Electronic Supplementary Information for Dalton Transactions

ELECTRONIC SUPPLEMENTARY INFORMATION

for the paper entitled

Interaction of 6,6''-bis(5,5,8,8-tetramethyl-5,6,7,8-tetrahydro-1,2,4-benzotriazin-3-yl)-2,2':6',2''-terpyridine ($CyMe_4$-BTTP) with some Trivalent Ions such as Lanthanide(III) Ions and Americium(III)

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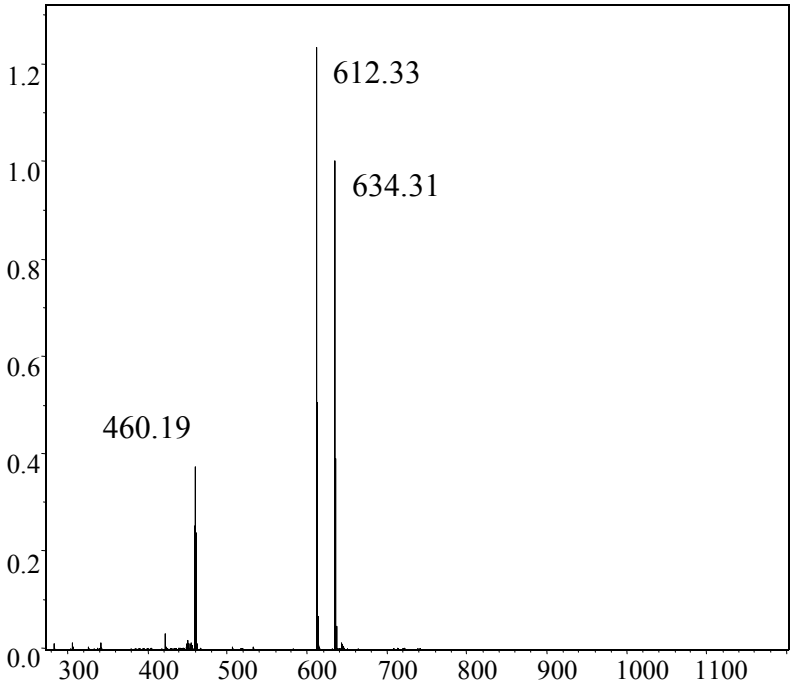

Figure S1. Mass spectrum of a **5**:$Gd(ClO_4)_3$ mixture (2.5:1 ratio). m/z = 460.19: $[Gd(\mathbf{5})_2]^{3+}$, m/z = 612.33: **5** + H^+, m/z = 634.31: **5** + Na^+.

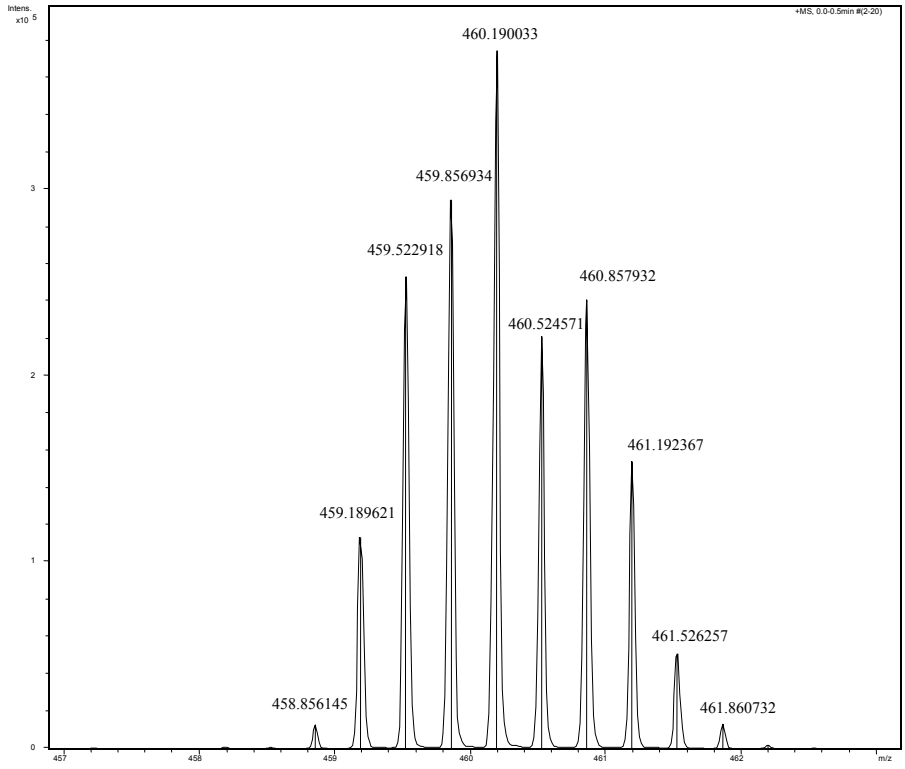

Figure S2. Expanded view of the mass peak at m/z = 460.19 of $[Gd(\mathbf{5})_2]^{3+}$.

