Imidazolyl-Phenyl (IMP) Anions: A Modular Structure for Tuning Solubility and Coordinating Ability.

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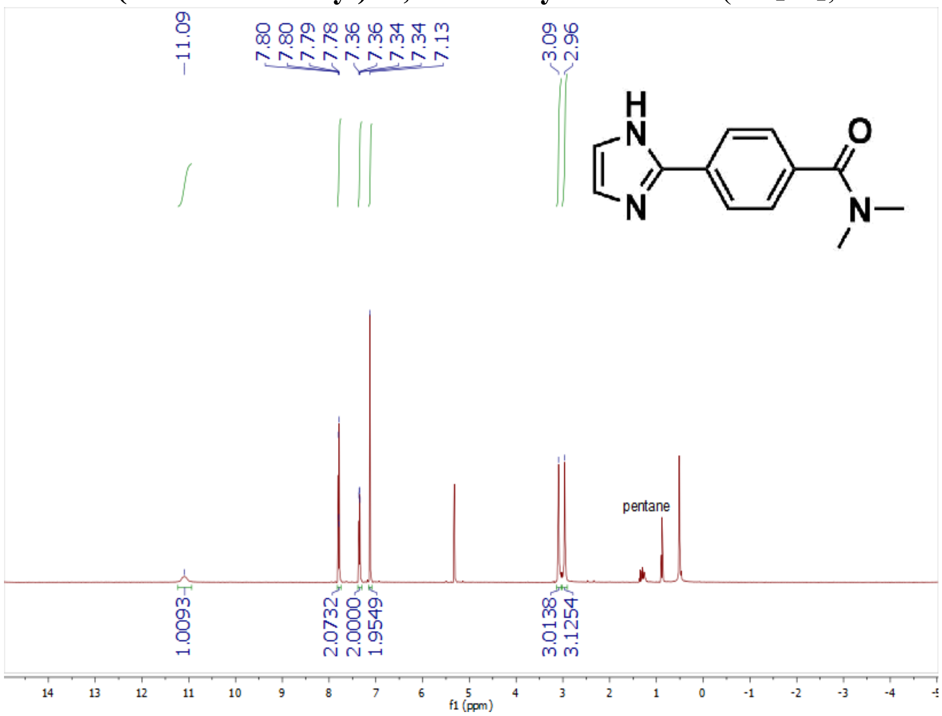
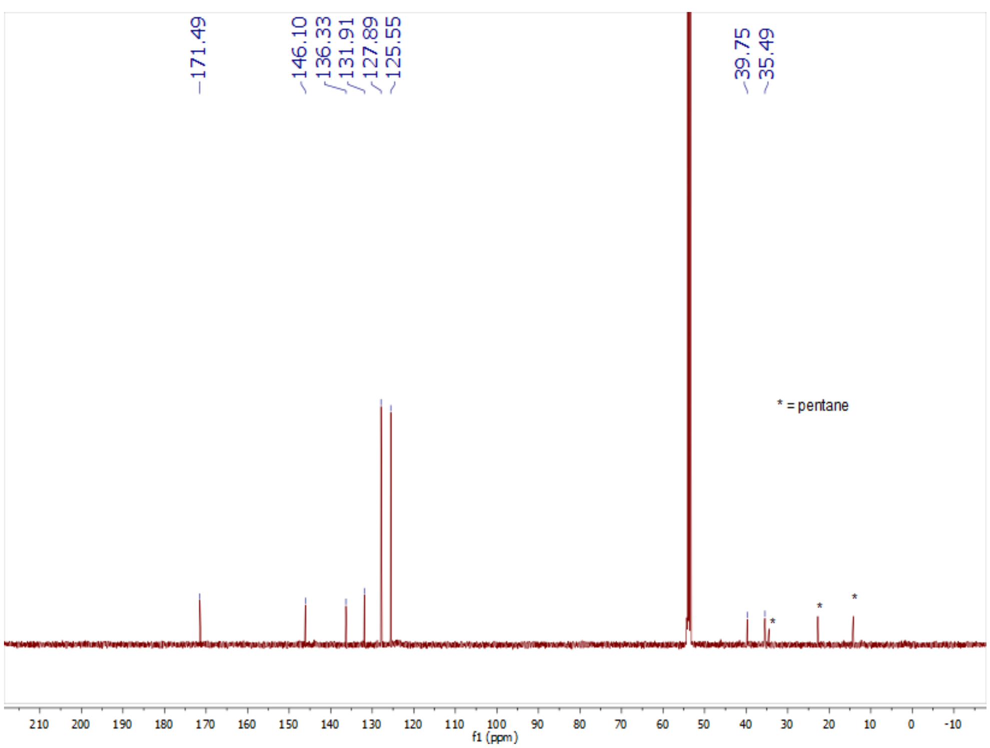
I. NMR Spectra

Impurities present in the following spectra were assigned based on literature precedent.[1]

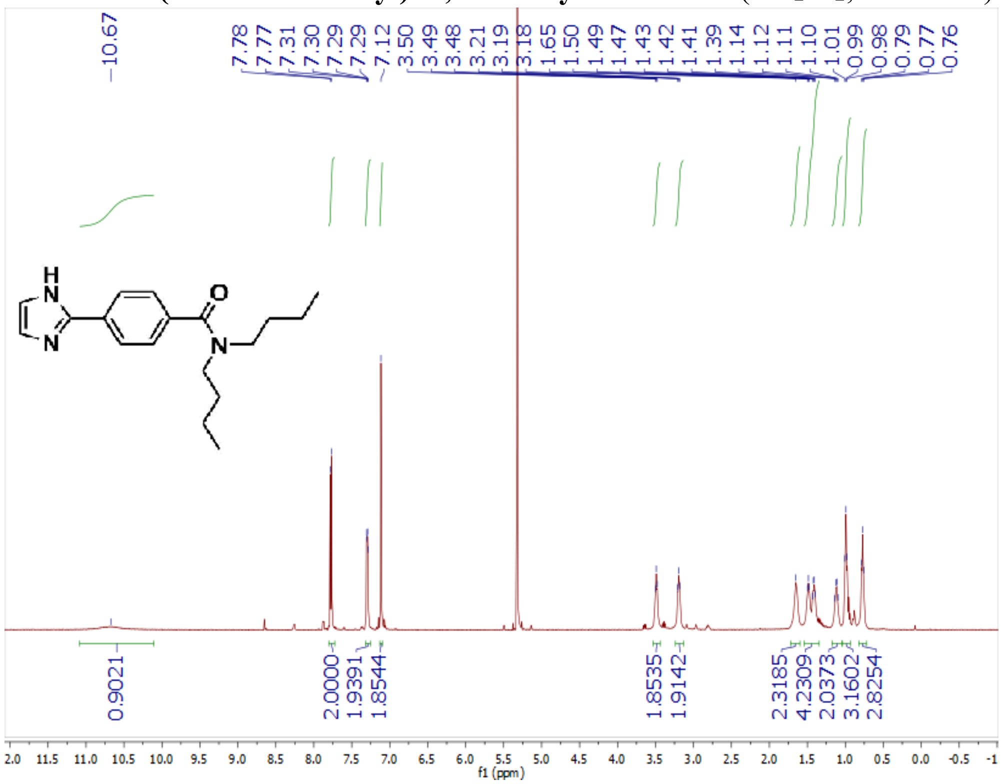
^{1}H NMR **4-(1H-imidazol-2-yl)-N,N-dimethylbenzamide** (CD_2Cl_2, 500 MHz)



