Supporting Information

"Click" Synthesis of Heteroleptic Tris-cyclometalated Iridium(III) Complexes: Cu(I) Triazolide Intermediates as Transmetalating Reagents

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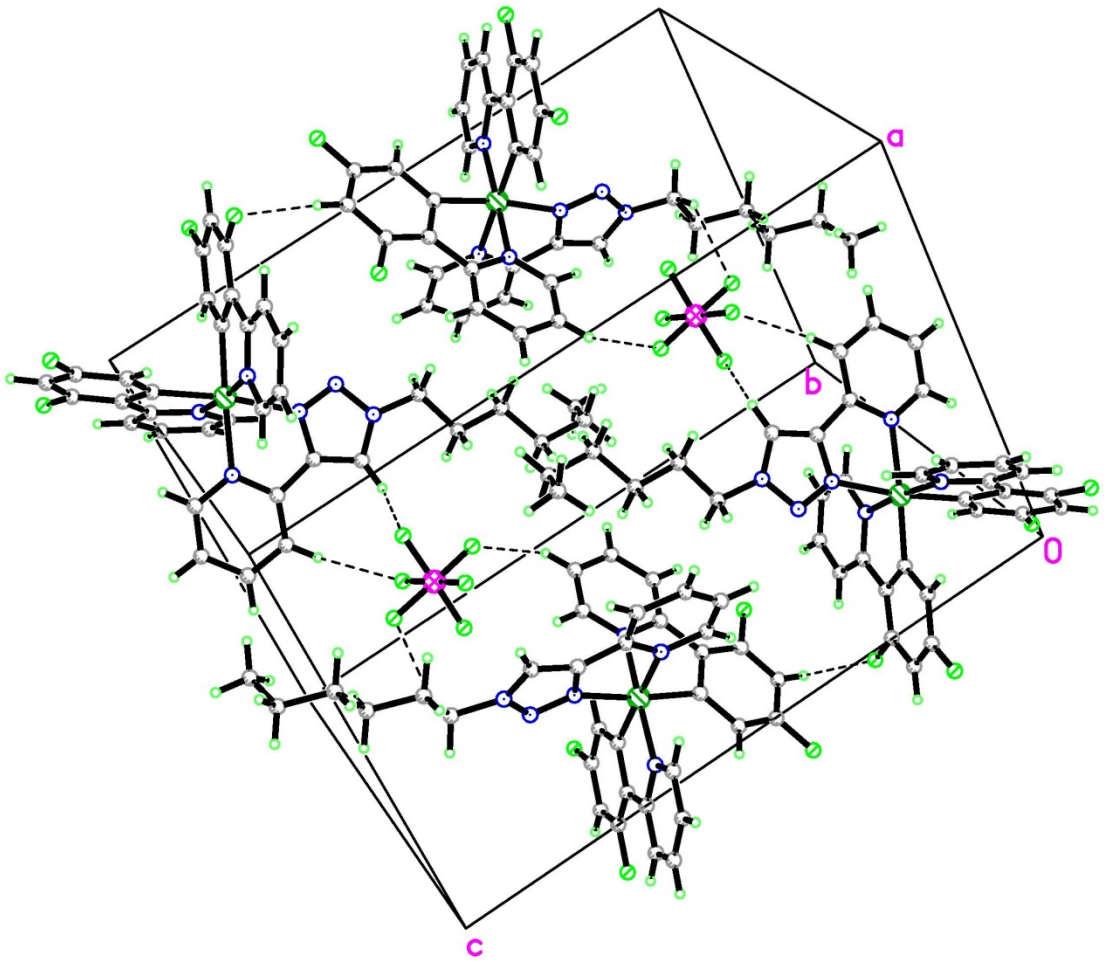


Figure S1. Packing diagram of **6b**.

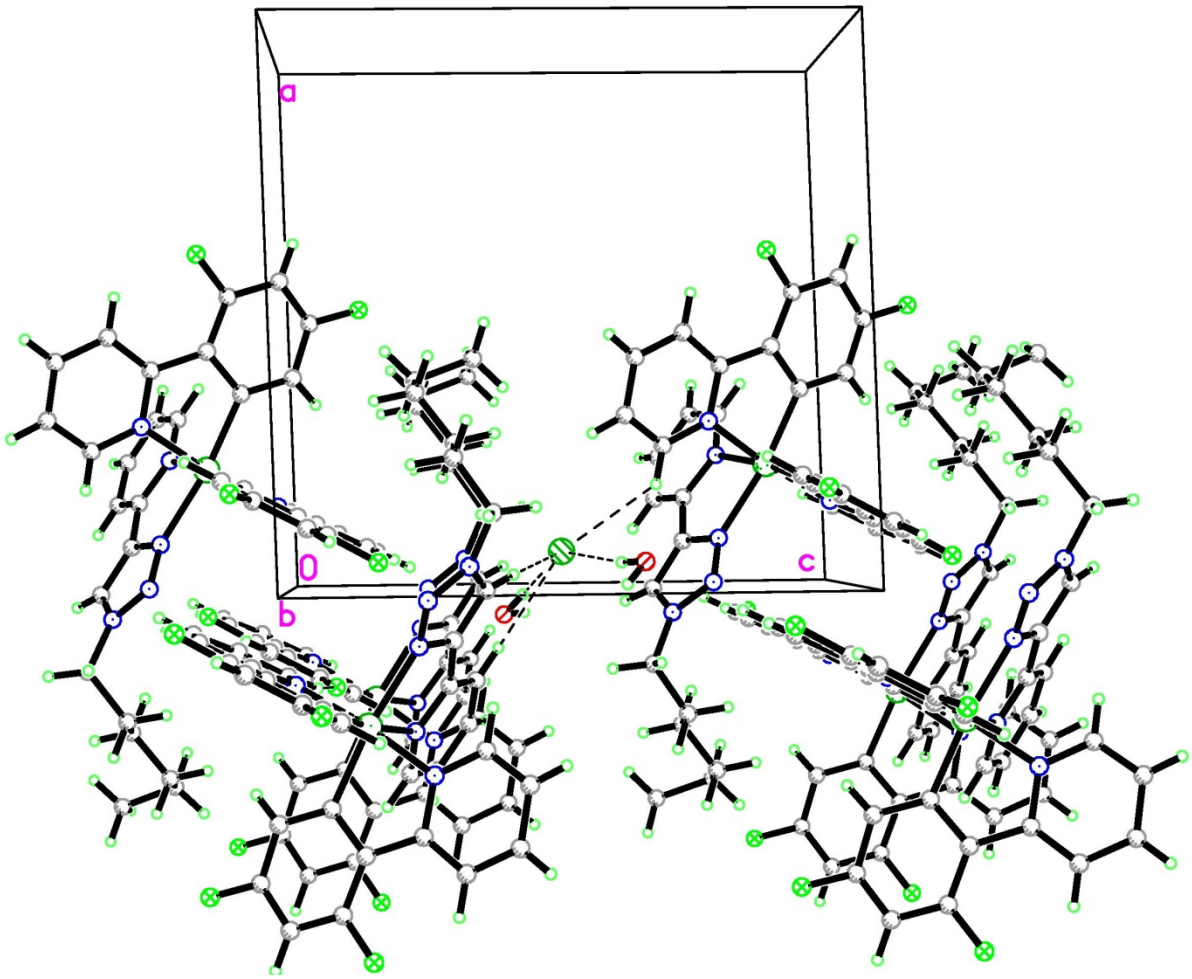


Figure S2. Packing diagram of **7b**.

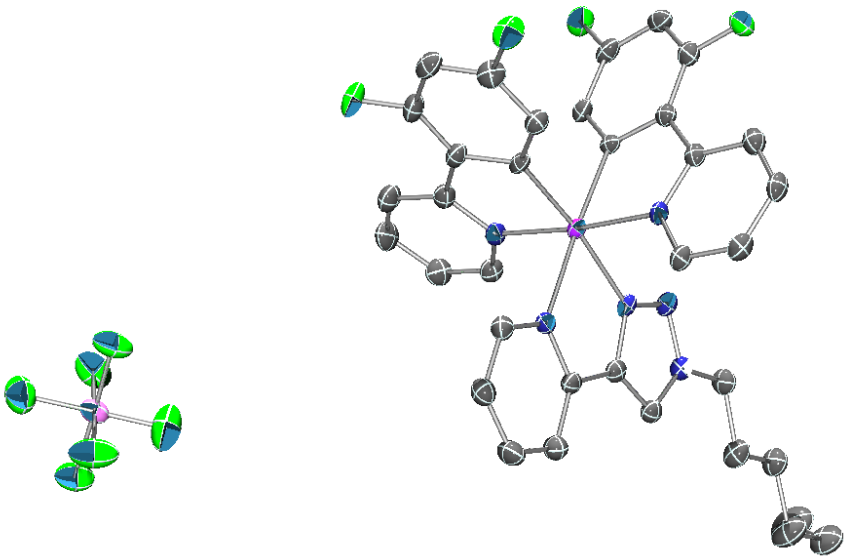


Figure S3. Ortep diagrams of **6b**. Thermal elliposoids are drawn at the 50% probability level.