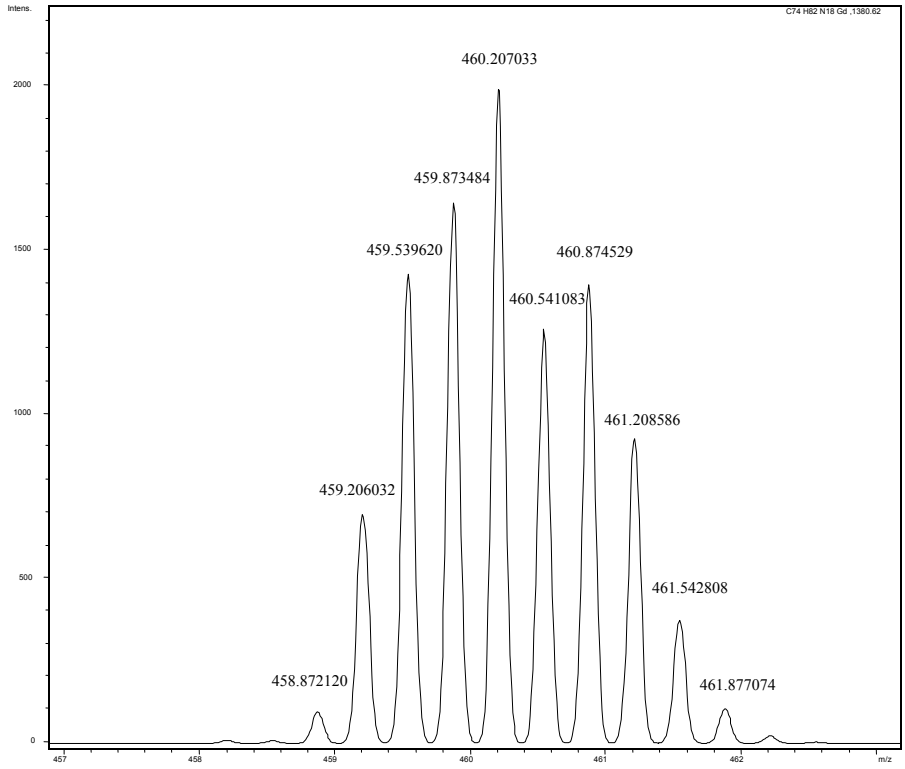

Figure S3. Computer simulation of the isotope distribution pattern of $[Gd(\mathbf{5})_2]^{3+}$.

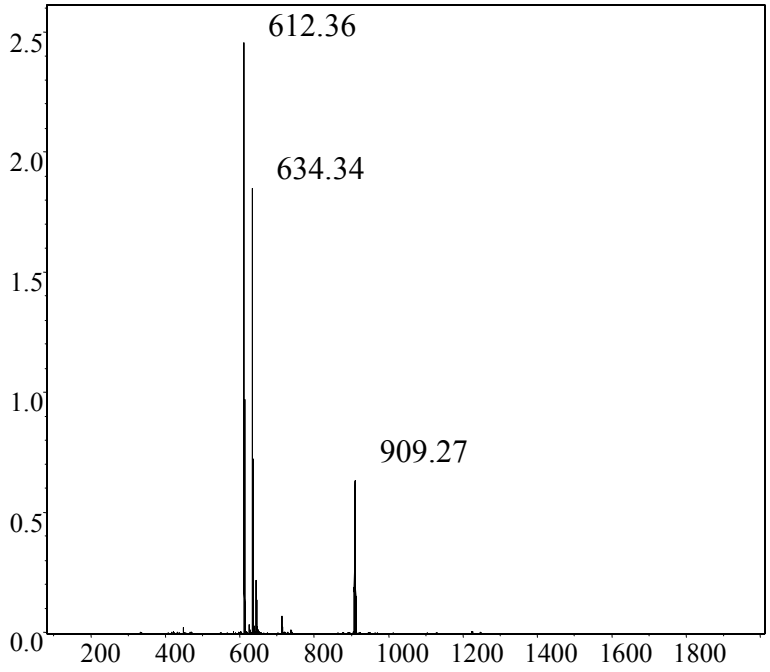

Figure S4. Mass Spectrum of a **5**:$Yb(NO_3)_3$ mixture (1:1 ratio). m/z = 612.36: **5** + H^+, m/z = 634.34: **5** + Na^+, m/z = 909.27: $[Yb(\mathbf{5})(NO_3)_2]^+$.

