Electronic Supplementary Material (ESI) for Dalton Transactions.

Supporting Information

Controllable Construction of Half-sandwich Octanuclear Complexes Based on Pyridyl-substituted Ligands with Conjugated Centers

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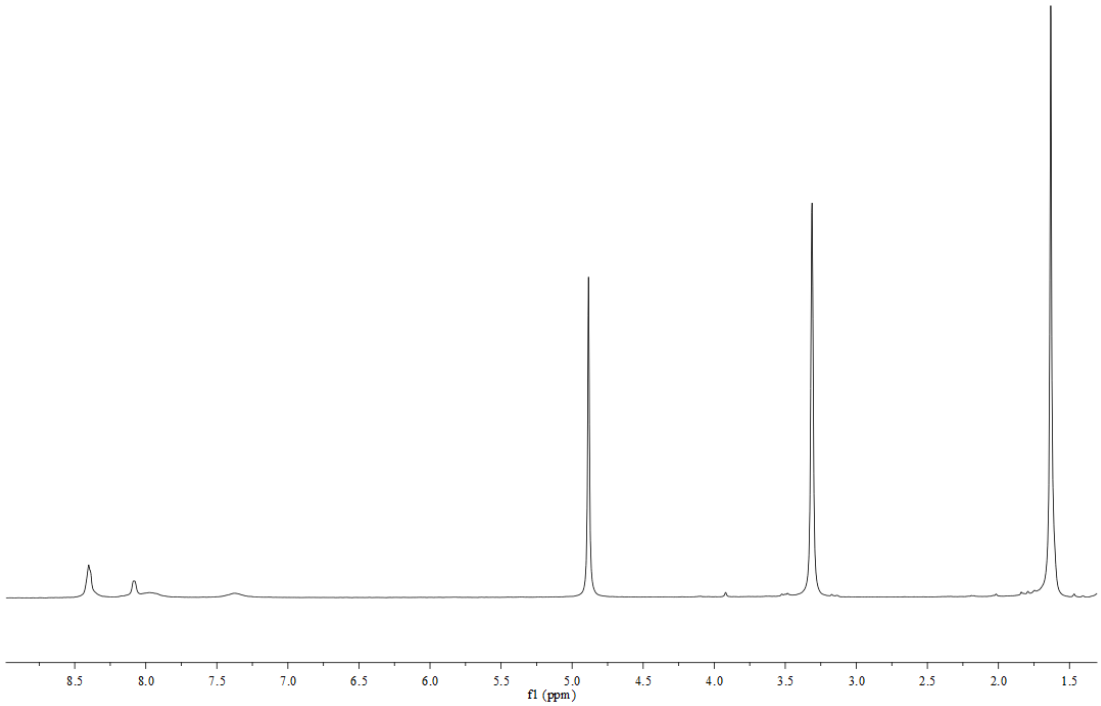


Figure S1. ^{1}H NMR (400 MHz, CD_3OD- d_4) of **4a**.

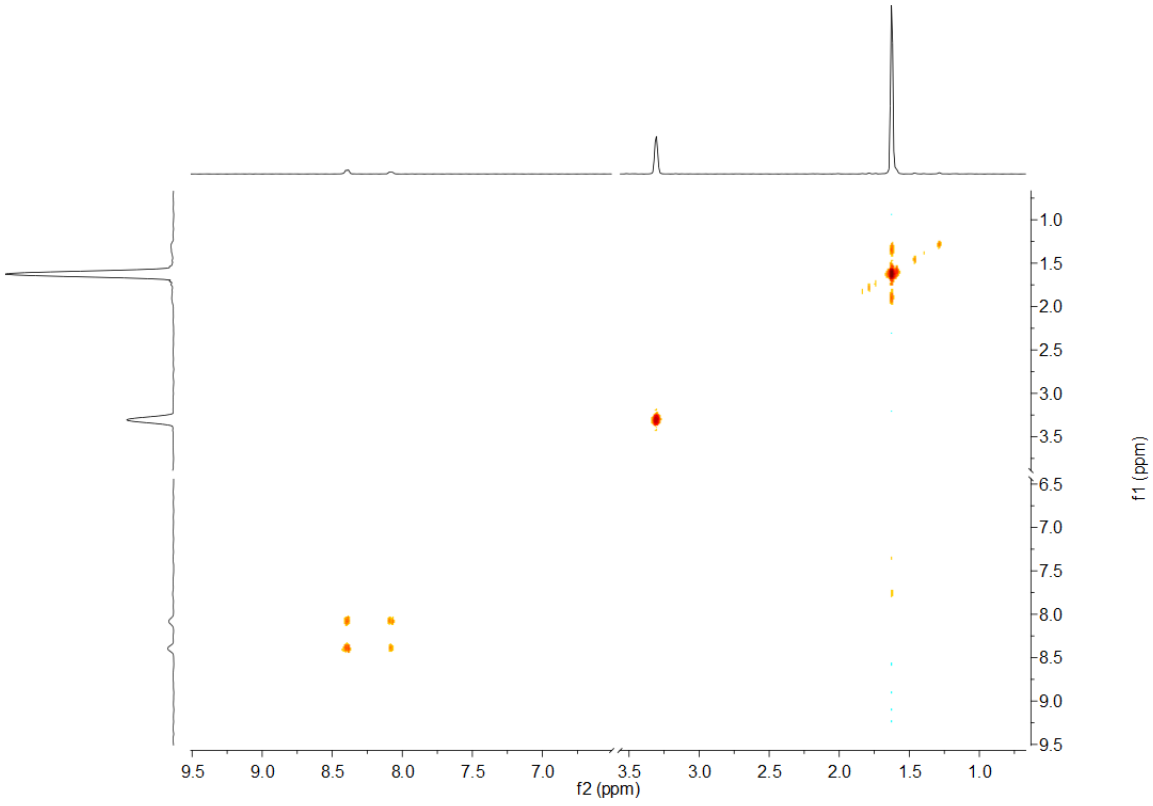


Figure S2. ^{1}H-^{1}H COSY NMR (400 MHz, CD_3OD- d_4) of **4a**.

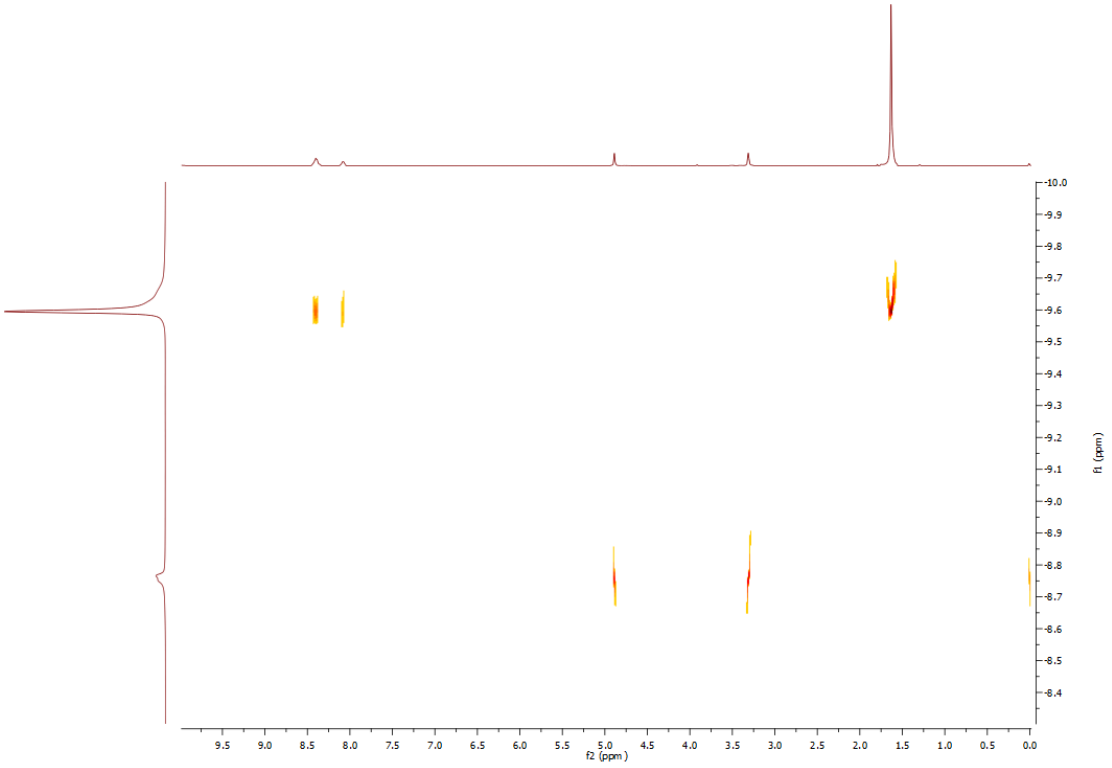


Figure S3. ^{1}H DOSY NMR (400 MHz, CD_3OD- d_4) of **4a**.