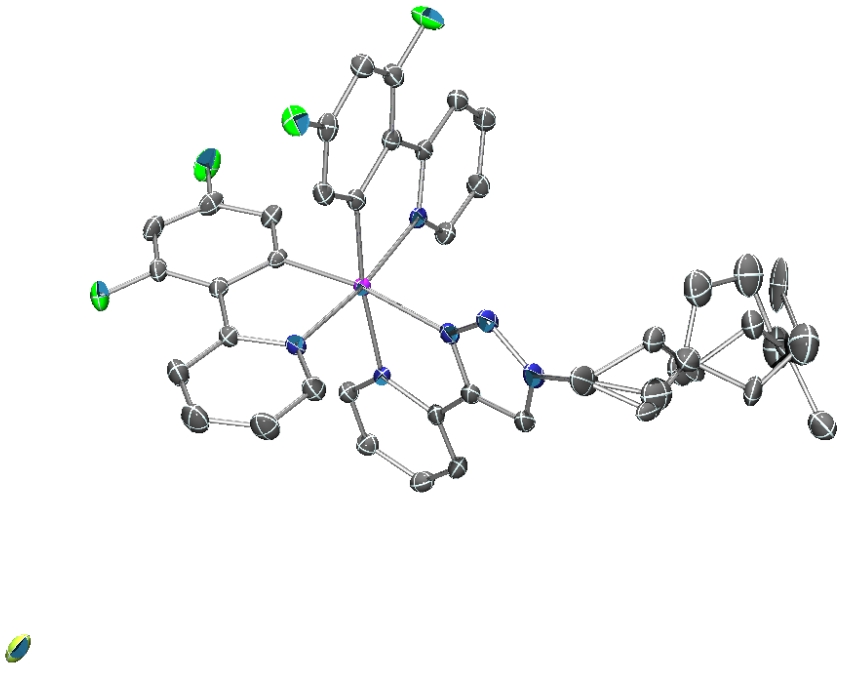
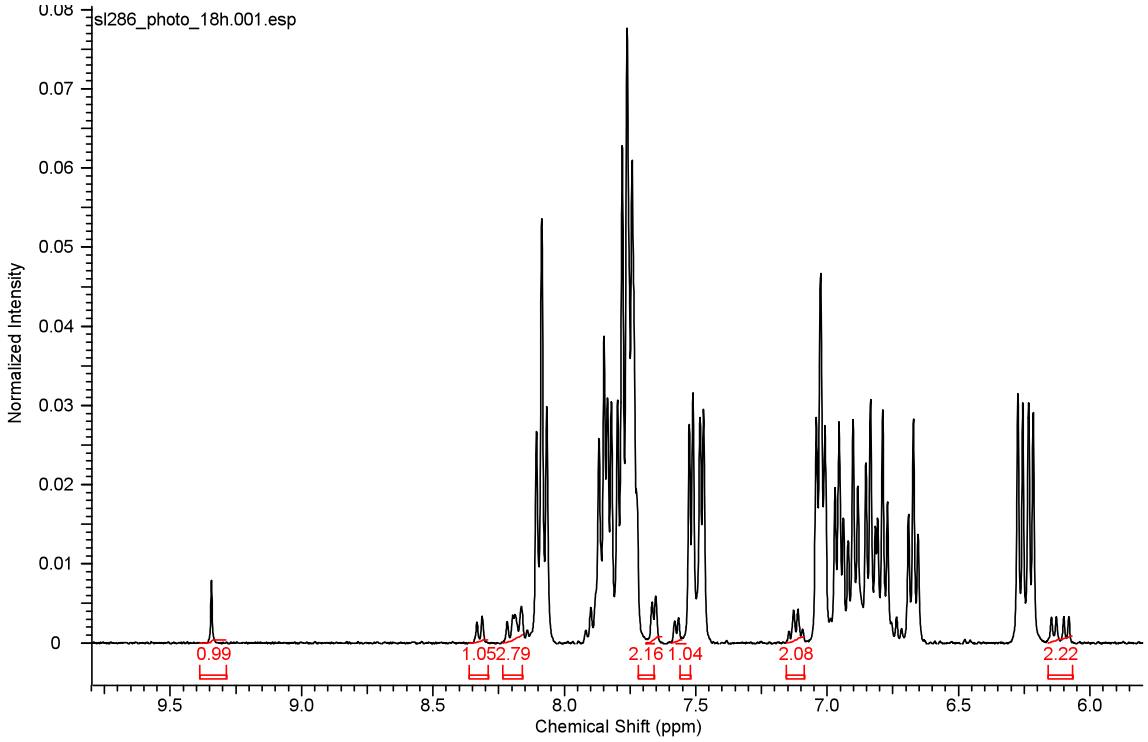


Figure S4. Ortep diagrams of **7b**. Thermal elliposoids are drawn at the 50% probability level.

(a)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0.03
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2.79
2.16
1.04
2.08
2.22
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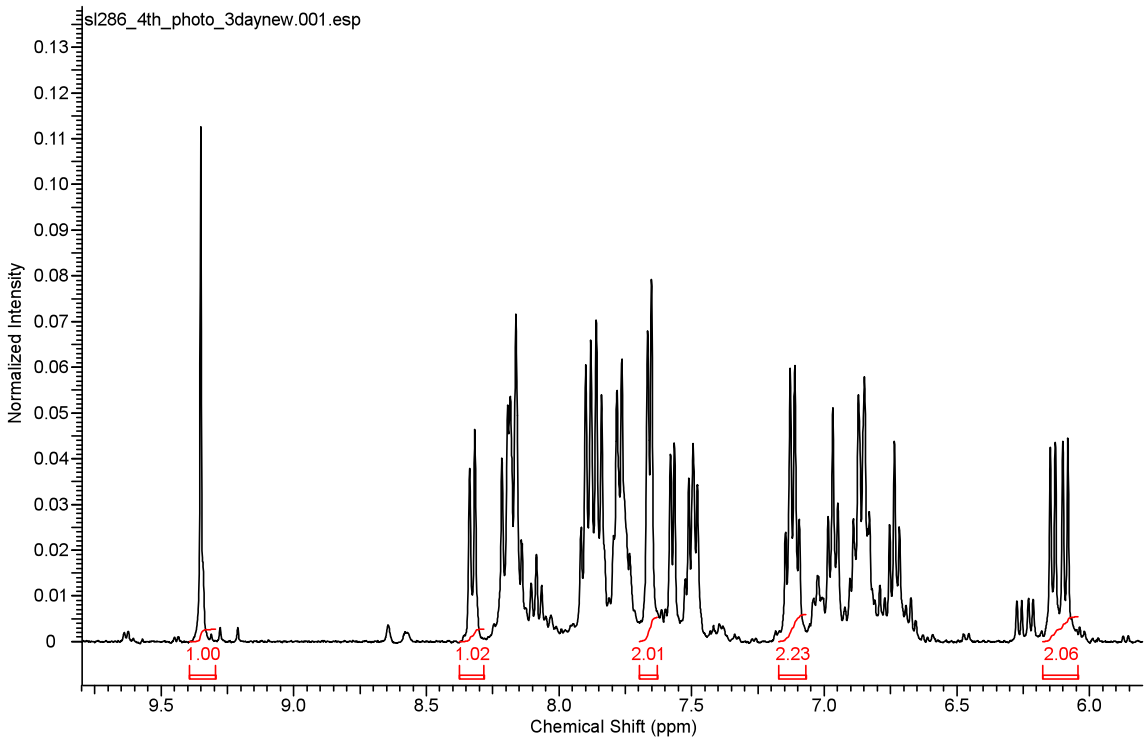
9.0
8.5
8.0
7.5
7.0
6.5
6.0
Chemical Shift (ppm)

(b)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0.07
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0.04
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0.02
0.01
0
1.00
1.02
2.01
2.23
2.06
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
Chemical Shift (ppm)

(c)

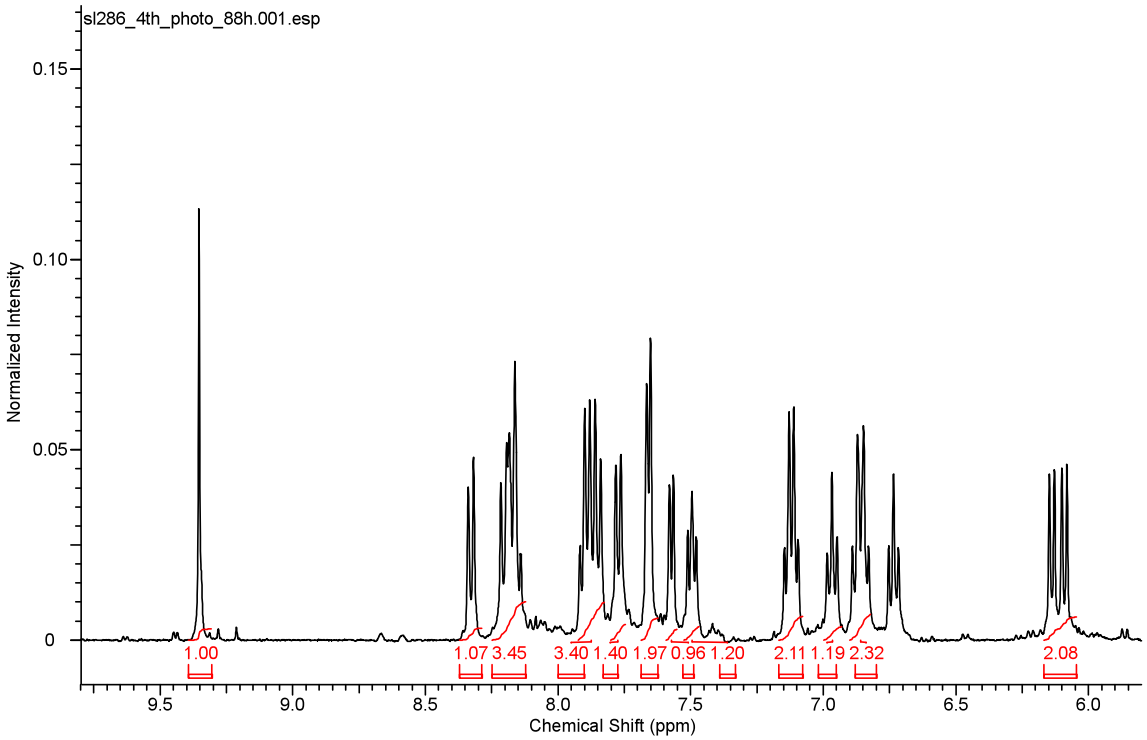

Figure S5. Photoisomerization of **2a** in DMSO-d_6, monitored by ^{1}H NMR after exposed to UV radiation for 18 h, 72 h and 88 h. The non-overlapping peaks corresponding to the newly formed $[Ir(C^N)_2(N^N\_trpy)]^+$ cation are integrated.

