

Catalytic properties of zirconocene-based systems in 1-hexene oligomerization and structure of metal hydride reaction centers

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Figure S1. ^1H and ^{13}C NMR of 1-hexene oligomers obtained in the system *rac*- $\text{Me}_2\text{CInd}_2\text{ZrCl}_2$ (**1g**) – HAlBu_2^i – $(\text{Ph}_3\text{C})[\text{B}(\text{C}_6\text{F}_5)_4]$

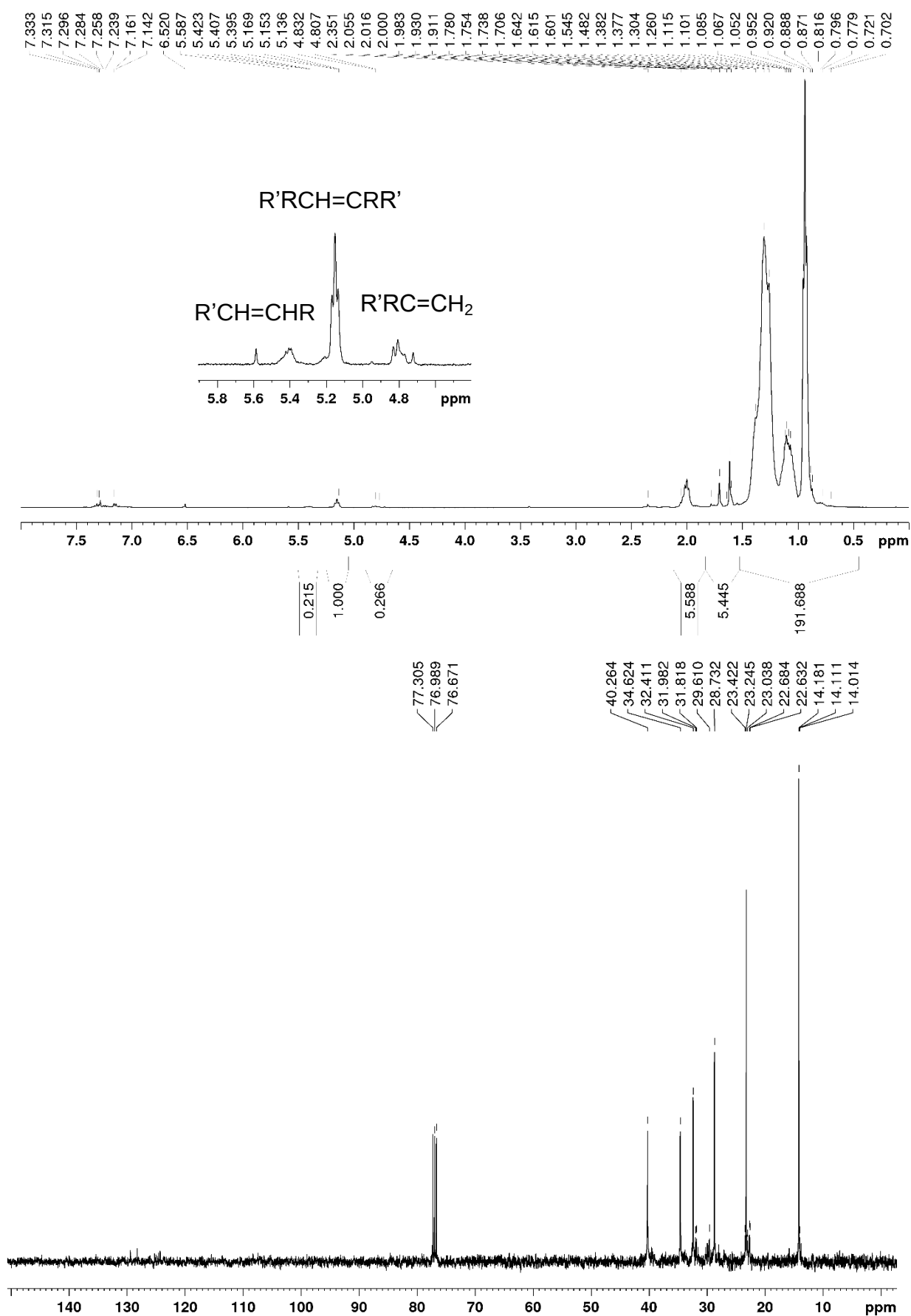


Figure S2. ^1H and ^{13}C NMR of 1-hexene oligomers obtained in the system *rac*- $\text{H}_4\text{C}_2[\text{Ind}]_2\text{ZrCl}_2$ (**1h**)- $\text{HAIBu}^i_2\text{-MMAO-12}$

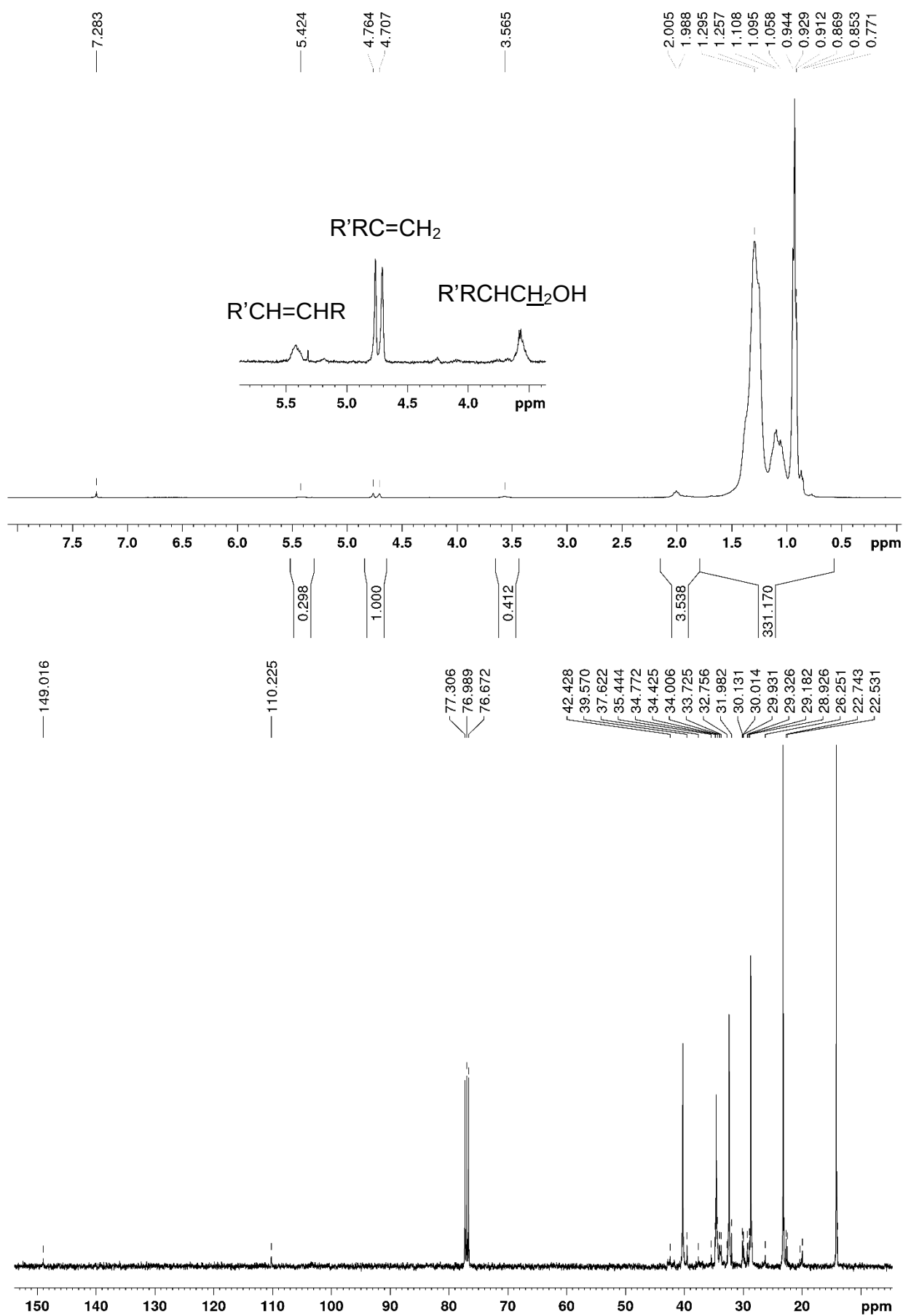


Figure S3. Comparison of ^{13}C NMR of 1-hexene oligomers obtained in the system $\text{Ind}_2\text{ZrCl}_2$ (**1f**)- HAlBu_2^i activated by MMAO-12 and $(\text{Ph}_3\text{C})[\text{B}(\text{C}_6\text{F}_5)_4]$.