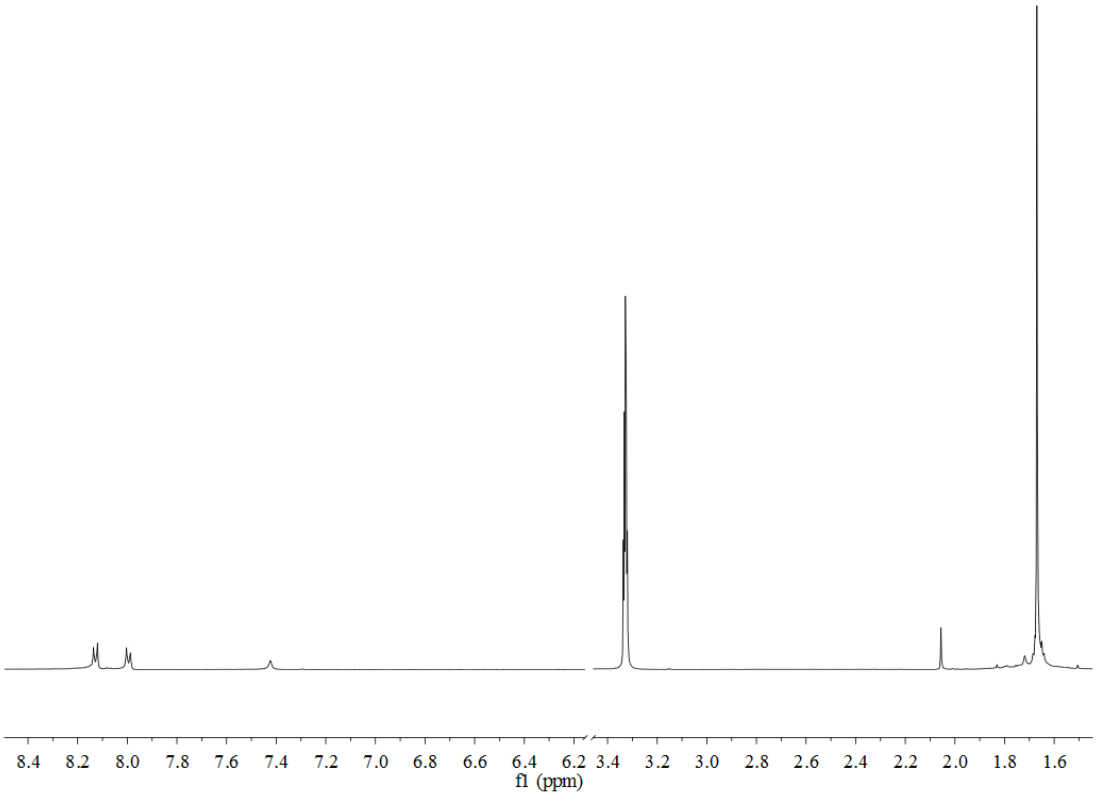


Figure S4. ^{1}H NMR (400 MHz, CD_3OD- d_4) of **4b**.

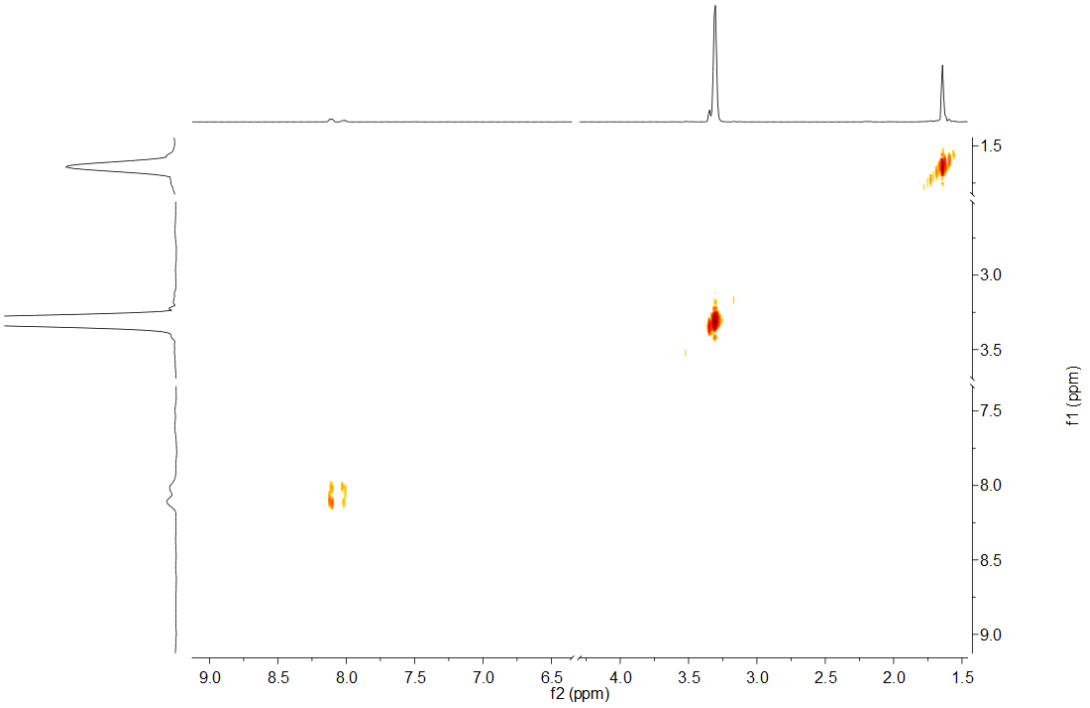


Figure S5. ^{1}H-^{1}H COSY NMR (400 MHz, CD_3OD- d_4) of **4b**.

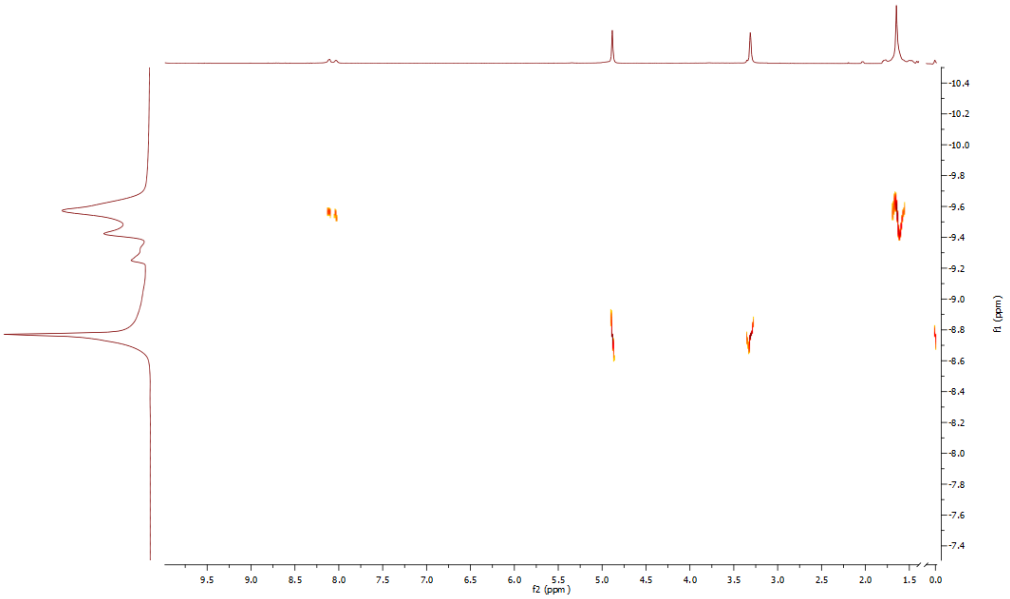


Figure S6. ^{1}H DOSY NMR (400 MHz, CD_3OD- d_4) of **4b**.