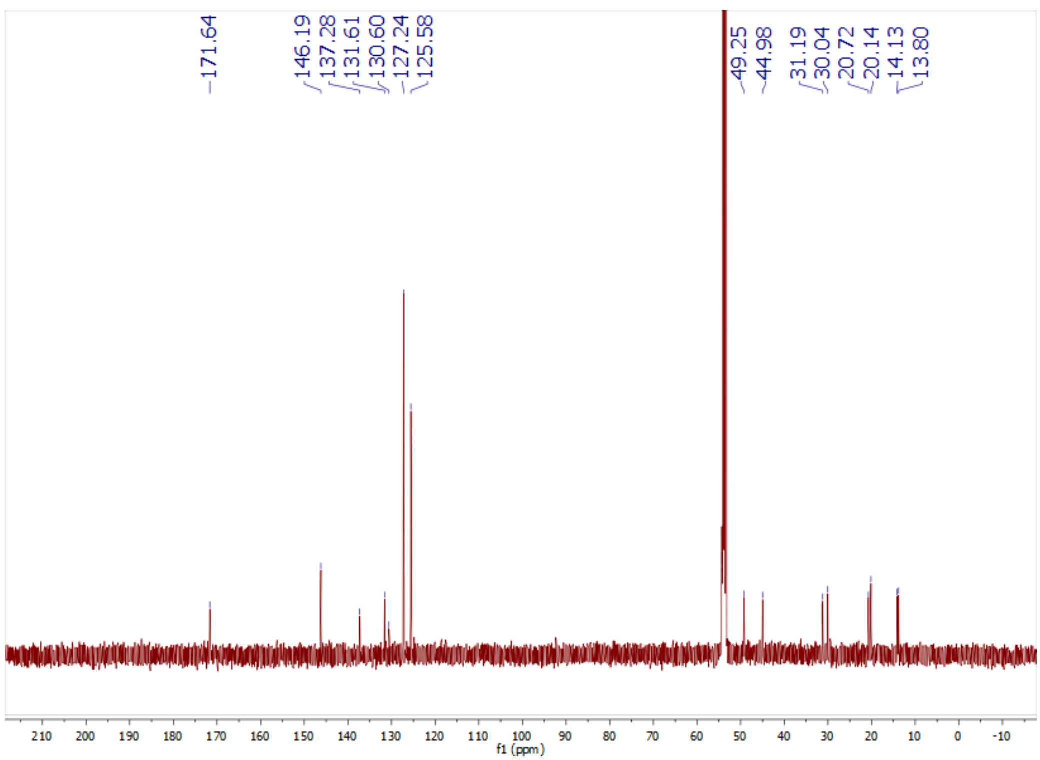
^{13}C NMR **4-(1H-imidazol-2-yl)-N,N-dimethylbenzamide** (CD_2Cl_2, 126 MHz)



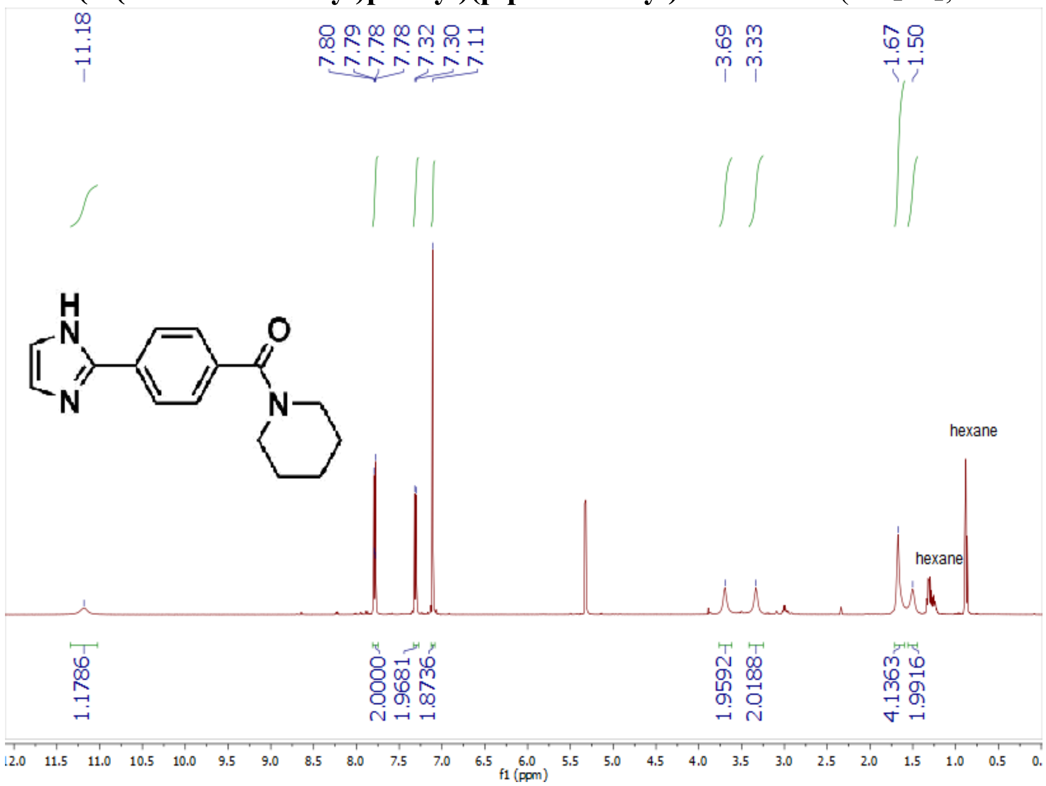
[1]H NMR **4-(1H-imidazol-2-yl)-N,N-dibutylbenzamide** (CD_2Cl_2, 500 MHz)



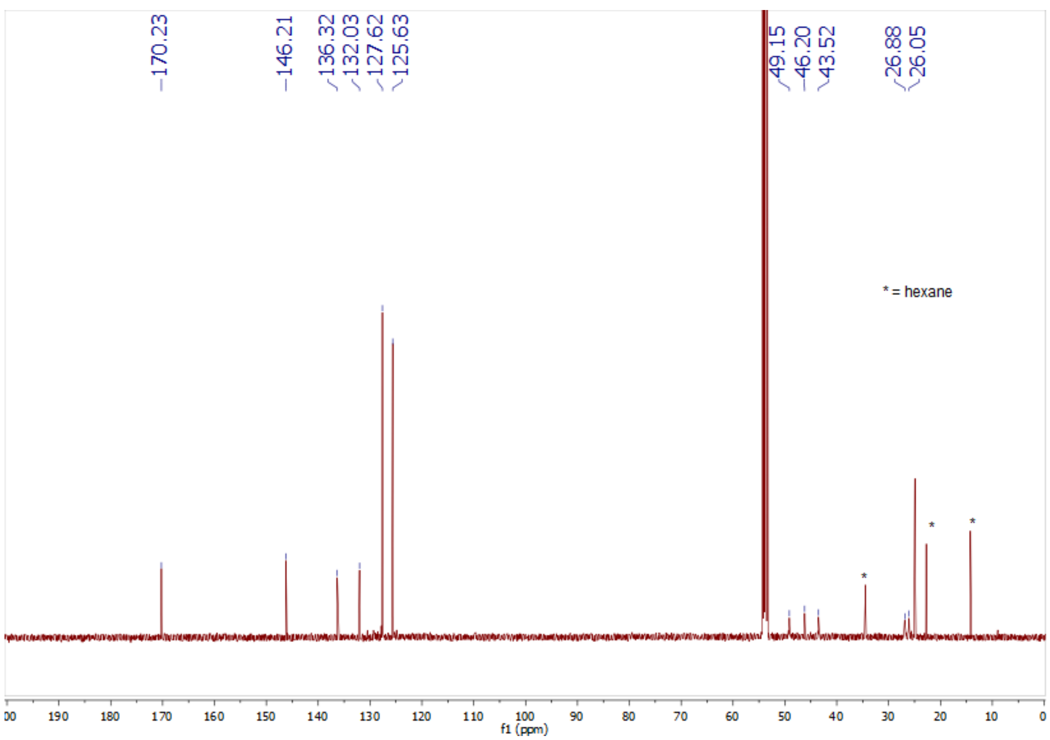
[13]C NMR **4-(1H-imidazol-2-yl)-N,N-dibutylbenzamide** (CD_2Cl_2, 126 MHz)