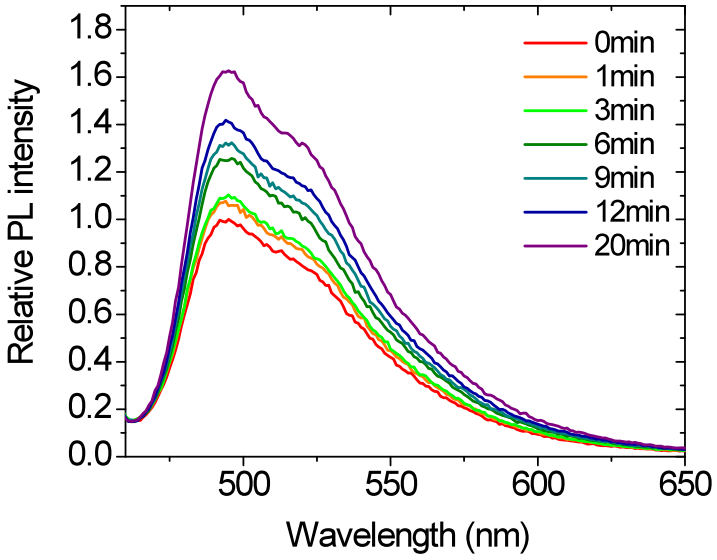

Figure S6. Enhanced photoluminescence of **2a** in deoxygenated THF solution upon broadband UV radiation.