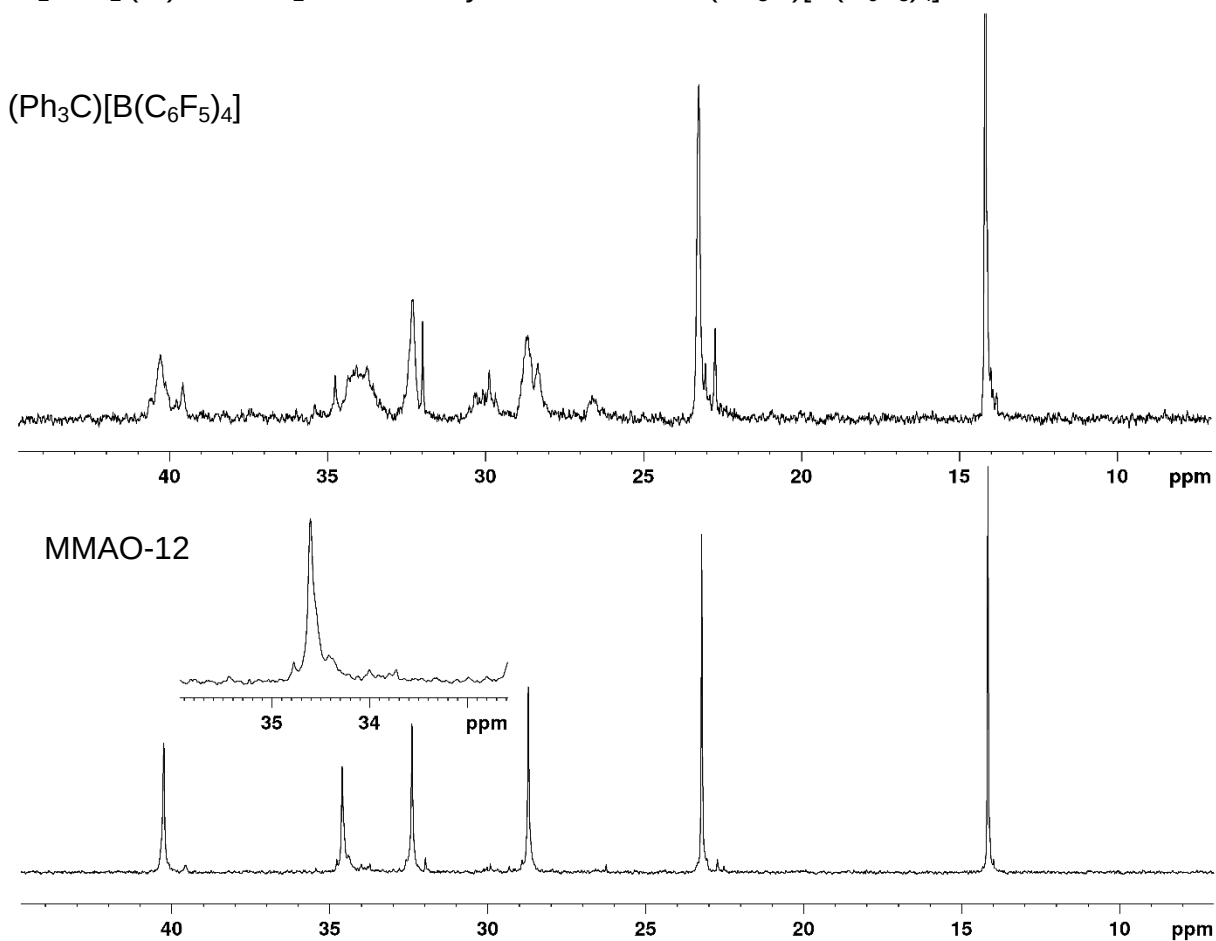


Figure S4. Comparison of ^{13}C NMR of 1-hexene oligomers obtained in the system $\text{rac-Me}_2\text{CInd}_2\text{ZrCl}_2$ (**1g**)- HAlBu_2^i activated by MMAO-12 and $(\text{Ph}_3\text{C})[\text{B}(\text{C}_6\text{F}_5)_4]$.

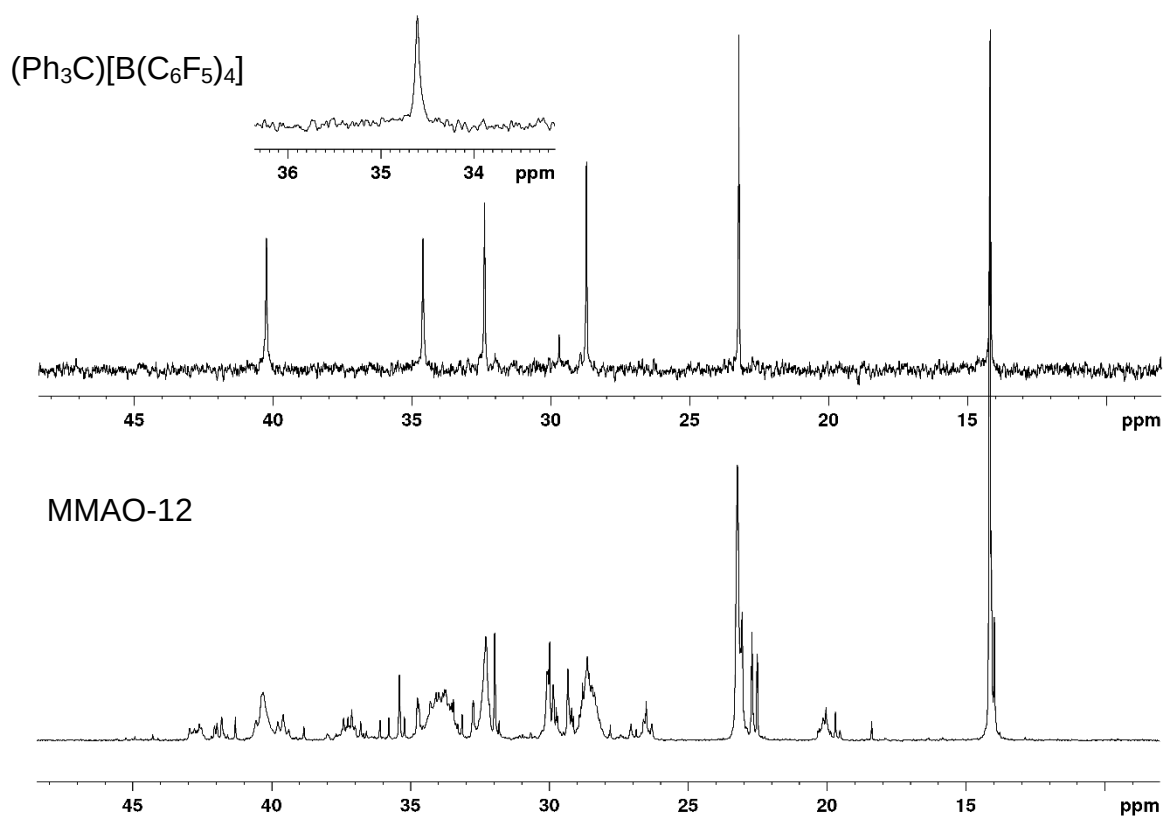


Figure S5. ^1H NMR of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAlBu_2 (1:3) in C_7D_8 (250 K).

