SUPPORTING INFORMATION

(1) MD movies made from the simulation trajectories:
cNTnC●Ca^{2+}●$cTnI_{147-163}$ structure simulations WT *vs*. L48Q
Apo cNTnC structure simulations WT *vs*. L48Q
cNTnC•Ca^{2+} structure simulations WT *vs*. L48Q

(2) Figures

Figure 1 The stabilizing role of L48. A. Cartoon representation of cNTnC•Ca^{2+} (PDB: 1AP4) is shown with helices labeled and the side chains of L48, F20, A23, and F27 are colored in orange. B. -90° rotation about the y-axis of A.

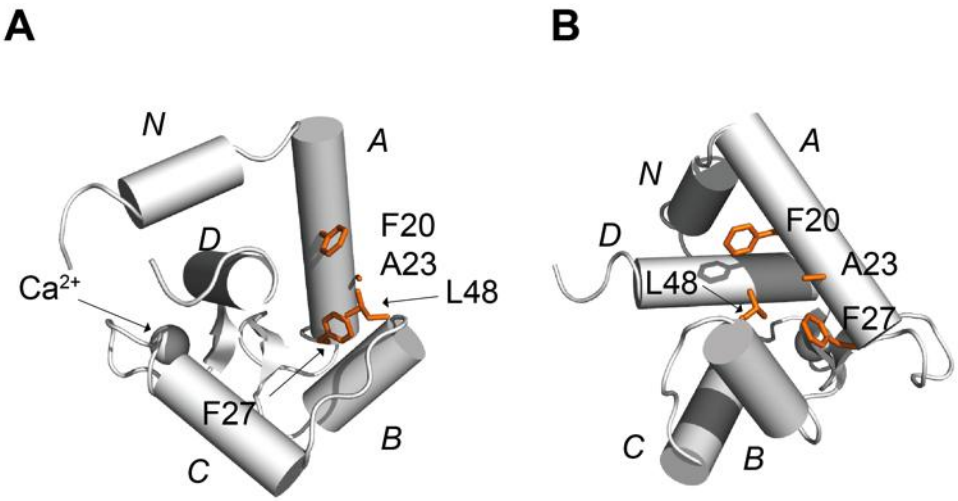


Figure 2. Plots of ^{15}N-T_2, ^{15}N-T_1, and $\{^1H\}^{15}N$ NOE (500 MHz and 600 MHz relaxation data are superimposed) for 0.33 mM cNTnC(L48Q)•Ca^{2+}. T_1 and T_2 increase with an increase internal motion, and NOE decreases with an increase in internal motion. Residues 87-89, at the C-terminus of cNTnC(L48Q) have high T_1 and T_2 and low NOE, which indicate that the C-terminus of cNTnC(L48Q) is disordered.

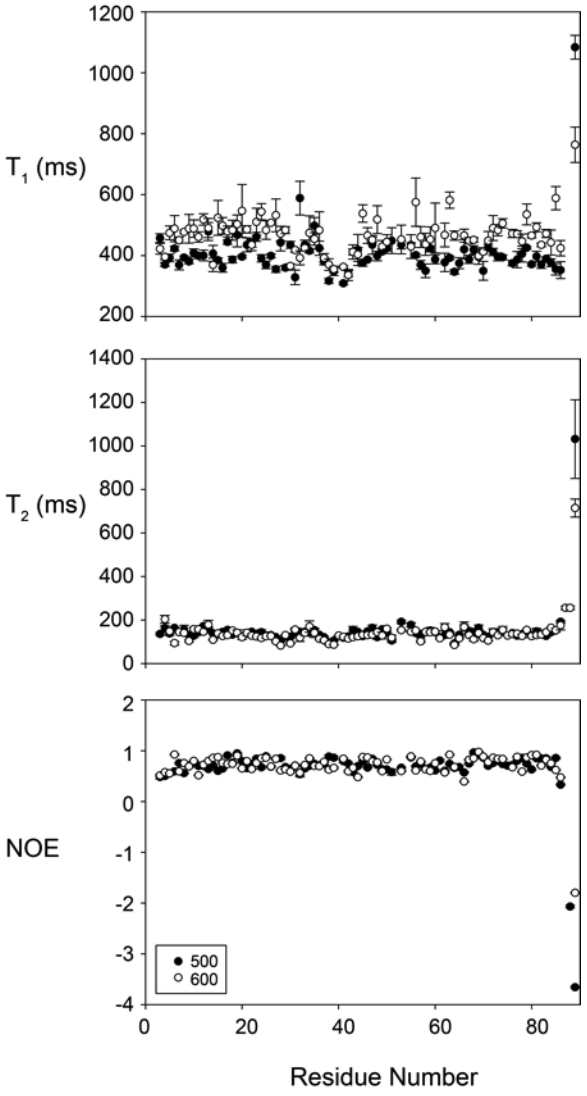


Figure 3. A. Plots of ^{15}N-T_2, ^{15}N-T_1, and $\{^1H\}^{15}N$ NOE of cNTnC•Ca^{2+} superimposed with cNTnC(L48Q)•Ca^{2+}. The concentrations of cNTnC(wt)•Ca^{2+} and cNTnC(L48Q)•Ca^{2+} were both 0.15 mM in order to limit the influence any aggregation may have on the relaxation data. B. Differences in T_1, T_2, and NOE data between cNTnC(L48Q)•Ca^{2+} and cNTnC•Ca^{2+} are plotted. Overall, the data are consistent; however, there are deviations between the two proteins in residues of site I (residues 29-40; highlighted in dashed box), which may represent a change in conformation and/or dynamics of this site.