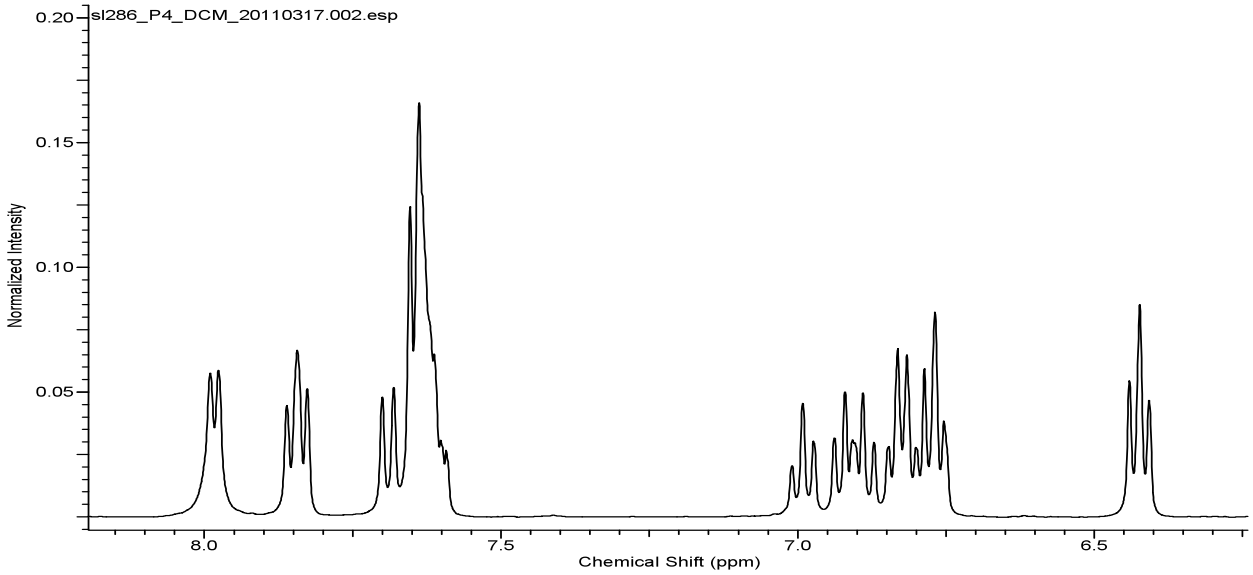

Figure S7. ^{1}H NMR of **2a** in DMOS-d_6

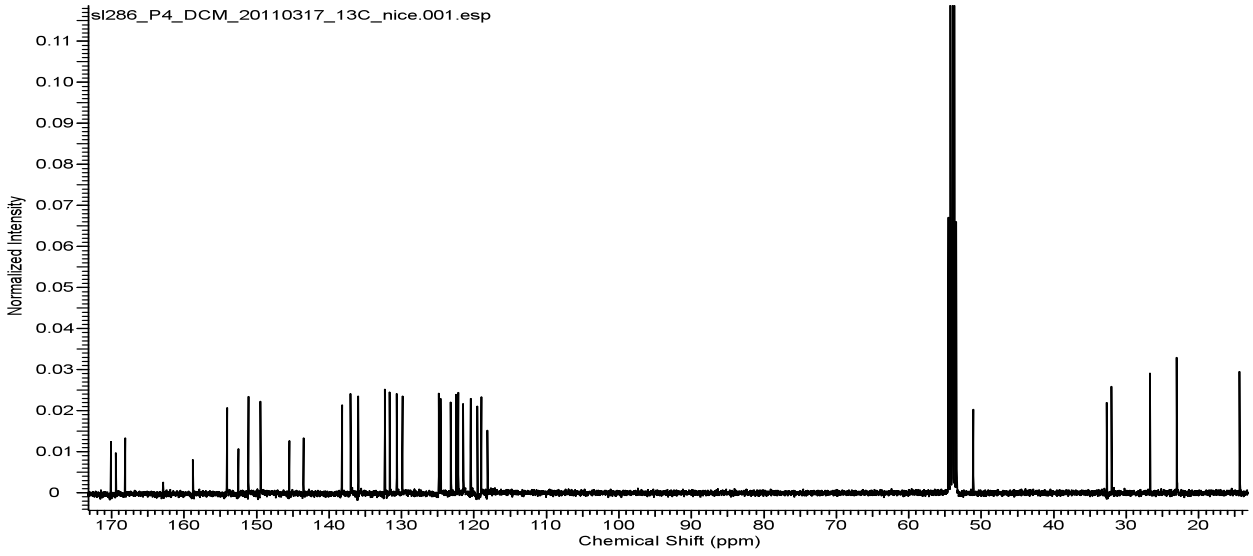

Figure S8. ^{13}C NMR of **2a** in CD_2Cl_2

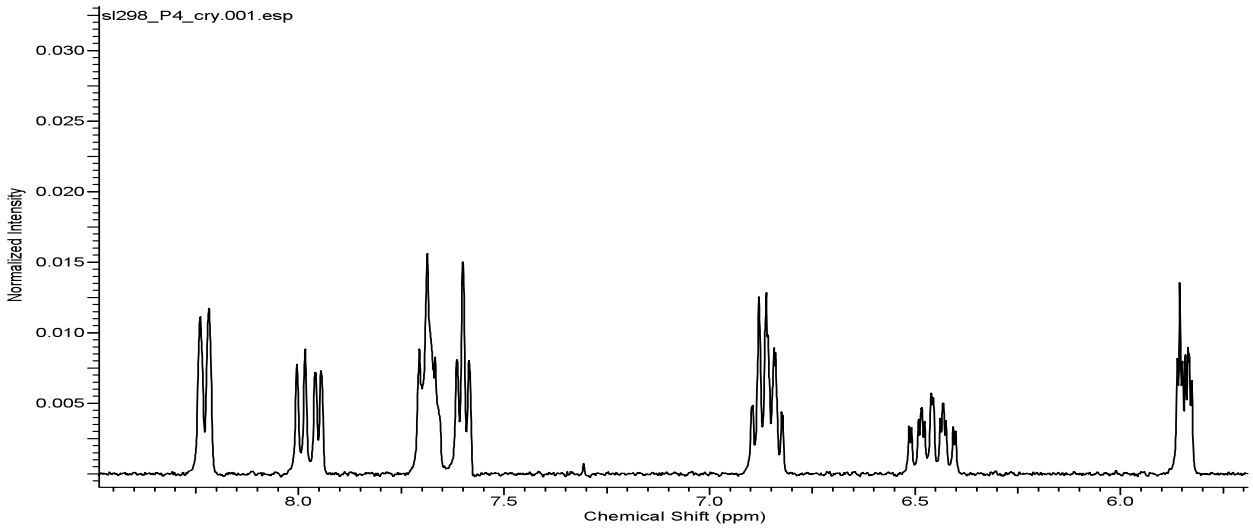

Figure S9. ^{1}H NMR of **2b** in CD_2Cl_2

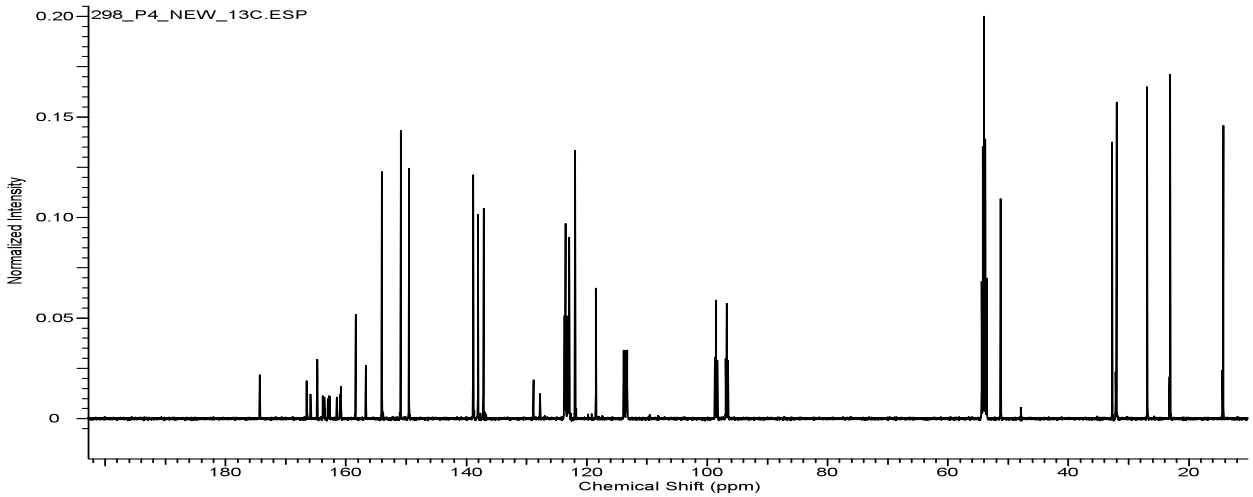

Figure S10. ^{13}C NMR of **2b** in CD_2Cl_2

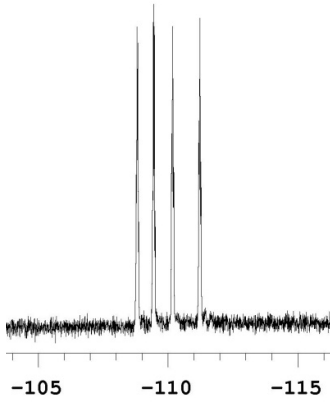

Figure S11. ^{19}F NMR of **2b** in CD_2Cl_2

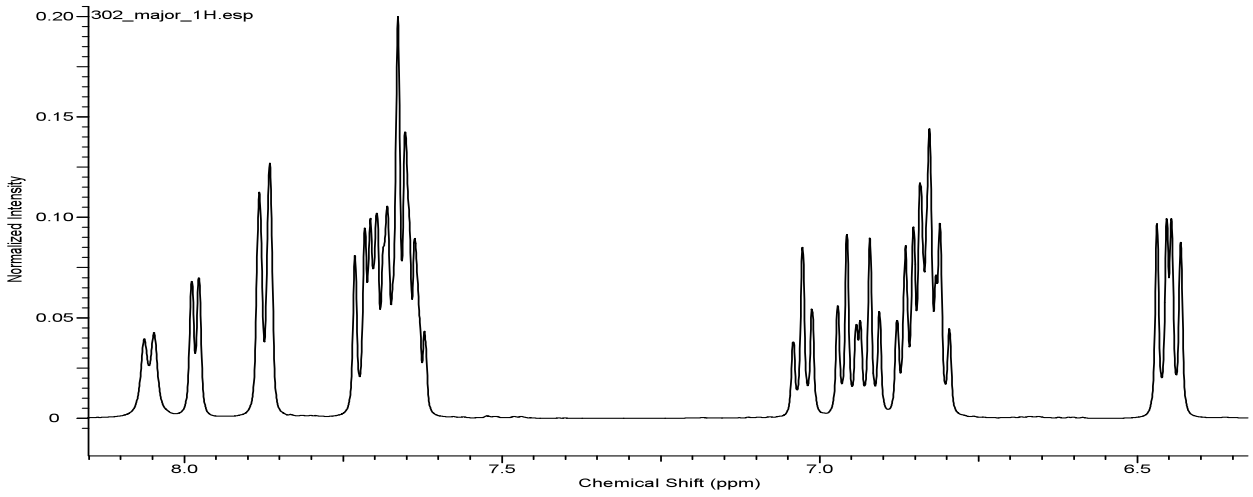