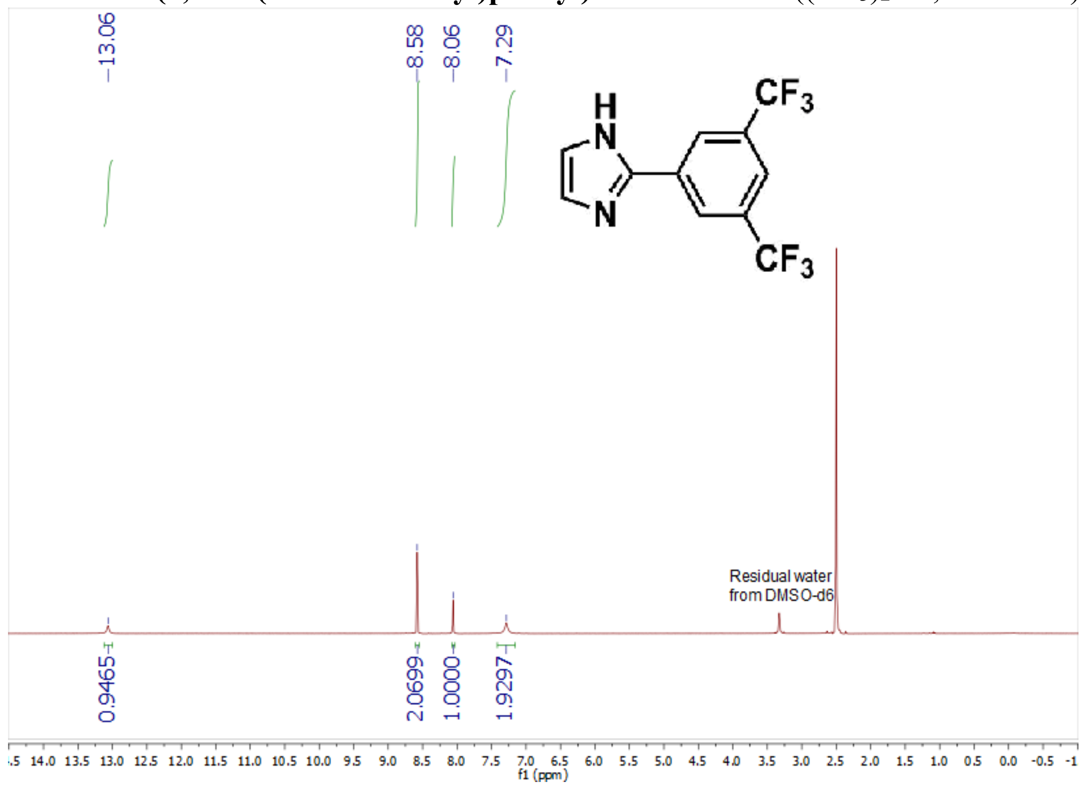
^{1}H NMR **(4-(1H-imidazol-2-yl)phenyl)(piperidin-1-yl)methanone** (CD_2Cl_2, 500 MHz)



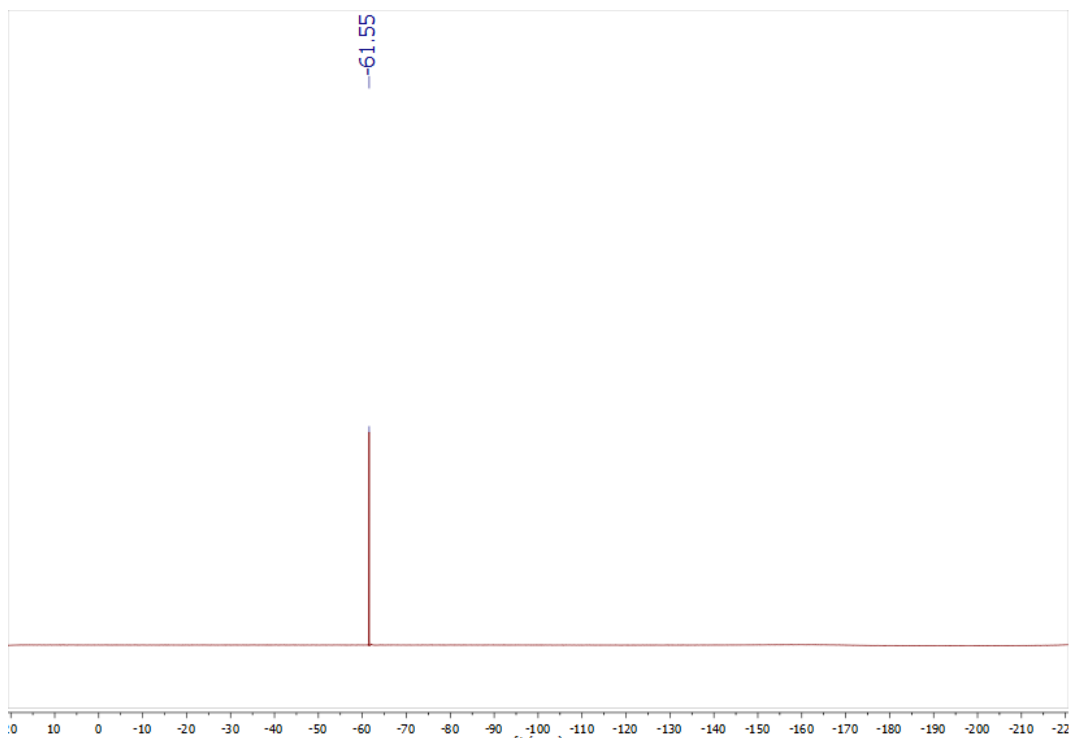
^{13}C NMR **(4-(1H-imidazol-2-yl)phenyl)(piperidin-1-yl)methanone** (CD_2Cl_2, 126 MHz)



