

Supplemental Information

Synthesis, Characterization, and Cellular uptake of a Glycylglycine Chelate of Magnesium

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Table of Contents

ESI Mass Spectrum of 1 (S1)	Page 2
Full Spectra ¹ H NMR of Glycylglycine (S2)	Page 3
¹ H NMR of 1 Full Spectra (S3)	Page 4
¹ H NMR Overlay of Glycylglycine and 1 (S4)	Page 5
¹ H NMR Overlay of Glycylglycine, 1 , Citric Acid and Magnesium Citrate (S5)	Page 6
¹³ C NMR of Glycylglycine (S6)	Page 7
¹³ C NMR Overlay of Glycylglycine and 1 (S7)	Page 8
¹³ C NMR Overlay of Glycylglycine, 1 , and Magnesium Citrate (S8)	Page 9
Full Spectra HSQC of Glycylglycine and 1 (S9)	Page 10
Full Spectra HMBC of Glycylglycine and 1 (S10)	Page 11
Elemental Analysis and ICP of 1 (S11)	Page 12
Linear Regression of Magnesium Uptake Standard (S12)	Page 13

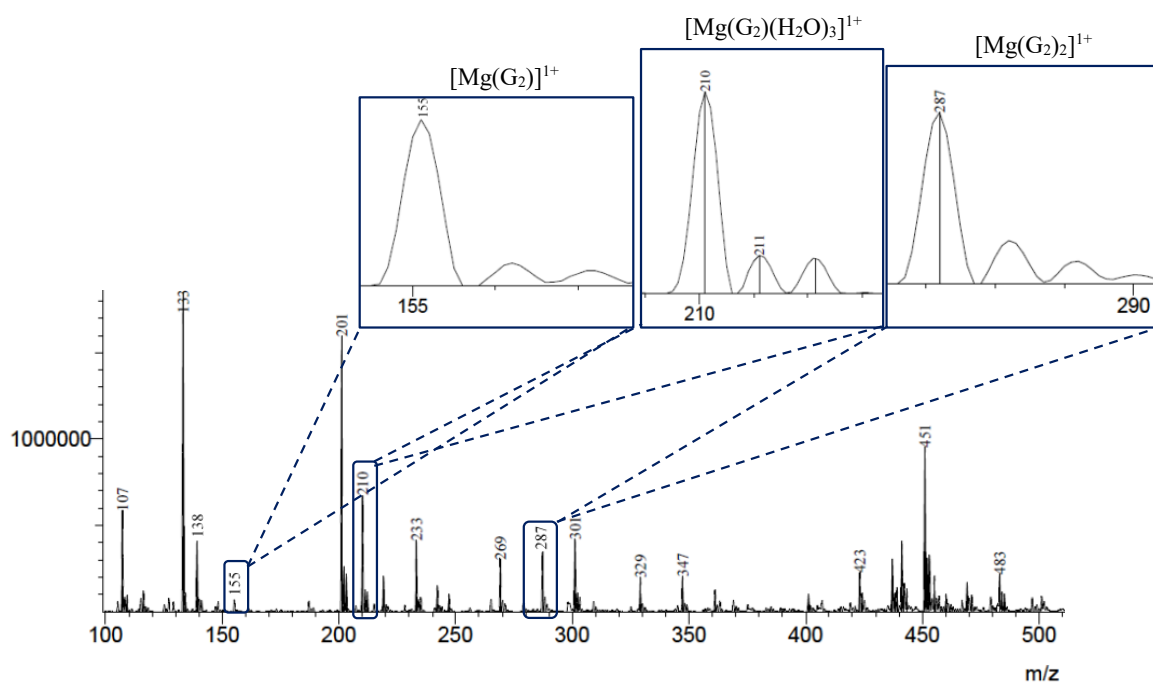


Figure S1. ESI-MS mass spectrum of **1** exhibiting an appropriate magnesium isotopic distribution pattern (IDP) and the presence of **1** along with an *in situ* formed 1:2 complex.