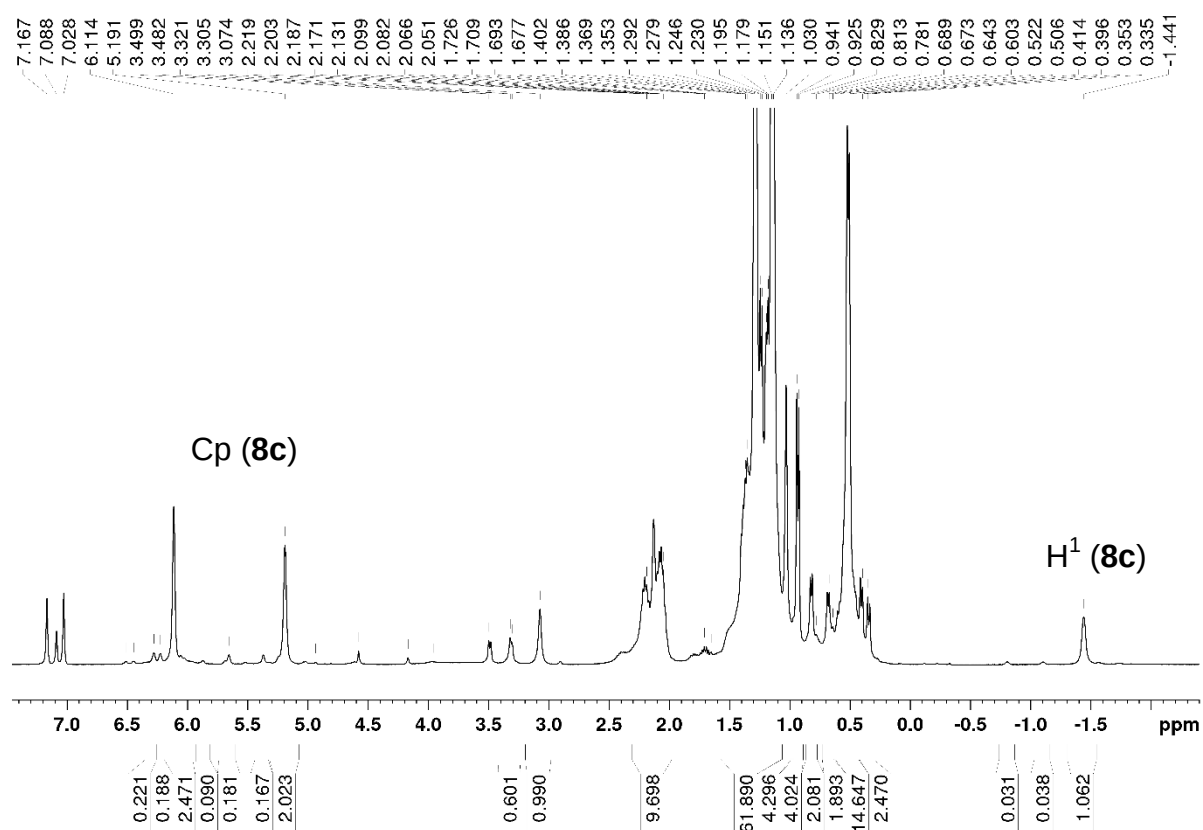


Figure S6. COSY HH of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAlBu_2 (1:3) in C_7D_8 (250 K).

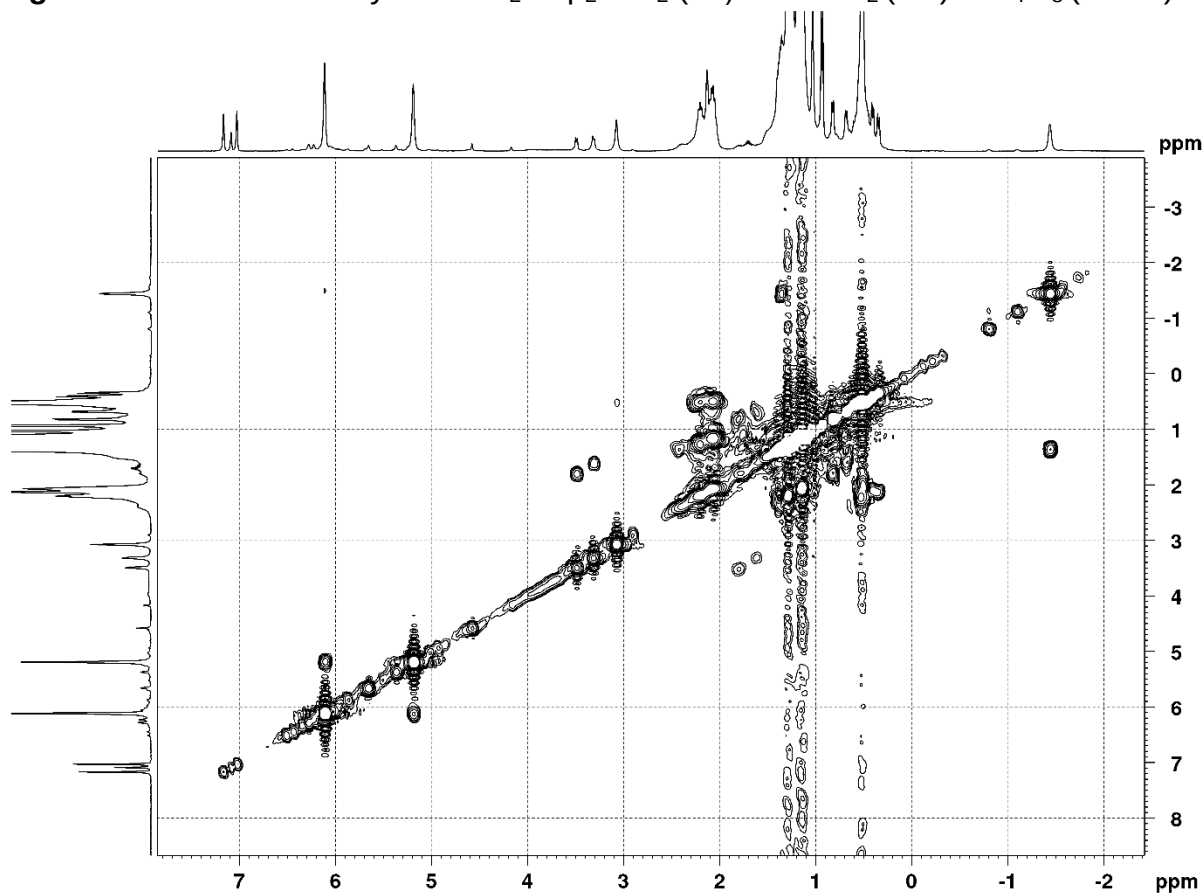


Figure S7. NOESY of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAlBu_2^i (1:3) in C_7D_8 (250 K).

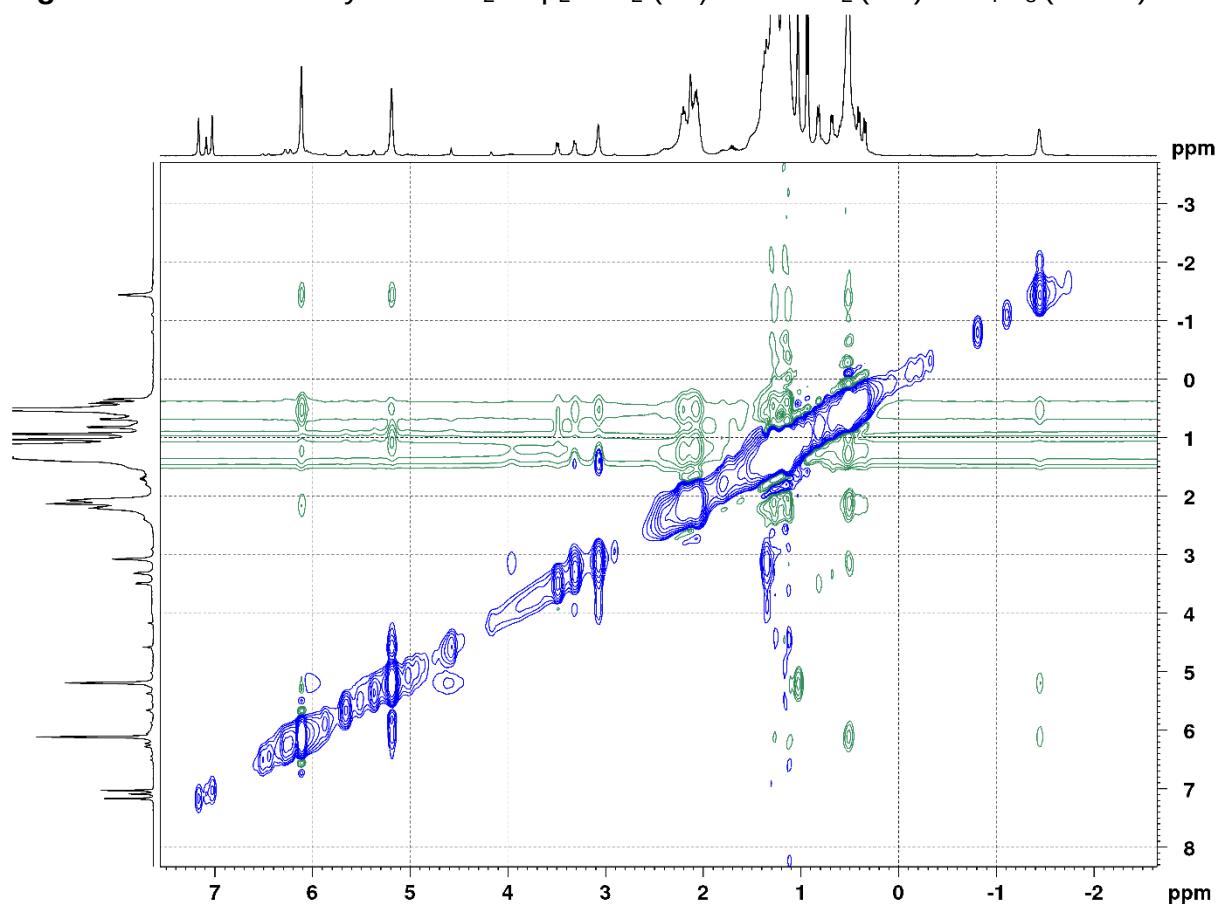


Figure S8. NOESY of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAlBu_3^i (1:8) in C_7D_8 (298 K).