Figure S12. ^{1}H NMR of **3a** in CD_2Cl_2

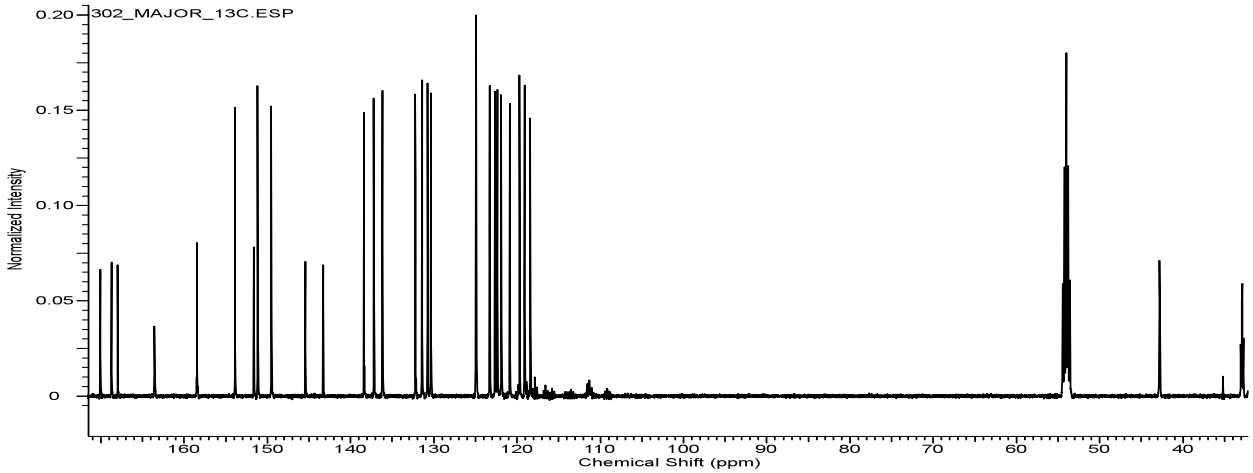

Figure S13. ^{13}C NMR of **3a** in CD_2Cl_2

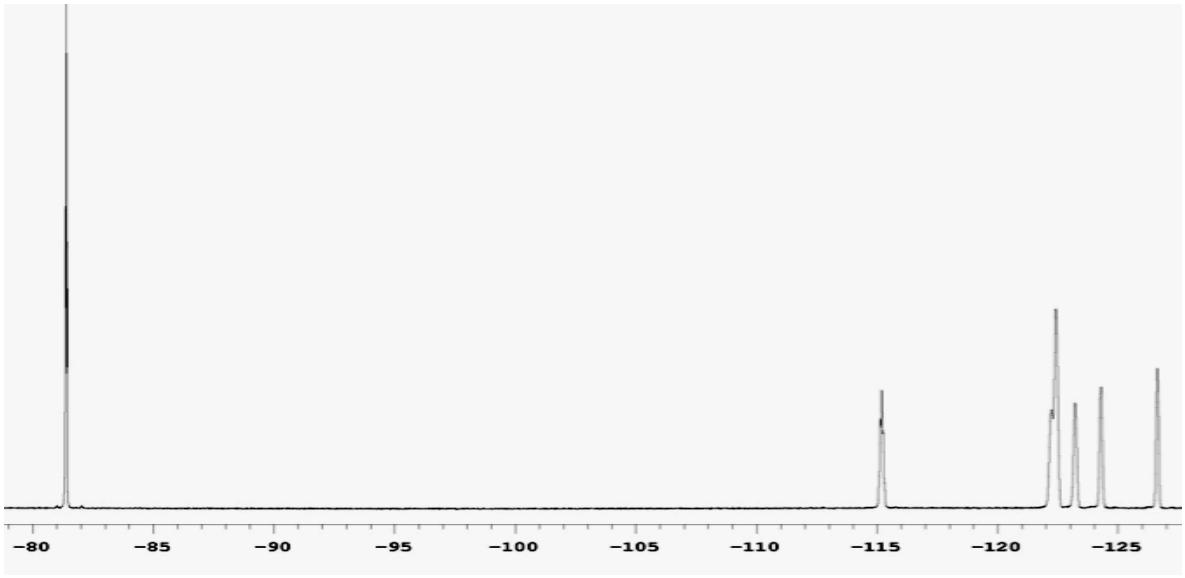

Figure S14. ^{19}F NMR of **3a** in CD_2Cl_2

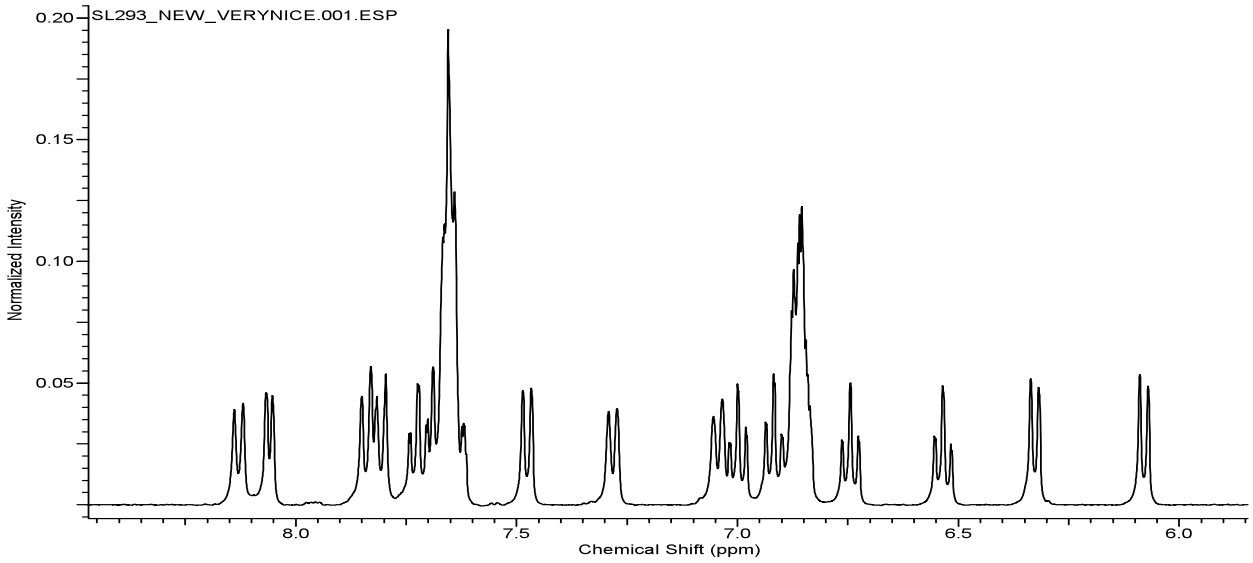

Figure S15. ^{1}H NMR of **4a** in CD_2Cl_2

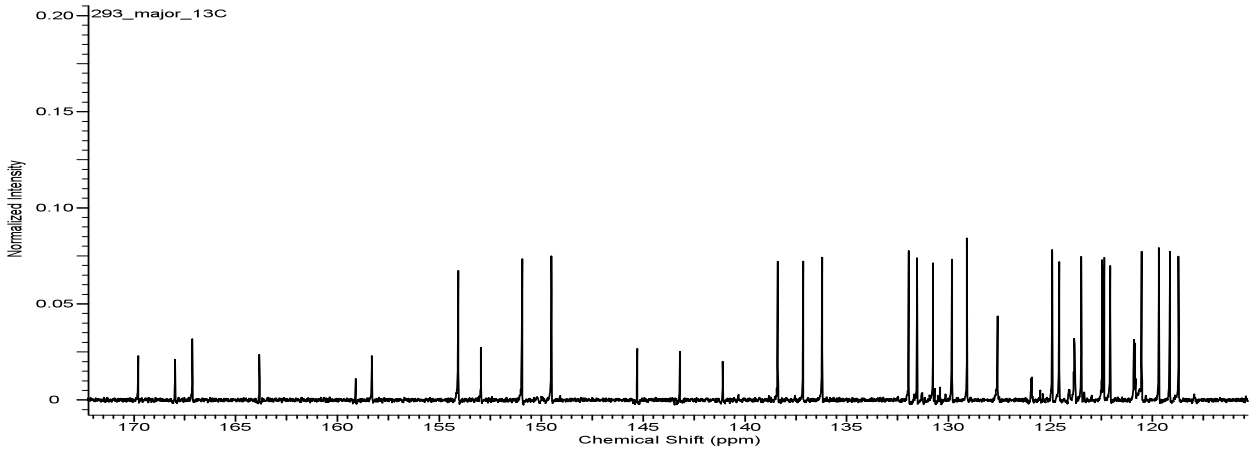

Figure S16. ^{13}C NMR of **4a** in CD_2Cl_2

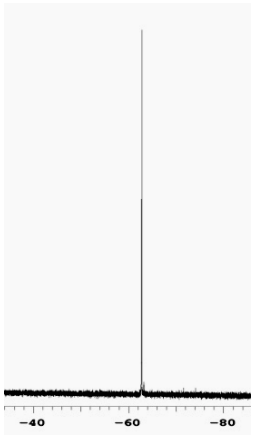

Figure S17. ^{19}F NMR of **4a** in CD_2Cl_2

