

Supplementary Information

Small Compound - Big Colors: Synthesis and Structural Investigation of Brightly Colored Alkaline Earth Metal 1,3-Dimethylviolurates

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1. IR spectra of all title compounds

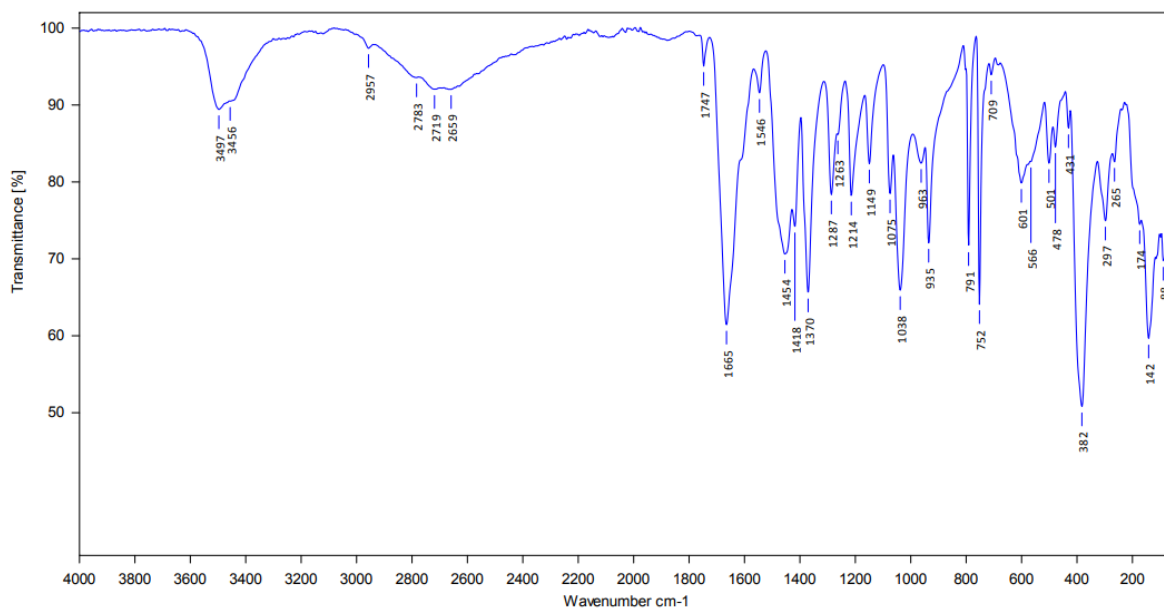


Figure S1. IR spectrum of $[(\text{Me}_2\text{Vio})(\text{H}_2\text{O})]$ (2)

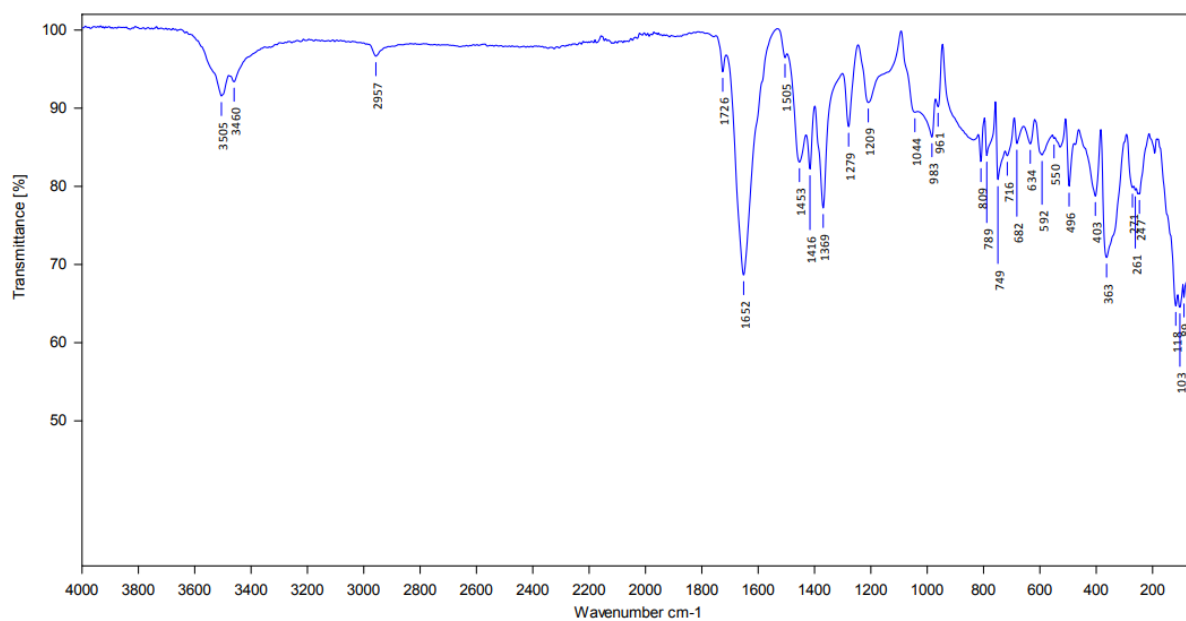


Figure S2. IR spectrum of $[(\text{Me}_2\text{Vio})(\text{H}_2\text{O})]$ (2a)

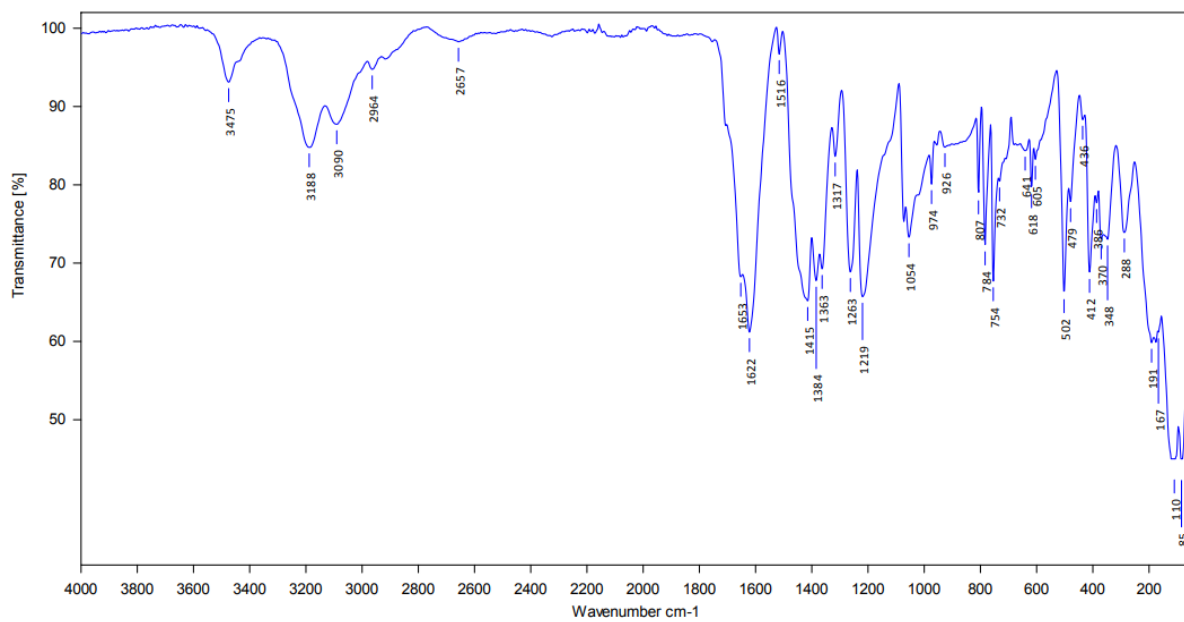


Figure S3. IR spectrum of $[\text{H}_3\text{O}]^+[(\text{Me}_2\text{Vio})(\text{H}_2\text{O})]^-$ (2b)

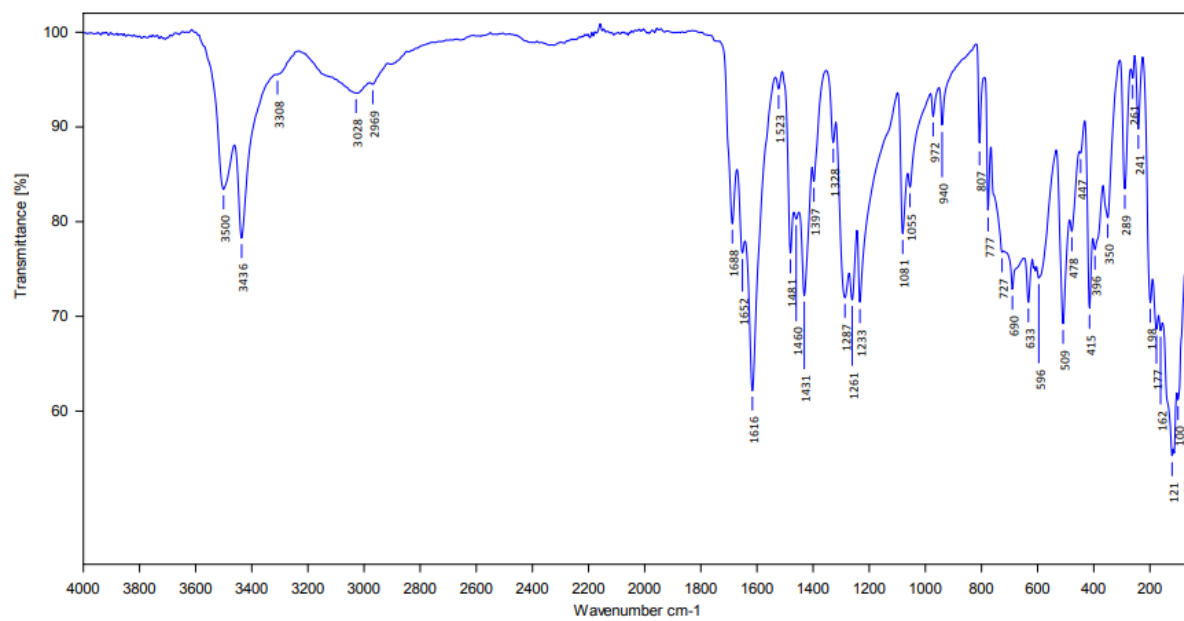


Figure S4. IR spectrum of $[\text{Mg}(\text{Me}_2\text{Vio})_2(\text{H}_2\text{O})_6]$ (3)