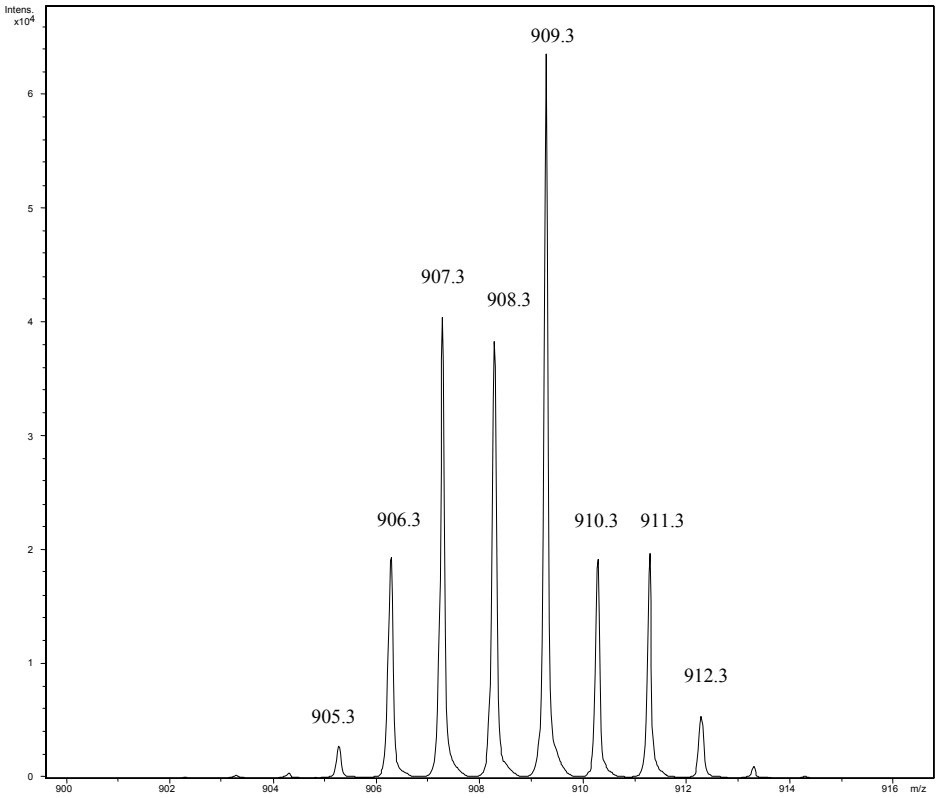

Figure S5. Expanded view of the mass peak at m/z = 909.27 of $[Yb(\mathbf{5})(NO_3)_2]^+$.

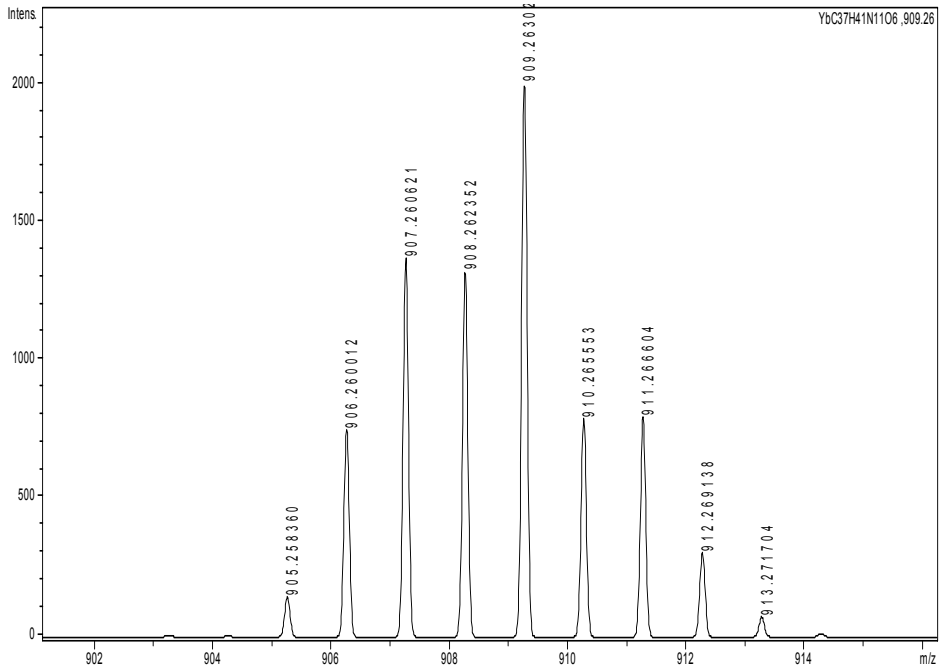

Figure S6. Computer simulation of the isotope distribution pattern of $[Yb(\mathbf{5})(NO_3)_2]^+$.

