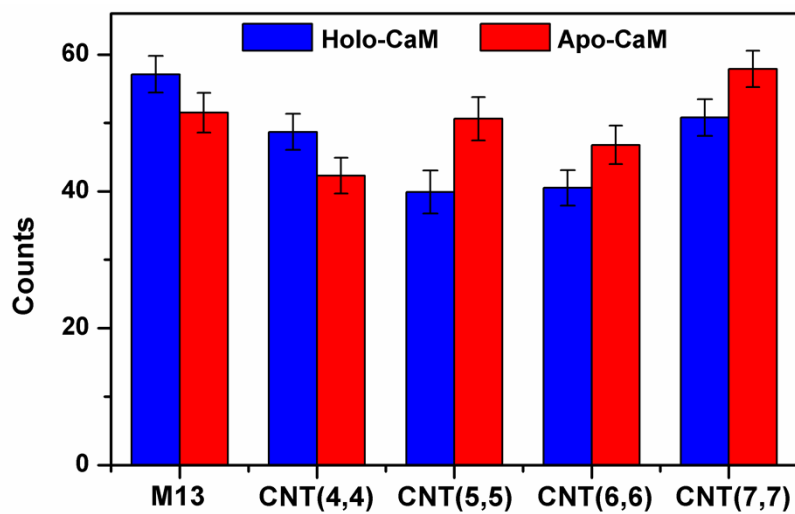


Figure S2. The average number of contact heavy atoms of CaM in complex with various ligands. For each ligand, the results of Holo-CaM and Apo-CaM are colored in blue and red, separately.

The interaction potentials of CaM/ligand complexes (kJ/mol)

	M13	CNT(4,4)	CNT(5,5)	CNT(6,6)	CNT(7,7)
Holo-CaM	-1602.0 ± 33.1	-583.1 ± 17.5	-552.5 ± 18.7	-605.1 ± 20.5	-735.8 ± 20.2
Apo-CaM	-1385.8 ± 33.9	-513.0 ± 16.5	-616.6 ± 17.0	-625.7 ± 19.8	-777.9 ± 19.2