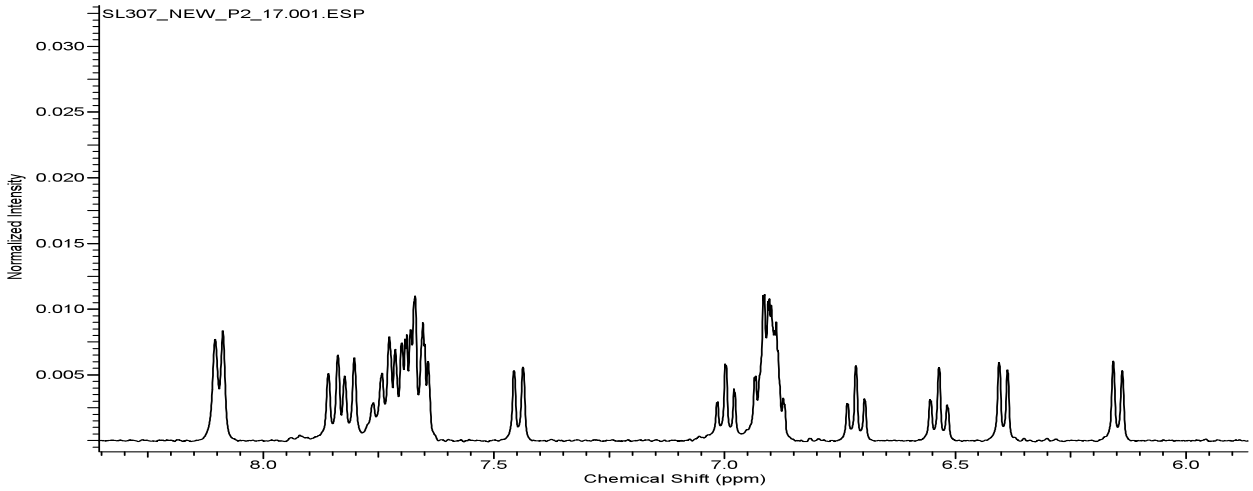

Figure S18. ^{1}H NMR of **5a** in CD_2Cl_2

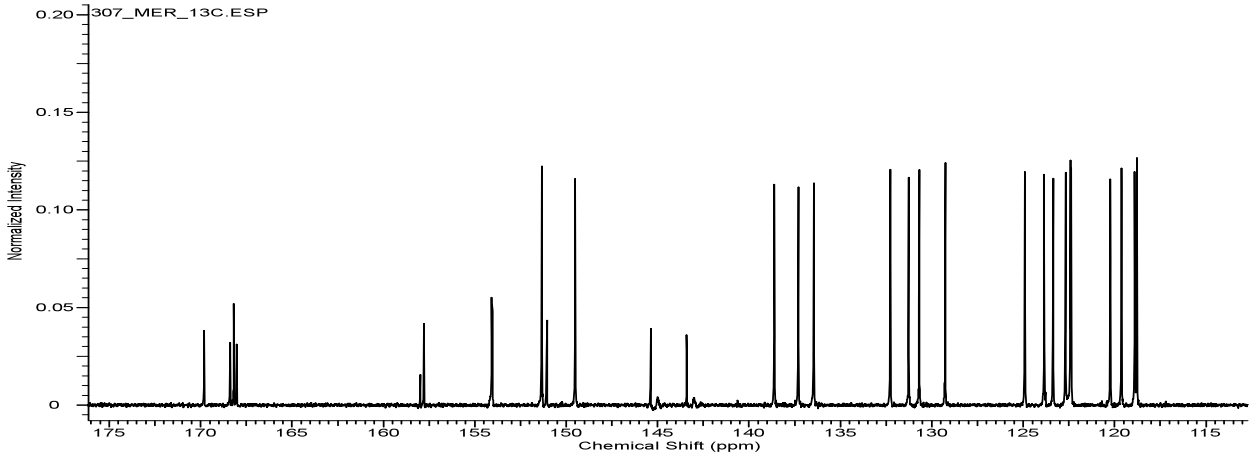

Figure S19. ^{13}C NMR of **5a** in CD_2Cl_2

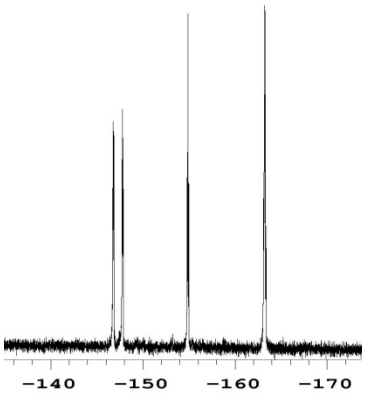

Figure S20. ^{19}F NMR of **5a** in CD_2Cl_2

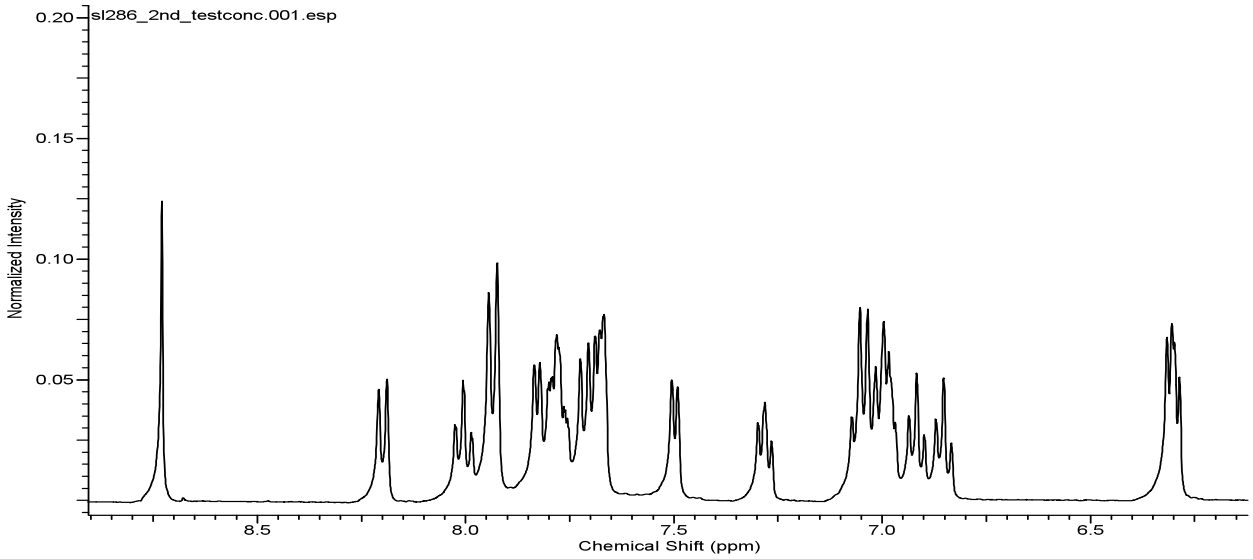

Figure S21. ^{1}H NMR of **6a** in CD_2Cl_2

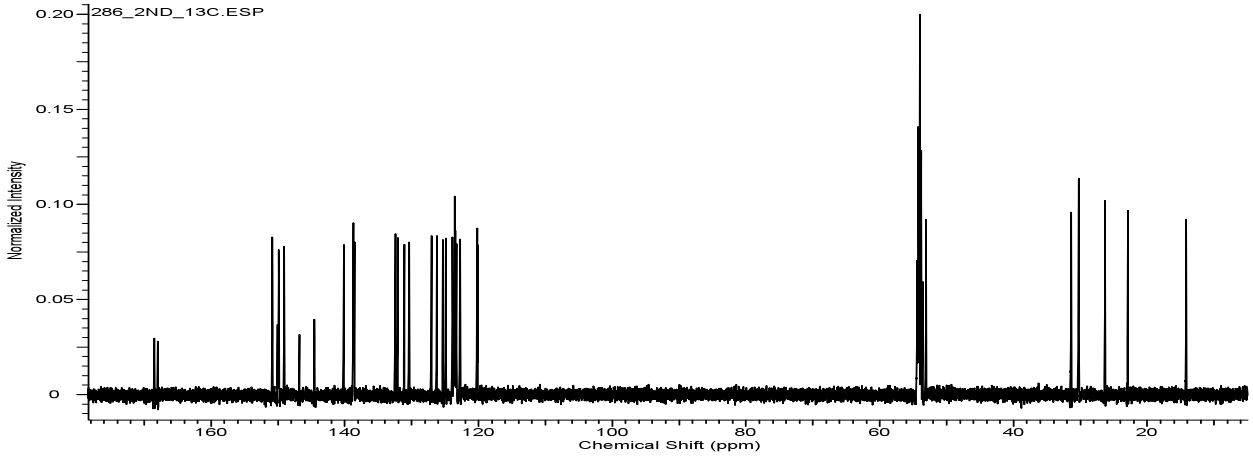

Figure S22. ^{13}C NMR of **6a** in CD_2Cl_2