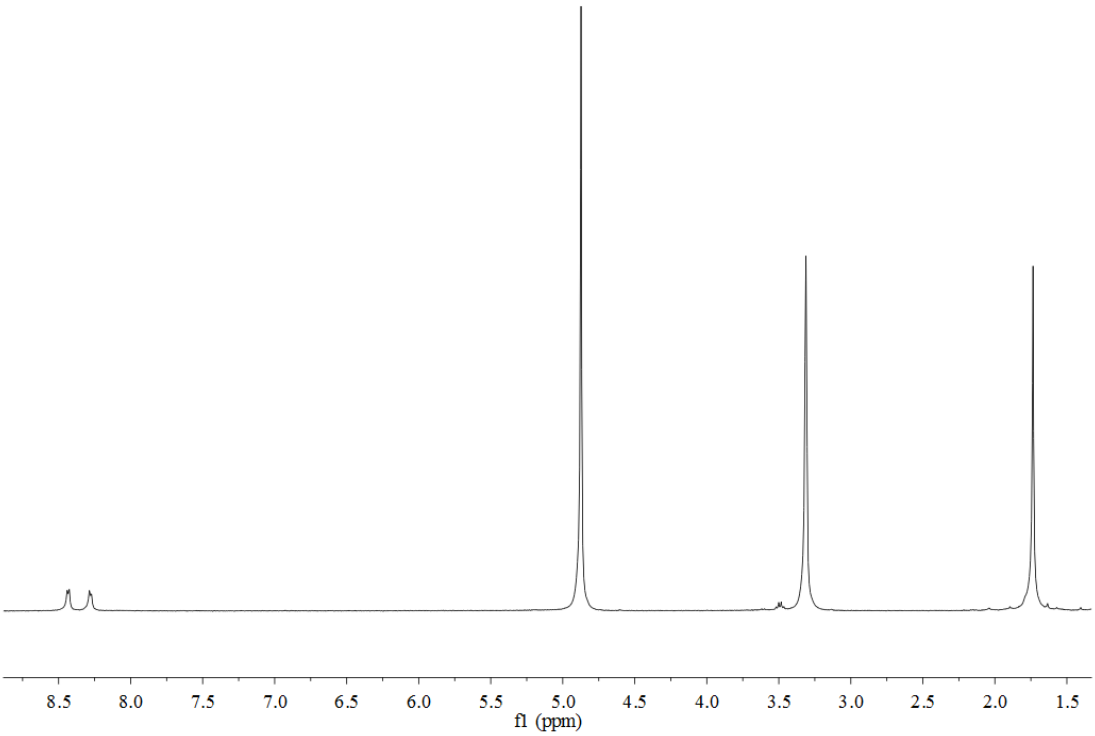


Figure S7. ^{1}H NMR (400 MHz, CD_3OD- d_4) of **4c**.

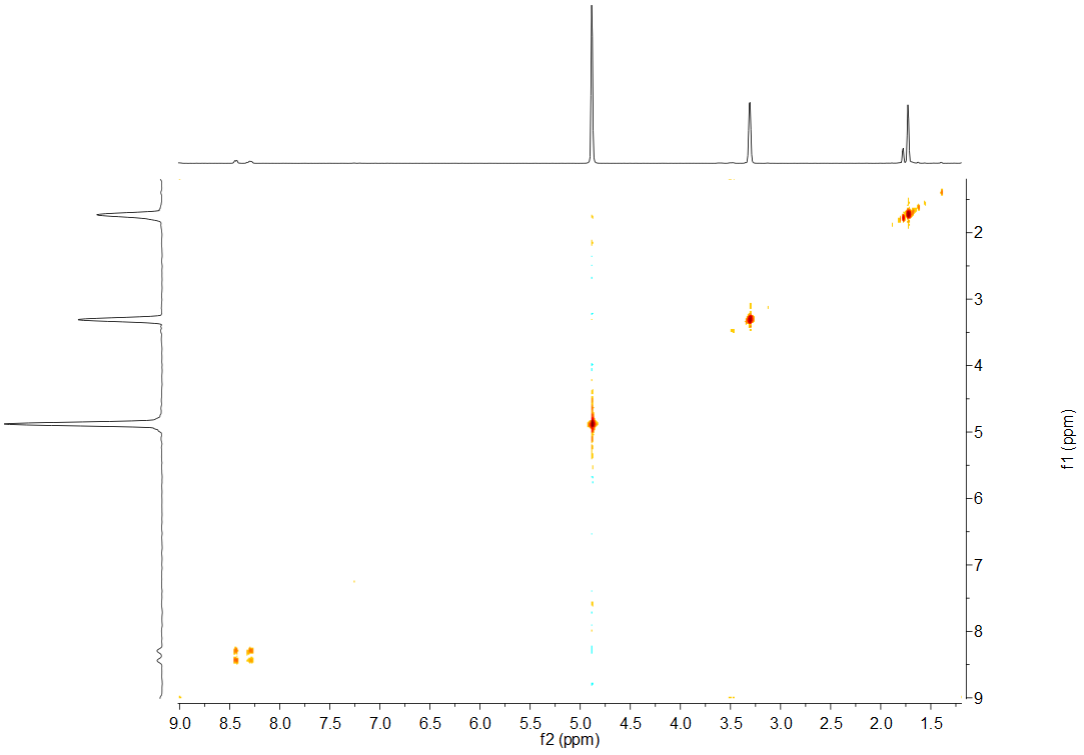


Figure S8. ^{1}H-^{1}H COSY NMR (400 MHz, CD_3OD- d_4) of **4c**.

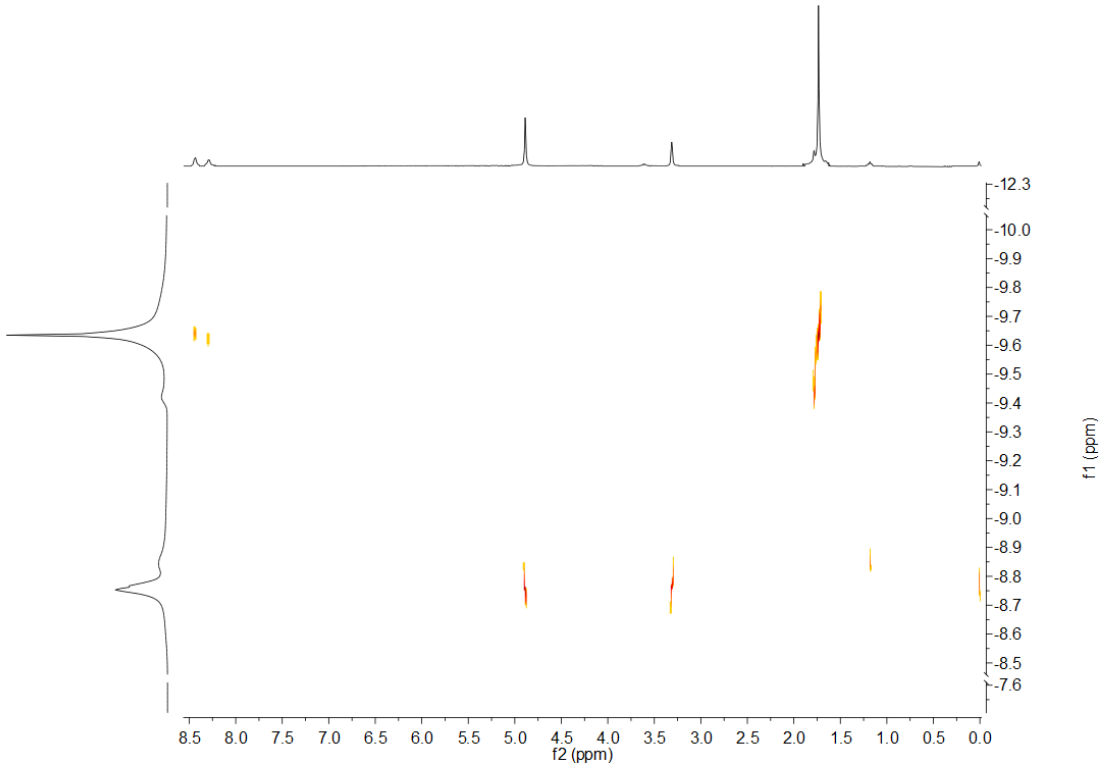


Figure S9. ^{1}H DOSY NMR (400 MHz, CD_3OD- d_4) of **4c**.