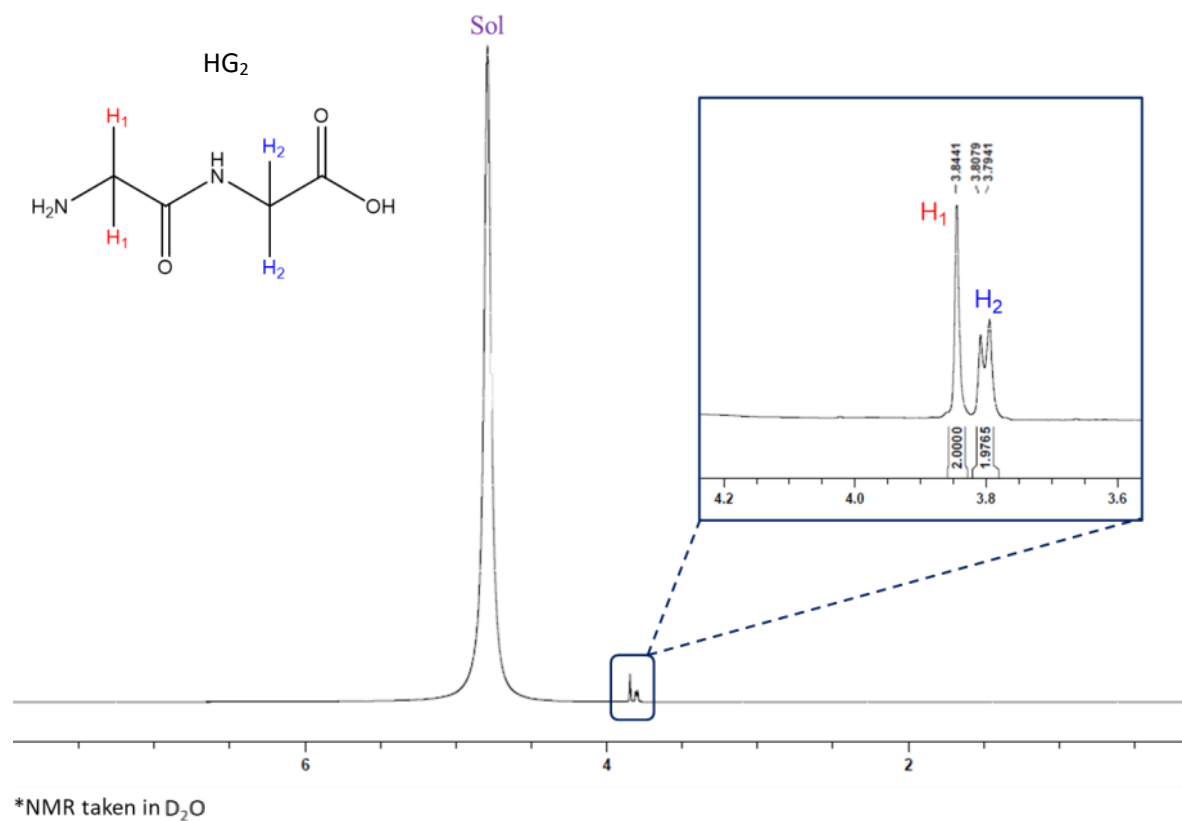
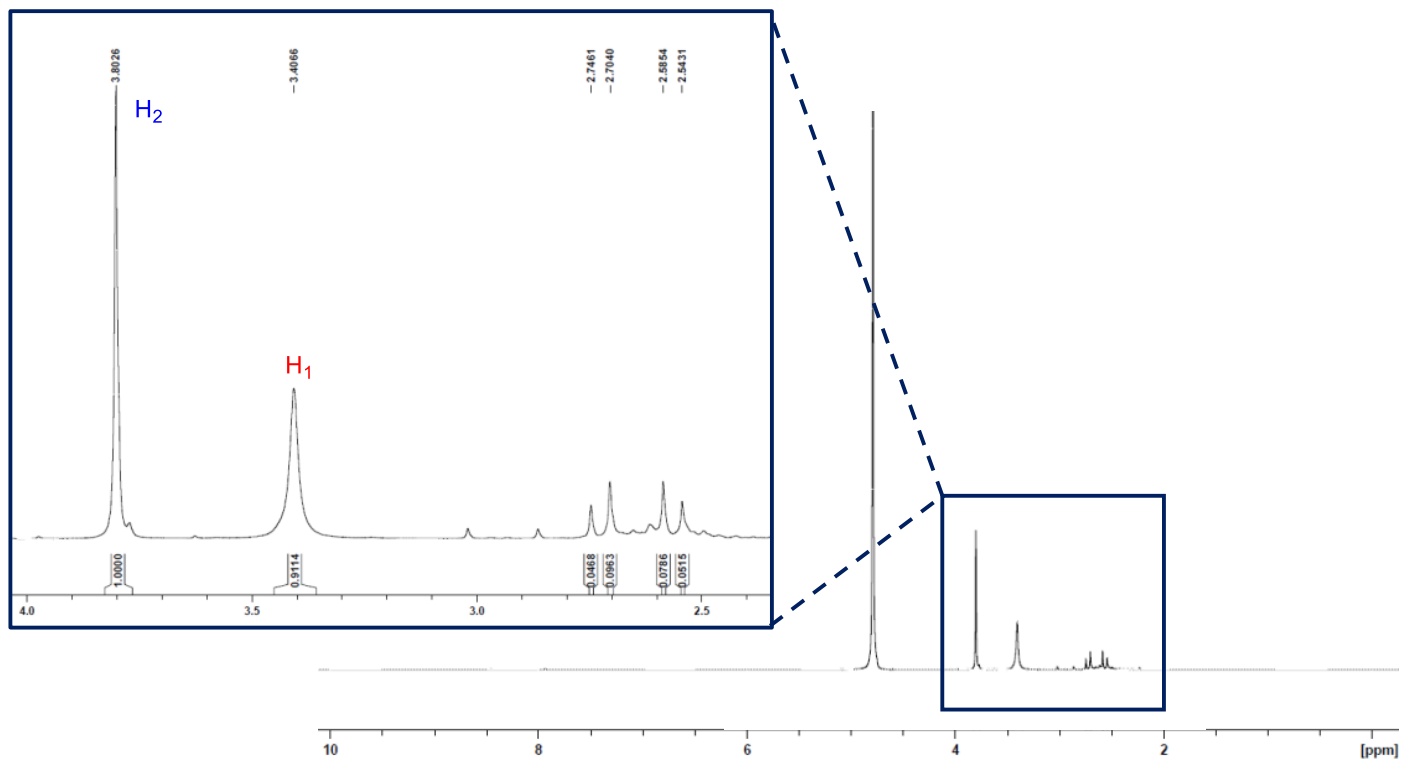