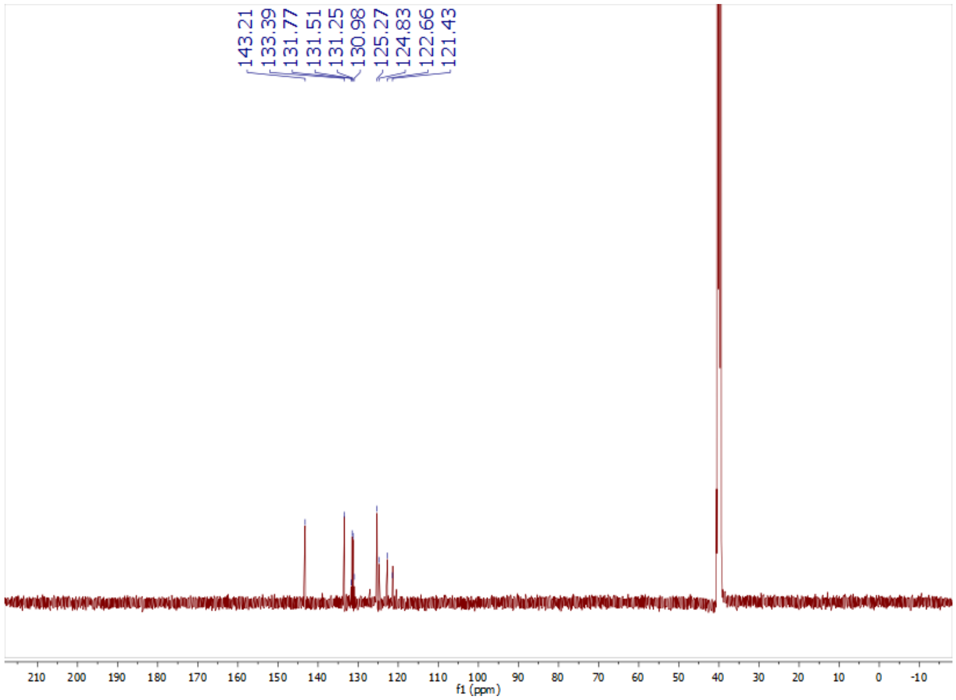
^{1}H NMR **2-(3,5-bis(trifluoromethyl)phenyl)-1H-imidazole** ($(CD_3)_2SO$, 500 MHz)



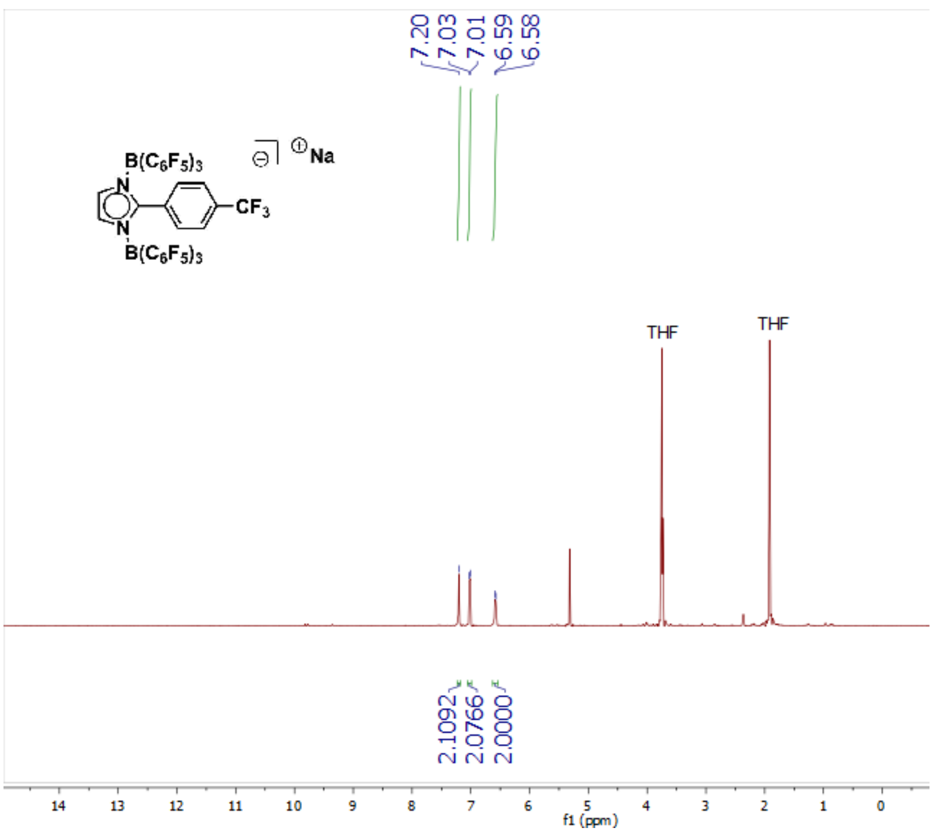
^{19}F NMR **2-(3,5-bis(trifluoromethyl)phenyl)-1H-imidazole** ($(CD_3)_2SO$, 471 MHz)



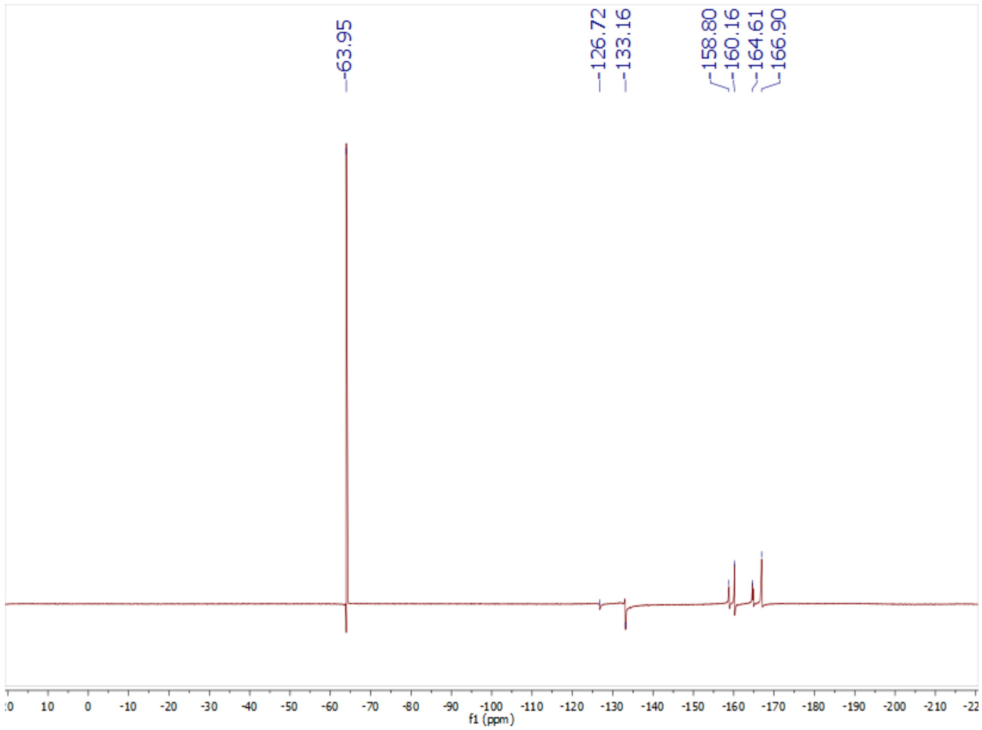
^{13}C NMR **2-(3,5-bis(trifluoromethyl)phenyl)-1H-imidazole** ($(CD_3)_2SO$, 126 MHz)