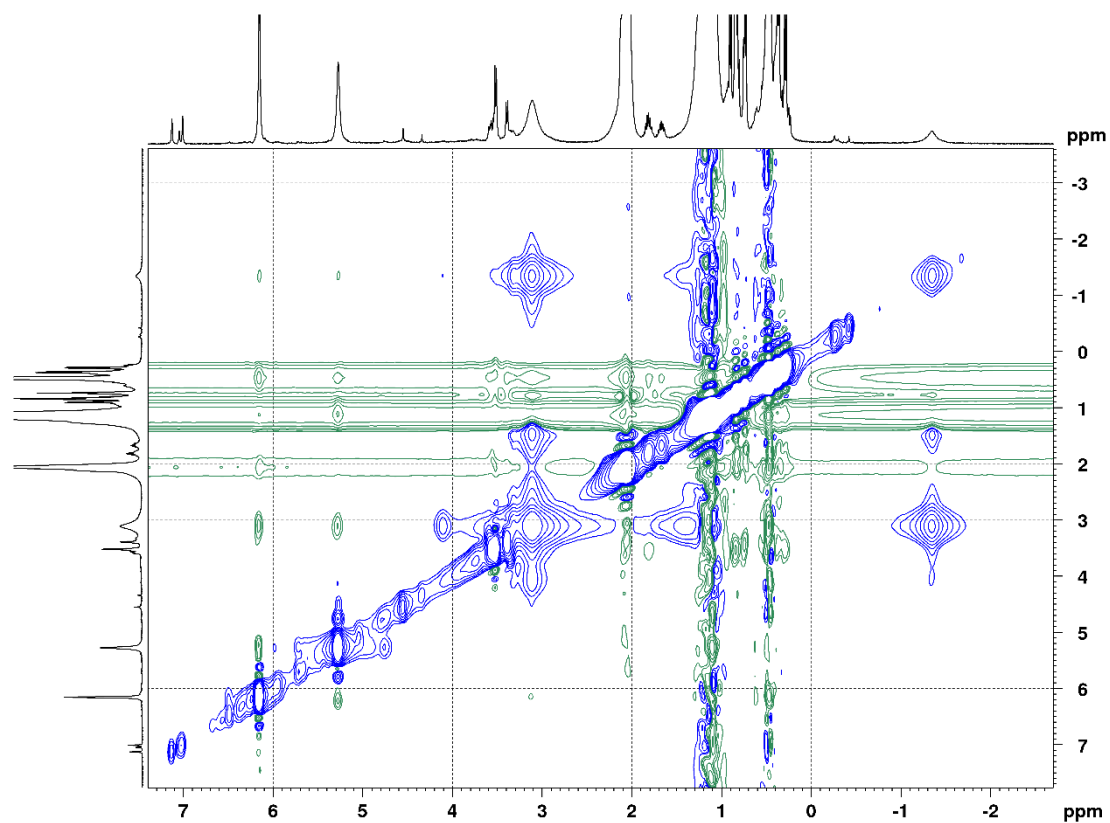


Figure S9. ^1H NMR of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAlBu^i_2 (1:1.7) in C_7D_8 (298 K).

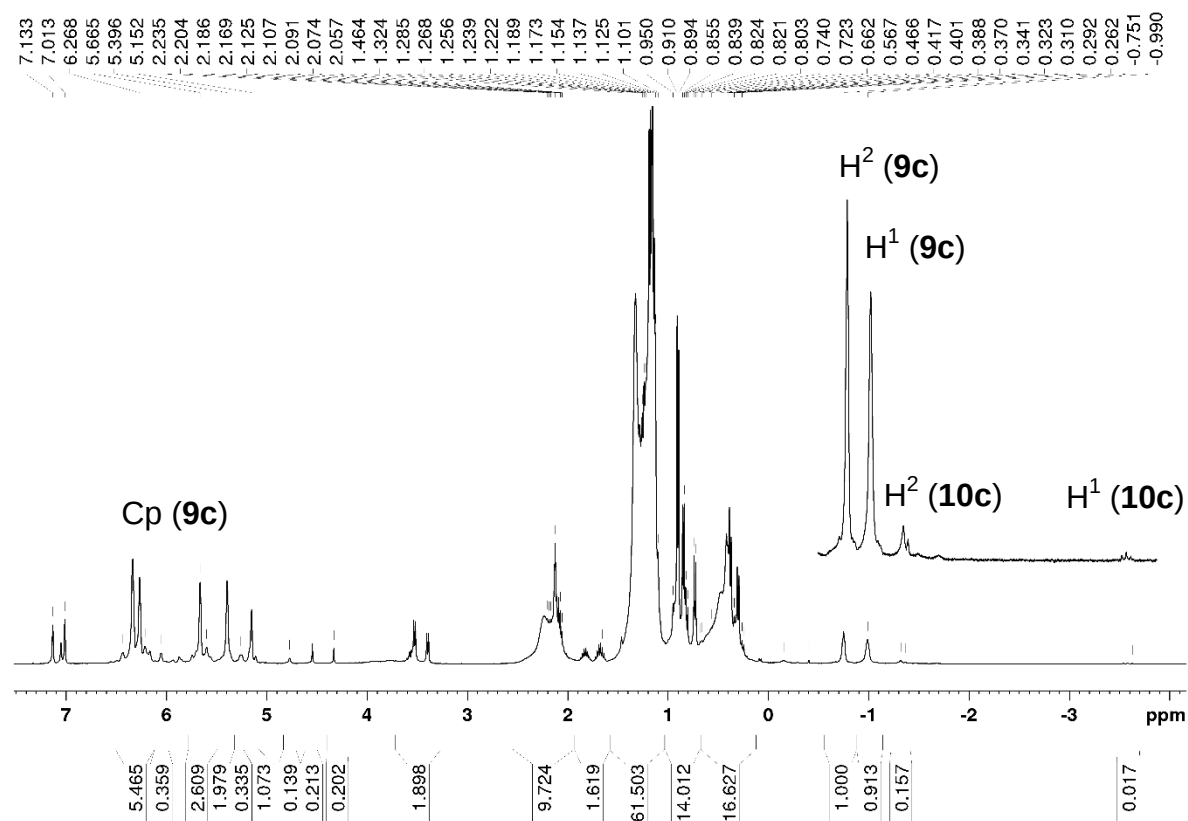


Figure S10. COSY HH of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAlBu^i_2 (1:1.7) in C_7D_8 (298 K).