Figure S2. The full spectrum ¹H NMR of HG₂ showing a clean singlet and a signal with observed coupling – the observed integration coincides with the expected integration.



*NMR taken in D₂O

Figure S3. Full spectrum ¹H NMR of **1** showing two singlets and the presence of magnesium citrate. The observed integration coincides with the expected integration values.

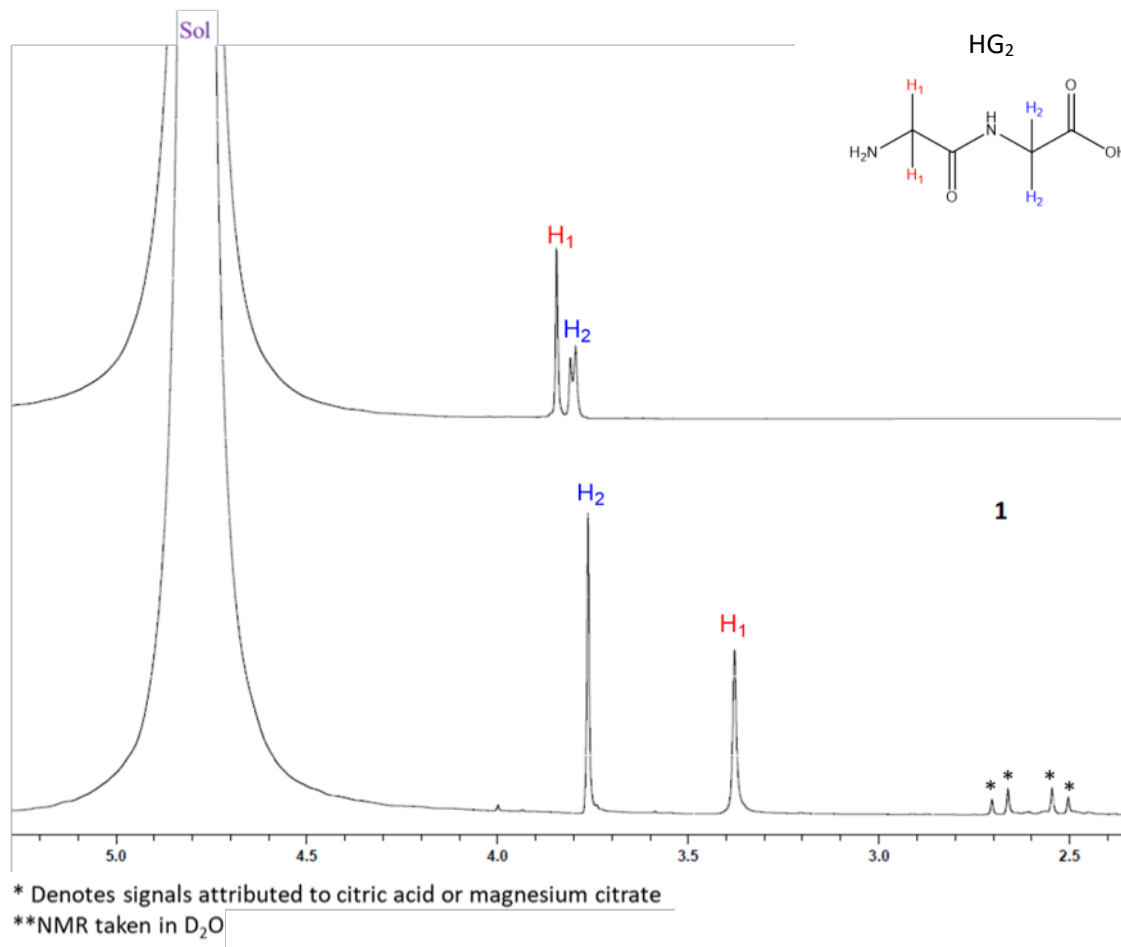


Figure S4. ¹H NMR spectra overlay of HG₂ (**Top**) and the **1** complex (**Bottom**) – the ¹H NMR spectrum of **1** shows the presence of magnesium citrate, but the desired integration is conserved between HG₂ and **1**. Observed coupling of the H₂ proton of HG₂ is no longer observed for **1**.