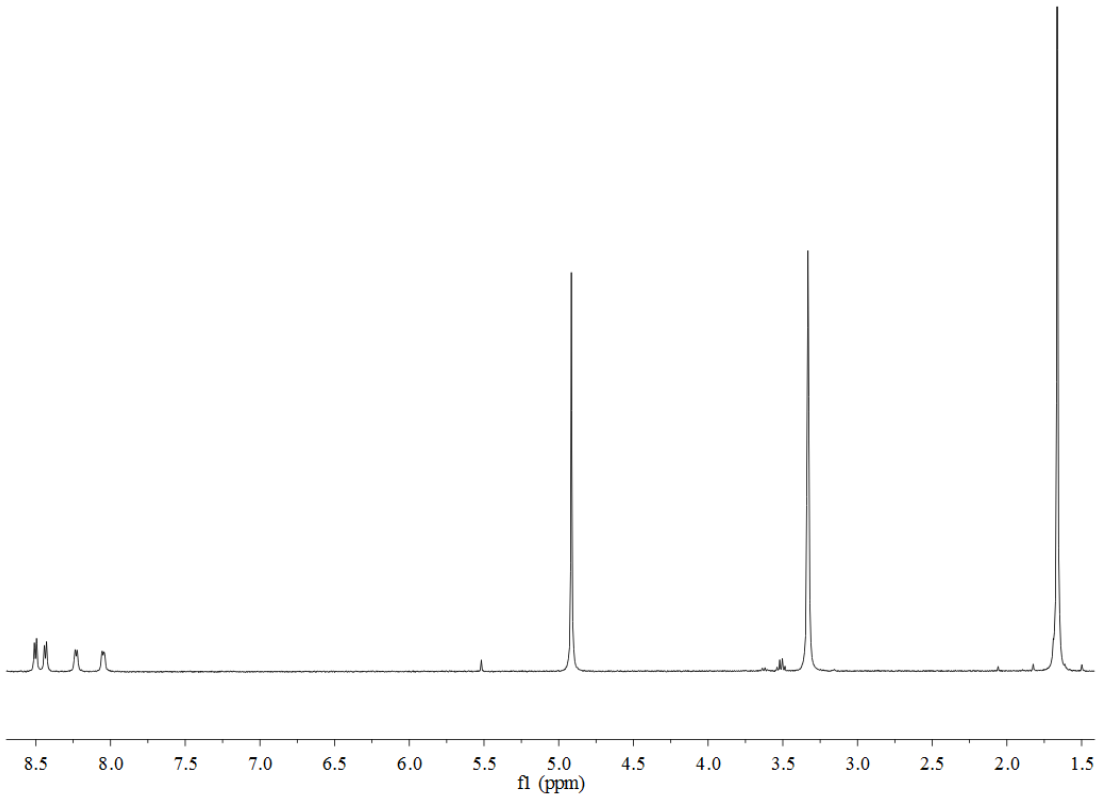


Figure S10. ^{1}H NMR (400 MHz, CD_3OD- d_4) of **5a**.

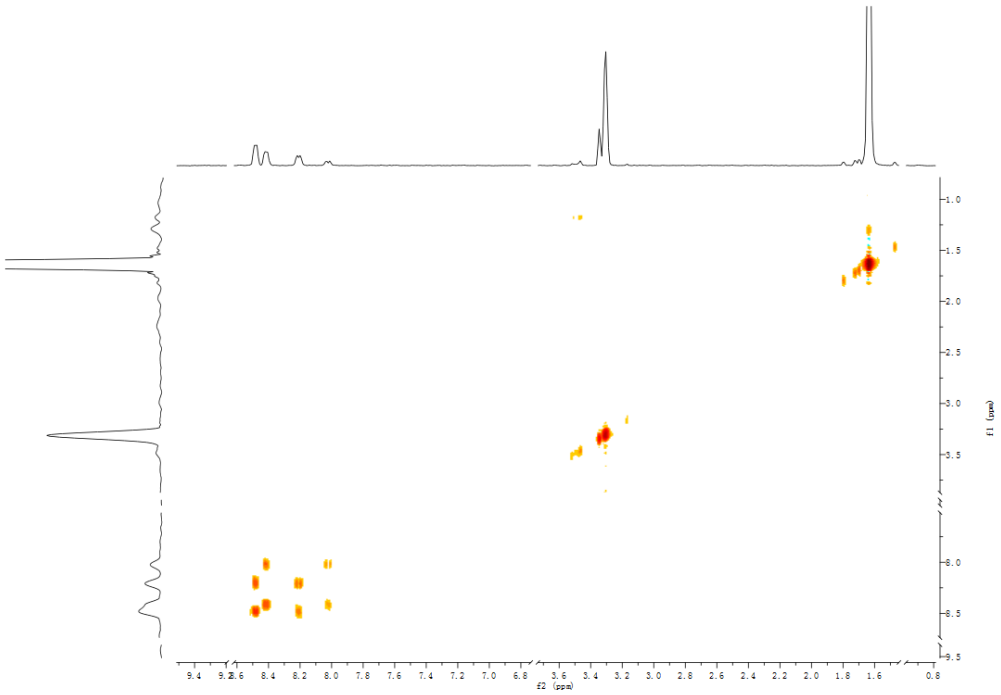


Figure S11. ^{1}H-^{1}H COSY NMR (400 MHz, CD_3OD- d_4) of **5a**.

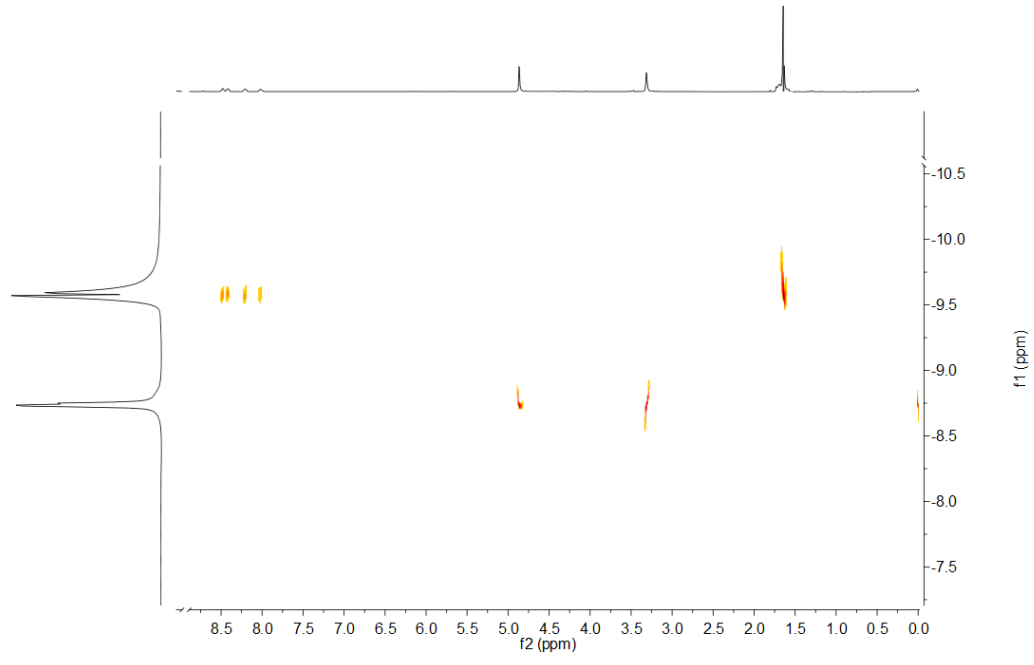


Figure S12. ^{1}H DOSY NMR (400 MHz, CD_3OD- d_4) of **5a**.