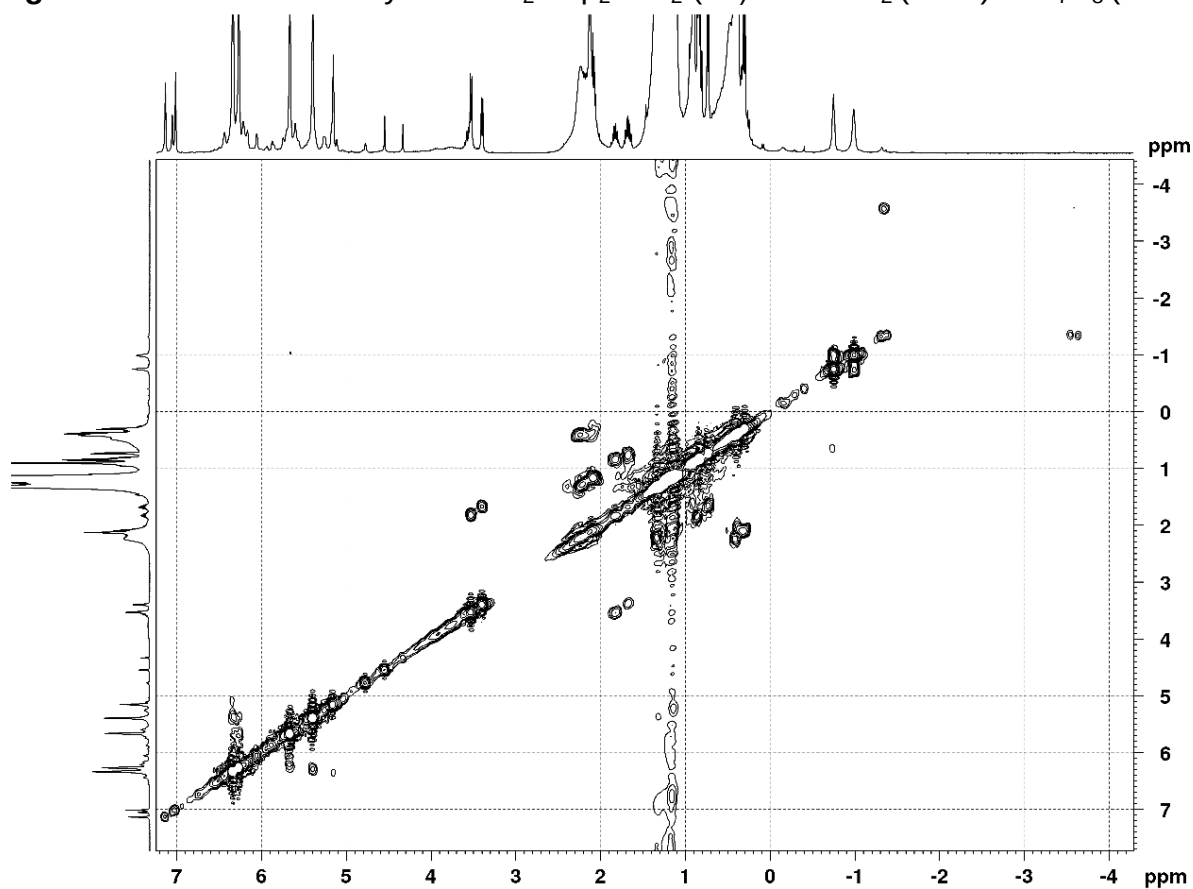


Figure S11. ^1H NMR of system MMAO-12 – HAIBu_2^i (1:3) in C_7D_8 (298 K).

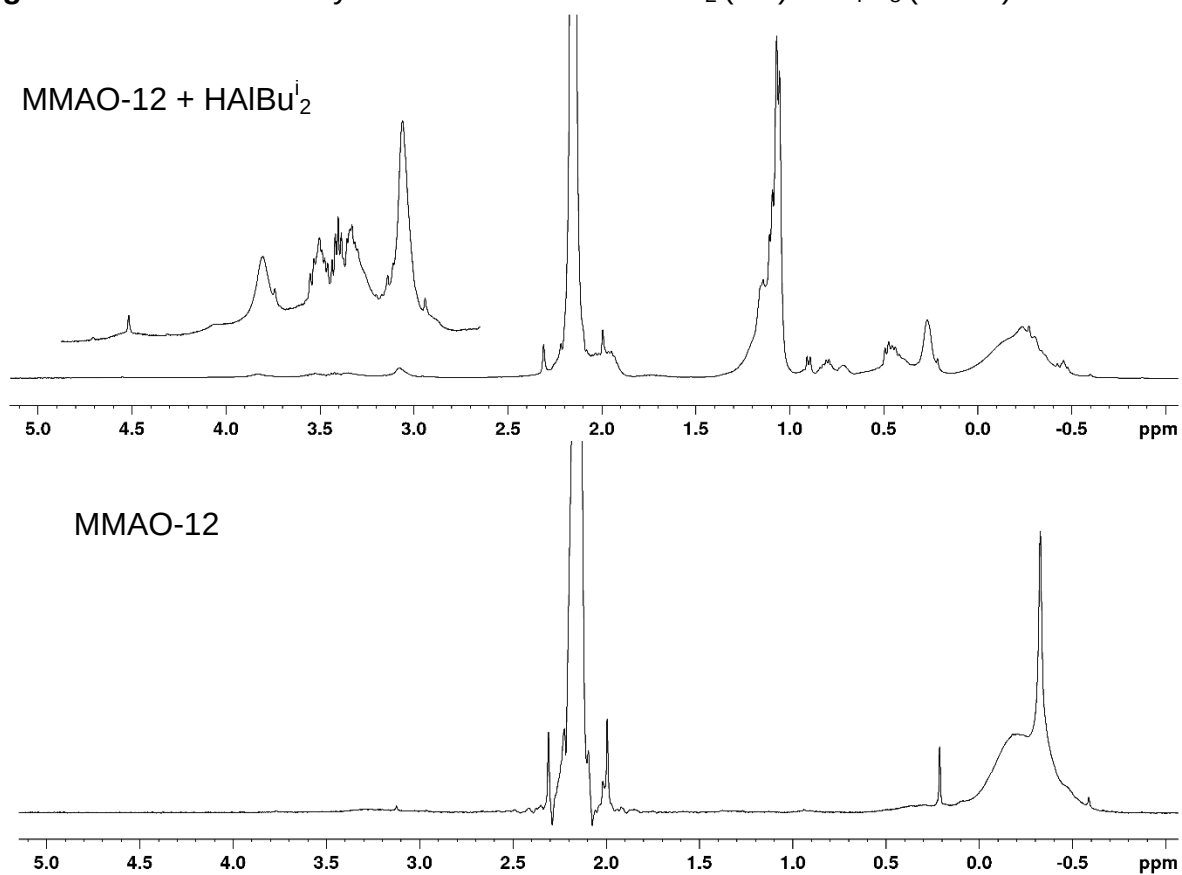


Figure S12. NOESY of system MMAO-12 – HAIBu_2^i (1:3) in C_7D_8 (298 K).

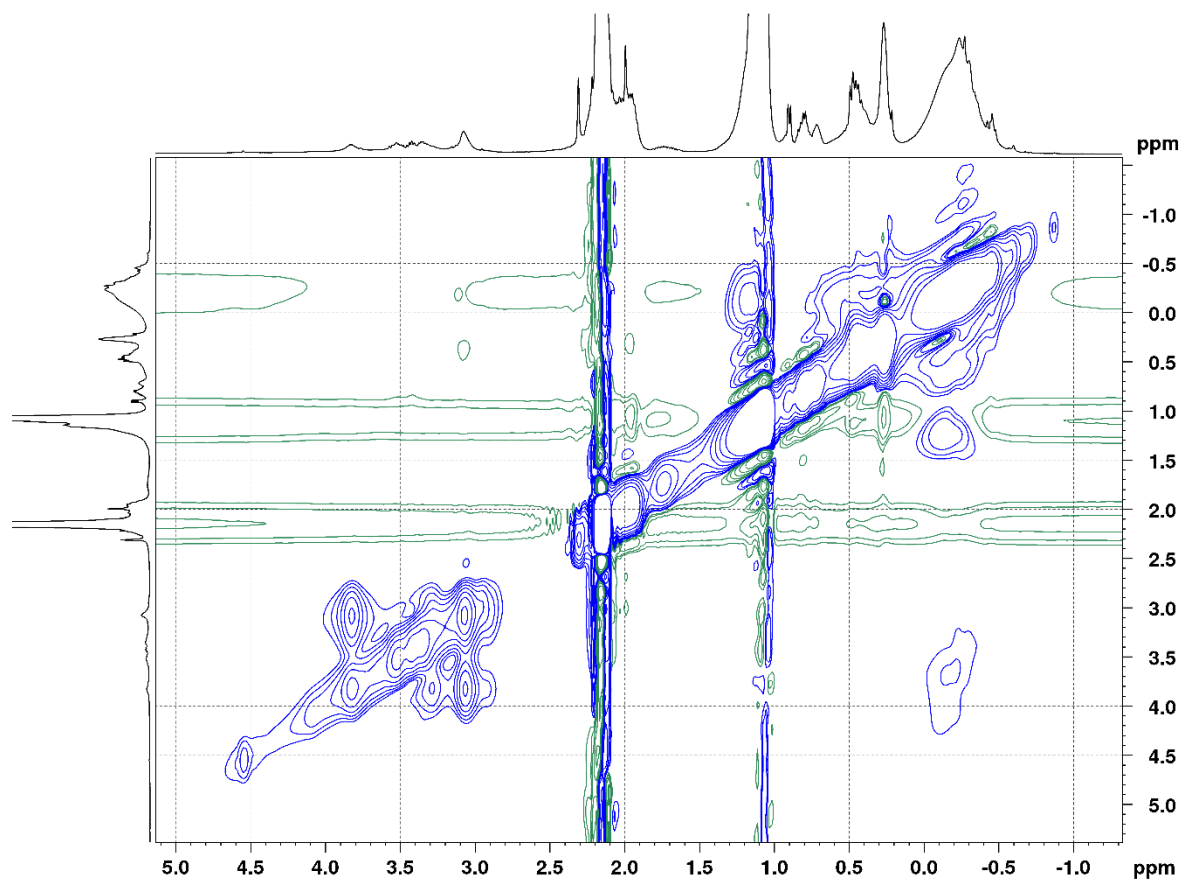


Figure S13. ^1H NMR of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAlBu_2^i – MMAO-12 (1:8:11) in C_7D_8 (298 K).

