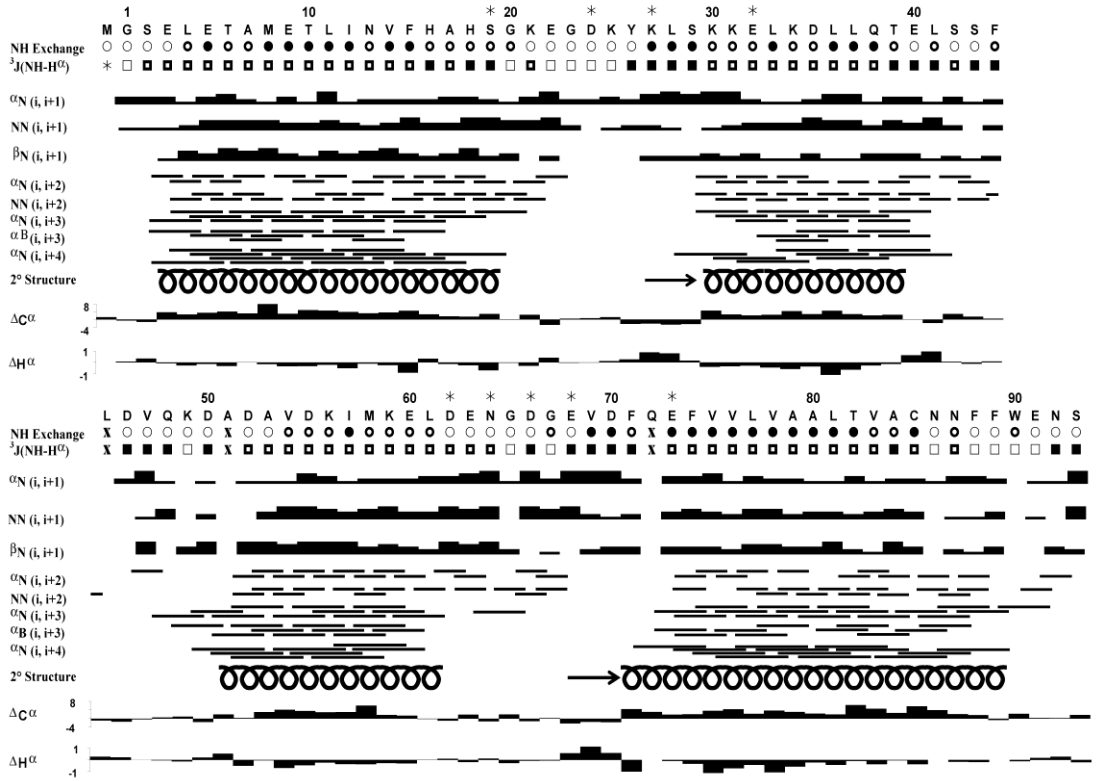
Supplementary Table 1

Table 1: Parameters for NMR Experiments[1]

			Parameters[2]		
			time	freq	Acq time
experiment	Dim	Nuc	pts	pts	(ms)
2D ^{1}H, ^{15}N	t_1	^{15}N	256	512	25.6
HSQC	t_2	^{1}H	1024	2048	106.5
3D ^{15}Nedited	t_1	^{15}N	64	128	27.4
HNCA	t_2	^{13}C	100	256	16.6
	t_3	^{1}H	1024	2048	122.1
3D ^{15}Nedited	t_1	^{1}H	256	512	5.2
NOESY[3]	t_2	^{15}N	84	256	5.7
	t_3	^{1}H	1024	2048	53.2
3D HNHA	t_1	^{1}H	128	256	10.0
	t_2	^{15}N	40	128	11.4
	t_3	^{1}H	1024	2048	122.1
3D	t_1	^{13}C[4]	100	256	4.4
CBCA(CO)NH	t_2	^{15}N	40	128	13.7
	t_3	^{1}H	1024	2048	106.5
3D	t_1	^{13}C	112	256	5.5
HNCACB	t_2	^{15}N	58	128	27.4
	t_3	^{1}H	1024	2048	61.0
3D HNCO	t_1	^{13}C[5]	100	256	16.5
	t_2	^{15}N	64	128	25.7
	t_3	^{1}H	1024	2048	122.1
3D	t_1	^{1}H	128	512	5.2
HC(CO)NH	t_2	^{15}N	44	128	25.7
	t_3	^{1}H	1024	2048	106.5
3D	t_1	^{13}C[4]	110	512	5.5
C(CO)NH	t_2	^{15}N	64	128	25.7
	t_3	^{1}H	1024	2048	61.1
4D ^{13}C, ^{15}N-	t_1	^{13}C[6]	36	128	13.8
edited [7]	t_2	^{1}H	128	256	8.3
NOESY	t_3	^{15}N	36	64	5.7
	t_4	^{1}H	512	1024	61.1
4D ^{13}C, ^{13}C-	t_1	^{13}C[6]	36	64	13.8
edited [7]	t_2	^{13}C[6]	36	64	13.8
NOESY	t_3	^{1}H	128	256	7.3
	t_4	^{1}H	1024	2048	71.3