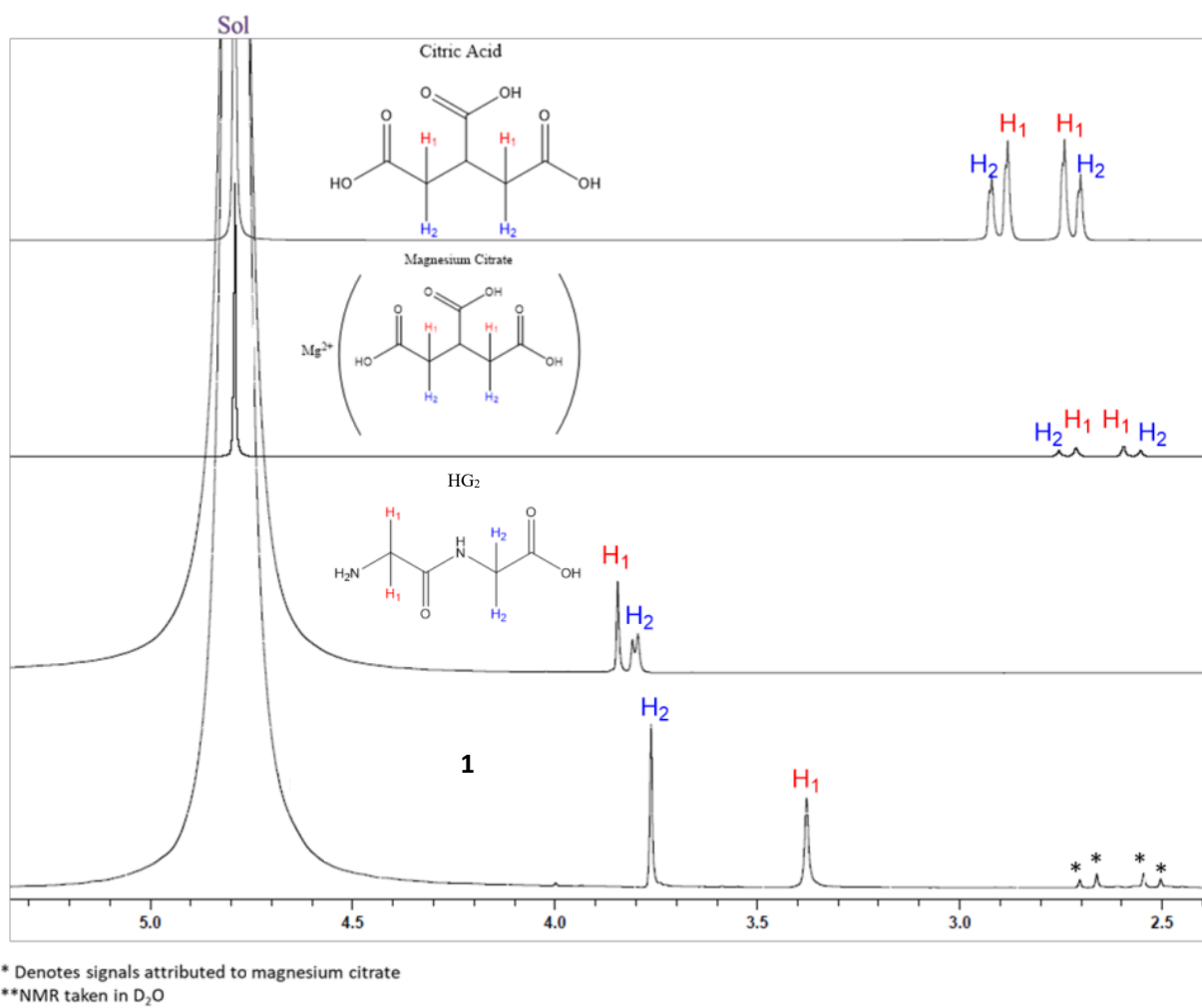


Figure S5. ¹H NMR spectra overlay for citric acid (**Top**), magnesium citrate (**Second from Top**), HG₂ (**Third from Top**), and **1** (**Bottom**). The integration is conserved between HG₂ and **1**, consistent with the formation of magnesium citrate.