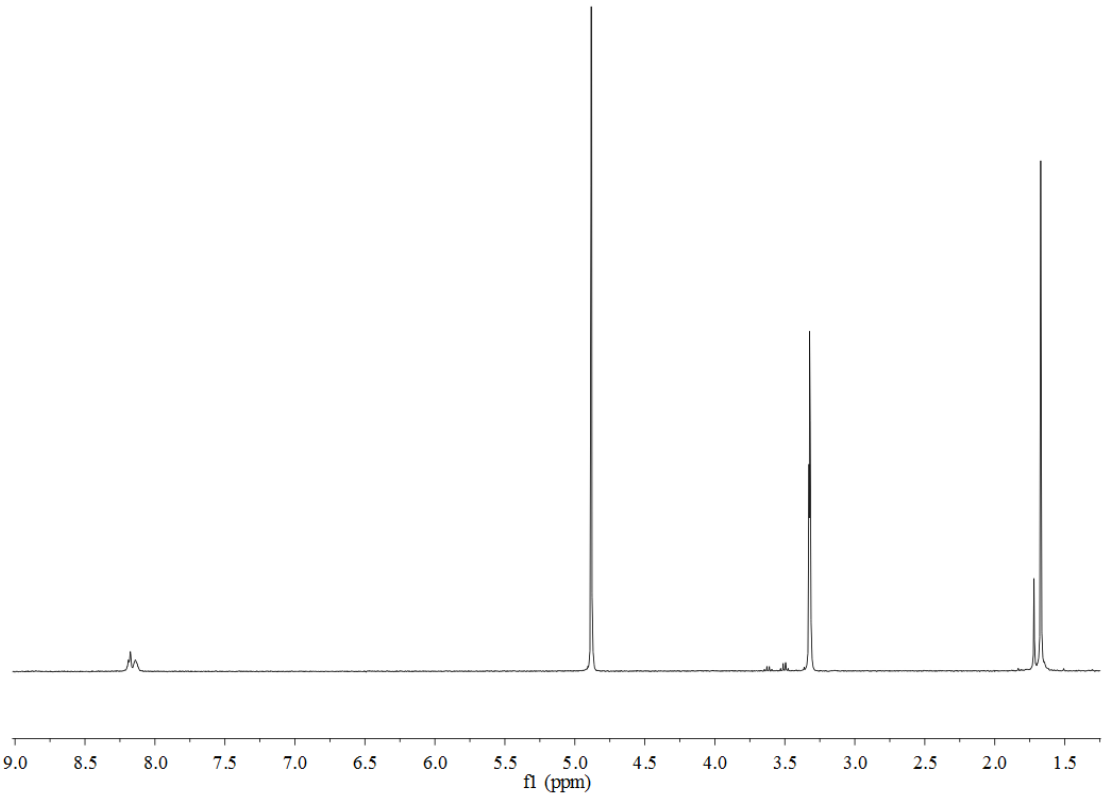


Figure S13. ^{1}H NMR (400 MHz, CD_3OD- d_4) of **5b**.

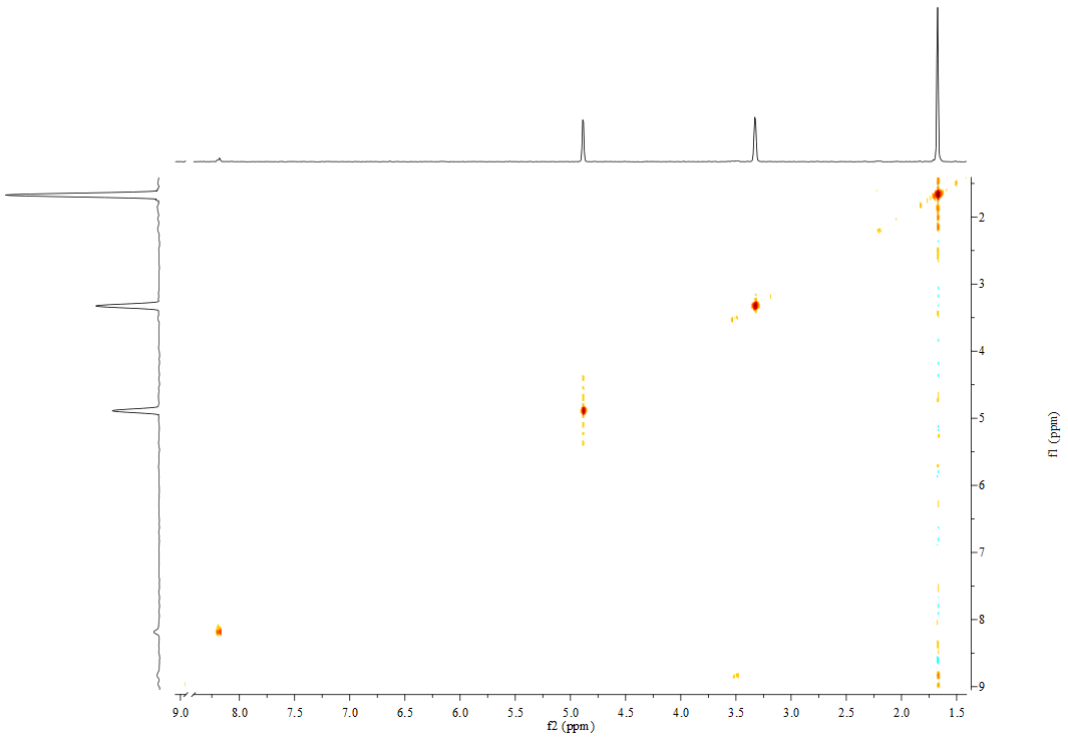


Figure S14. ^{1}H-^{1}H COSY NMR (400 MHz, CD_3OD- d_4) of **5b**.

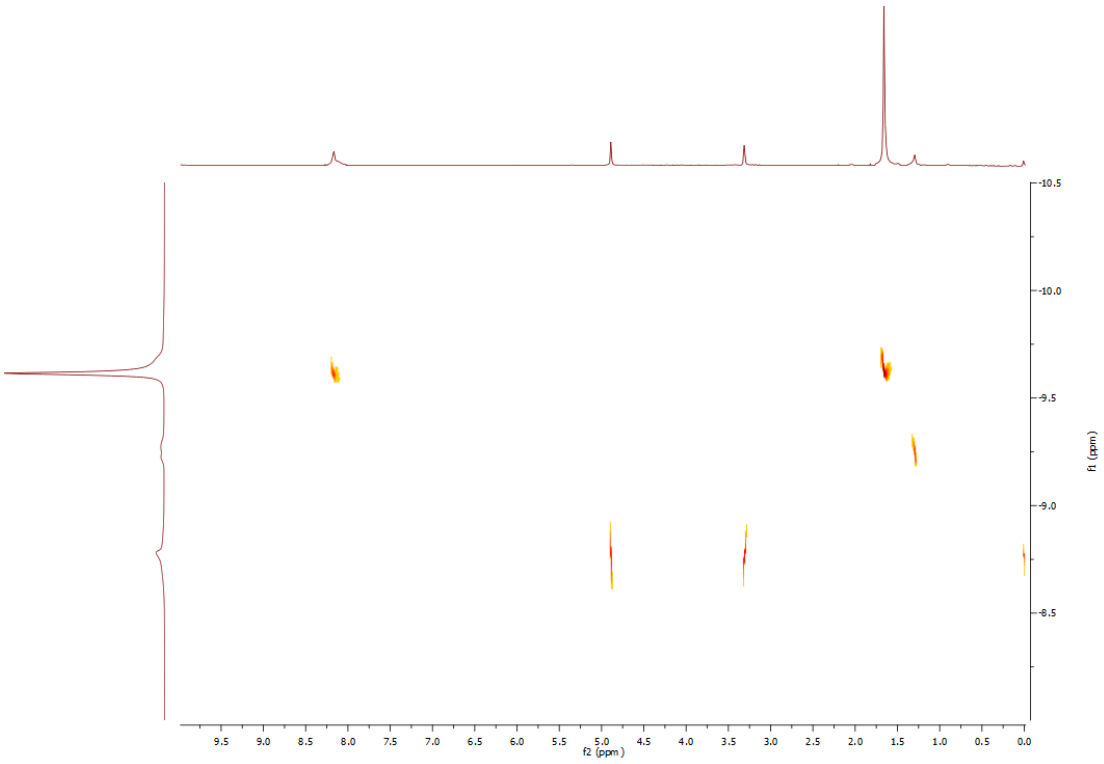


Figure S15. ^{1}H DOSY NMR (400 MHz, CD_3OD- d_4) of **5b**.

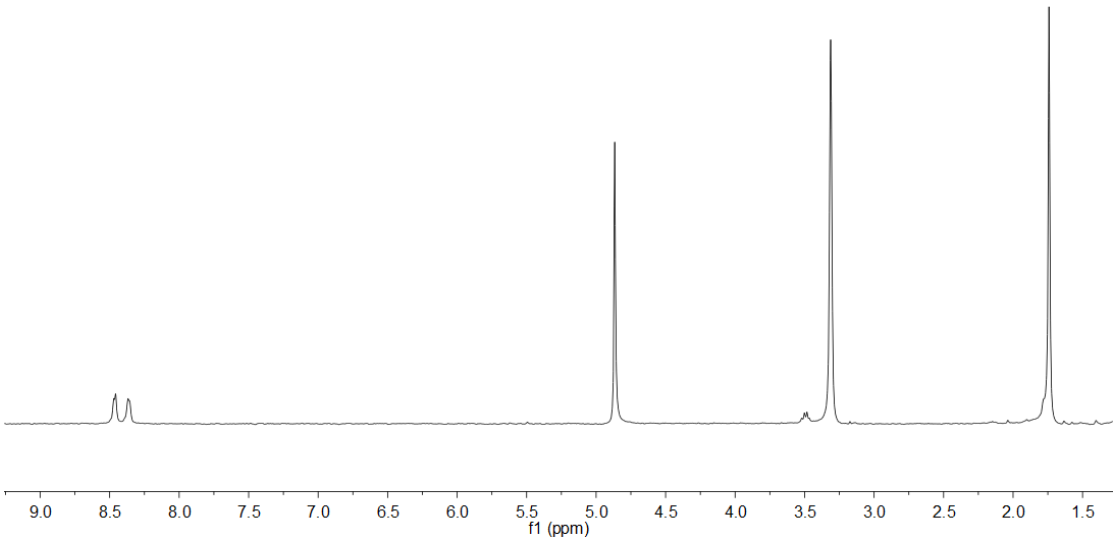


Figure S16 ^{1}H NMR (400 MHz, CD_3OD- d_4) of **5c**.

