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Supporting Information

Calcium Regulates S100A12 Zinc Sequestration by Limiting Structural Variations

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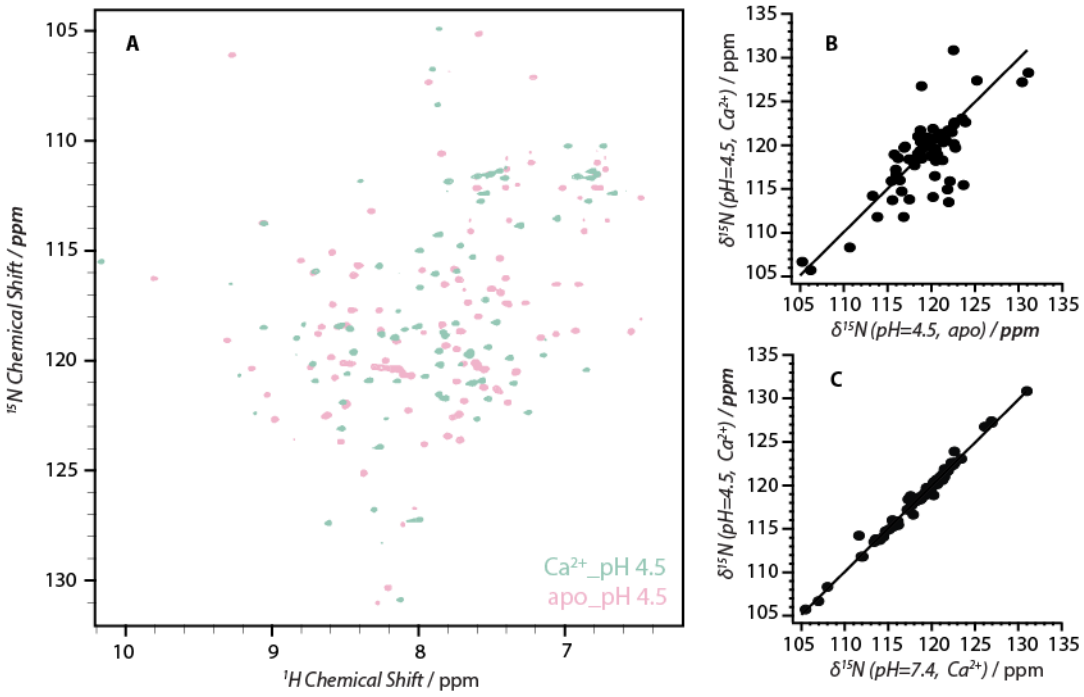

Figure S1. A) Overlay of 14.1 T HSQC spectra of apo (pink) and calcium (green) bound S100A12 at pH 4.5. Plots of ^{15}N amide chemical shift of calcium bound S100A12 at pH 4.5 vs B) apo S100A12 at pH 4.5 with correlation coefficient value of 0.625, and C) calcium bound S100A12 at pH 7.4 with correlation coefficient value of 0.987.

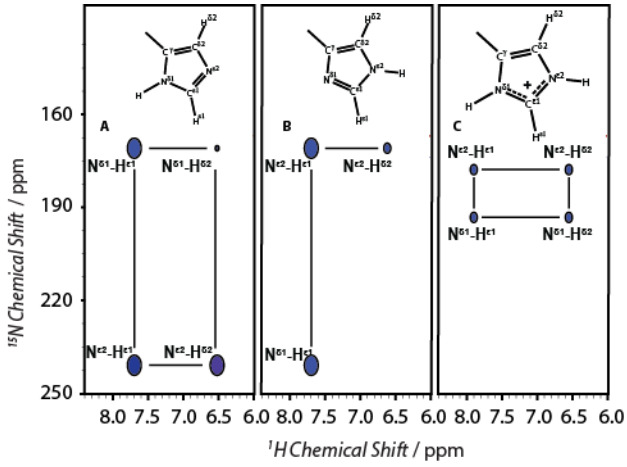

Figure S2. Schematic representation of the three histidine tautomeric states showing approximate $N^{\delta1/\varepsilon2}$ and H^N chemical shifts and expected cross-peak pattern in long range ^{1}H-^{15}N HMQC spectra for the A) $N^{\delta1}$H tautomer, B) $N^{\varepsilon2}$H tautomer and; C) the protonated form of histidine.