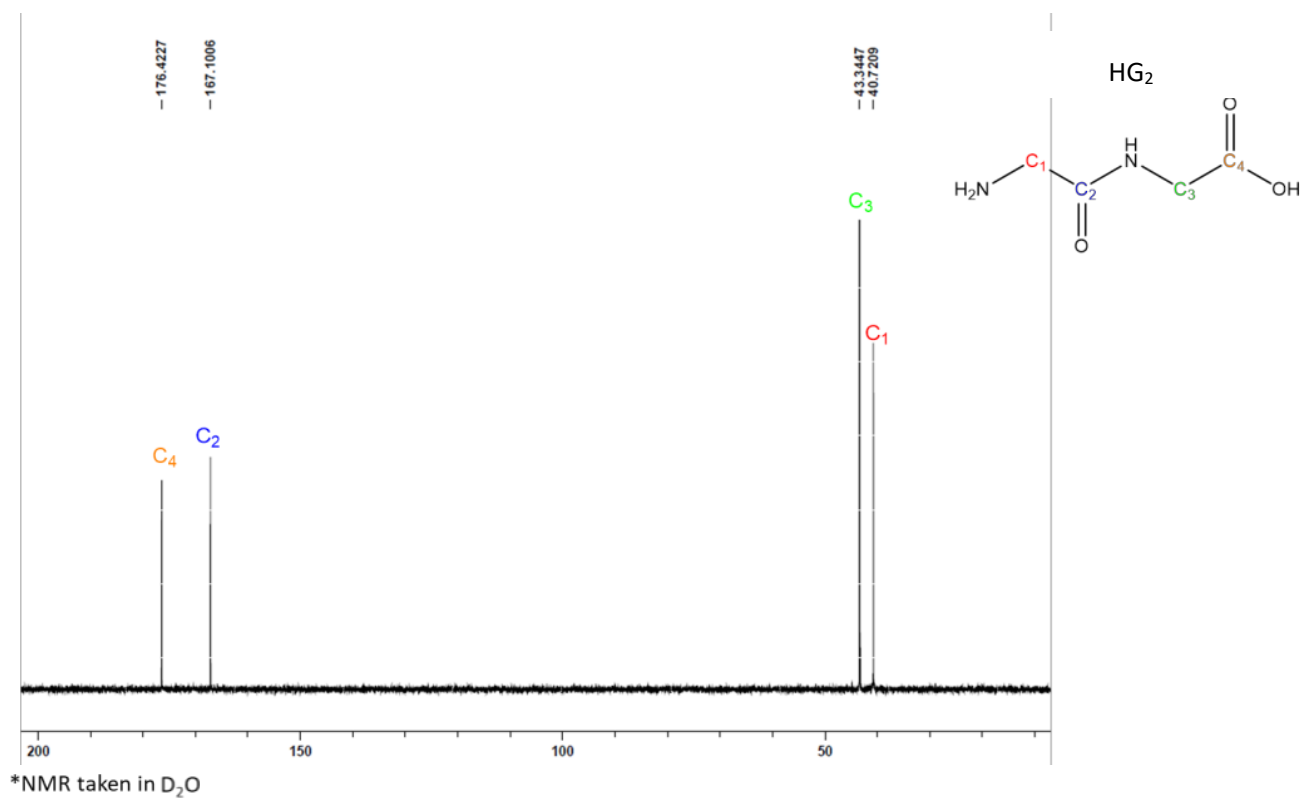


Figure S6. Full spectrum ^{13}C NMR of HG_2 .