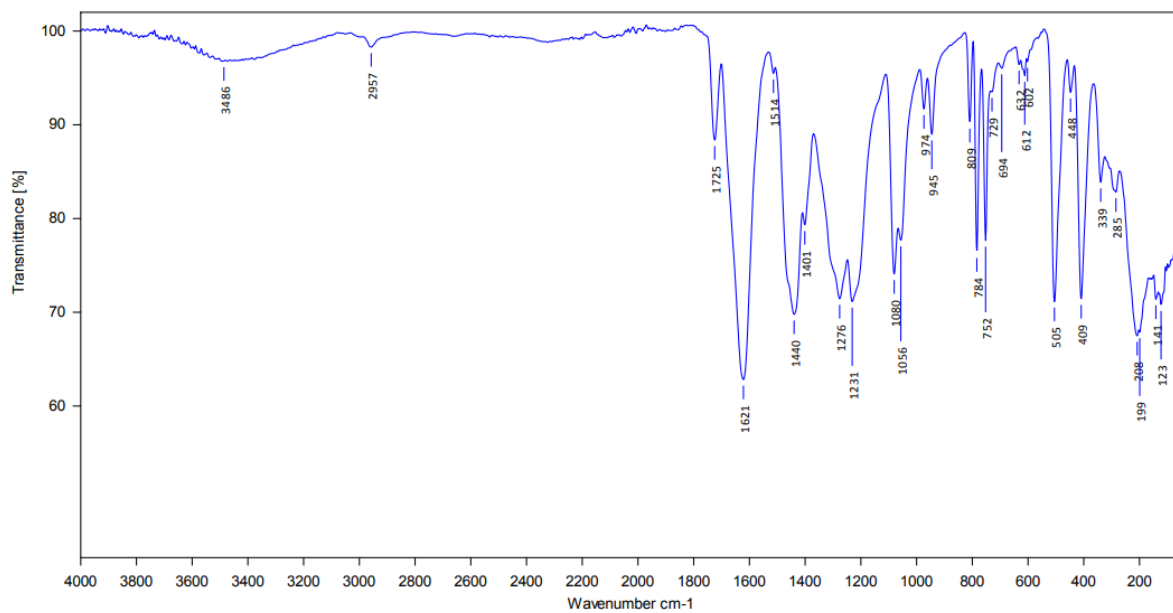


Figure S5. IR spectrum of [Ca(Me₂Vio)(H₂O)₈] (4)

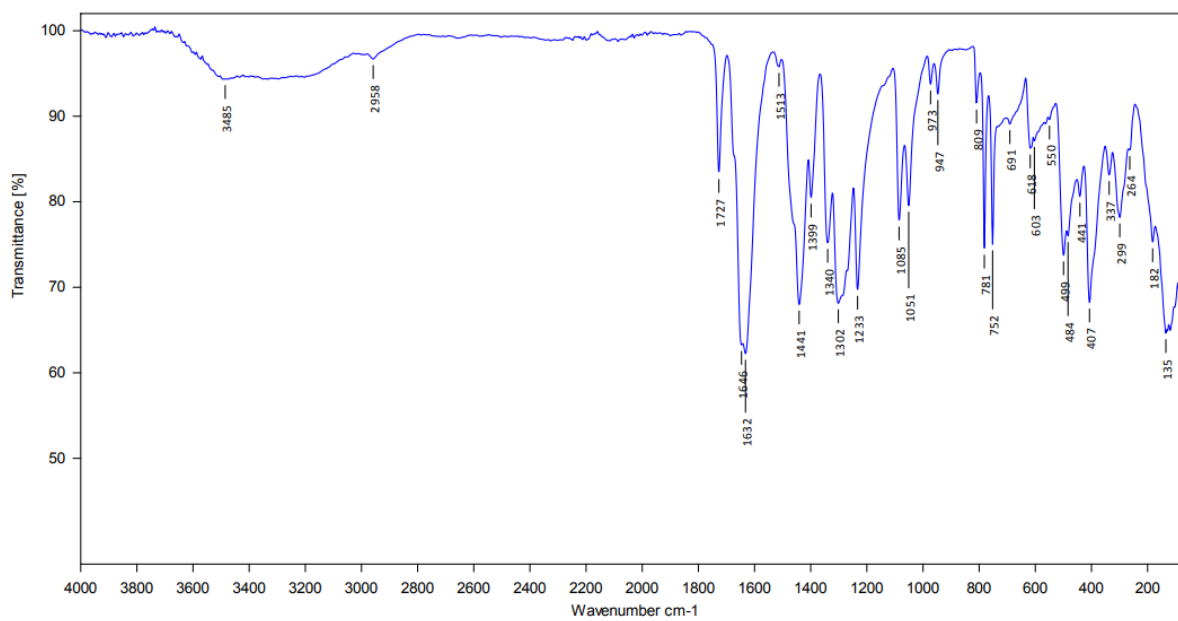


Figure S6. IR spectrum of [Sr(Me₂Vio)₂(H₂O)₆] (5)

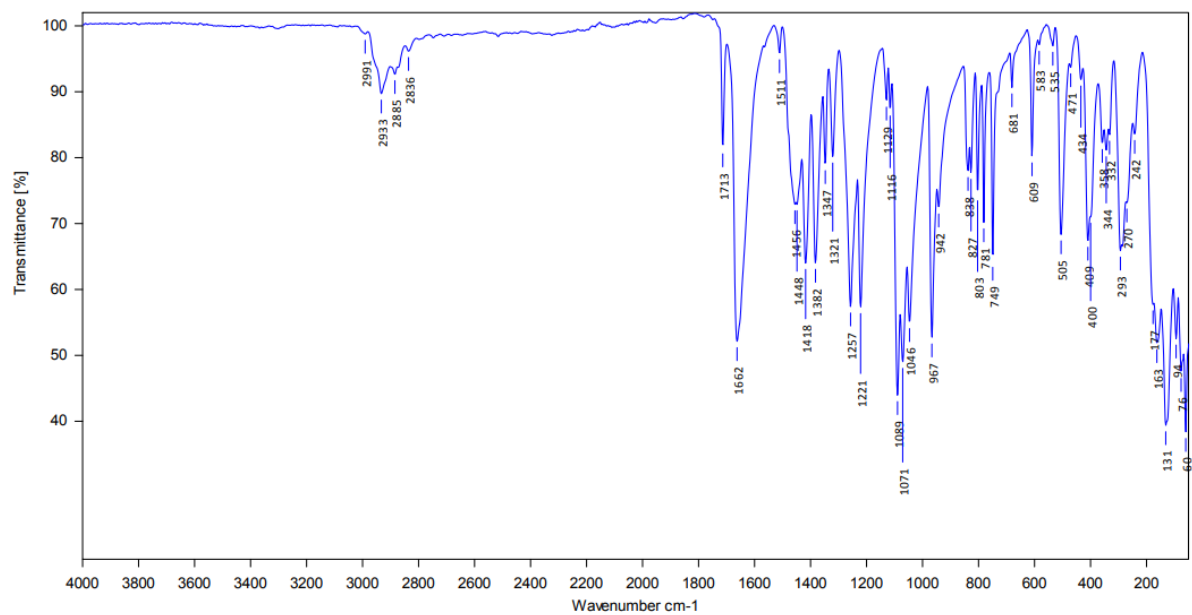


Figure S7. IR spectrum of [Sr(Me₂Vio)₂(18-crown-6)] (5a)

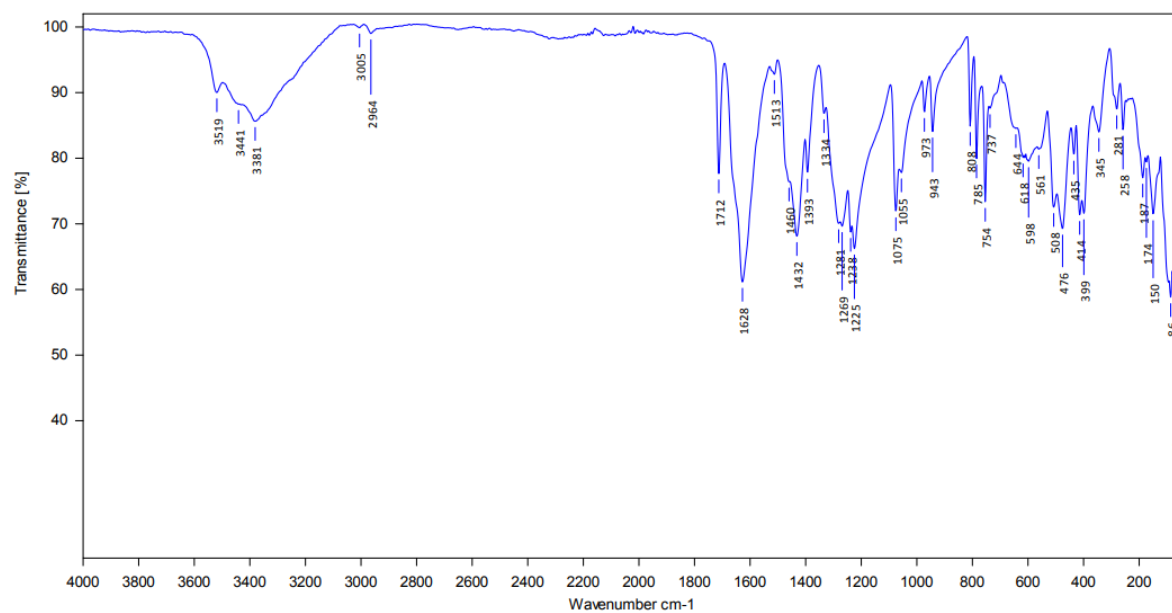


Figure S8. IR spectrum of [Ba(Me₂Vio)₂(H₂O)₄] (6)

