Supporting Information

Direct NMR evidence for Ca^{2+} ion binding to G-quartets

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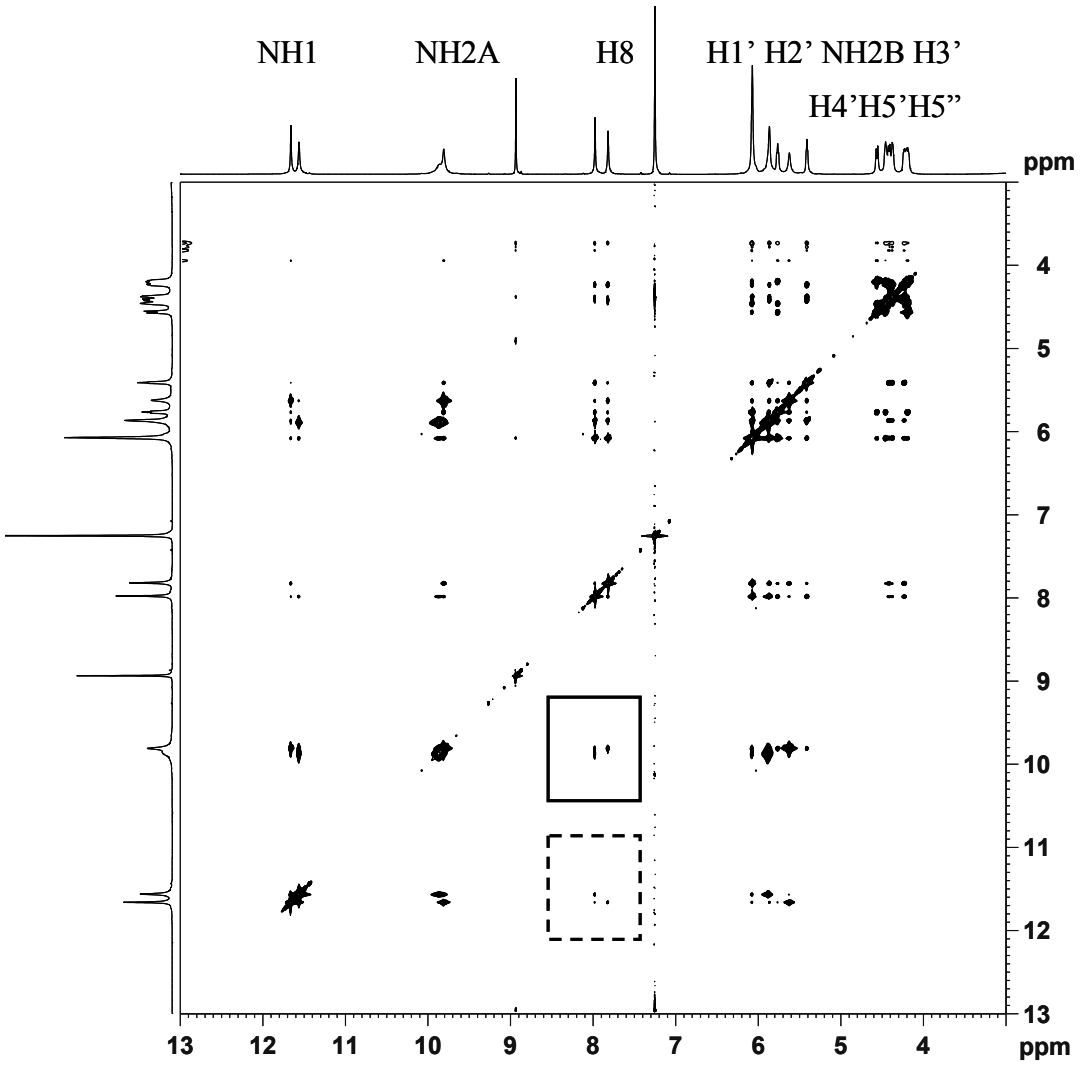

Figure 1S. 600-MHz ^{1}H NOESY spectrum of the TAG-Ca^{2+} complex in CDCl3 at 268 K. Cross peaks formed between NH2A and H8 were highlighted in the solid box while those formed between NH1 and H8 were enclosed in the dashed box.