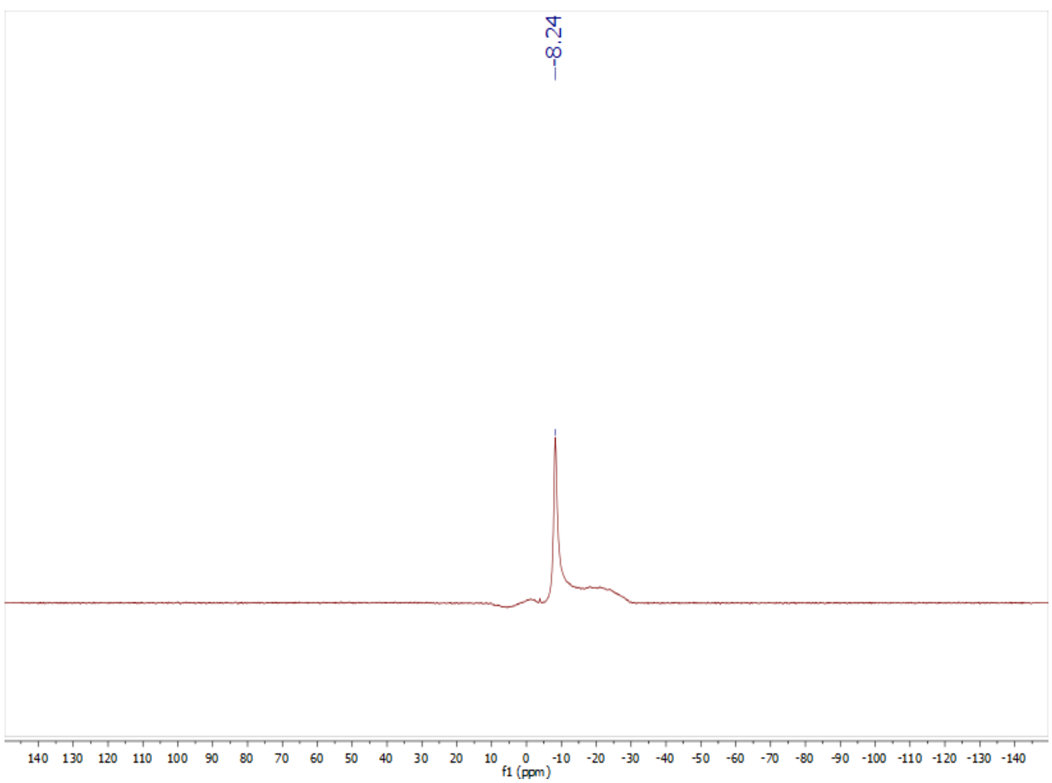
^{1}H NMR **Na[IMP-CF$_3$]** (CD_2Cl_2, 500 MHz)



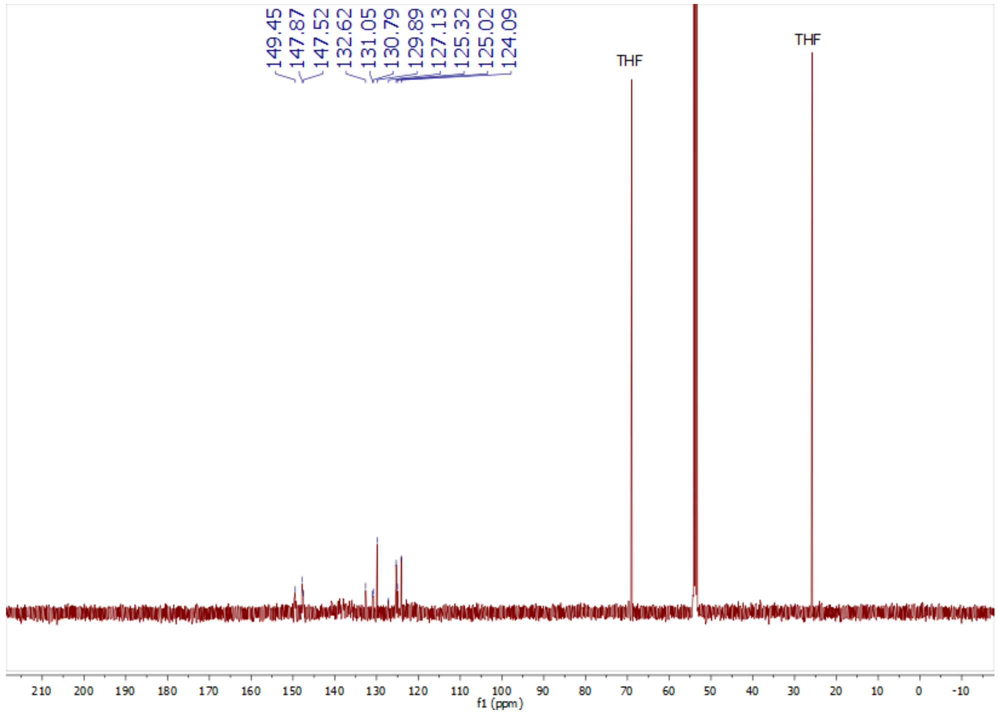
^{19}F NMR **Na[IMP-CF$_3$]** (CD_2Cl_2, 471 MHz)



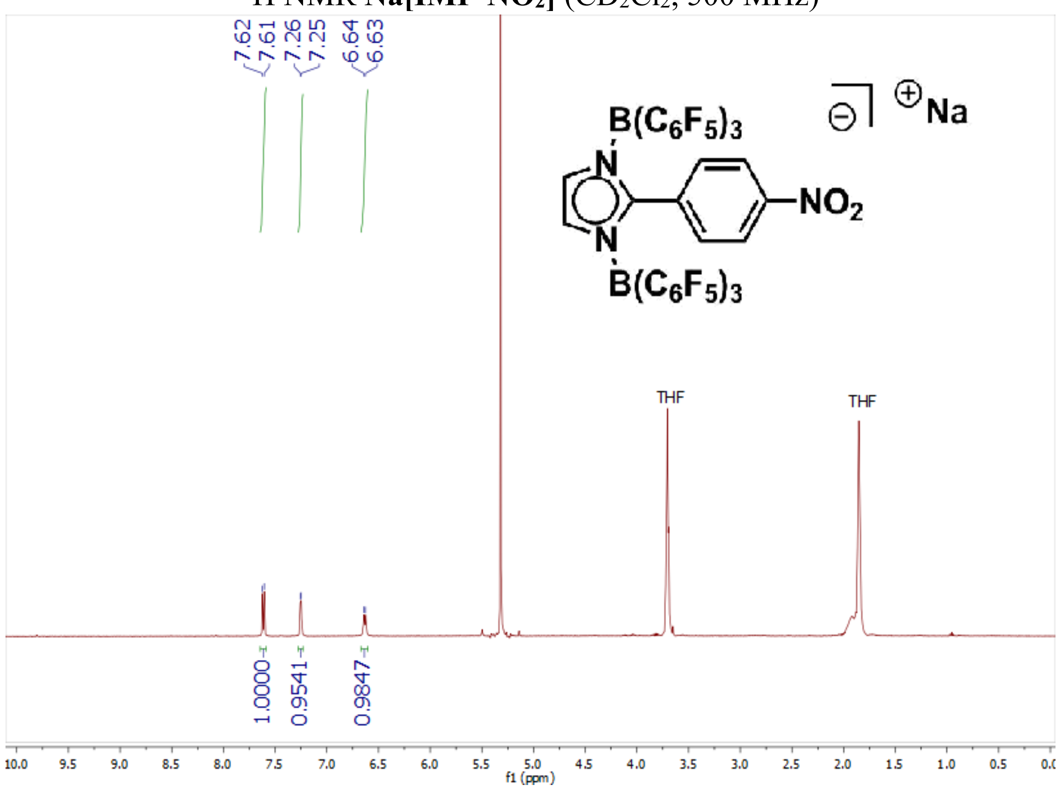
^{11}B NMR **Na[IMP-CF$_3$]** (CD_2Cl_2, 161 MHz)