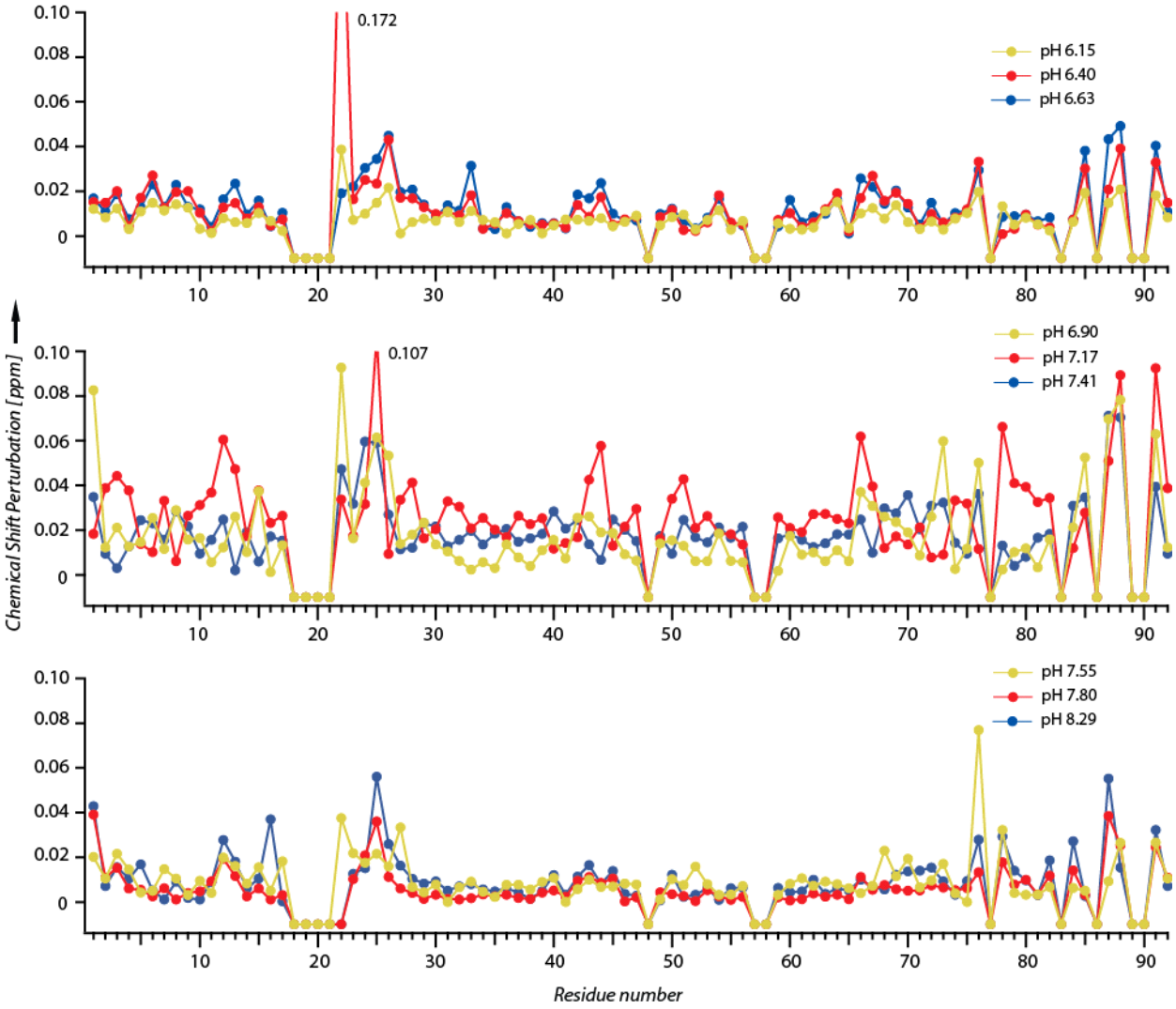

Figure S3. Combined site specific $^{15}N^{H}$ and ^{1}H CSPs for apo- S100A12 as at various pH conditions. Top: CSP between pH 6.0 and 6.15 (yellow); CSP between pH 6.15 and 6.40 (red); CSP between pH 6.40 and 6.63 (blue). Middle: CSP between pH 6.63 and 6.90 (yellow); CSP between pH 6.90 and 7.17 (red); CSP between pH 7.17 and 7.41 (blue). Bottom: CSP between pH 7.41 and 7.55 (yellow); CSP between pH 7.55 and 8.0 (red); CSP between pH 8.0 and 8.29 (blue). The CSP were calculated according to:

$$CSP = \sqrt{\Delta H^2 + \left(\frac{\Delta N}{5.0}\right)^2}$$