[1] Data were collected in H_2O at 37 ^{o}C at 600.13 MHz for ^{1}H.
[2] The number of points in the time domain is complex. The number of points in the frequency domain is real. The carrier frequency is 4.658 and 118.0 ppm for ^{1}H and ^{15}N, respectively, unless otherwise stated.
[3] The NOE mixing time was 150 ms.
[4] The ^{13}C carrier position was set at 43.78 ppm.
[5] The ^{13}C carrier position was set at 173.78 ppm.
[6] The ^{13}C carrier position was set at 40.78 ppm.
[7] The NOE mixing time was 130 ms.

Supplementary Figure 1



Supplementary Fig. 1. Secondary structure of S100A1 in the Ca^{2+}-S100A1-RyRP12 complex. Diagram of amide exchange, HNHA *J*-couplings, sequential connectivities, NOE connectivities, and the secondary structure for reduced, Ca^{2+}-loaded, RyRP12 bound S100A1. Stars above the sequence represent Ca^{2+}binding residues. Circles indicate relative amide hydrogen exchange rates at 37°C as determined using 2D ^{1}H ^{15}N HSQC spectra. Open circles (T<10 min.) are arbitrarily referred to as fast exchanging amide protons. Residues with partially filled circles are arbitrarily referred to as medium exchanging amide protons (T<16 h). Residues with solid circles are referred to as slowly exchanging protons (T>16 h). Squares refer to ^{3}J(HN-H^{α}) coupling from a 3D HNHA experiment, where open squares represent data not obtained, partially filled squares refer to ^{3}J-coupling <6 Hz, and closed squares represent 3J coupling >6 Hz. The NOE correlations were determined from 3D ^{15}N-edited NOESY-HSQC, 4D ^{13}C, ^{15}N-edited NOESY, and 4D ^{13}C, ^{13}C-edited NOESY experiments. The height of the bars indicates the strength of the NOE (strong, medium, medium-weak, weak, and very weak). NOE correlations from non-neighboring residues are indicated by lines connecting the residues. Deviations in the $^{13}C^{\alpha}$ and $^{1}H^{\alpha}$ chemical shift from those of a random coil are illustrated such that regions of contiguous upfield-shifted $^{13}C^{\alpha}$ chemical shifts (positive values) and downfield $^{1}H^{\alpha}$ chemical shifts (negative values) are indicative of helical regions. Likewise, regions of contiguous downfield-shifted $^{13}C^{\alpha}$ chemical shifts (negative values) and upfield-shifted $^{1}H^{\alpha}$ chemical shifts (positive values) are indicative of β-sheet. The secondary structure, as derived from all of the data presented here, is represented by α-helices (spirals) β-sheets (arrows) and loops (no symbol), as indicated under the appropriate residues in the sequence of S100A1.

S100A1 Binds to the Calmodulin-binding Site of Ryanodine Receptor and Modulates Skeletal Muscle Excitation-Contraction Coupling

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