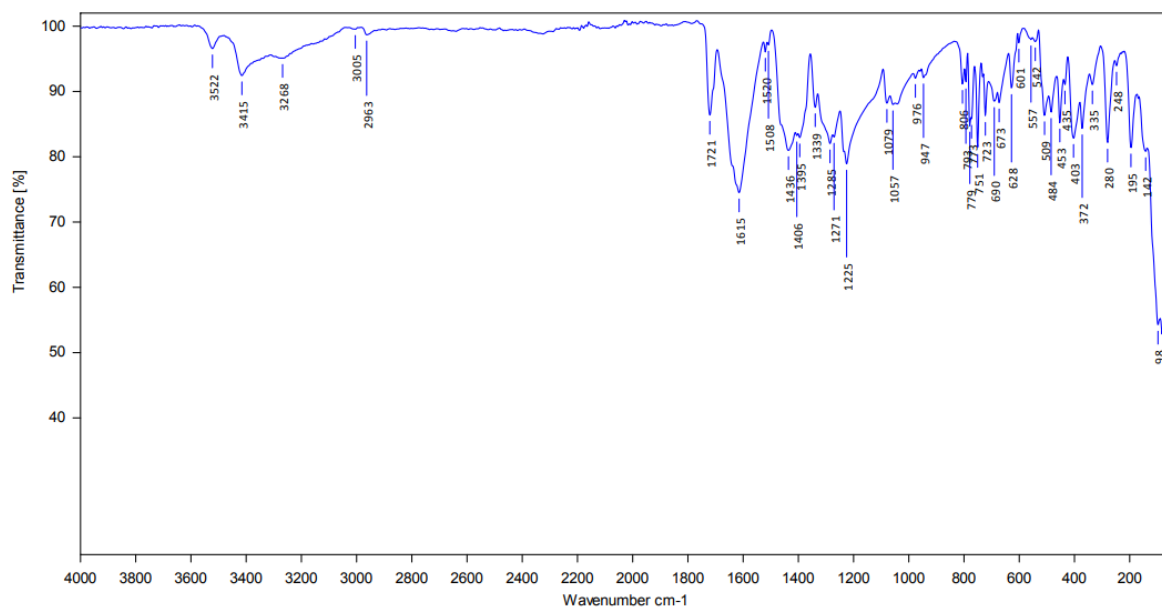
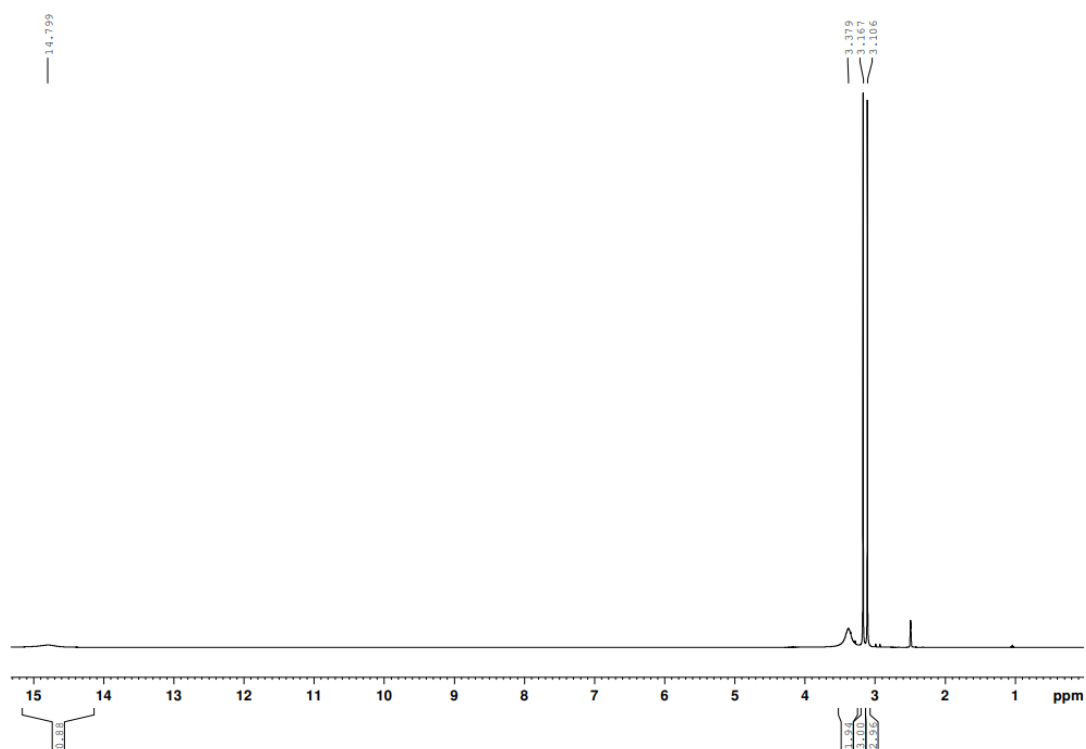


Figure S9. IR spectrum of $[\text{Ba}(\text{Me}_2\text{Vio})(\text{NO}_2\text{Barb}) \cdot 4\text{H}_2\text{O}]$ (**8**)

2. NMR spectra of all title compounds

^1H NMR in $\text{DMSO-}d_6$:



^{13}C NMR in $\text{DMSO-}d_6$:

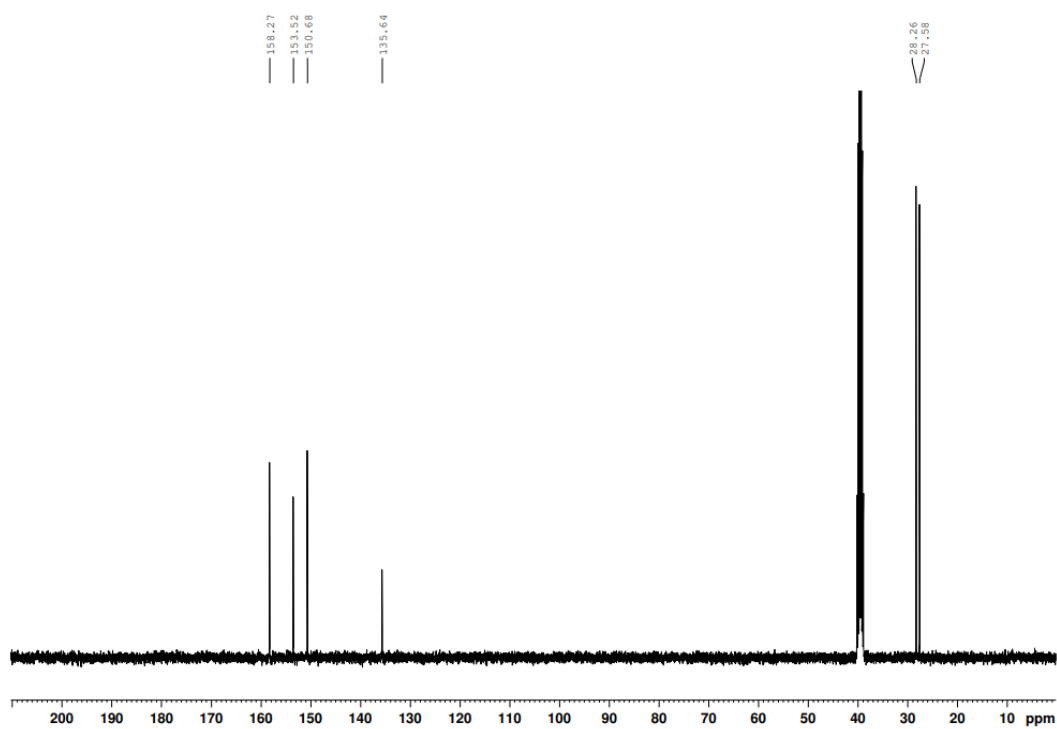
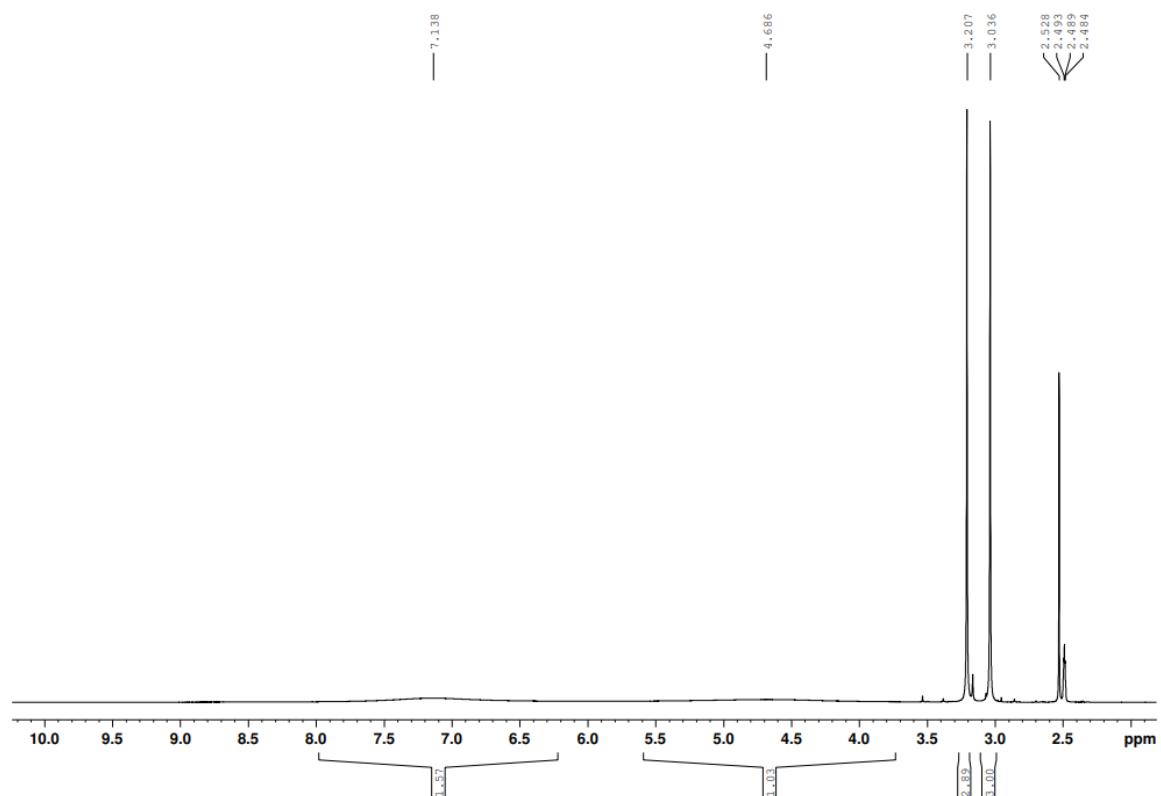


Figure S10. ^1H and ^{13}C NMR spectra of original (colorless) $\text{H}(\text{Me}_2\text{Vio})\cdot\text{H}_2\text{O}$ (**2**) in $\text{DMSO-}d_6$

^1H NMR in $\text{DMSO-}d_6$:



^{13}C NMR in $\text{DMSO-}d_6$:

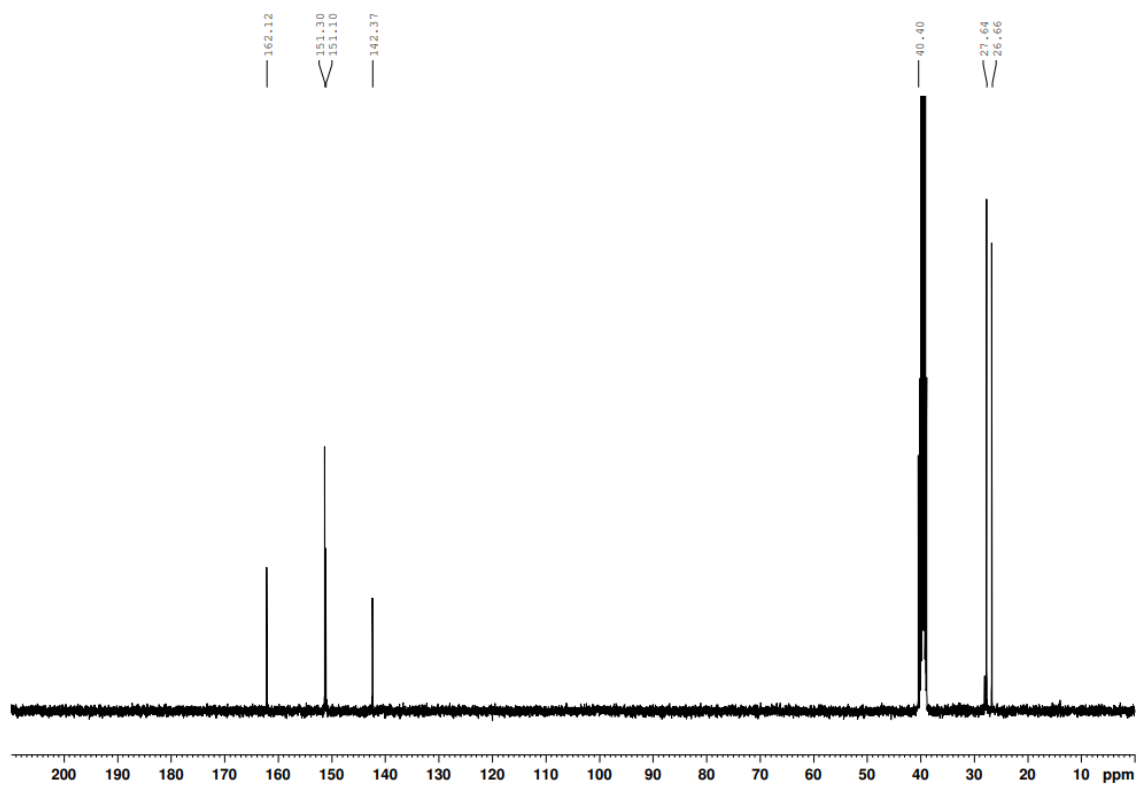
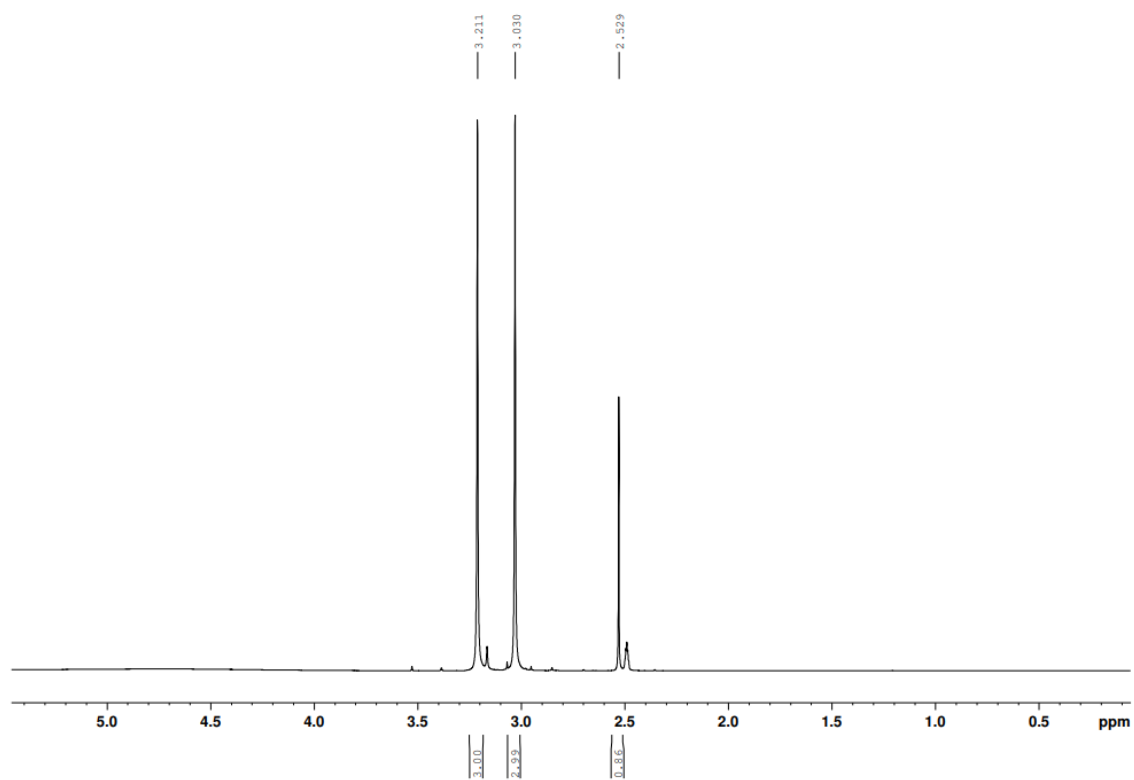


Figure S11. ^1H and ^{13}C NMR spectra of orange $\text{H}(\text{Me}_2\text{Vio})\cdot\text{H}_2\text{O}$ (**2a**) in $\text{DMSO-}d_6$

^1H NMR in $\text{DMSO-}d_6$:



^{13}C NMR in $\text{DMSO-}d_6$:

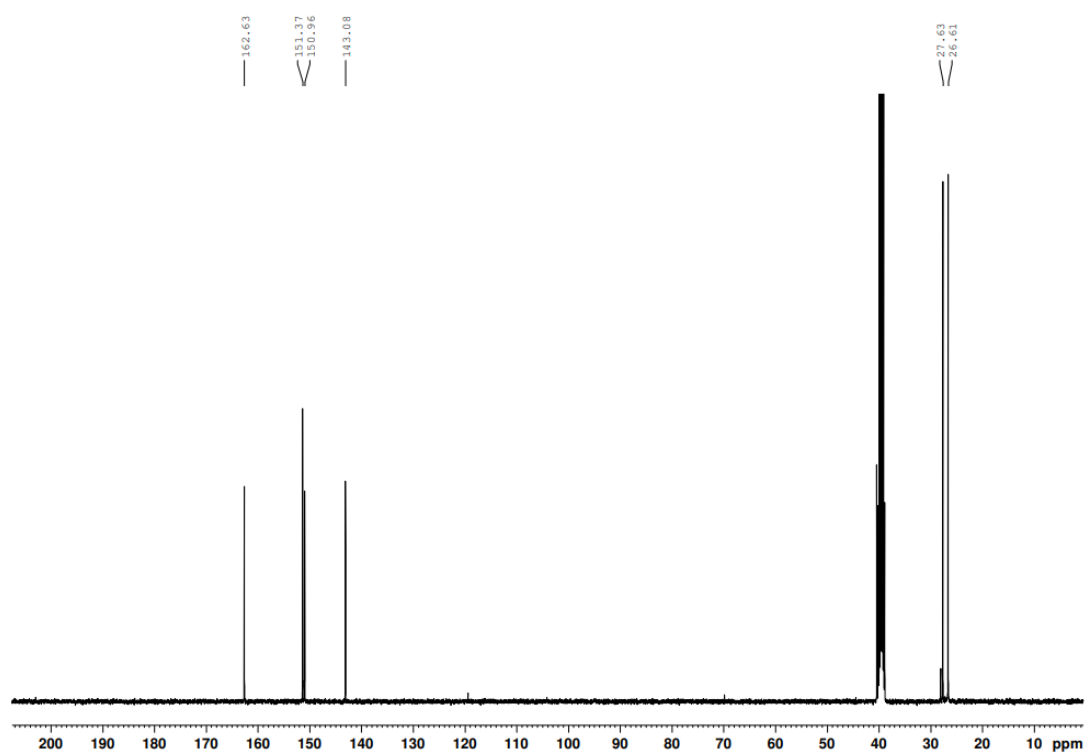
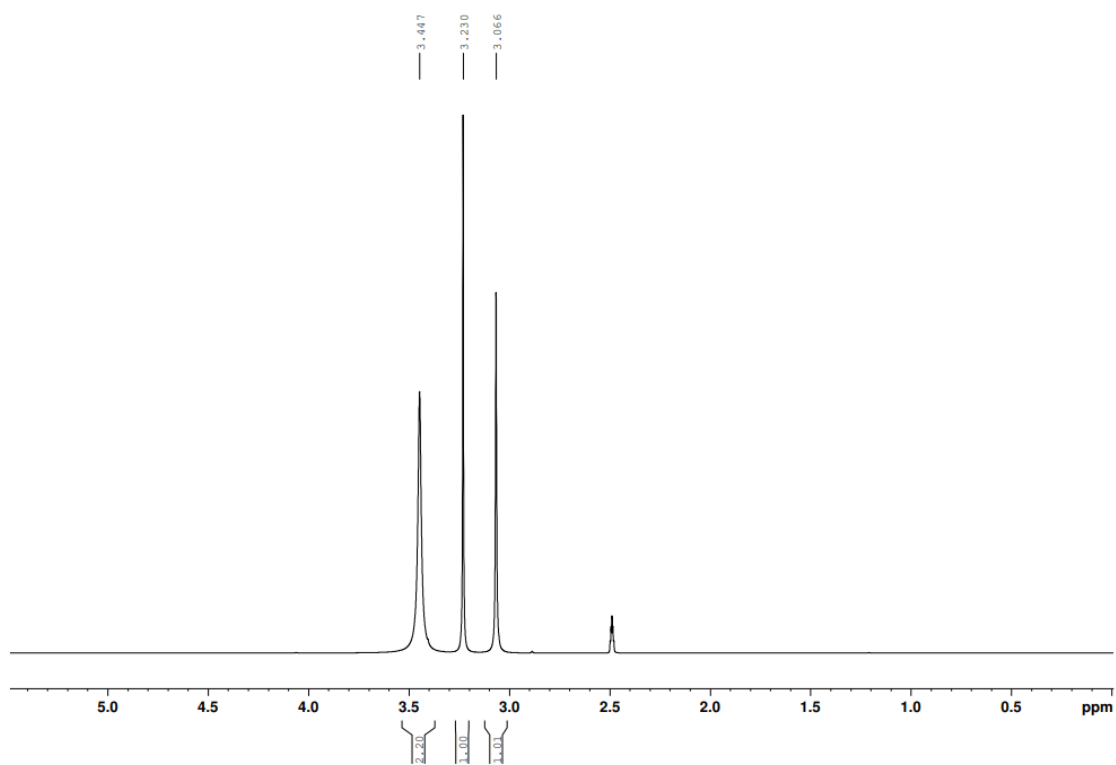


Figure S12. ^1H and ^{13}C NMR spectra of $[\text{H}_3\text{O}][\text{Me}_2\text{Vio}]$ (**2b**) in $\text{DMSO-}d_6$