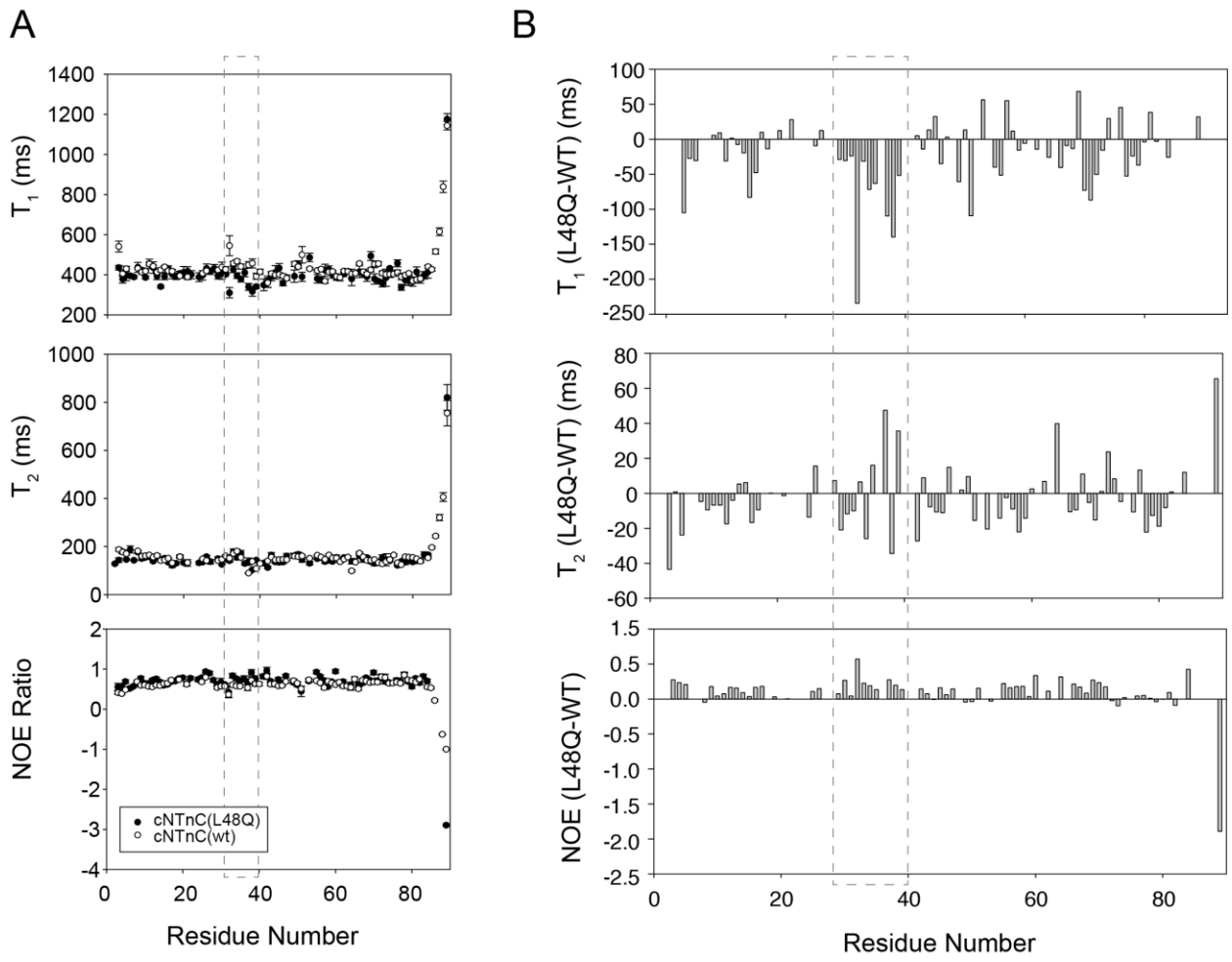
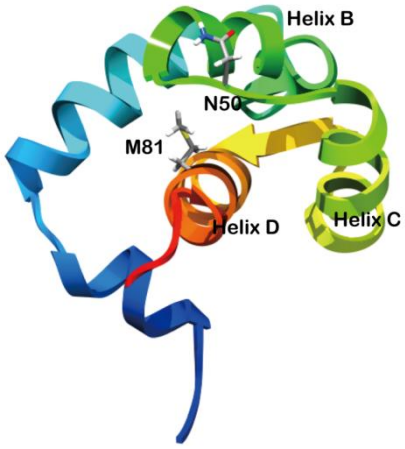


Figure 4. Residue N50 and M80 in cNTnC indicating the opening of the cNTnC



(3)Tables:

Table 1. Distances between residue M81 and N50 in cNTnC .

			WT	L48Q
Protein	Original NMR PDB code	Original NMR(Å)	70ns MD Simulations* (Å)	70ns MD Simulations* (Å)
cNTnC●Ca^{2+} ●$cTnI_{147-163}$	1MXL	17.5	16.11±1.5	17.97±1.3
cNTnC apo	1SPY	8	9.81±1.3	11.66±1.9
cNTnC●Ca^{2+}	1AP4	10	10.66±1.3	13.54±1.9

*Averaged from multiple runs of simulations (0-70ns).

Table 2 Total (main-chain and side-chain) SASA of the selected hydrophobic patch residues in cNTnC*

	WT ($Å^2$)	L48Q ($Å^2$)
Apo cNTnC	611±39	685±38
cNTnC.Ca^{2+}	630±43	642±39
cNTnC·Ca^{2+}·$cTnI_{147-163}$	722±42	748±39

*Averaged from multiple (n ≥3) simulations at last 45-70ns.