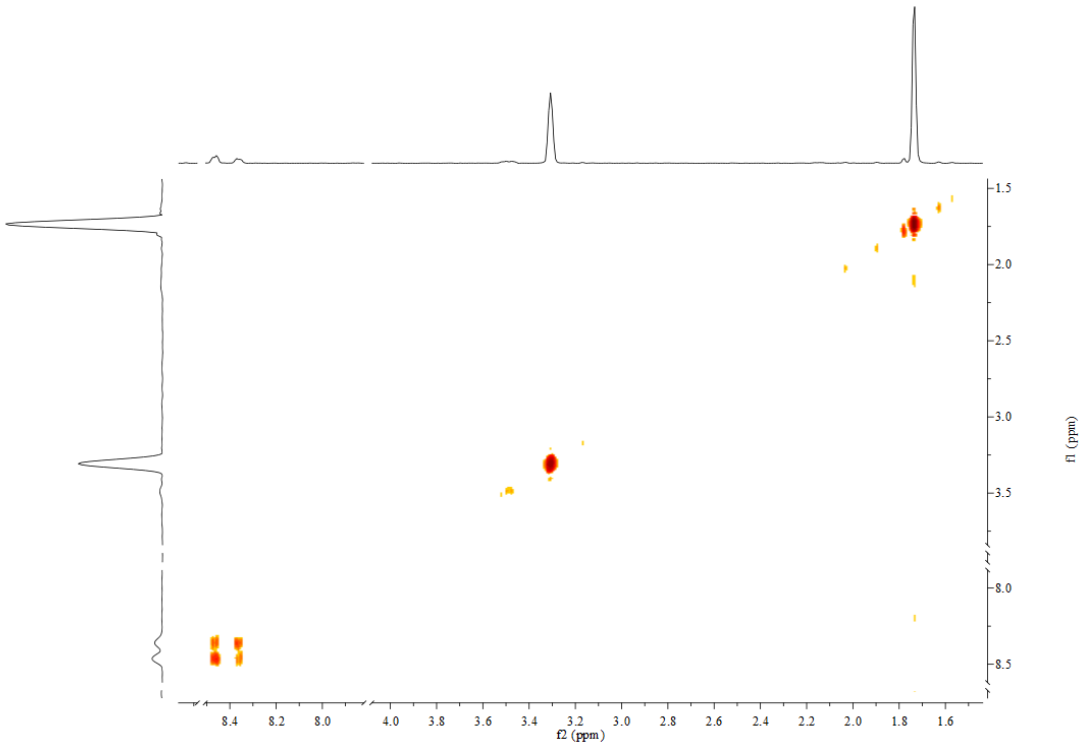


Figure S17. ^{1}H-^{1}H COSY NMR (400 MHz, CD_3OD- d_4) of **5c**.

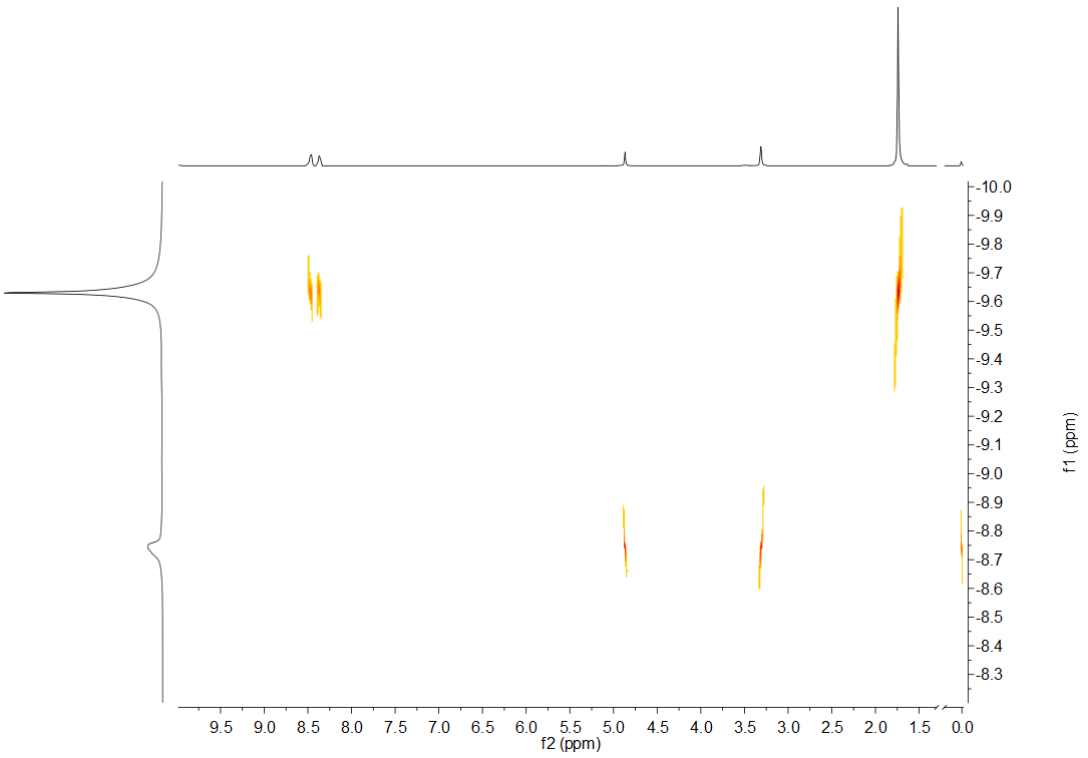


Figure S18. ^{1}H DOSY NMR (400 MHz, CD_3OD- d_4) of **5c**.

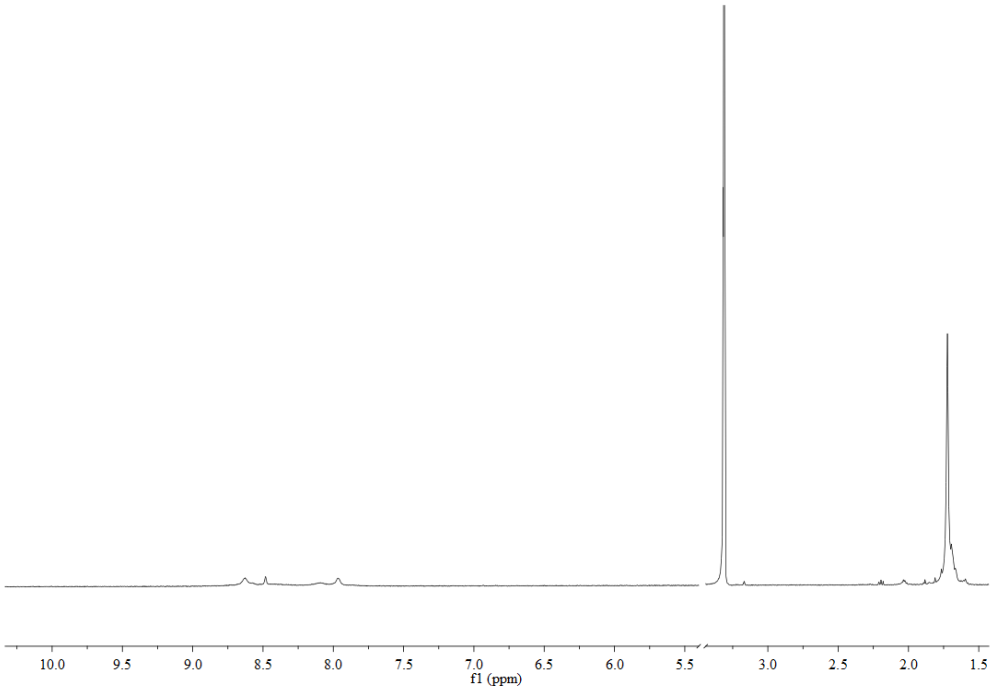


Figure S19. ^{1}H NMR (400 MHz, CD_3OD- d_4) of **6**.