^1H NMR in in $\text{DMSO-}d_6$:



^{13}C NMR in $\text{DMSO-}d_6$:

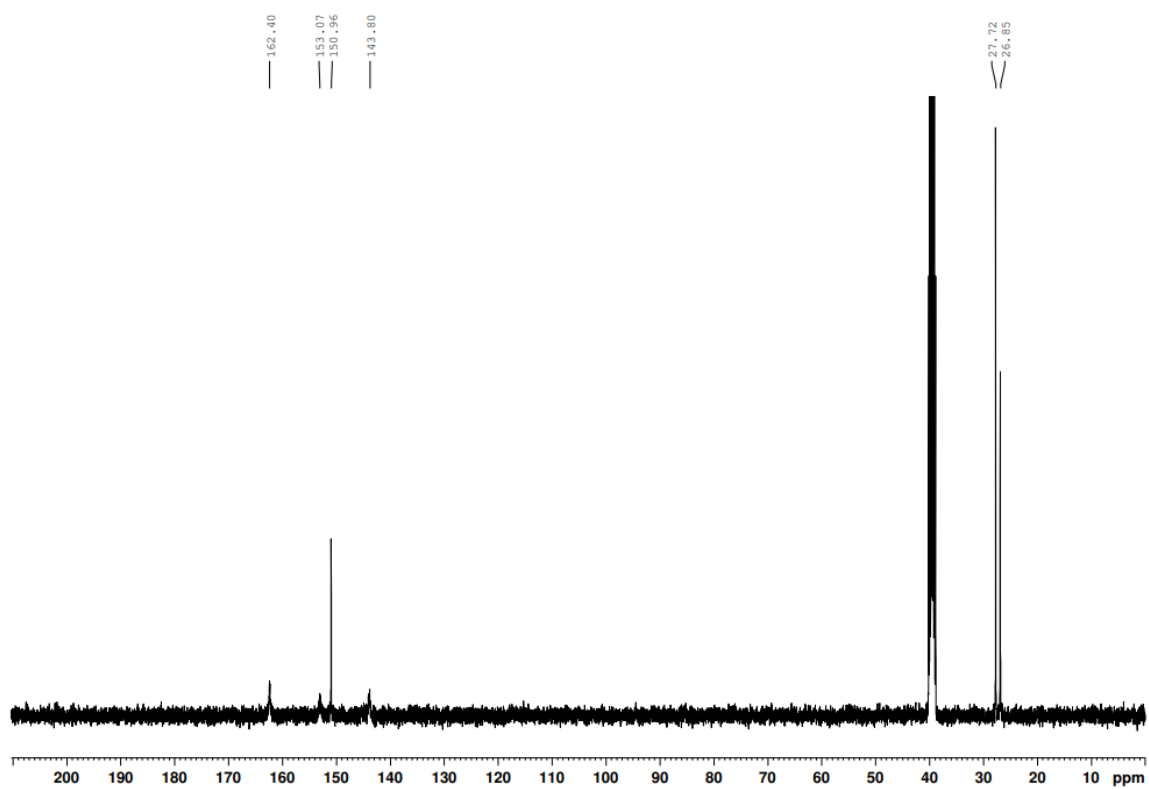
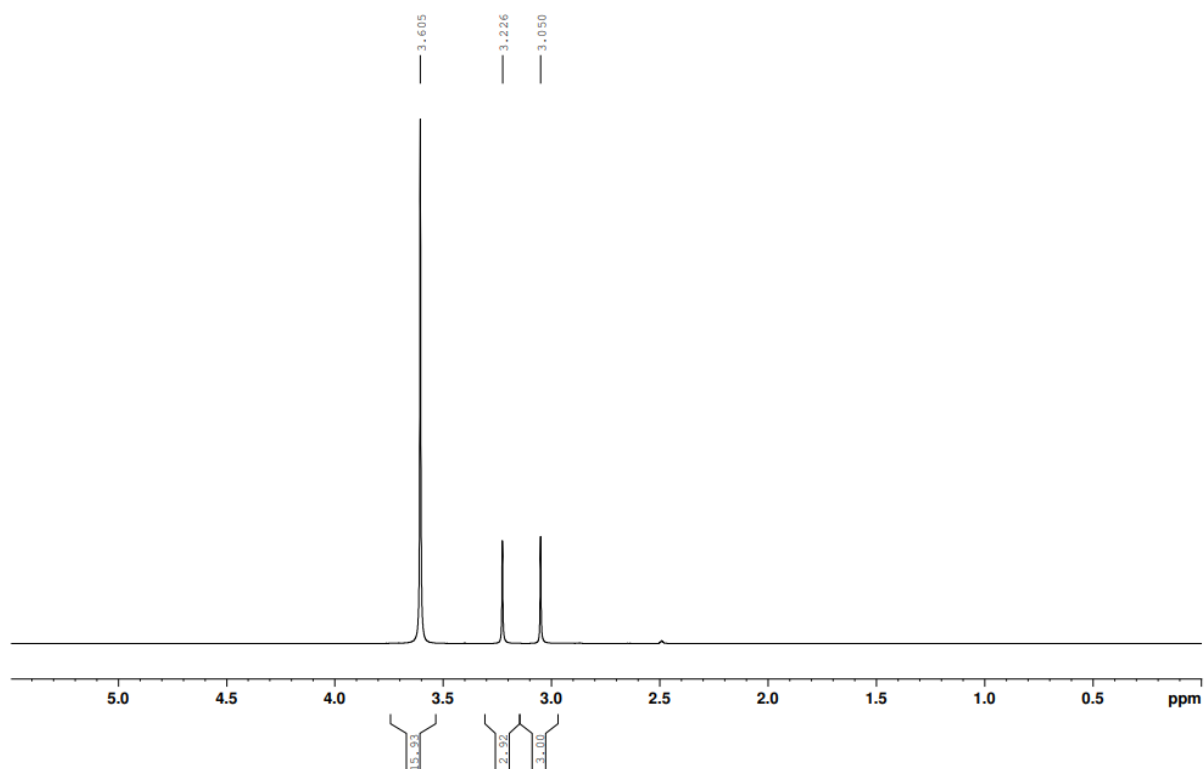


Figure S13. ^1H and ^{13}C NMR spectra of $[\text{Mg}(\text{H}_2\text{O})_6](\text{Me}_2\text{Vio})_2$ (**3**) in $\text{DMSO-}d_6$

^1H NMR in $\text{DMSO-}d_6$:



^{13}C NMR in $\text{DMSO-}d_6$:

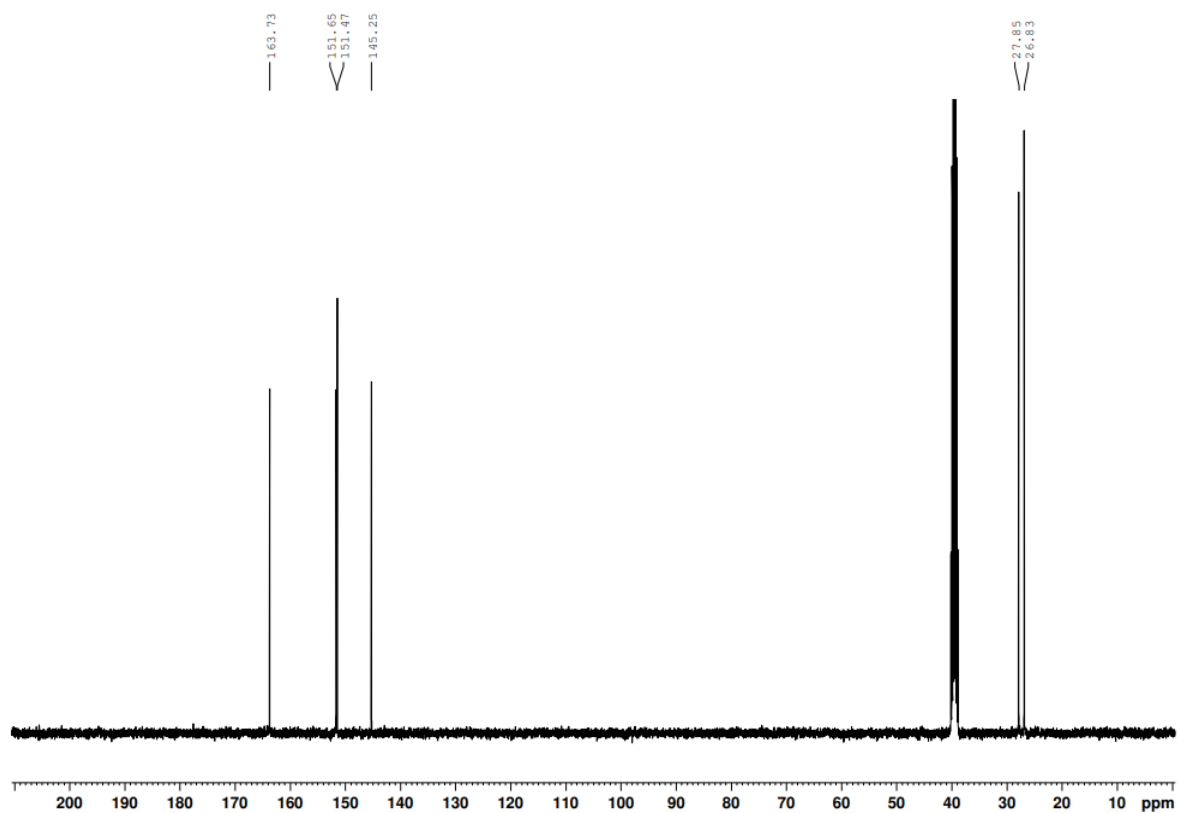
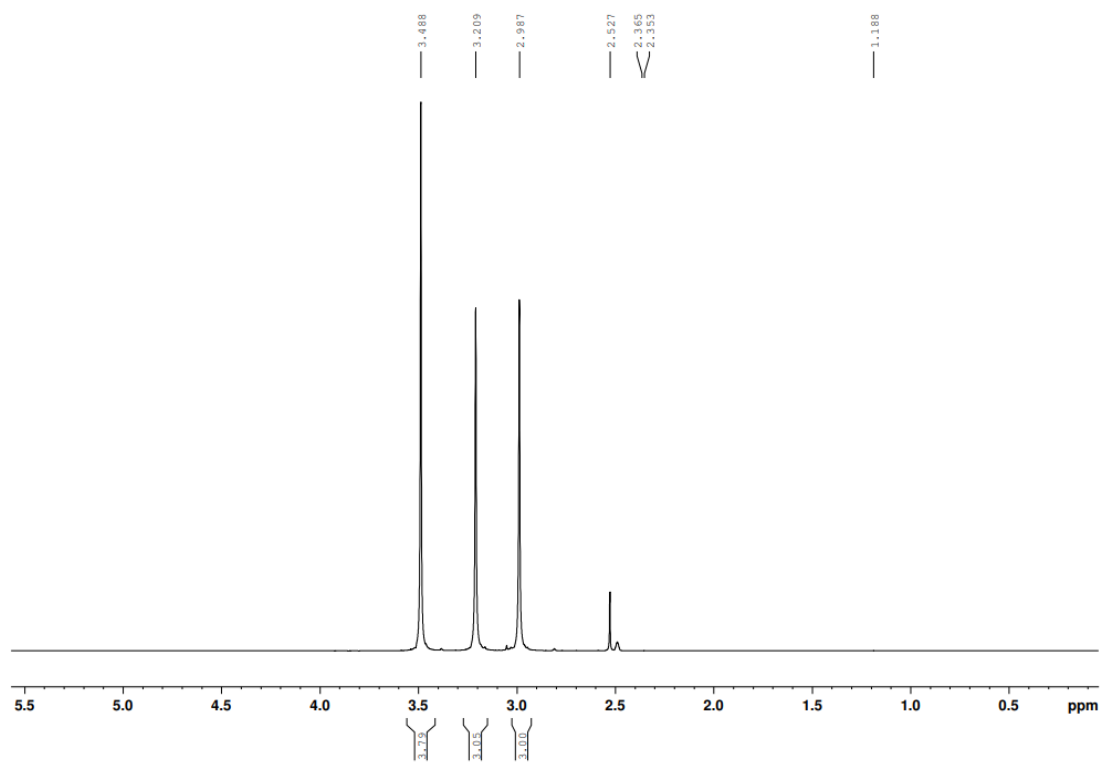