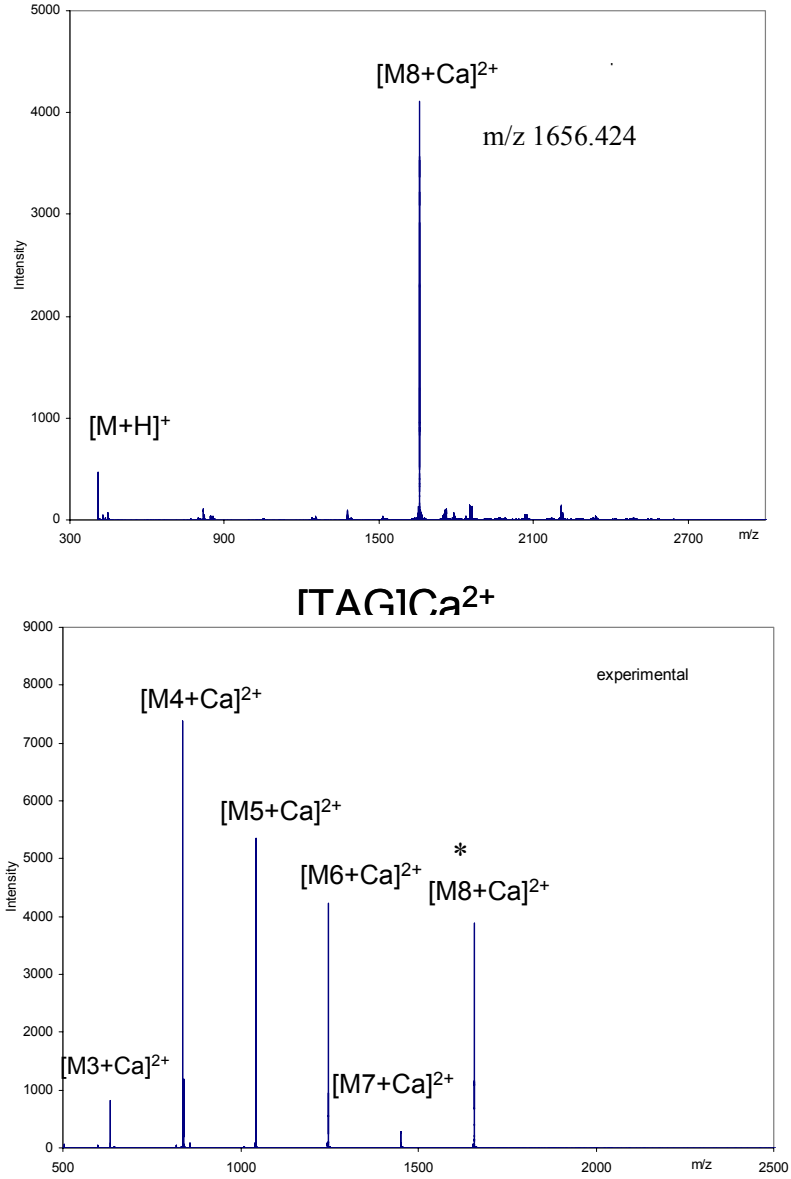

Figure 2S. (Top) ESI MS spectrum and (Bottom) ESI MS/MS (* parent ion, m/z 1656.424)spectrum of the TAG-Ca^{2+} complex. ESI MS spectra were recorded with an Applied Biosystems QSTAR XL quadrupole time-of-flight (QqTOF) mass spectrometer using the positive mode. ESI-MS data were acquired using the Analyst QS 1.1 software. Samples were dissolved in anhydrous nitromethane (CH_3NO_2) and injected with a syringe pump at a flow rate of 5.0 •L/min. The mass range of single MS measurements was set at m/z 300 to 6000. The declustering potential (DP) was set to 20 V during the MS experiment. Subsequent tandem mass spectrometry (MS/MS) measurements were performed using nitrogen as the collision gas. Collision induced dissociation (CID) energy of 35 eV was applied to break down the G dodecamers and G octamers. The mass range of MS/MS measurements was set at m/z 100 to 4000. For spectral assignment, theoretical MS peaks were generated using Data Explorer v. 4.0.0.0 (1997–2000) by Applied Biosystems.