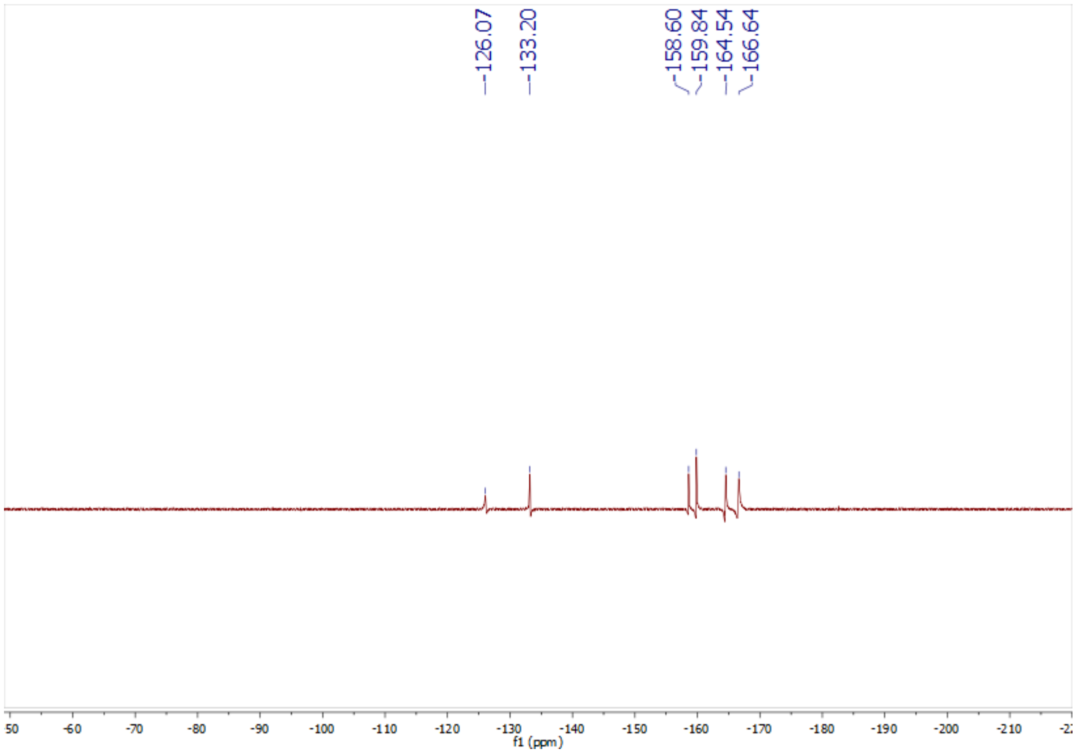
^{13}C NMR **Na[IMP-CF$_3$]** (CD_2Cl_2, 126 MHz)



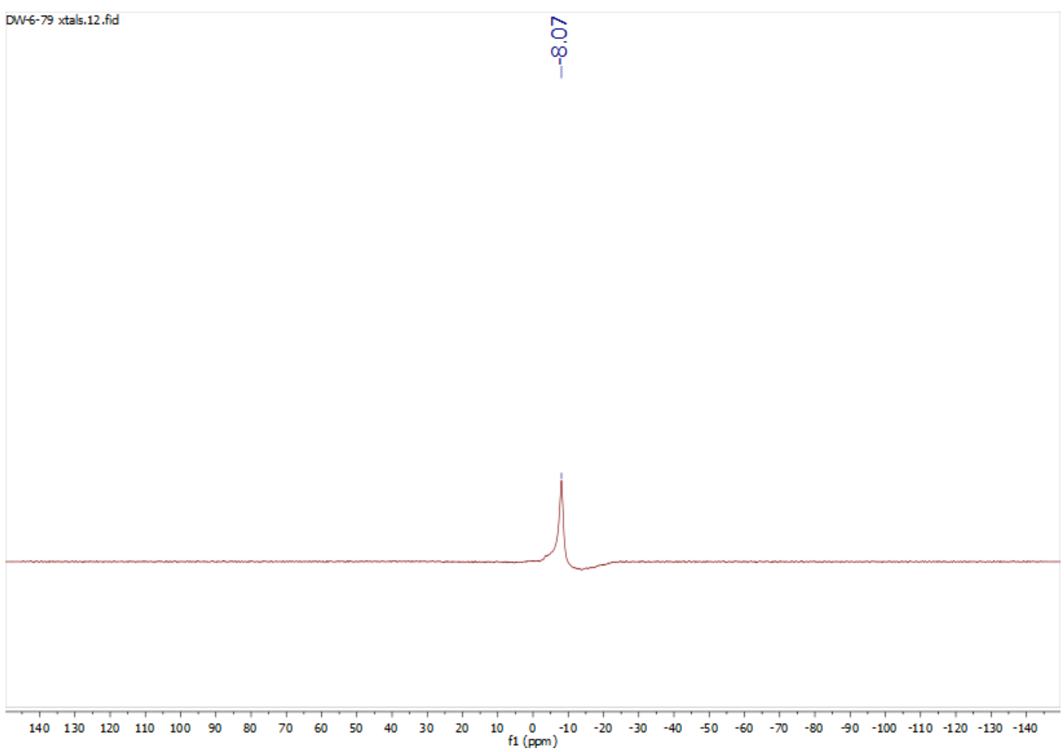
^{1}H NMR **Na[IMP-NO$_2$]** (CD_2Cl_2, 500 MHz)



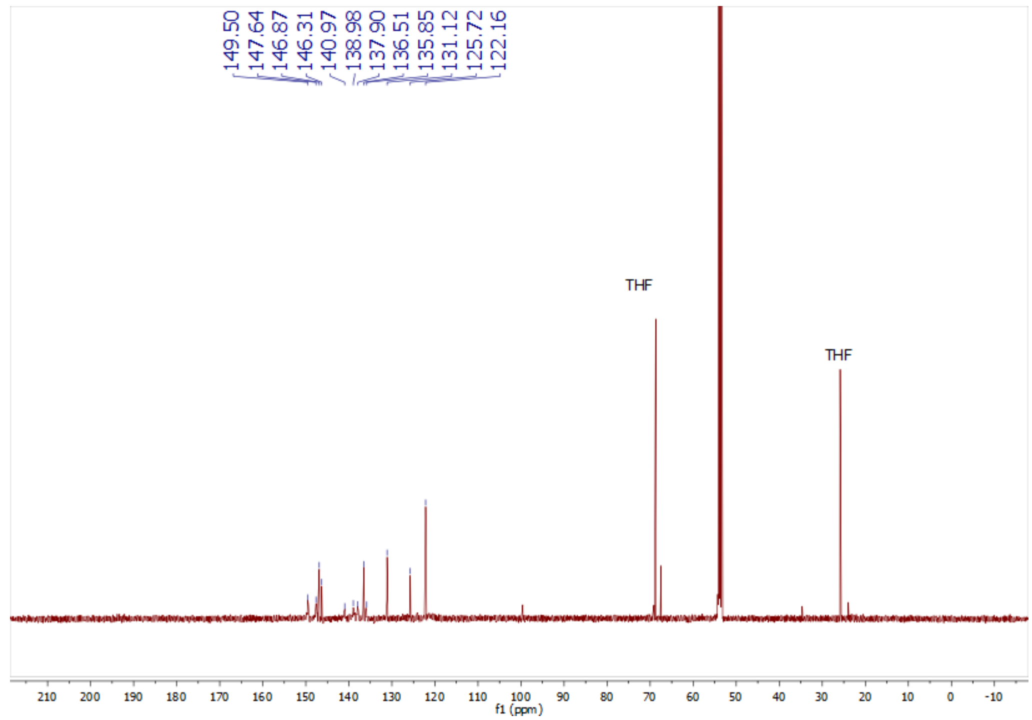
^{19}F NMR **Na[IMP-NO$_2$]** (CD_2Cl_2, 471 MHz)