Figure S14. ^1H and ^{13}C NMR spectra of $\text{Ca}(\text{Me}_2\text{Vio})\cdot 8\text{H}_2\text{O}$ (4) in $\text{DMSO-}d_6$

^1H NMR in $\text{DMSO-}d_6$:



^{13}C NMR in $\text{DMSO-}d_6$:

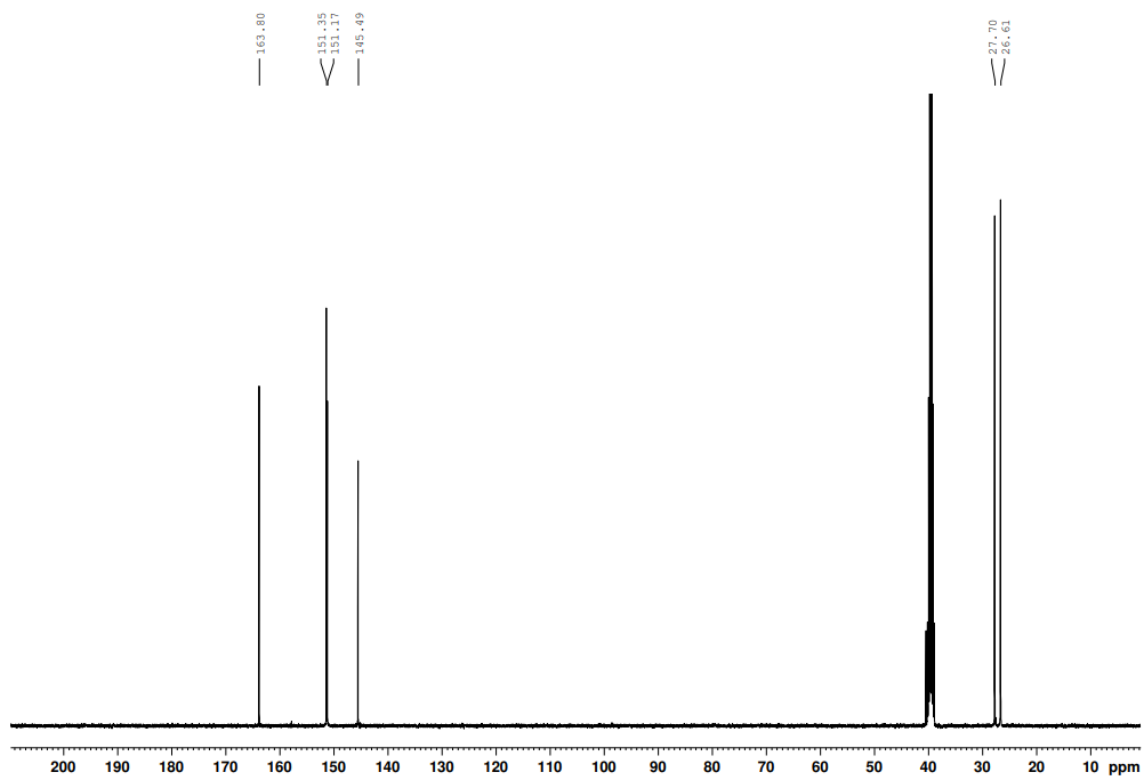
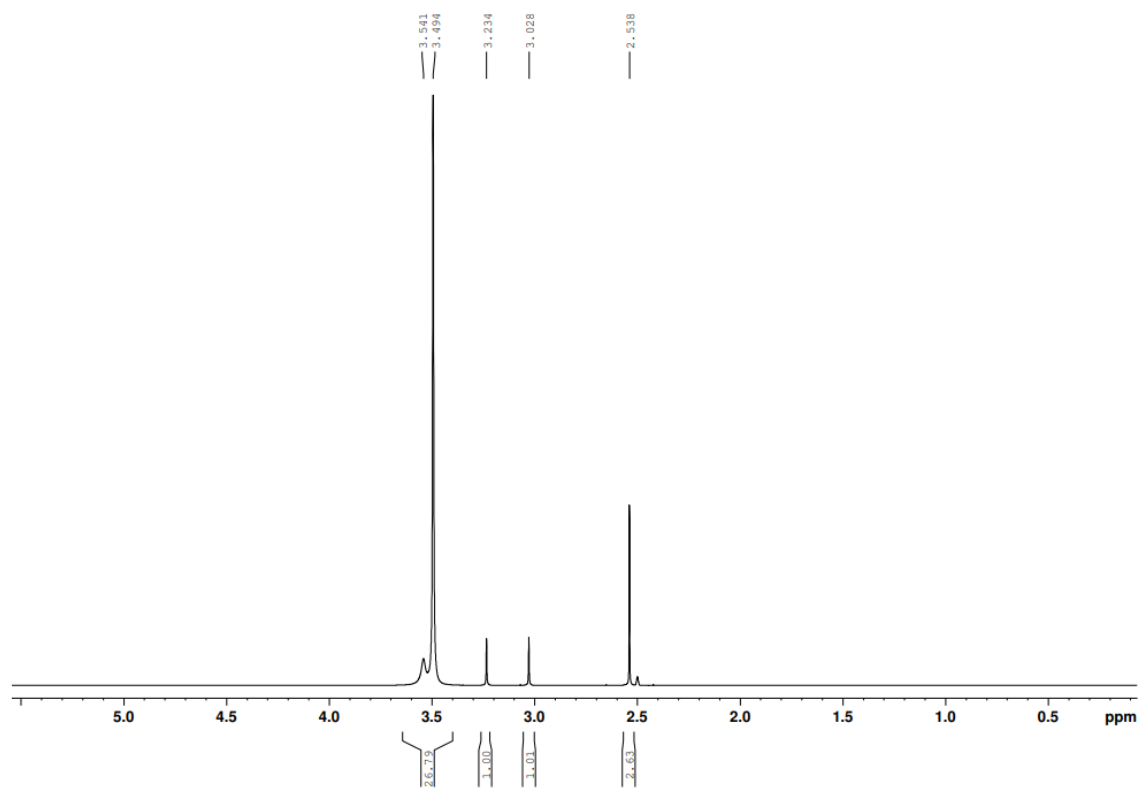


Figure S15. ^1H and ^{13}C NMR spectra of $\text{Sr}(\text{Me}_2\text{Vio})_2 \cdot 6\text{H}_2\text{O}$ (5) in $\text{DMSO-}d_6$

^1H NMR in $\text{DMSO-}d_6$:



^{13}C NMR in in $\text{DMSO-}d_6$:

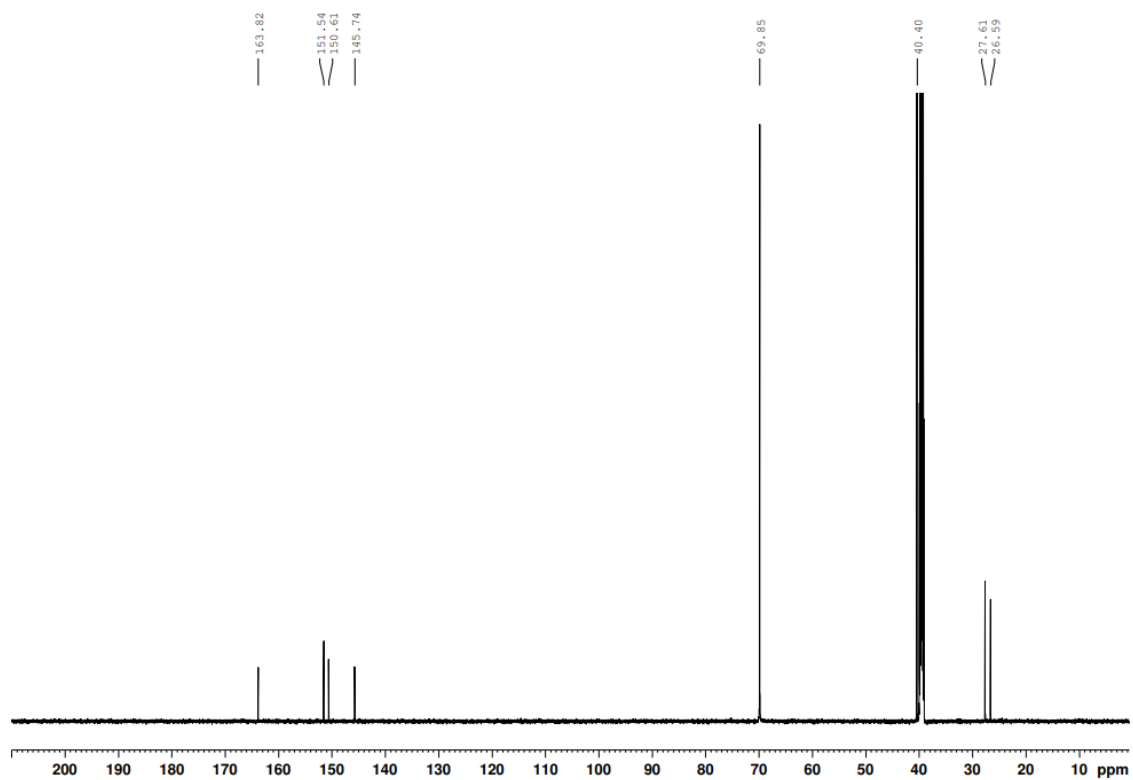
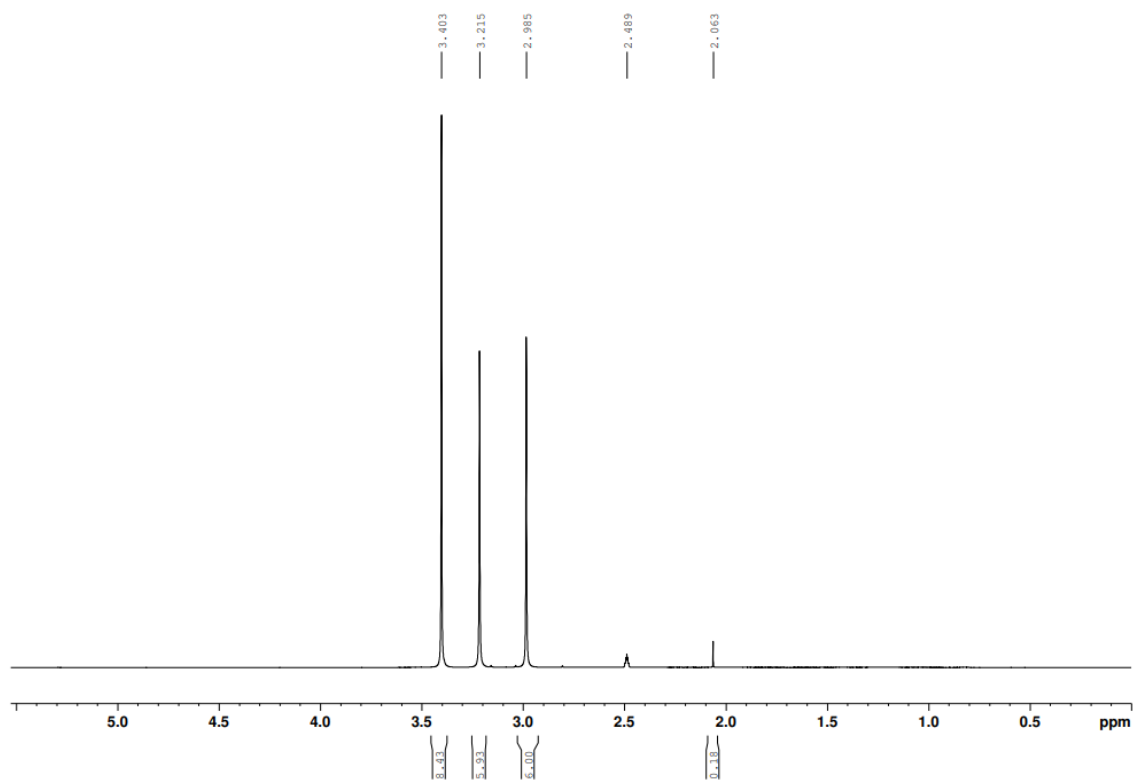


Figure S16. ^1H and ^{13}C NMR spectra of $\text{Sr}(\text{Me}_2\text{Vio})_2(18\text{-crown-}6)$ (**5a**) in $\text{DMSO-}d_6$

^1H NMR in $\text{DMSO-}d_6$:



^{13}C NMR in $\text{DMSO-}d_6$:

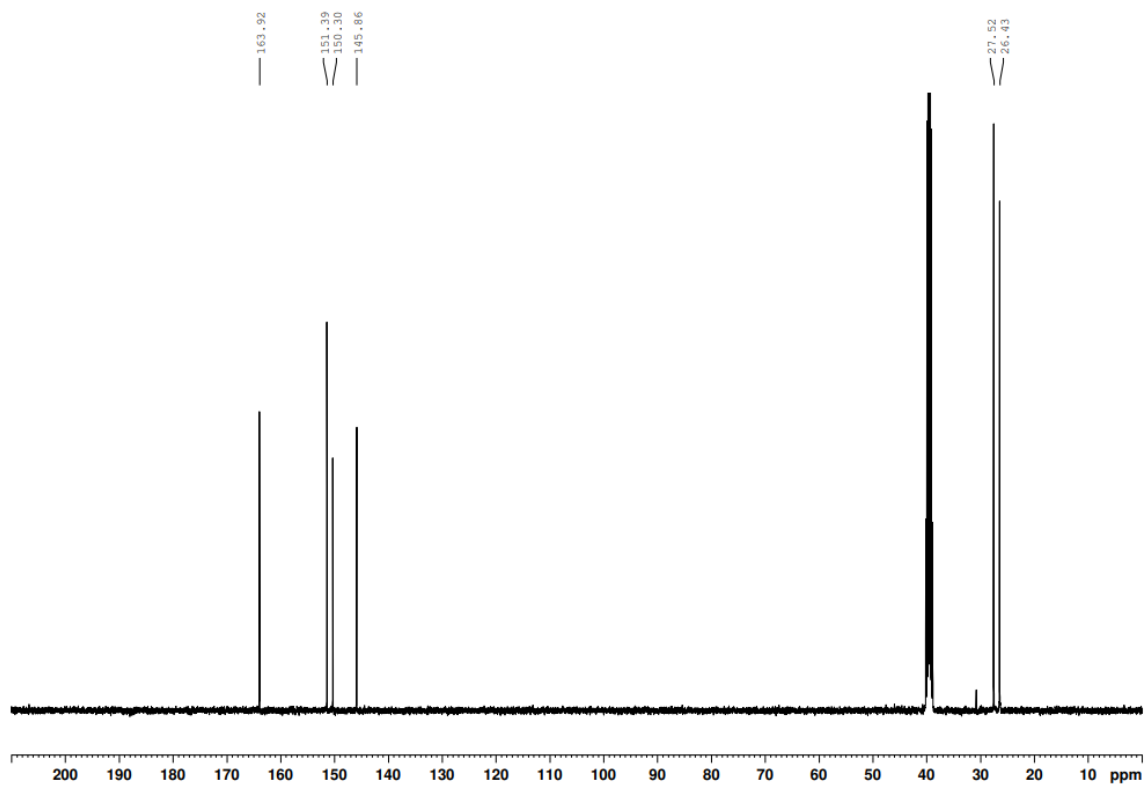
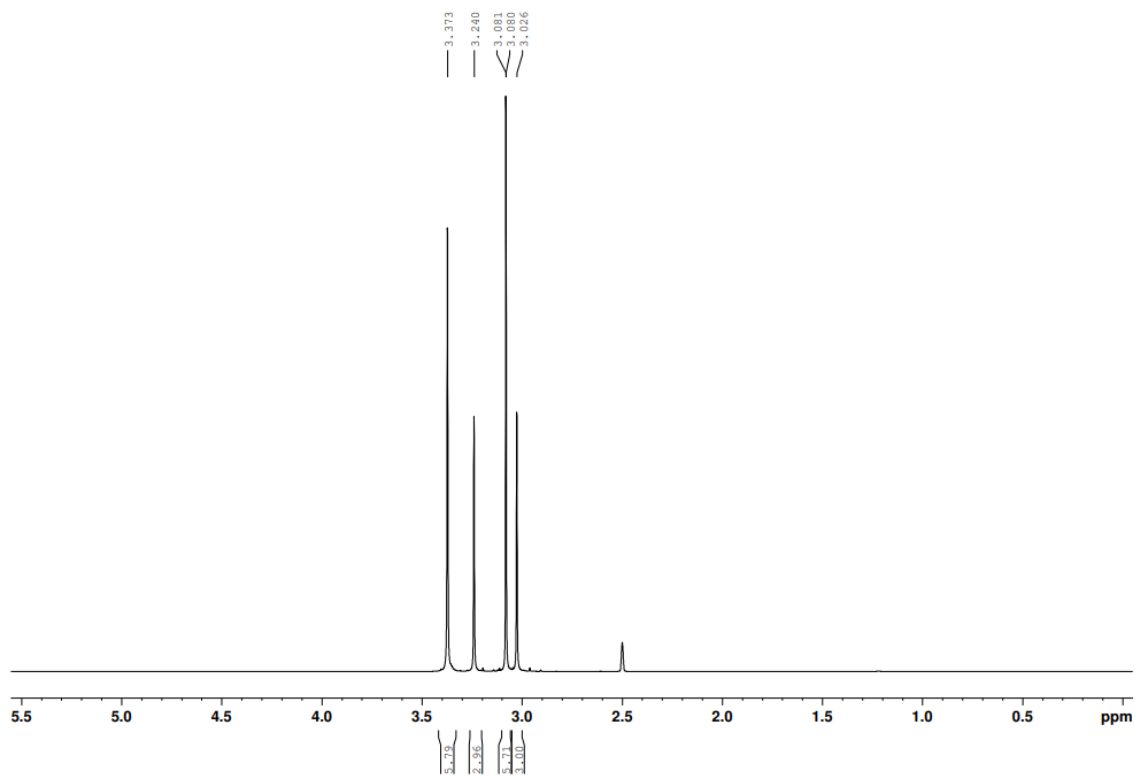


Figure S17. ^1H and ^{13}C NMR spectra of $\text{Ba}(\text{Me}_2\text{Vio})_2 \cdot 4\text{H}_2\text{O}$ (6) in $\text{DMSO-}d_6$

^1H NMR in $\text{DMSO-}d_6$:



^{13}C NMR in $\text{DMSO-}d_6$:

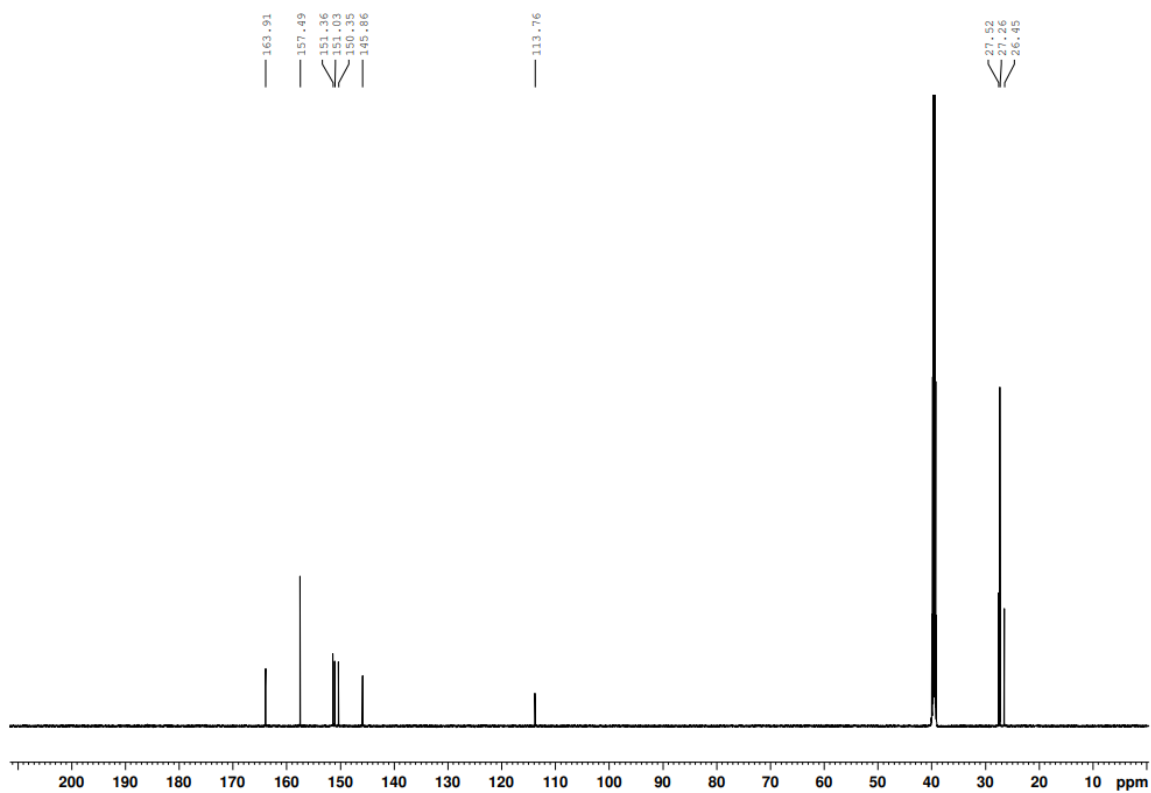


Figure S18. ^1H and ^{13}C NMR spectra of $\text{Ba}(\text{Me}_2\text{Vio})(\text{Me}_2\text{NO}_2\text{Barb})\cdot 2\text{H}_2\text{O}$ (**8**) in $\text{DMSO-}d_6$

3. Raman Spectra

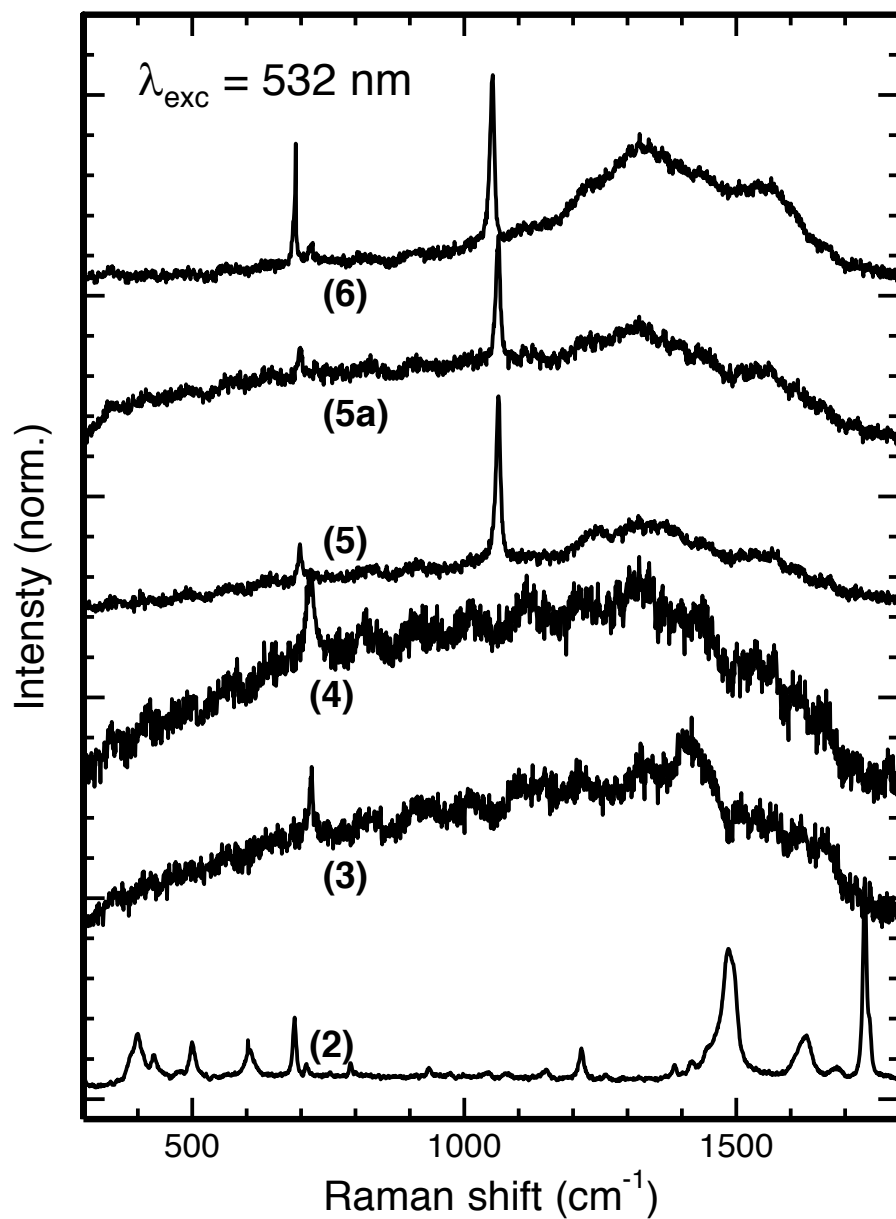


Figure S19. Raman spectra of compounds 2-6 from bottom to top. Laser wavelength was 532 nm, the detection was unpolarized. All spectra were normalized to their respective maximum and shifted vertically for better visibility.

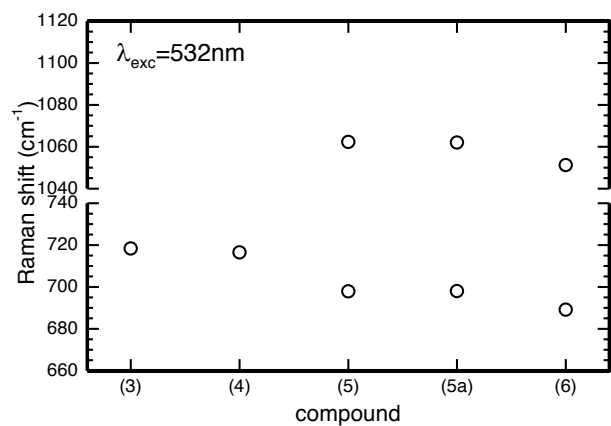


Figure S20. Raman peak positions for compounds **3-6** as determined from the spectra shown in Fig. S19. Only the sharp features around 700 cm⁻¹ and 1050 cm⁻¹ for **5** and **6** are shown. The results for compound **5** and **5a** are identical. A decrease of Raman shift with increasing AE atomic mass is observed (AE = Mg–Ba).

4. UV-vis Spectra

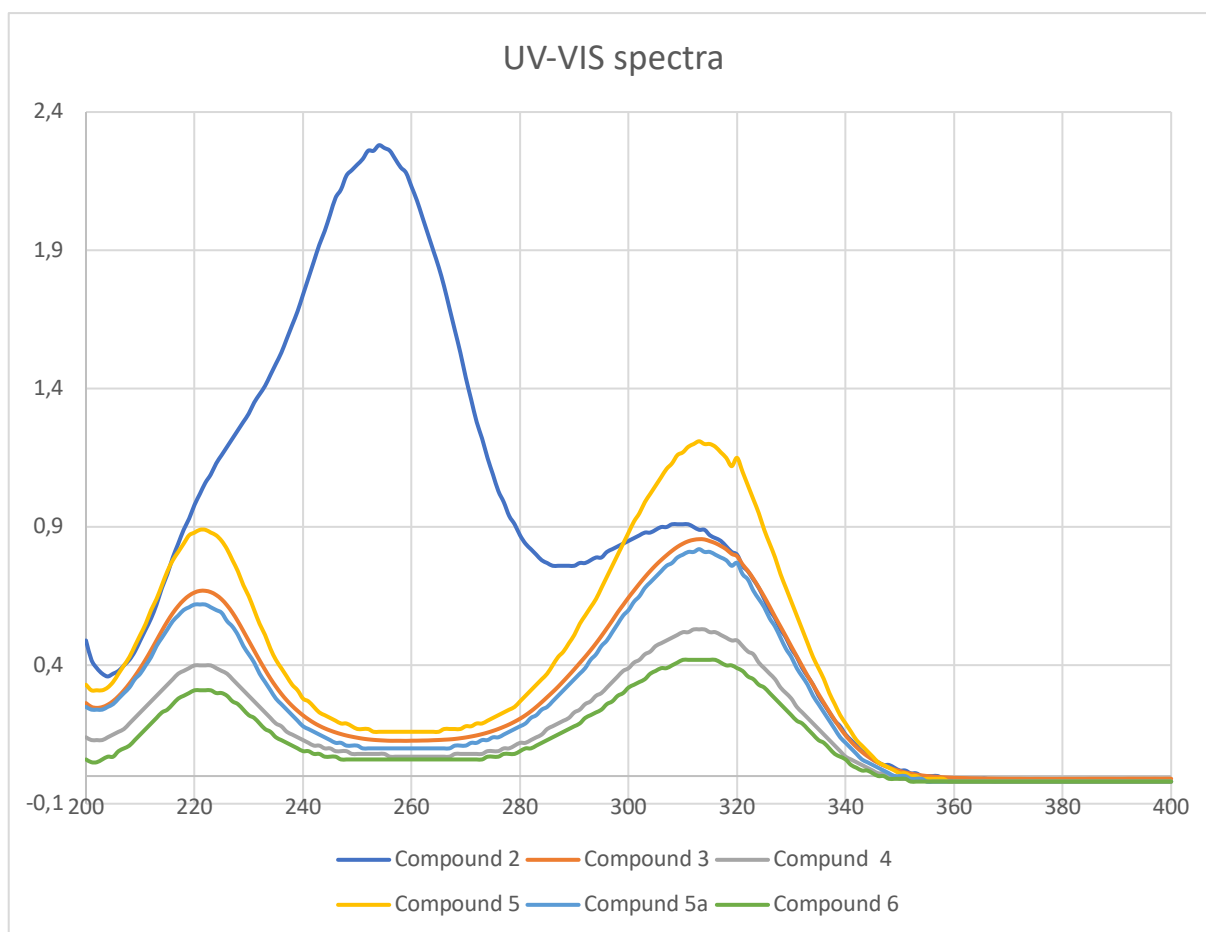


Figure S21. UV-vis spectra of compounds 2-6 in aqueous solution.