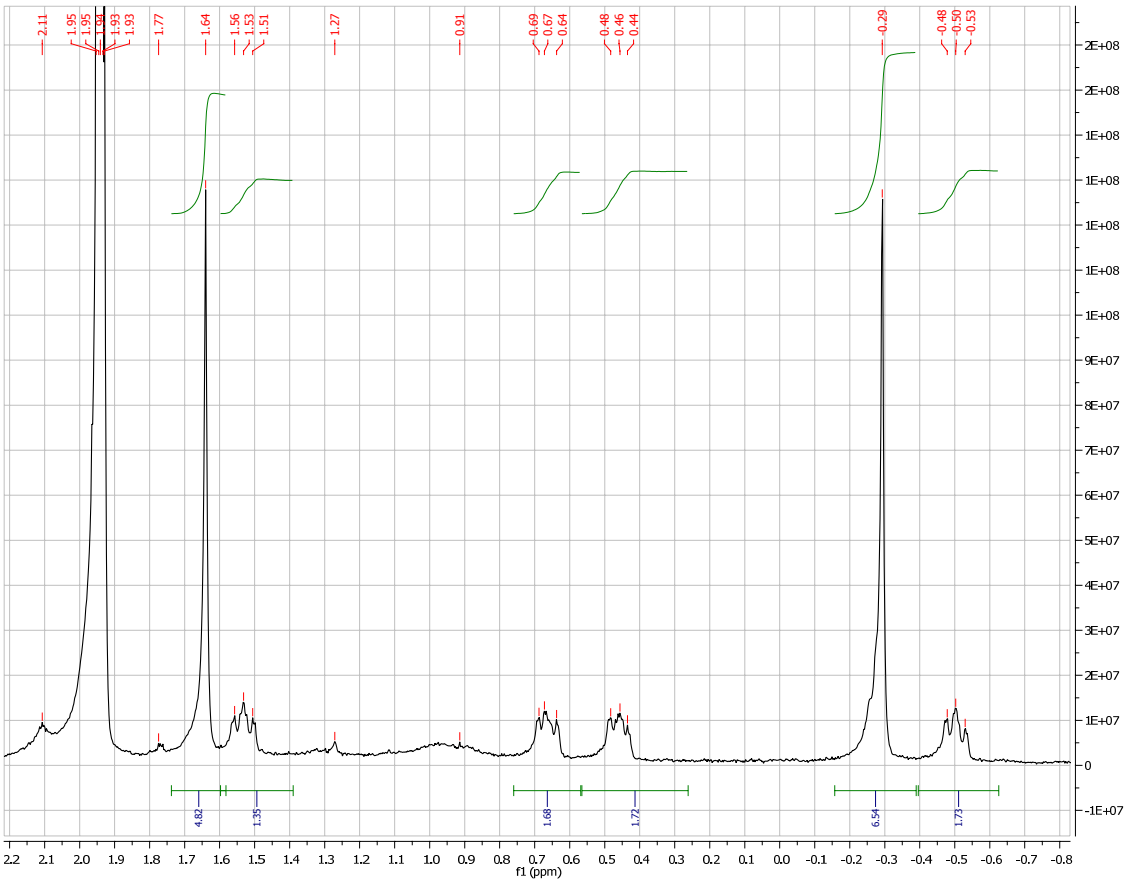

Figure S7. Expanded view of the methylene resonances in the ^{1}H NMR spectrum of a 2:1 **5**:$Eu(ClO_4)_3$ mixture in anhydrous CD_3CN.