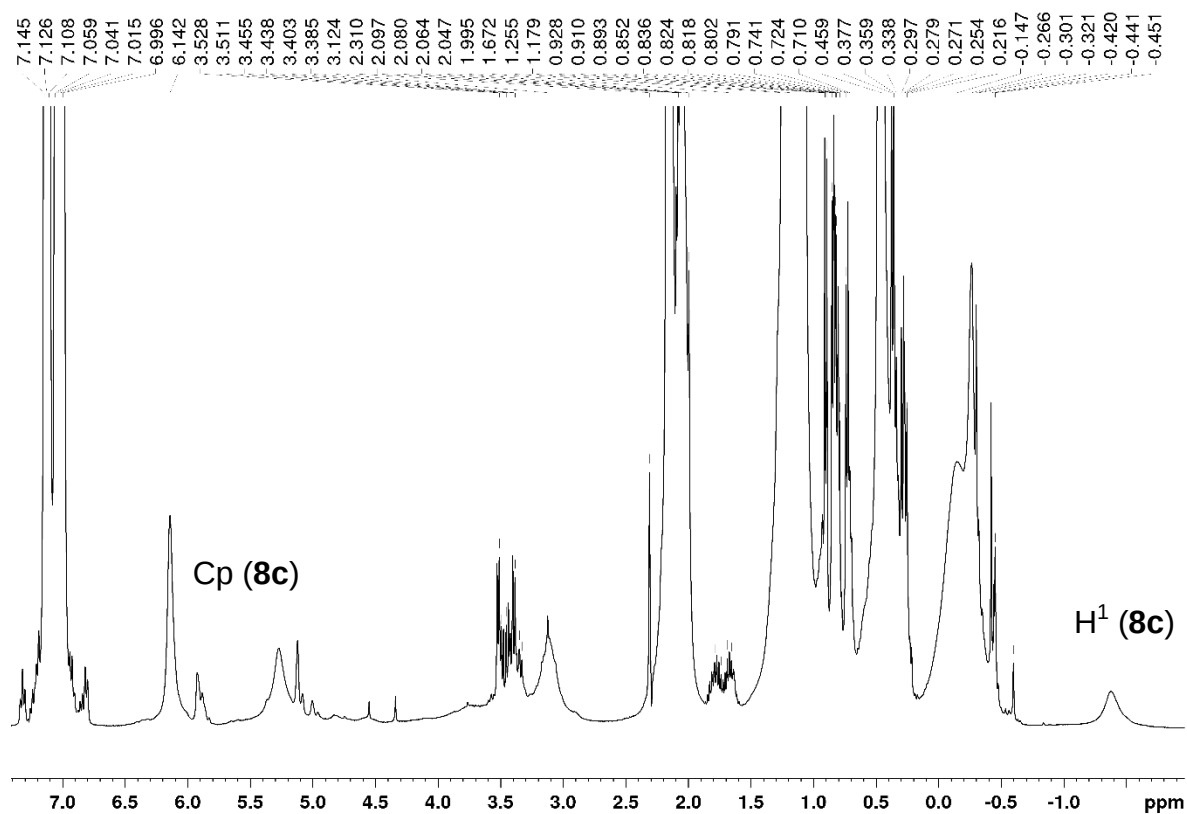


Figure S14. NOESY of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAlBu_2^i – MMAO-12 (1:8:11) in C_7D_8 (298 K).

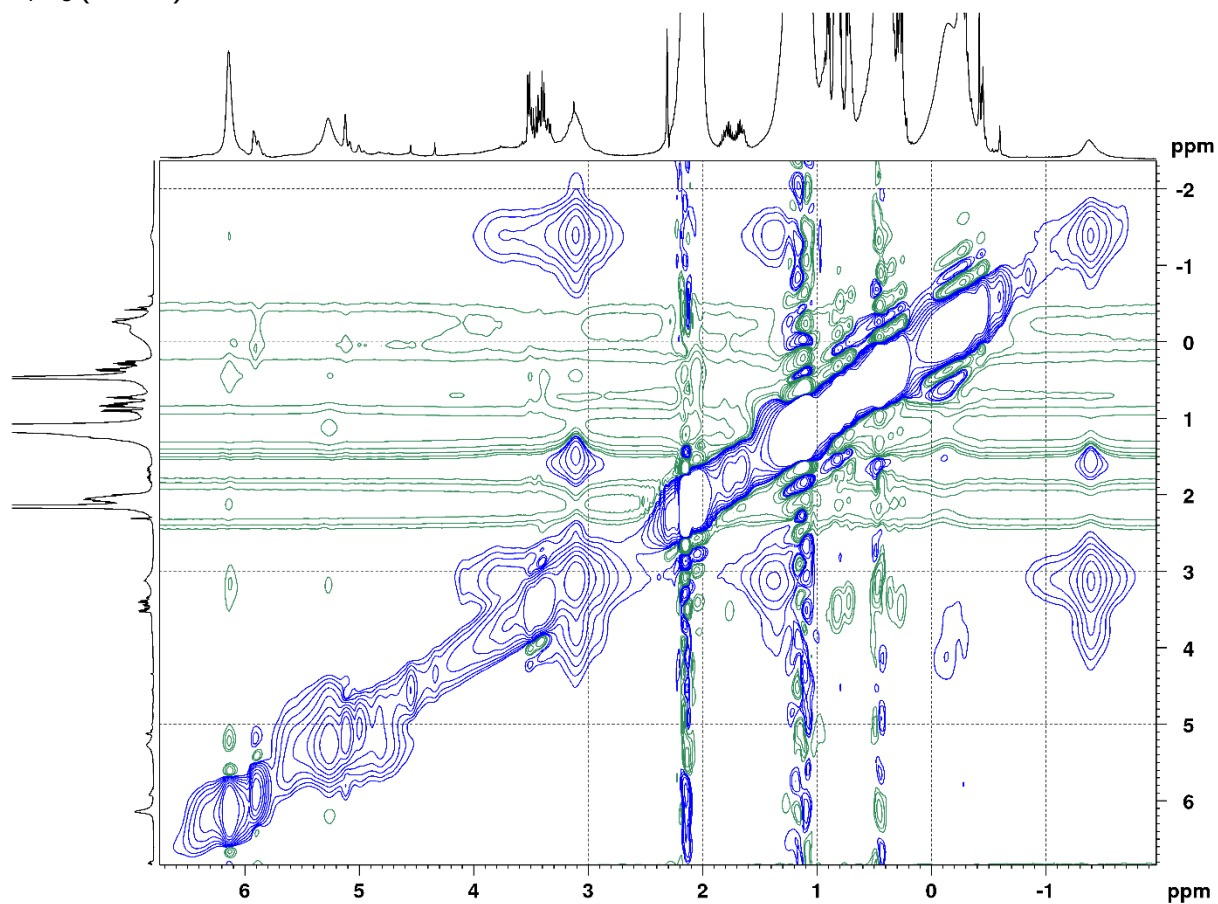


Figure S15. ^1H NMR of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAIBu_2^i – MMAO-12 (1:1.7:7) in C_7D_8 (298 K).