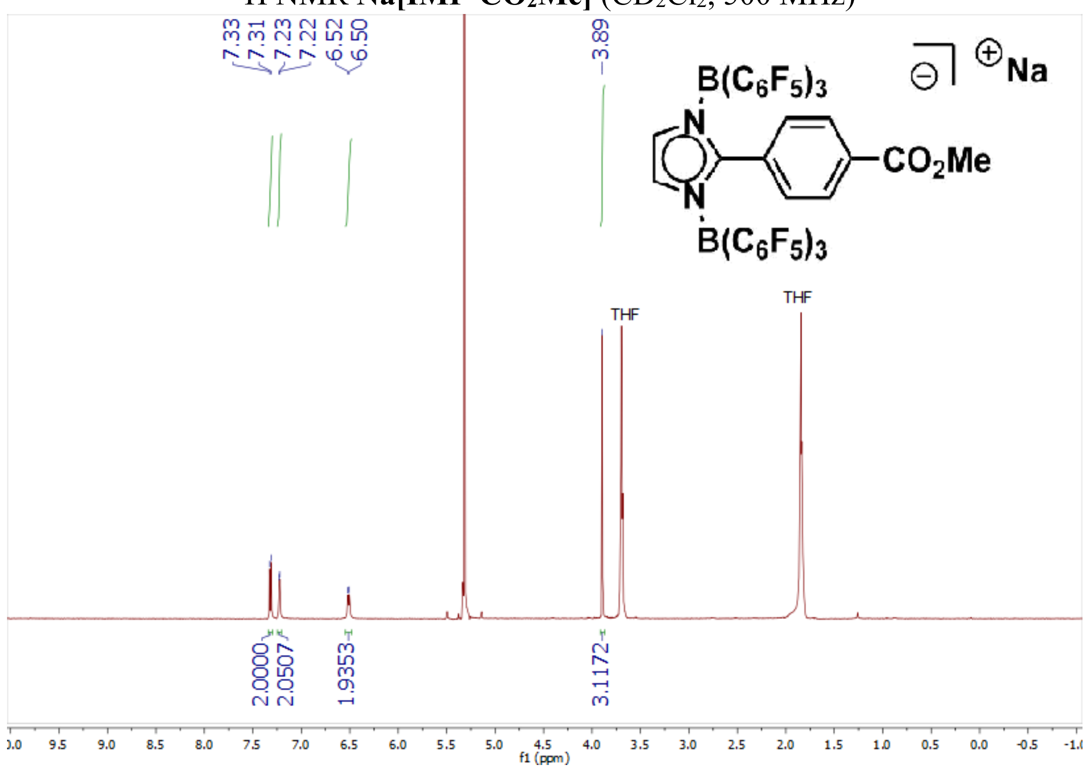
^{11}B NMR **Na[IMP-NO$_2$]** (CD_2Cl_2, 161 MHz)



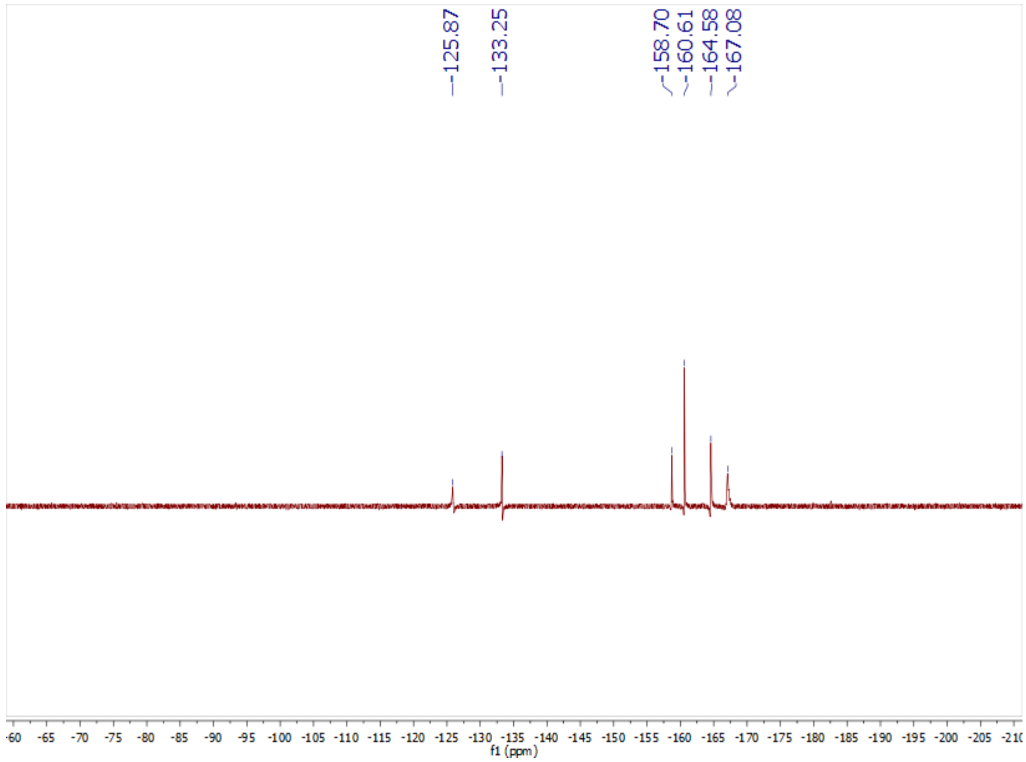
^{13}C NMR **Na[IMP-NO$_2$]** (CD_2Cl_2, 126 MHz)