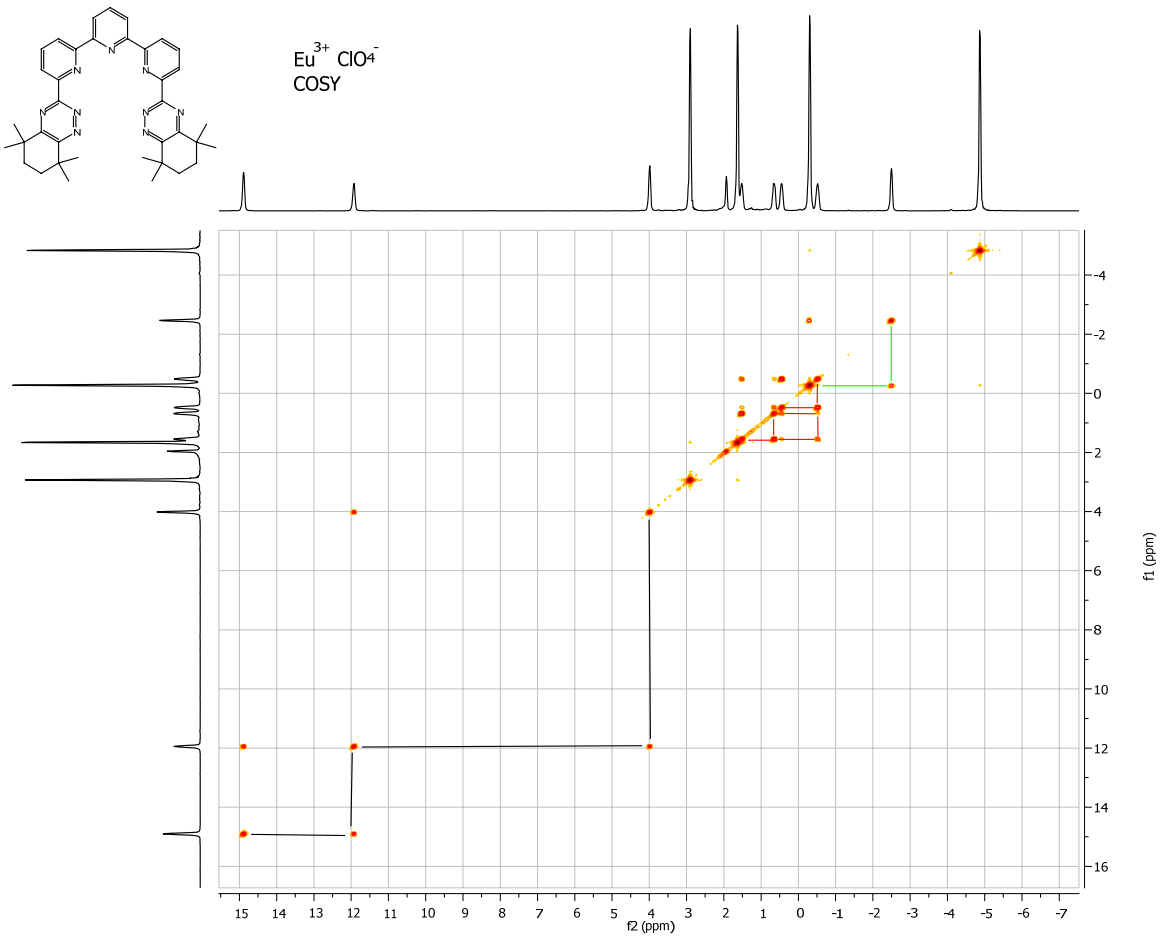

Figure S8. ^{1}H-^{1}H COSY spectrum of a 2:1 **5**:Eu(ClO_4)$_3$ mixture in anhydrous CD_3CN. Correlations between the central pyridine protons are in green, between the side pyridine protons in black and between the methylene protons in red.

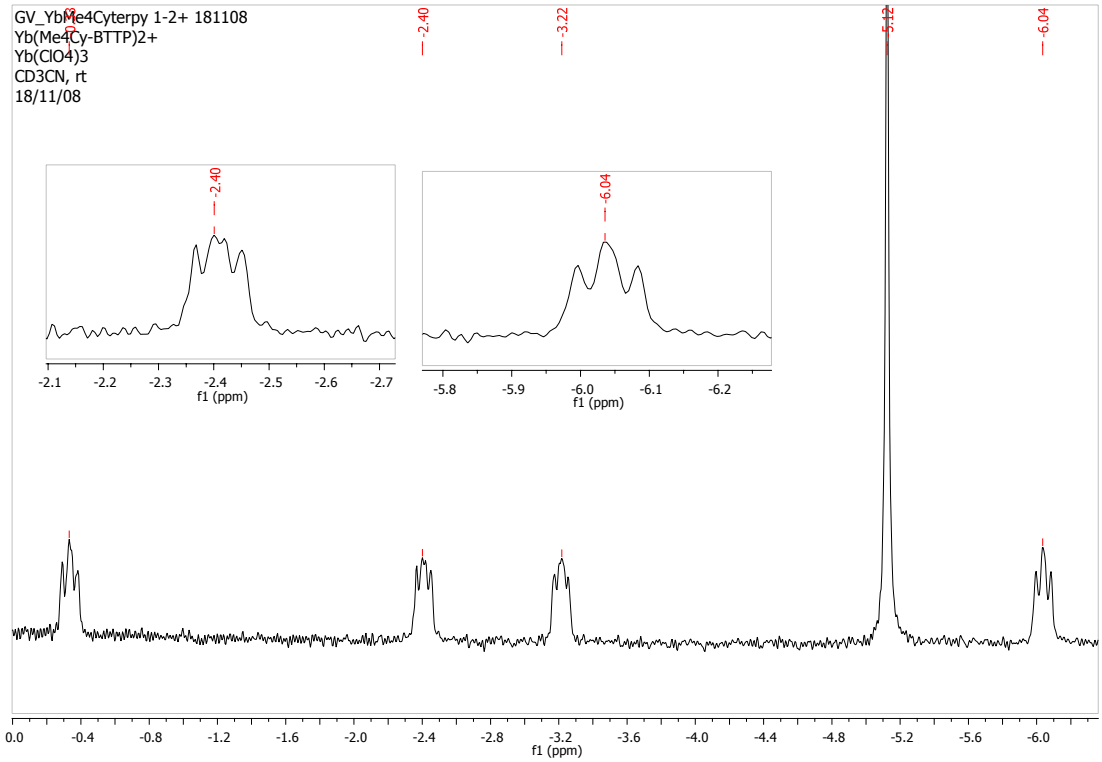

Figure S9. Expanded view of the methylene resonances in the ^{1}H NMR spectrum of a 2:1 **5**:Yb(ClO_4)$_3$ mixture in anhydrous CD_3CN.