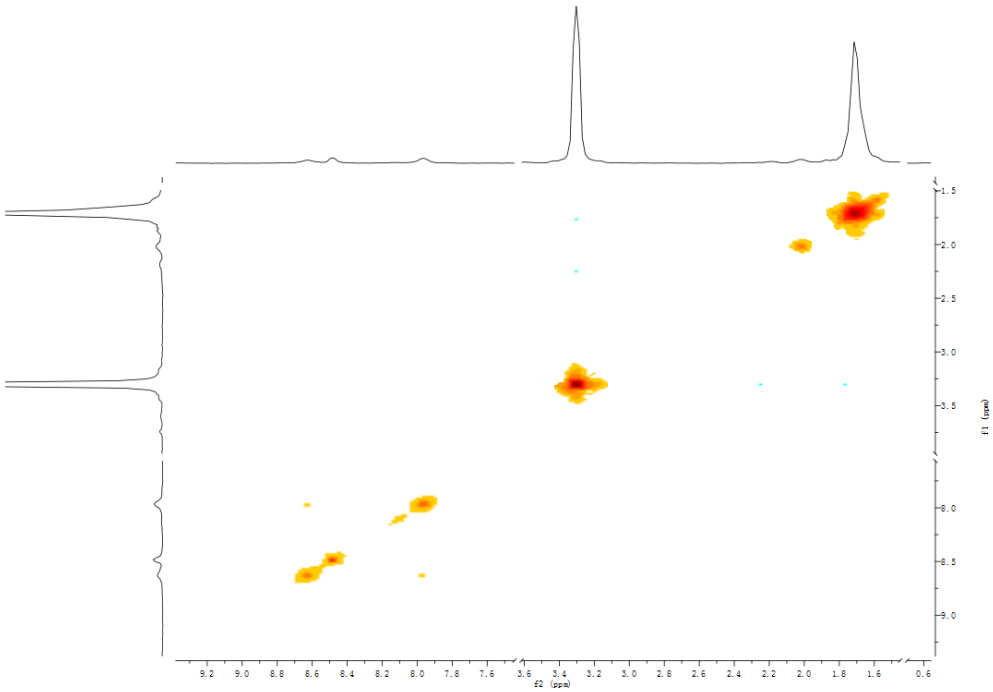
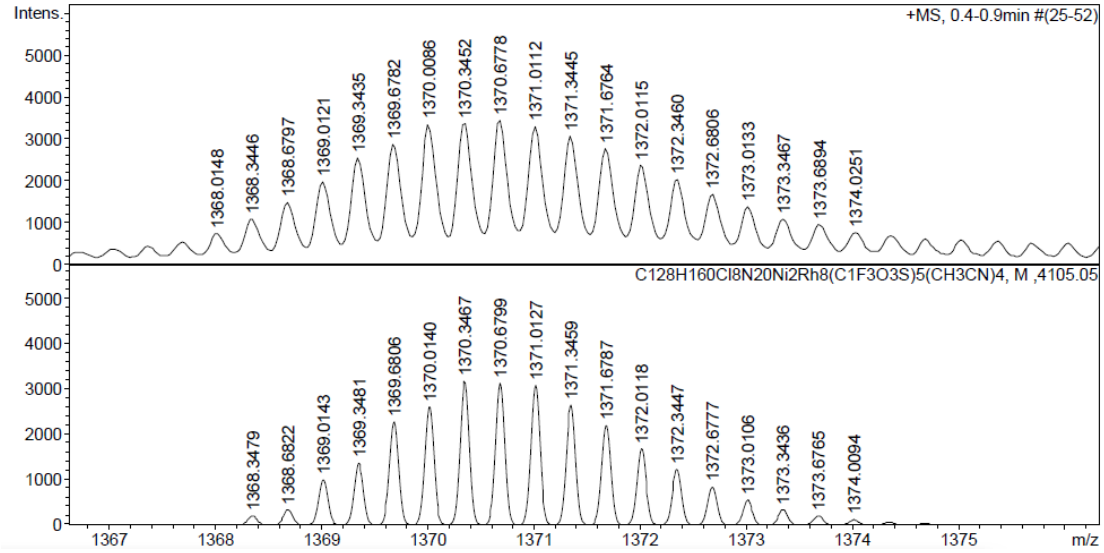
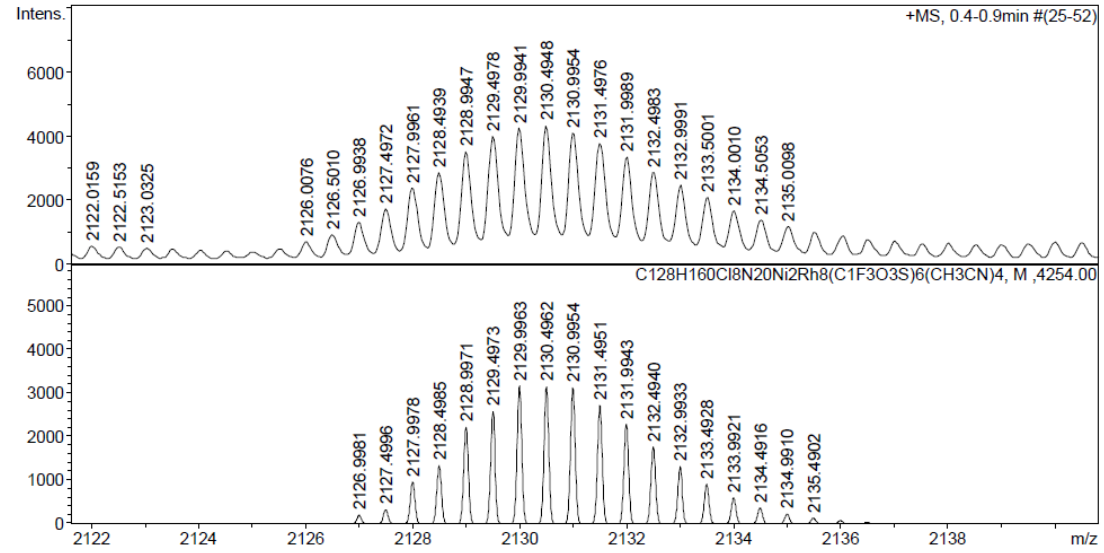


Figure S20. ^{1}H-^{1}H COSY NMR (400 MHz, CD_3OD- d_4) of **6**.

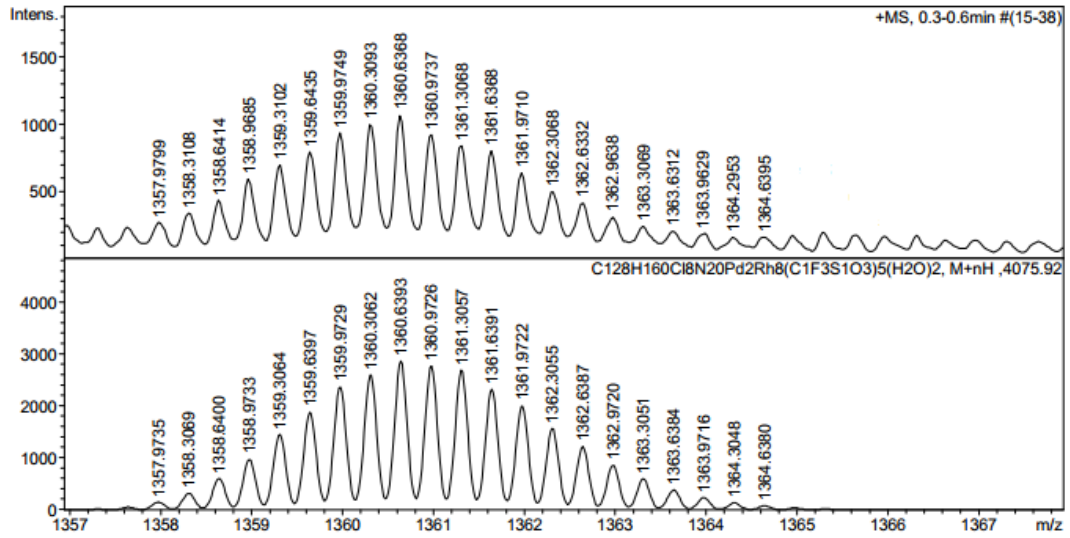


ESI-MS (positive ions) for $[M\text{-}(CH_3CN)_4, 5OTf]^{3+}$: Top (tested) and bottom (Calcd)