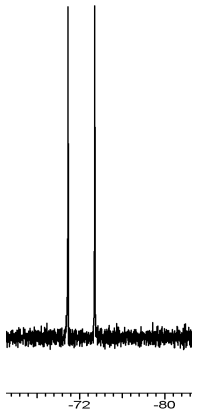

Figure S23. ^{19}F NMR of **6a** in CD_2Cl_2

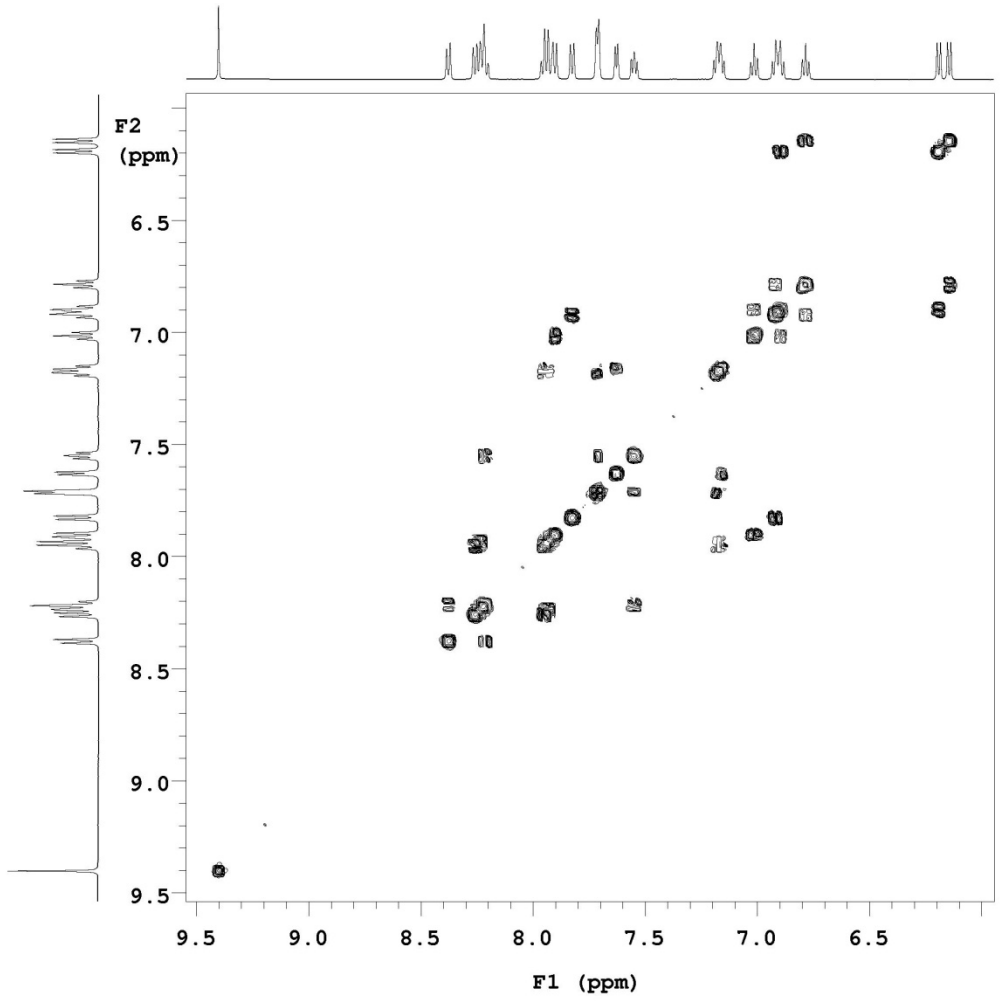

Figure S24. gCOSY of **6a** in DMOS-d_6

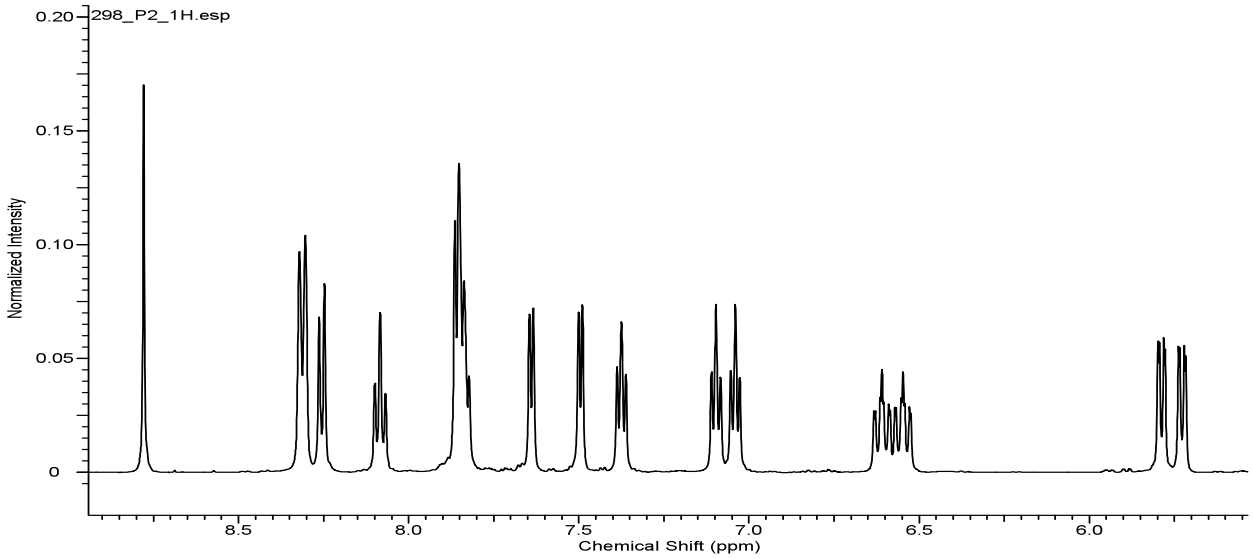

Figure S25. ^{1}H NMR of **6b** in CD_2Cl_2

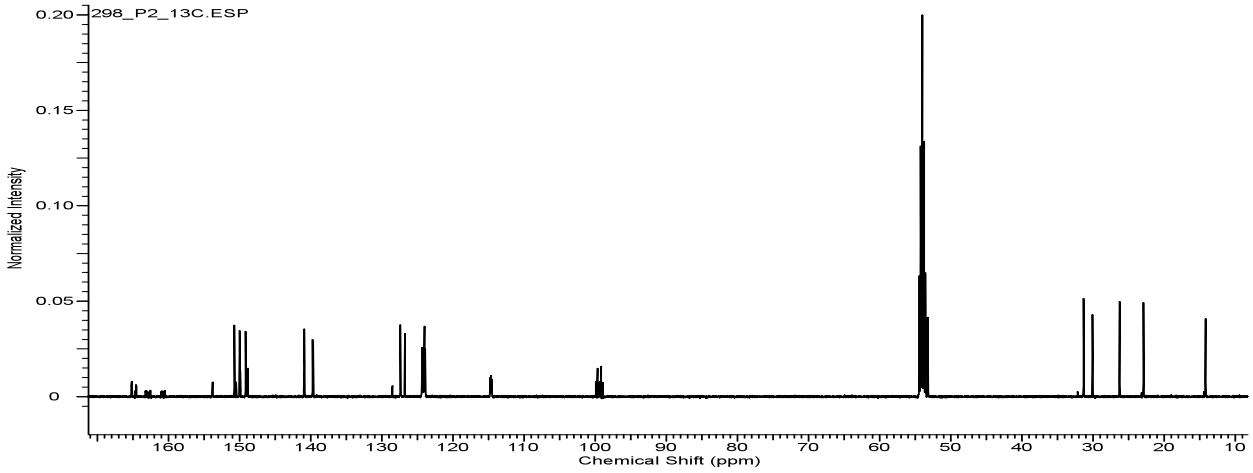

Figure S26. ^{13}C NMR of **6b** in CD_2Cl_2

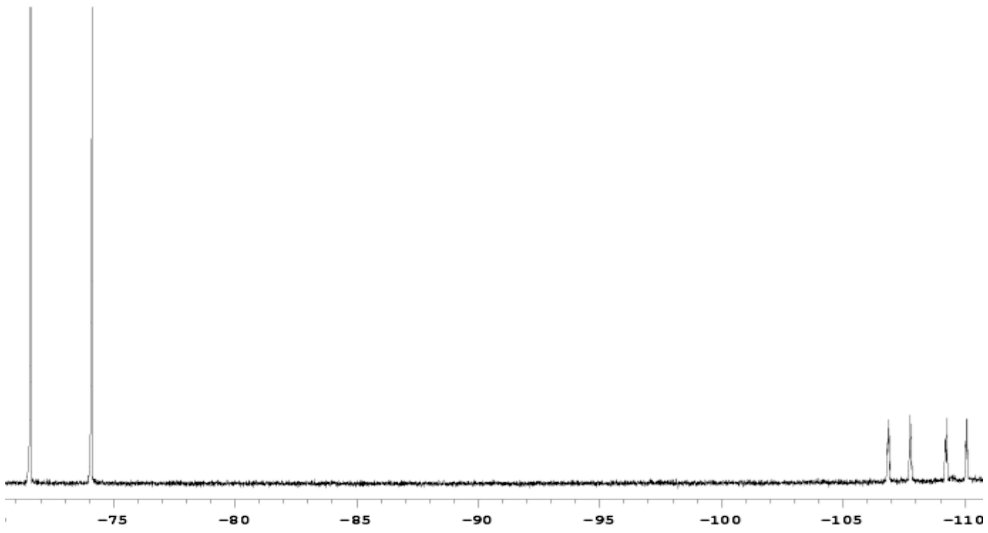

Figure S27. ^{19}F NMR of **6b** in CD_2Cl_2

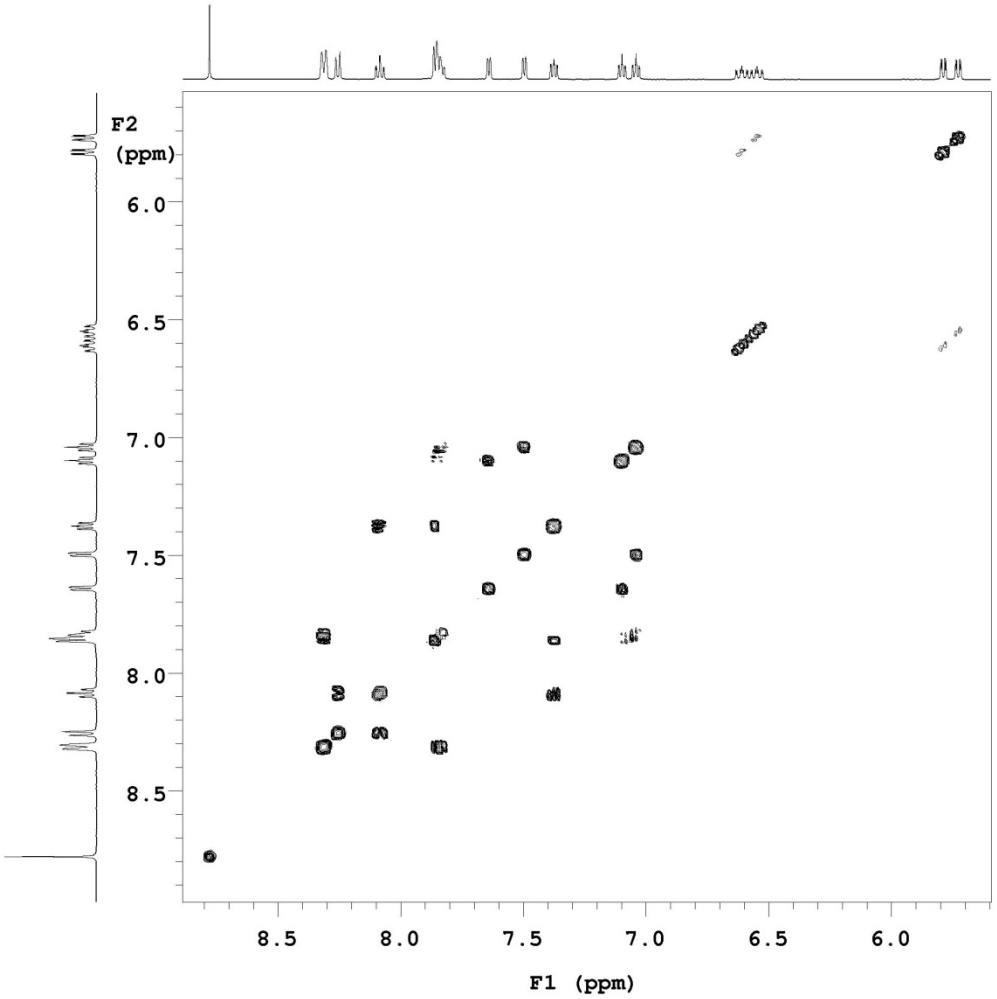