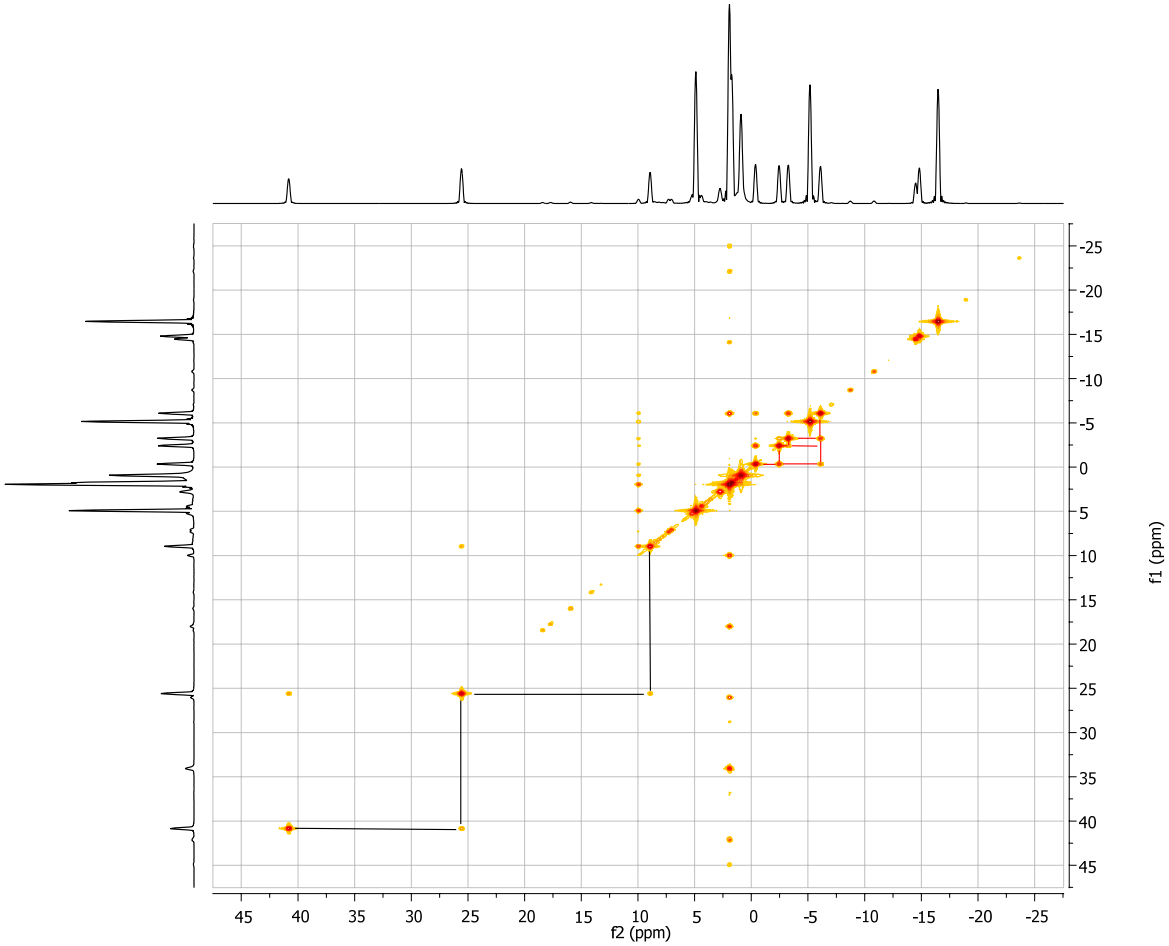

Figure S10. ^{1}H-^{1}H COSY spectrum of a 2:1 **5**:Yb(ClO_4)$_3$ mixture in anhydrous CD_3CN. Correlations between the protons in the outer pyridine rings in the terpyridine unit are indicated by black lines. Correlations between the methylene protons are in red.