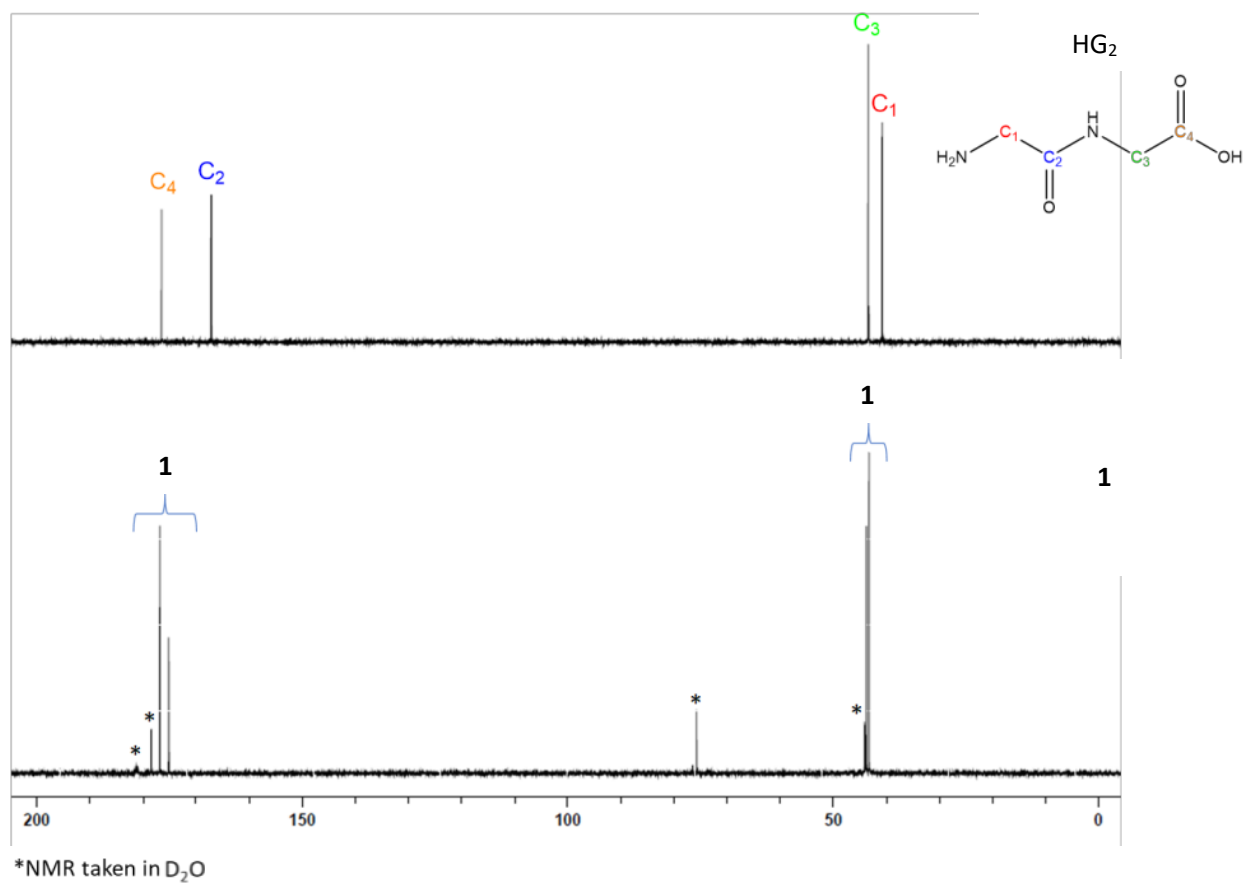


Figure S7. Full spectra ^{13}C NMR overlay of HG_2 (**Top**) and **1** (**Bottom**). **1** showed four signals attributed to magnesium citrate as marked by the asterisks, but the observation of four carbon signals attributed to HG_2 are conserved.

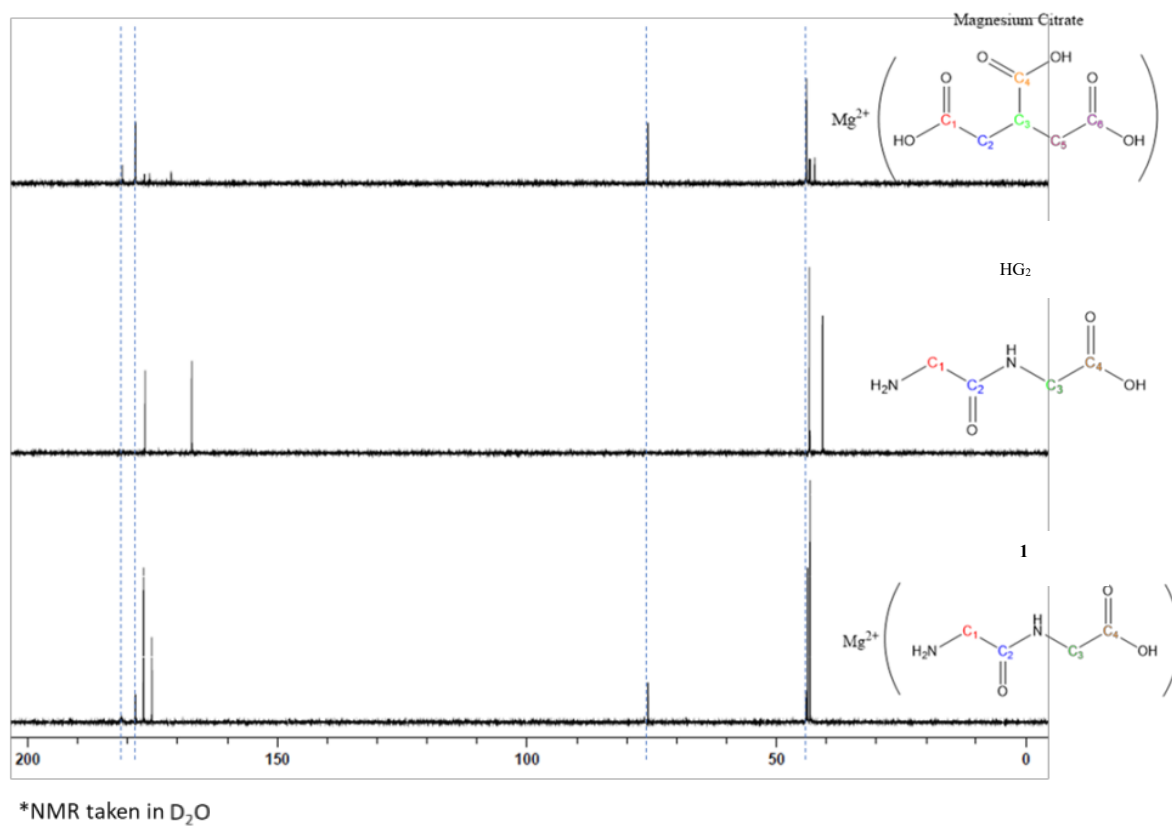


Figure S8. Full spectra ^{13}C NMR overlay of magnesium citrate (**Top**), HG_2 (**Middle**), and **1** (**Bottom**). The overlay illustrates the impurity observed in the spectra of **1** attributed to magnesium citrate, while the carbon signals attributed to HG_2 are conserved.