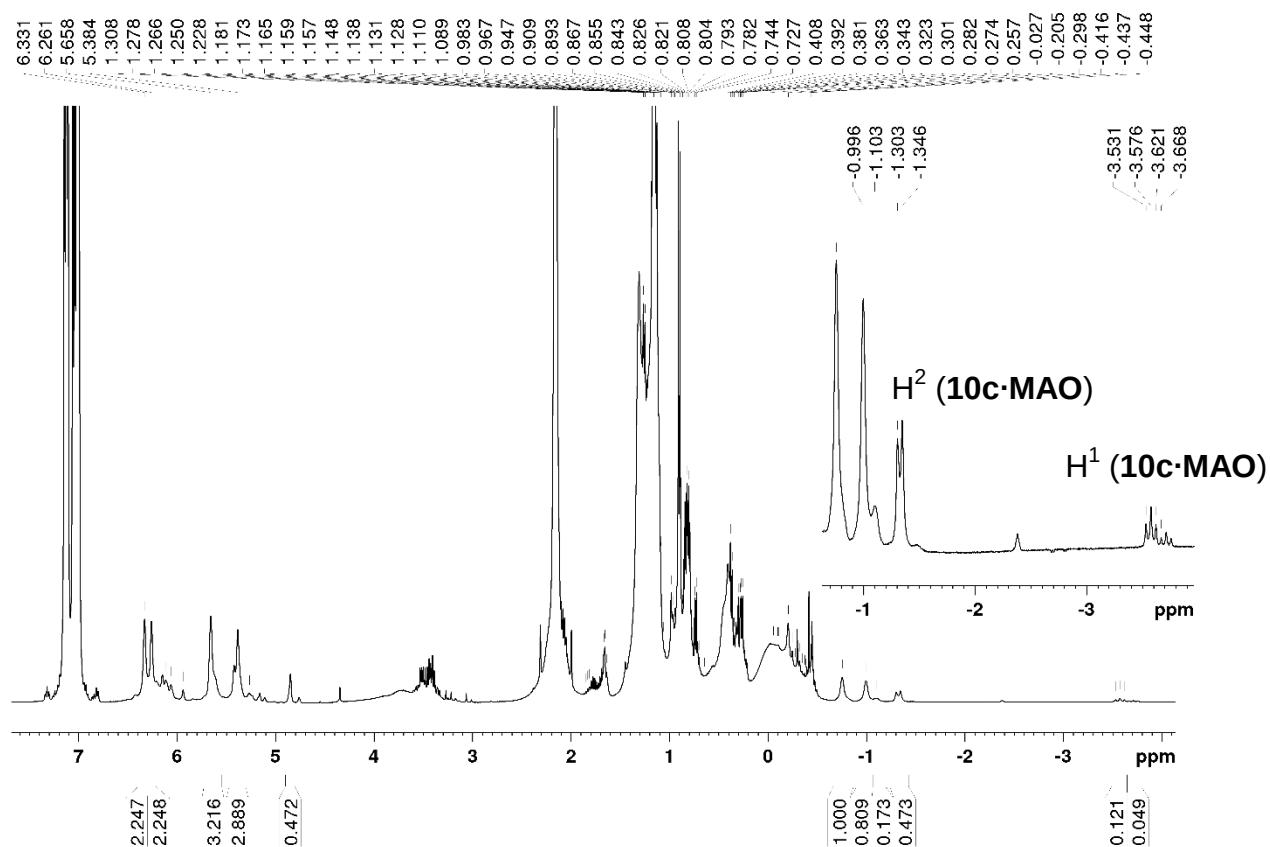


Figure S16. COSY HH of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAIBu_2^i – MMAO-12 (1:1.7:7) in C_7D_8 (298 K).

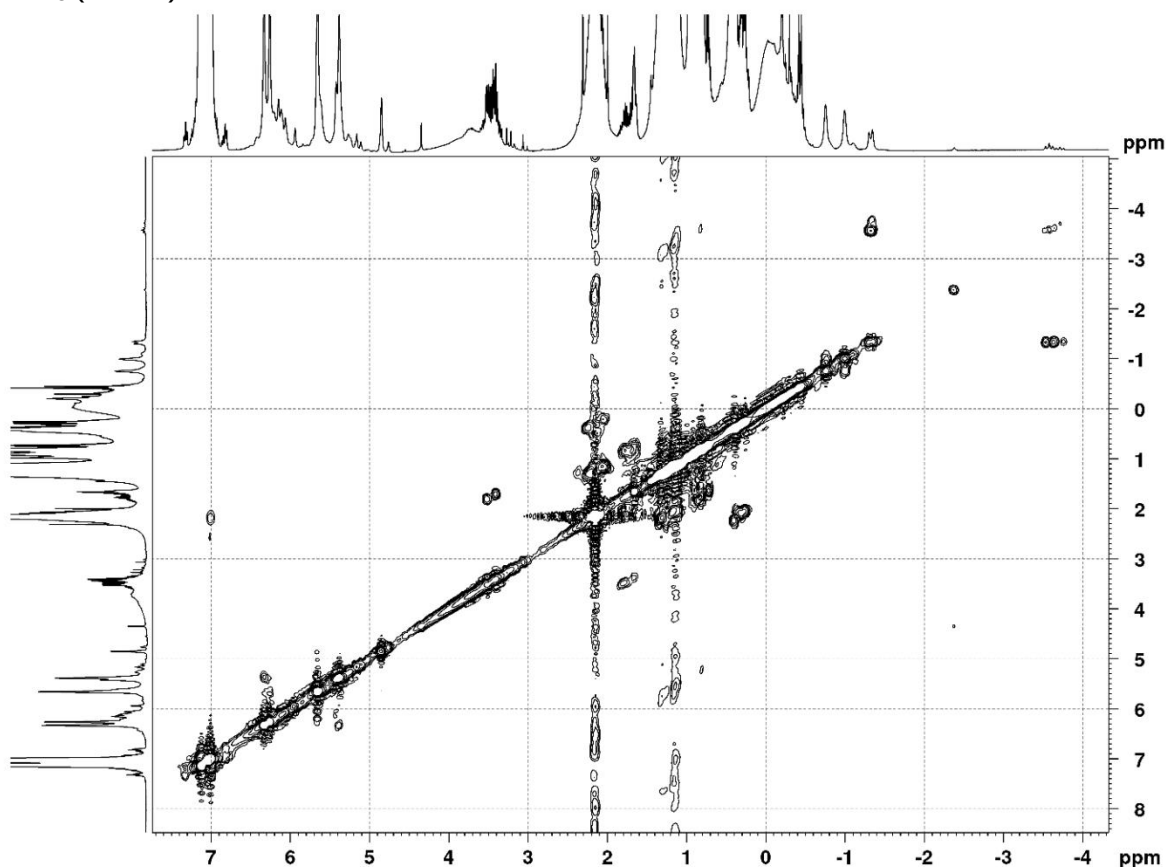


Figure S17. NOESY of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAlBu_2^i – MMAO-12 (1:1.7:7) in C_7D_8 (298 K).