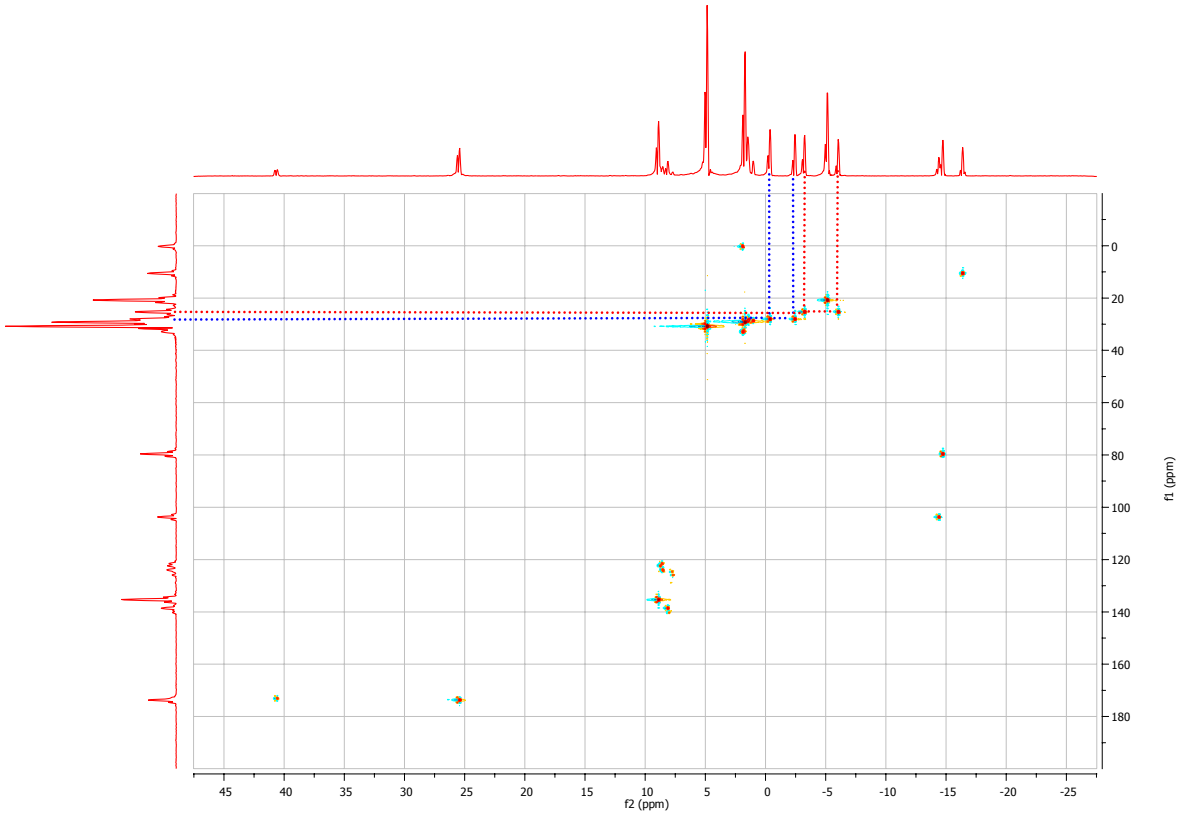

Figure S11. ^{1}H-^{13}C HSQC correlation of a 2:1 **5**:$Yb(ClO_4)_3$ mixture in anhydrous CD_3CN (X axis: ^{1}H NMR spectrum, Y axis: ^{13}C NMR spectrum). The correlation between the two types of each methylene carbon and its two protons are shown in red and in blue.

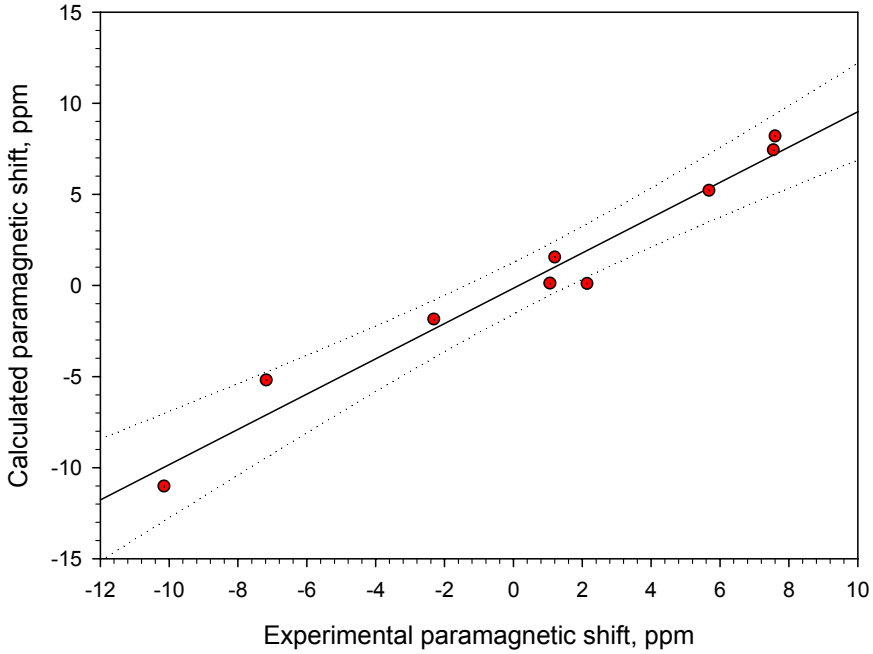

Figure S12. Correlation between the calculated and experimental paramagnetic shifts in the ^{1}H NMR spectrum of [Yb(**5**)](NO$_3$)$_3$. 99% confidence intervals are shown with dotted lines. (slope: 0.97, intercept: -0.15).

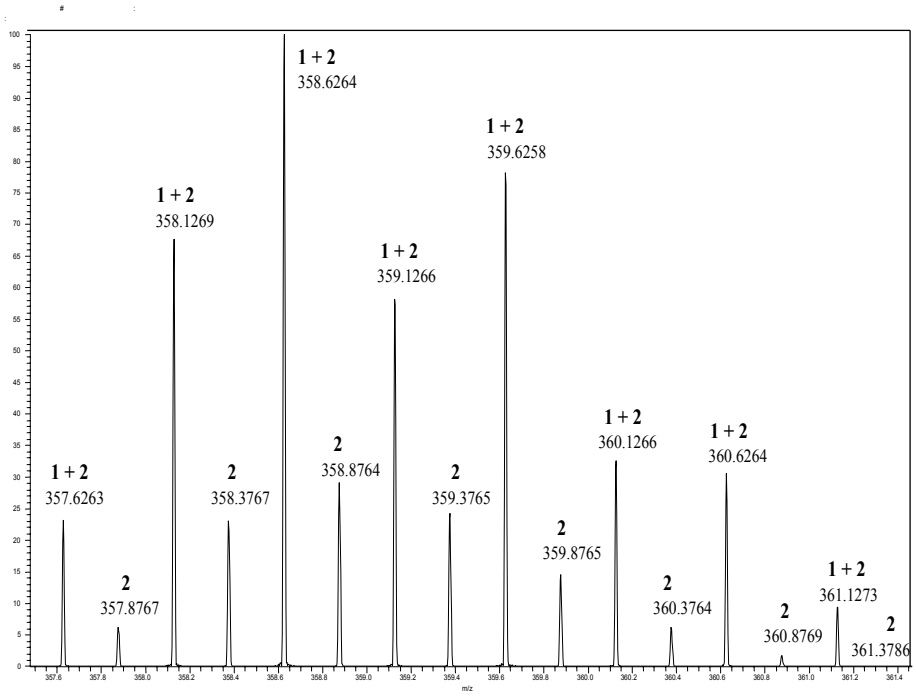

Figure S13. Expanded view of the mass peak at m/z = 358.6264 of the Pd(II) complex of CyMe$_4$-BTTP **5**. Assignments: Peaks labeled 1: [Pd(**5**)]$^{2+}$; Peaks labeled 2: [Pd$_2$(**5**)$_2$]$^{4+}$.