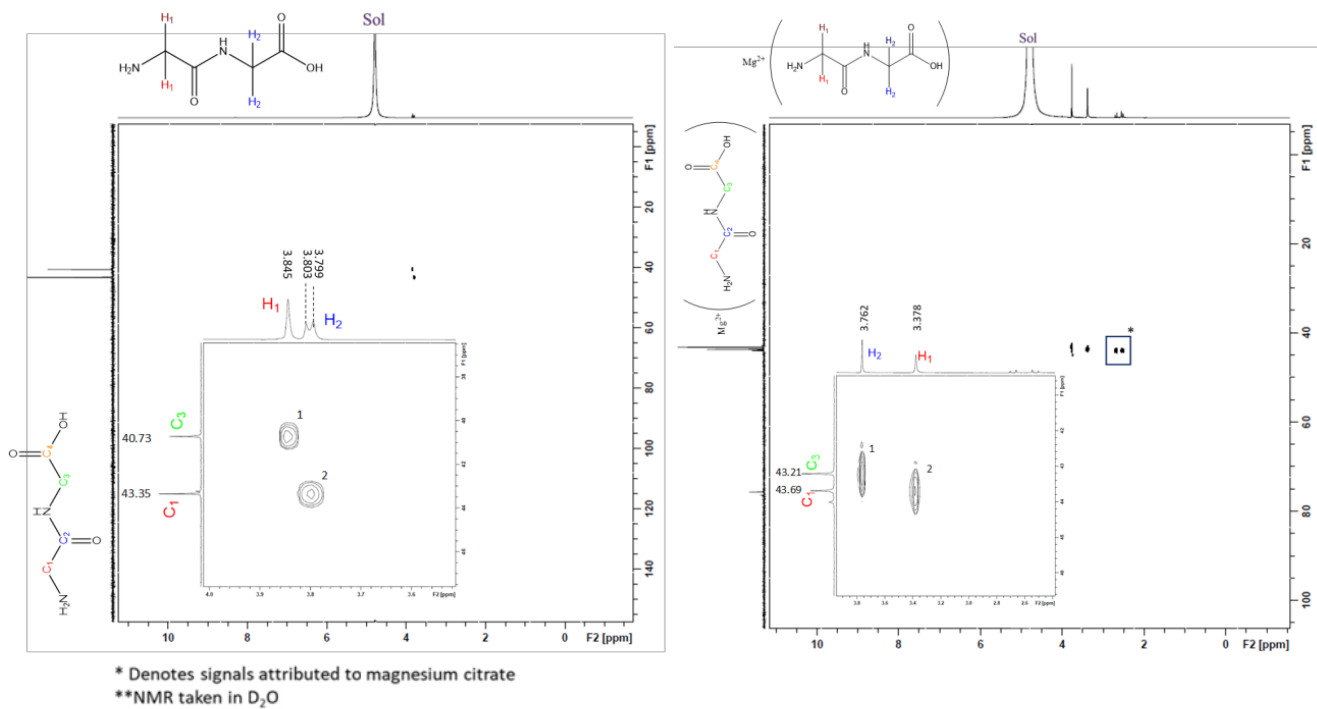


Figure S9. Full spectra HSQC of HG₂ (Left) and HSQC of **1** (Right) utilized to confirm the proton and carbon assignments of HG₂ and **1**.