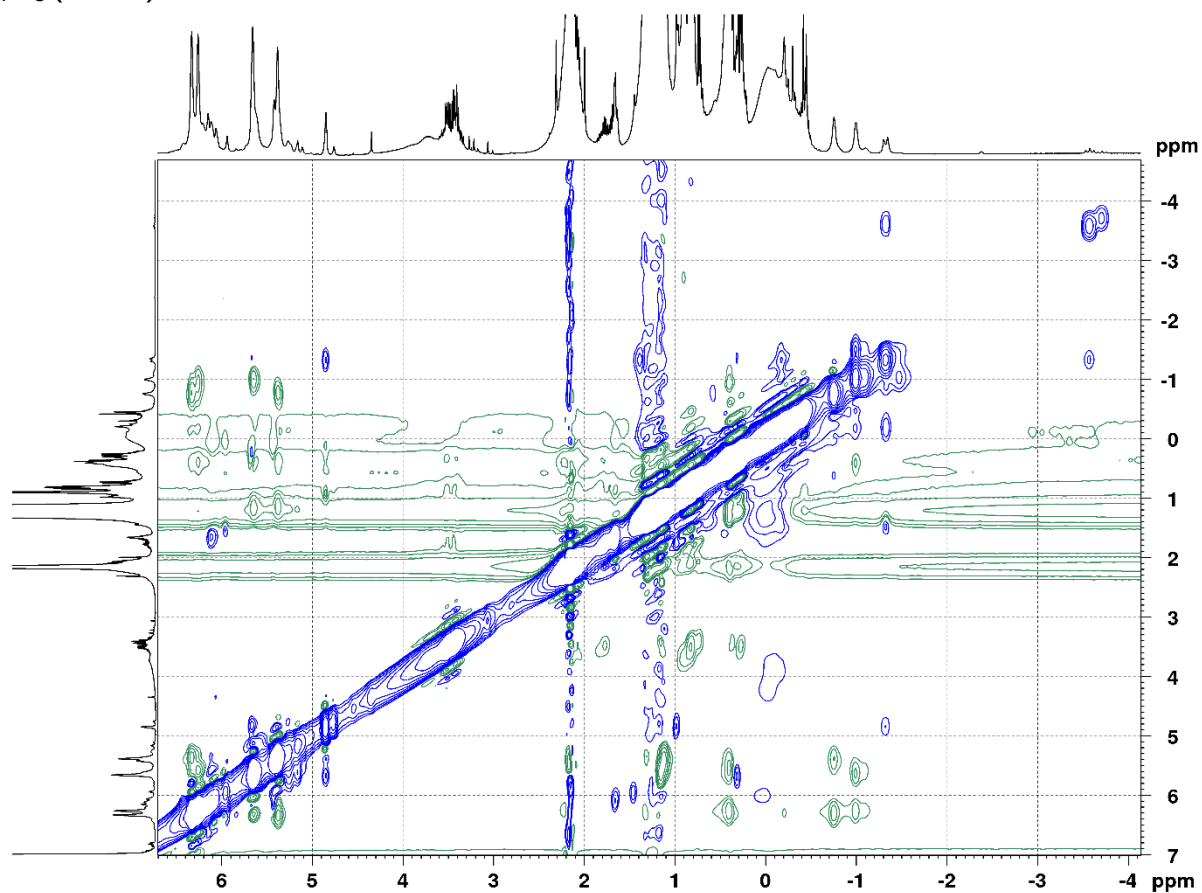


Figure S18. ^1H NMR of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAlBu^i_2 – $(\text{Ph}_3\text{C})[\text{B}(\text{C}_6\text{F}_5)_4]$ (1:1:0.1) in C_7D_8 (298 K).

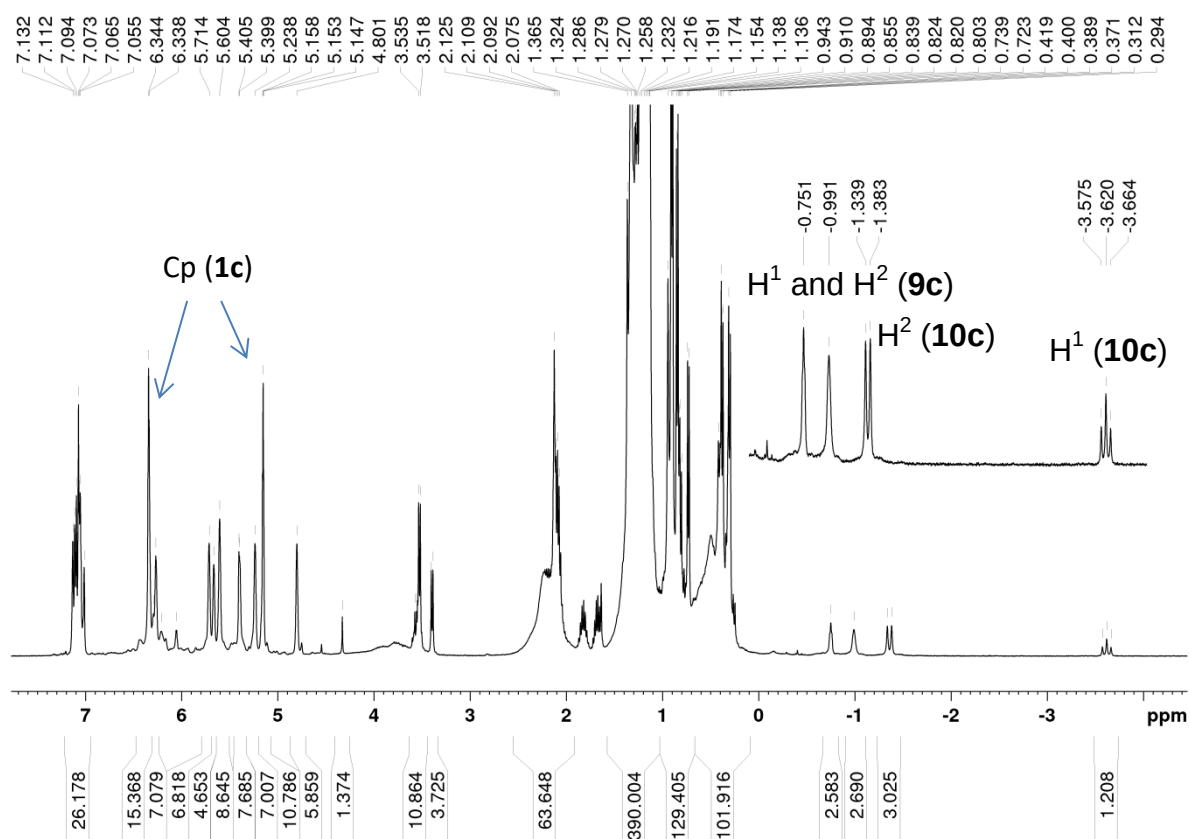


Figure S19. COSY HH of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAlBu^i_2 – $(\text{Ph}_3\text{C})[\text{B}(\text{C}_6\text{F}_5)_4]$ (1:1:0.1) in C_7D_8 (298 K).

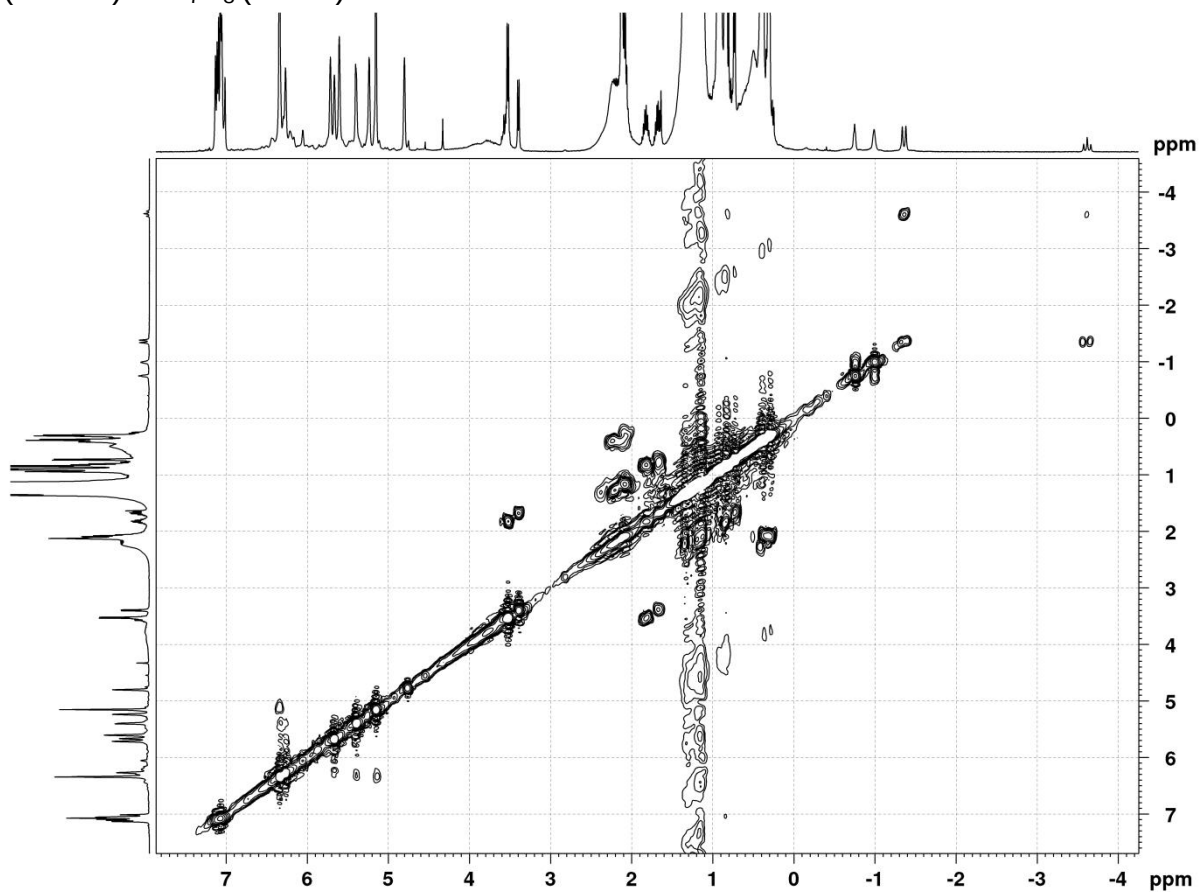


Figure S20. NMR monitoring of system $\text{Me}_2\text{CCp}_2\text{ZrCl}_2$ (**1c**) – HAlBu_2^i – MMAO-12 – 1-hexene (1:8:11:2) in C_7D_8 .