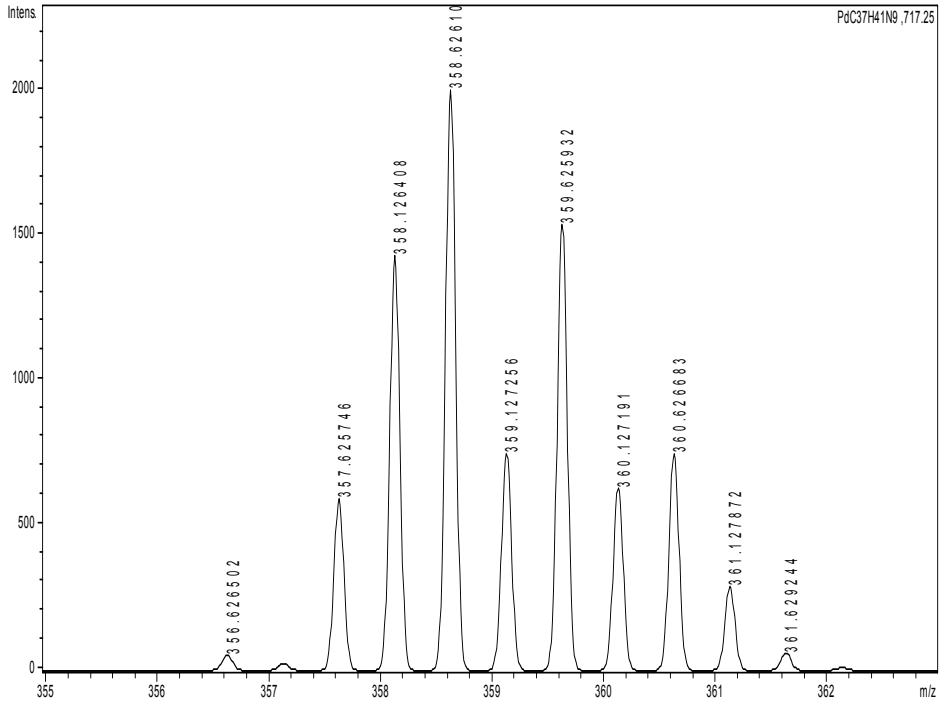

Figure S14. Computer simulation of the isotope distribution pattern of the 1:1 complex $[Pd(\mathbf{5})]^{2+}$.

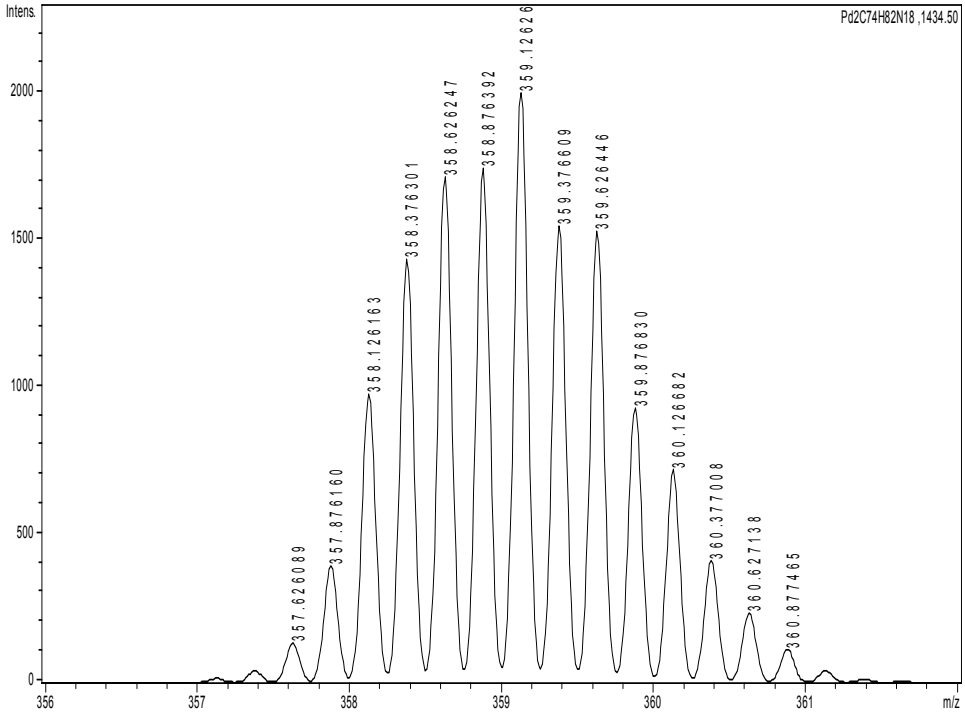

Figure S15. Computer simulation of the isotope distribution pattern of the 2:2 complex $[Pd_2(\mathbf{5})_2]^{4+}$.