Figure S28. gCOSY of **6b** in CD_2Cl_2

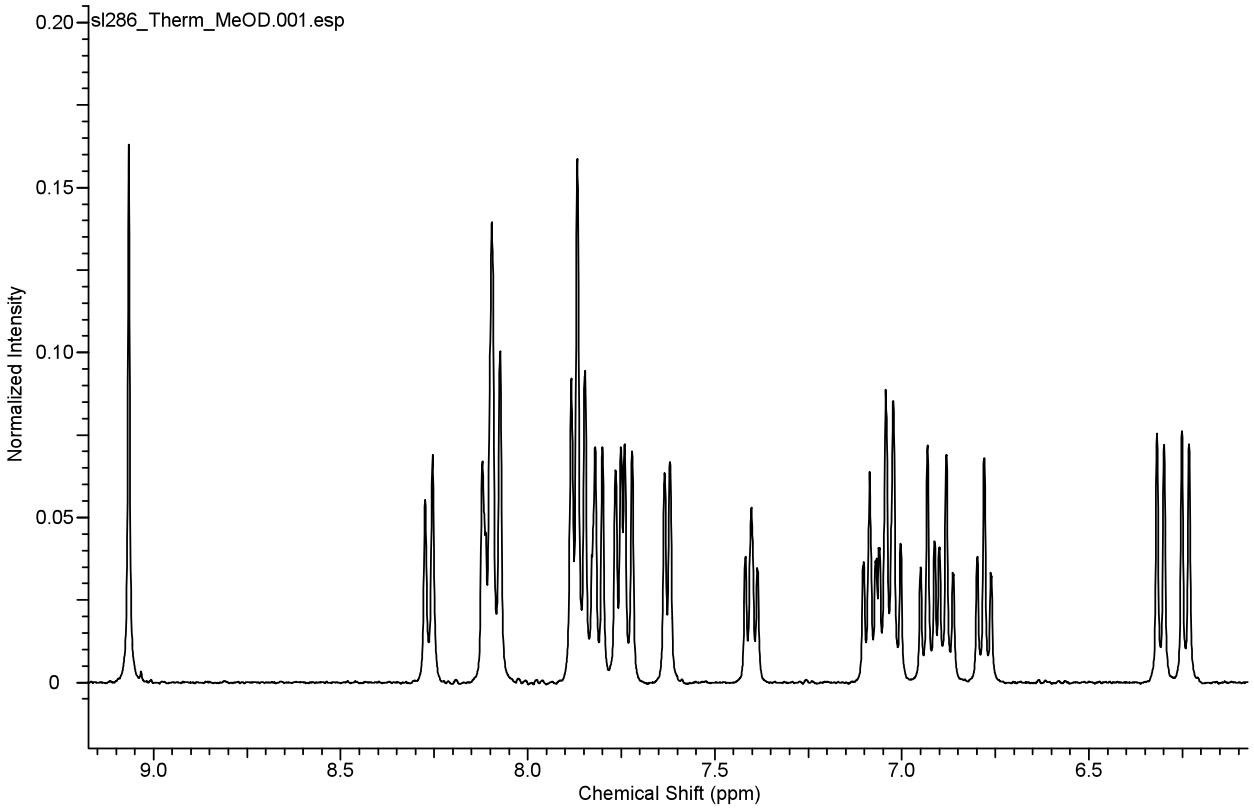

Figure S29. ^{1}H NMR of **7a** in CD_3OD

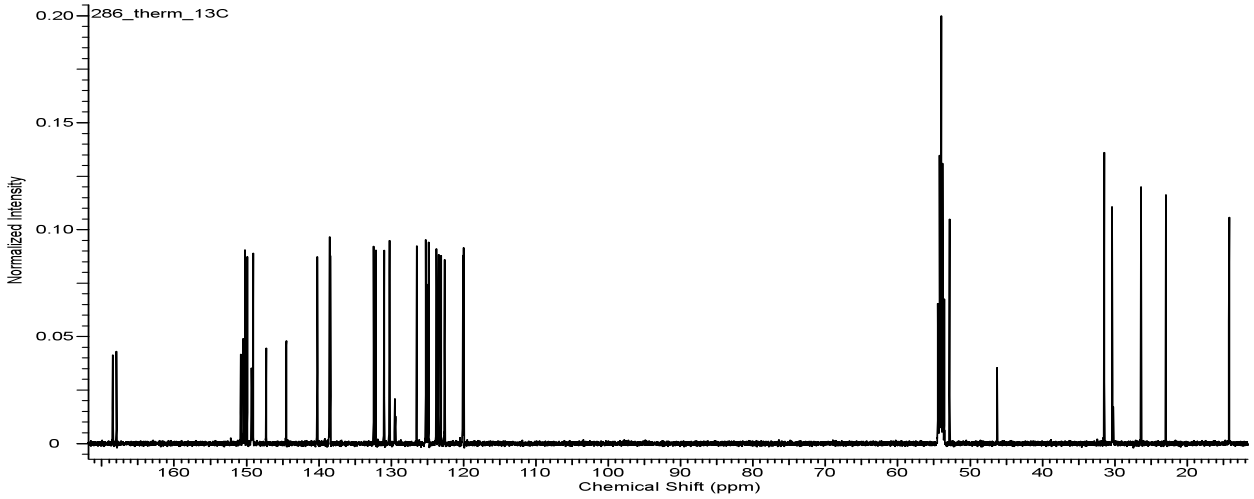

Figure S30. ^{13}C NMR of **7a** in CD_2Cl_2

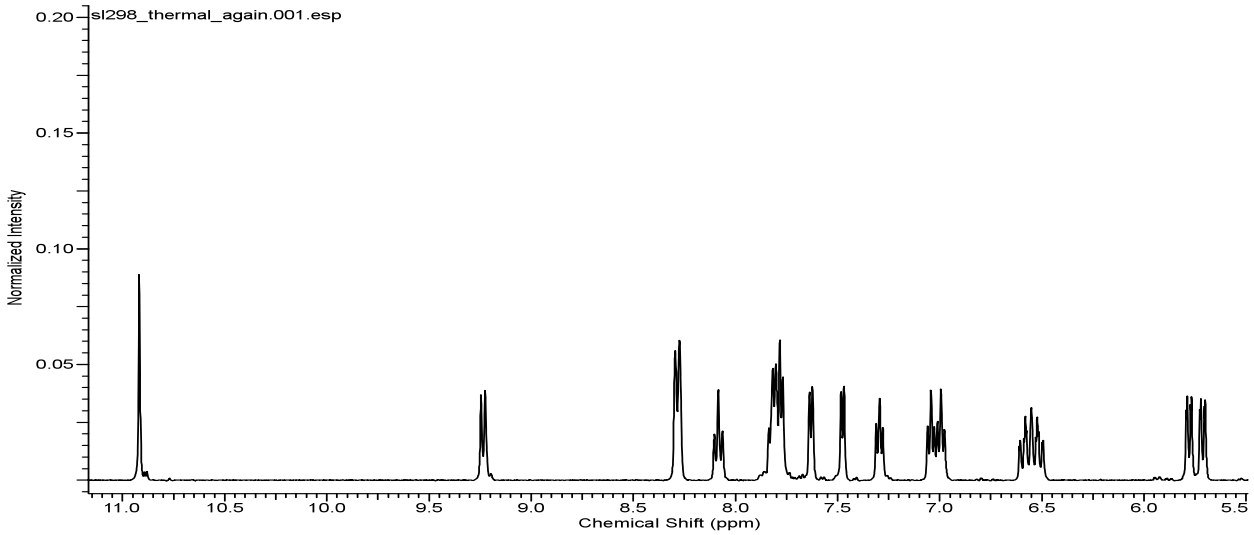

Figure S31. ^{1}H NMR of **7b** in CD_2Cl_2

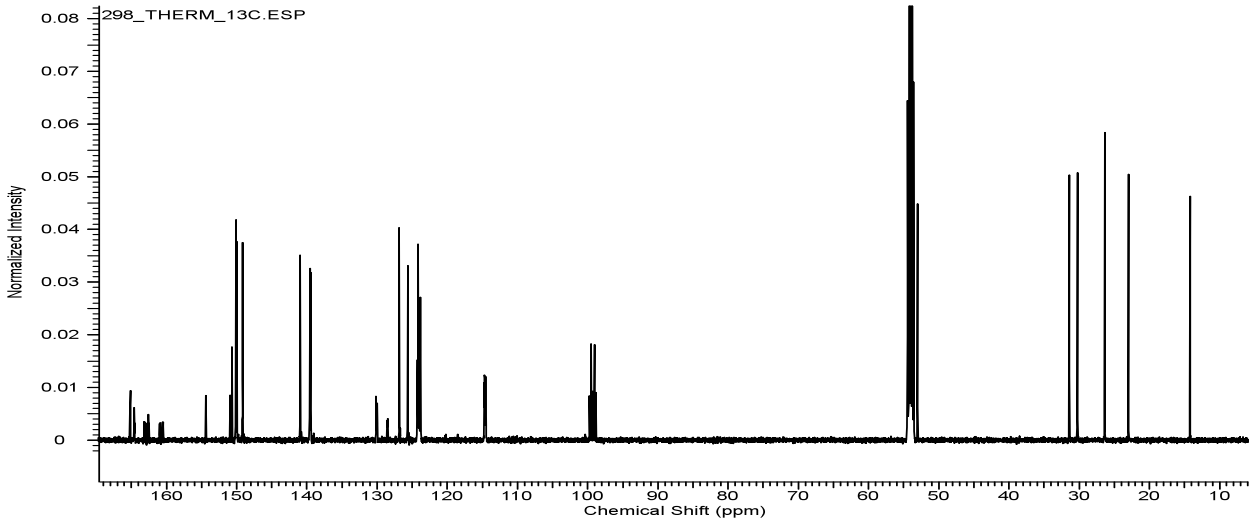

Figure S32. ^{13}C NMR of **7b** in CD_2Cl_2

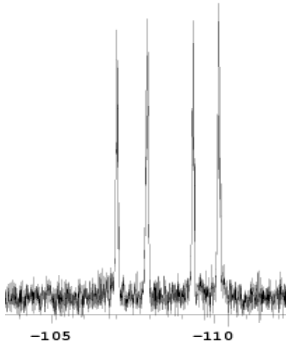

Figure S33. ^{19}F NMR of **7b** in CD_2Cl_2