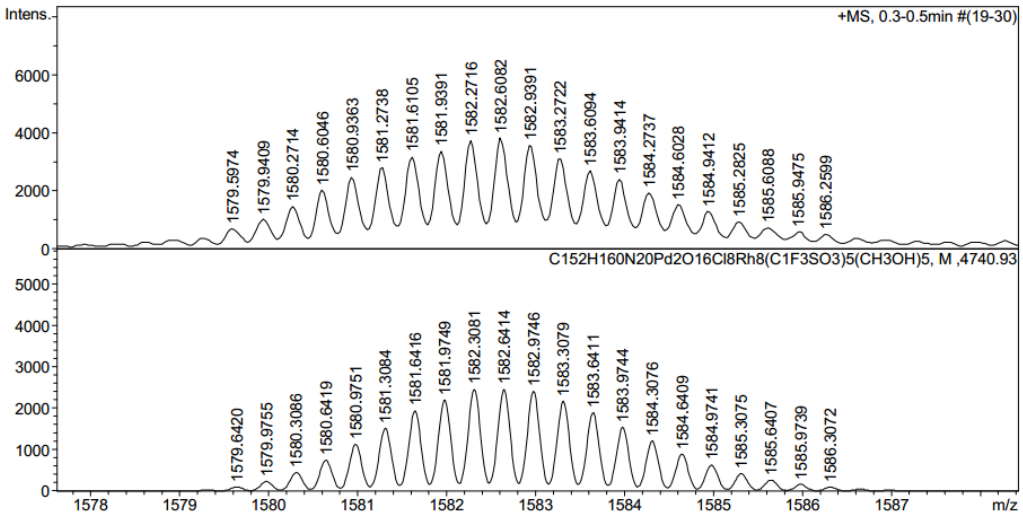
ESI-MS (positive ions) for $[M\text{-}(CH_3CN)_4, 6OTf]^{2+}$: Top (tested) and bottom (Calcd)

Figure S21. ESI-MS spectra of **4a**.

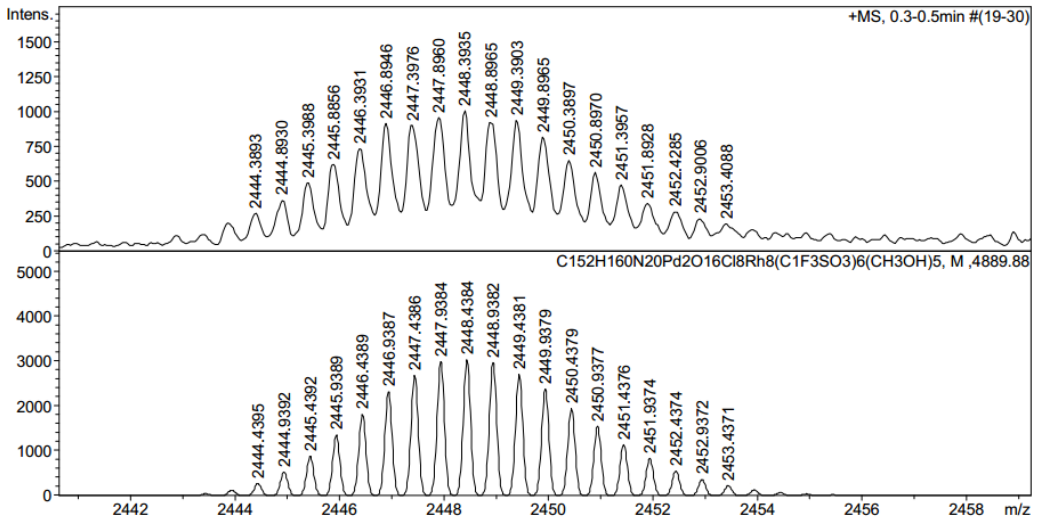


ESI-MS (positive ions) for $[M-(H_2O)_2, 5OTf]^{3+}$: Top (tested) and bottom (Calcd)

Figure S22. ESI-MS spectra of **5a**.

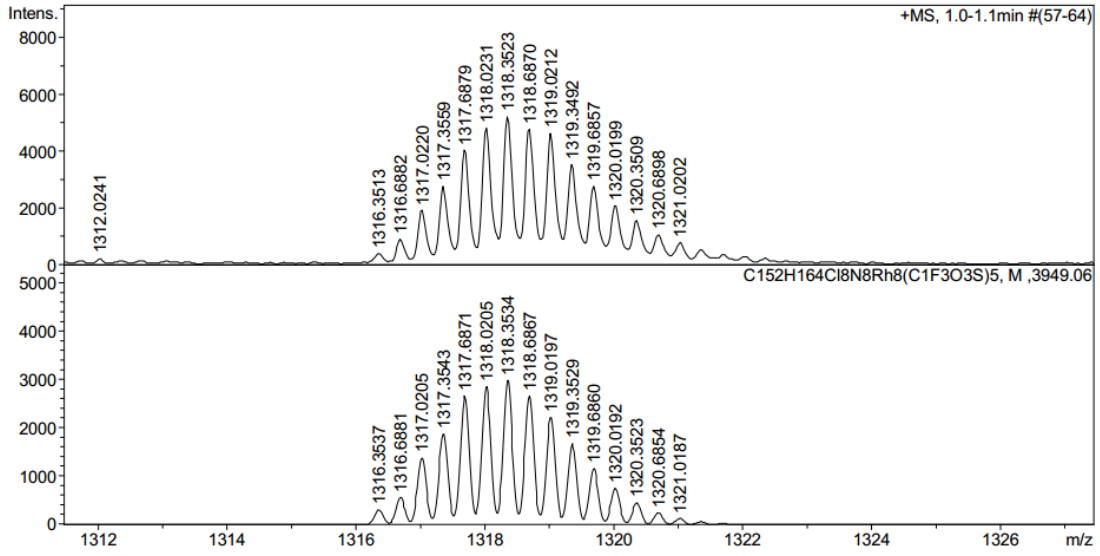


ESI-MS (positive ions) for $[M-(CH_3OH)_5, 5OTf]^{3+}$: Top (tested) and bottom (Calcd)

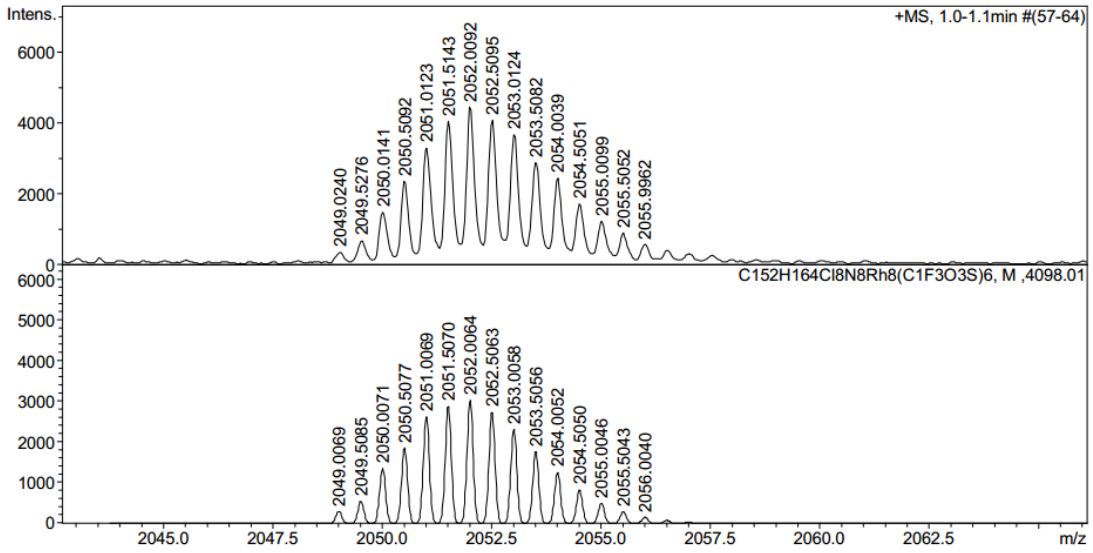


ESI-MS (positive ions) for $[M\text{-}(CH_3OH)_5, 6OTf]^{2+}$: Top (tested) and bottom (Calcd)

Figure S23. ESI-MS spectra of **5c**.



ESI-MS (positive ions) for $[M, 5OTf]^{3+}$: Top (tested) and bottom (Calcd)



ESI-MS (positive ions) for $[M, 6OTf]^{2+}$: Top (tested) and bottom (Calcd)

Figure S24. ESI-MS spectra of **6**.