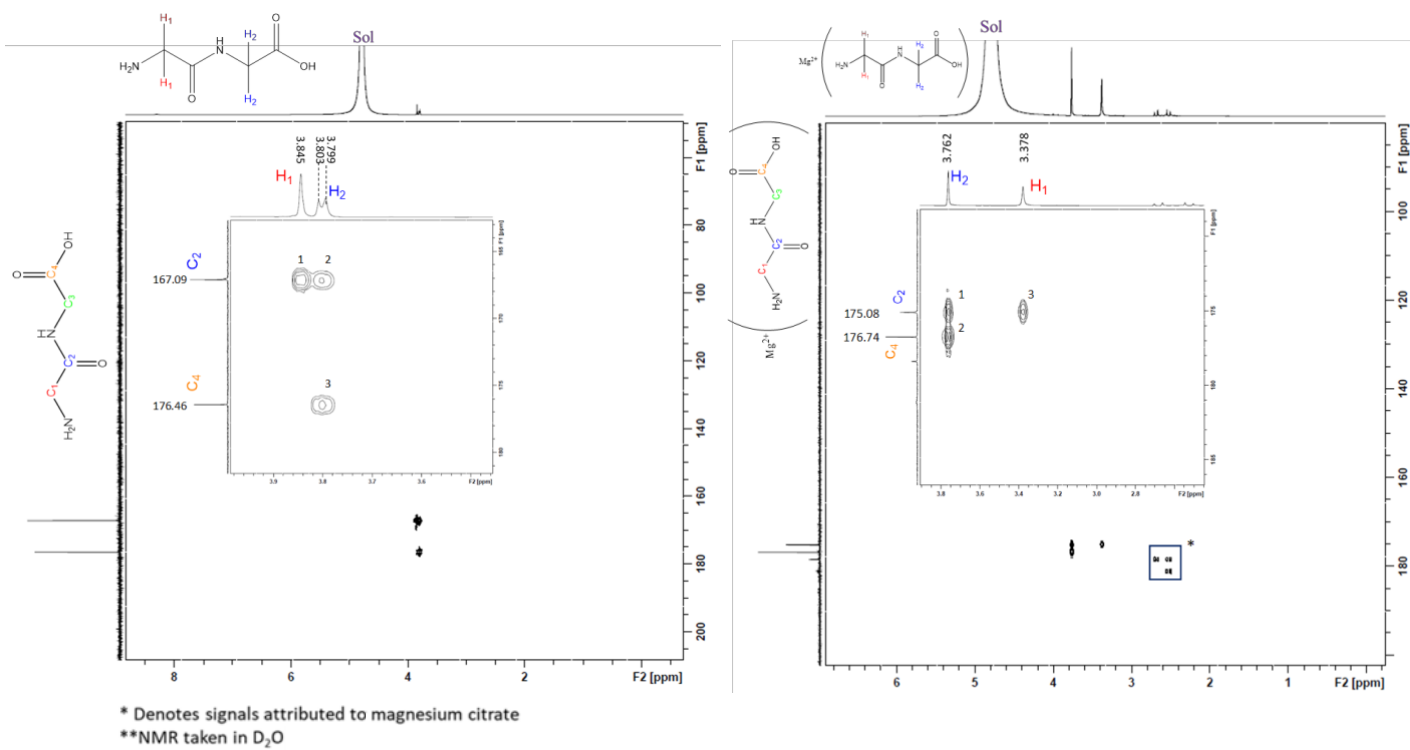


Figure S10. Full spectra HMBC of HG₂ (Left) and HMBC (Right) of **1** utilized to confirm the proton and carbon assignments of HG₂ and **1**.

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Mg	N
8.78 %	9.85 %
	9.92 %

Figure S11. ICP analysis of 1.

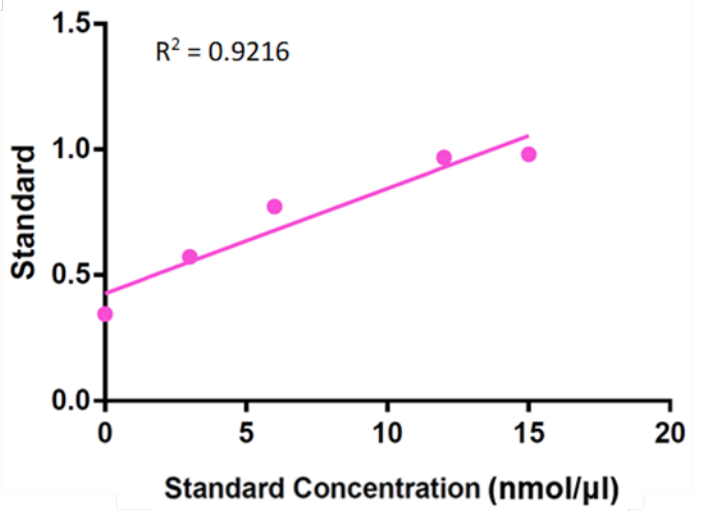
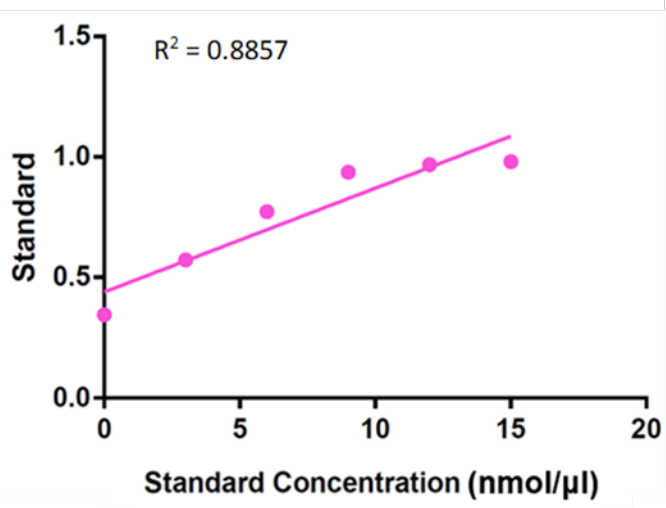


Figure S12. Plot of the linear regression of magnesium assay kit standard to confirm linearity.