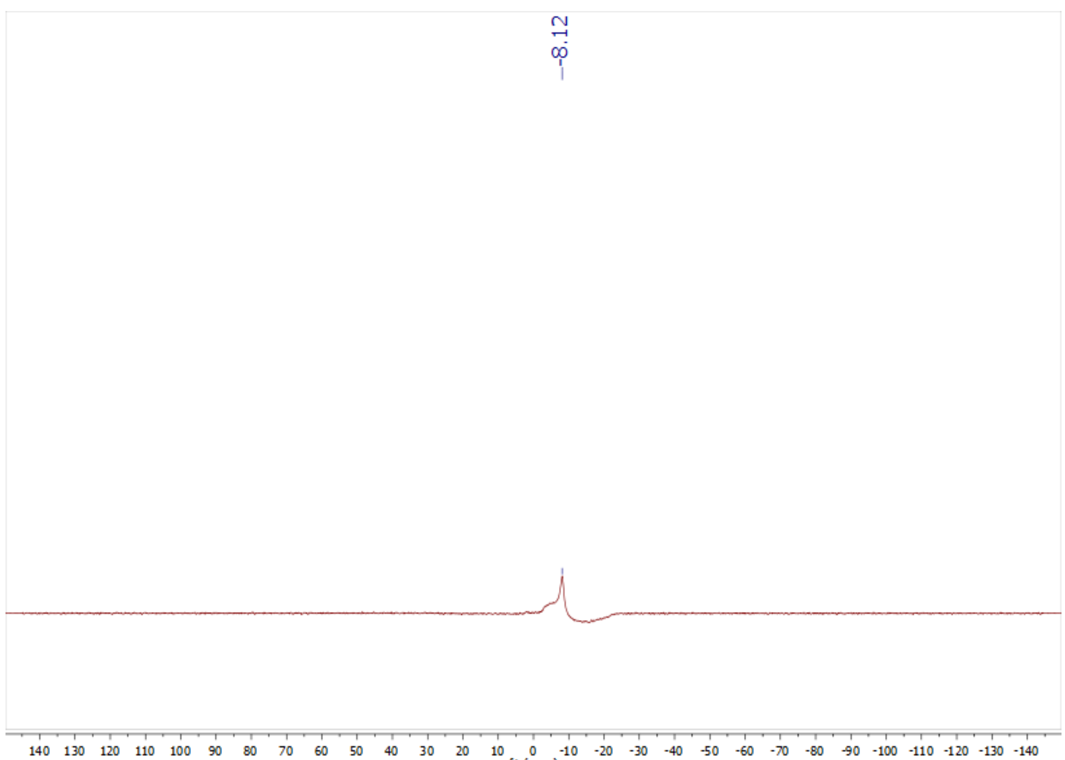
^{1}H NMR **Na[IMP-CO$_2$Me]** (CD_2Cl_2, 500 MHz)



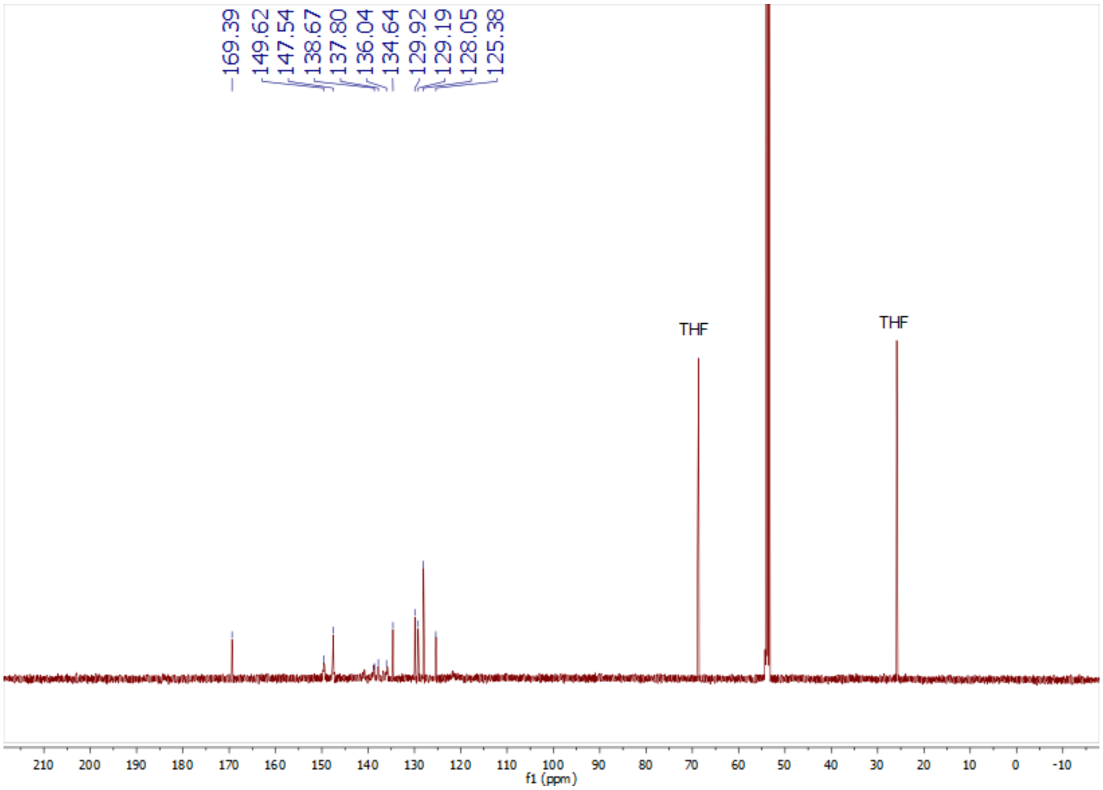
^{19}F NMR **Na[IMP-CO$_2$Me]** (CD_2Cl_2, 471 MHz)



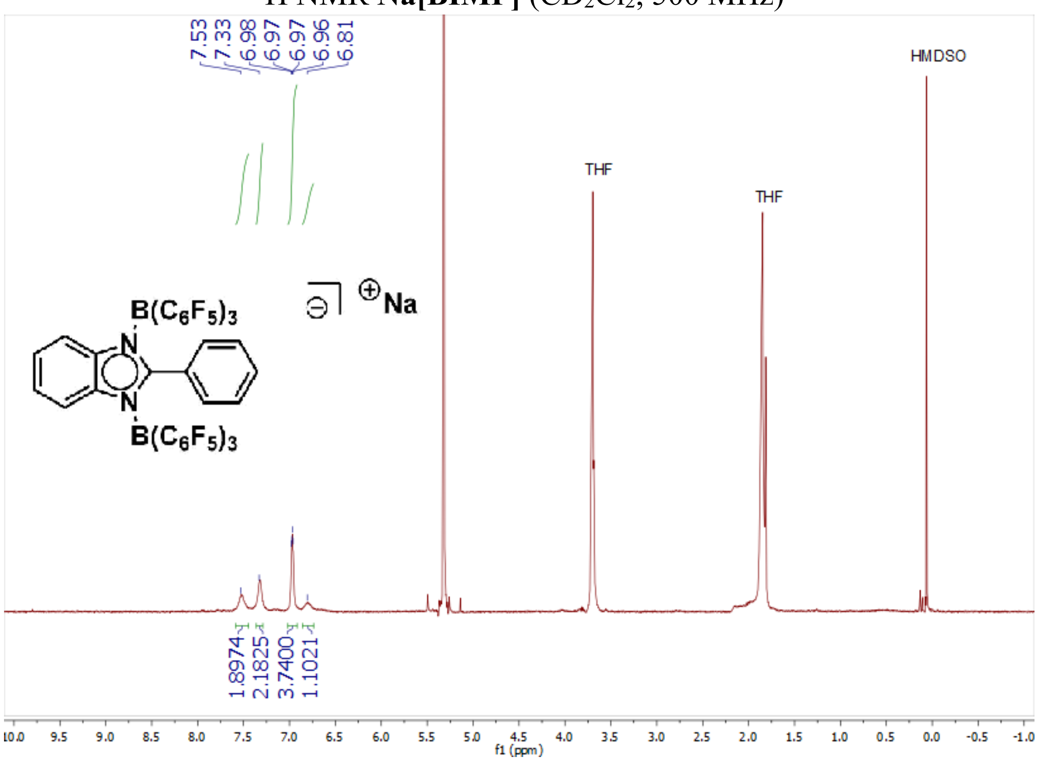
^{11}B NMR **Na[IMP-CO$_2$Me]** (CD_2Cl_2, 161 MHz)



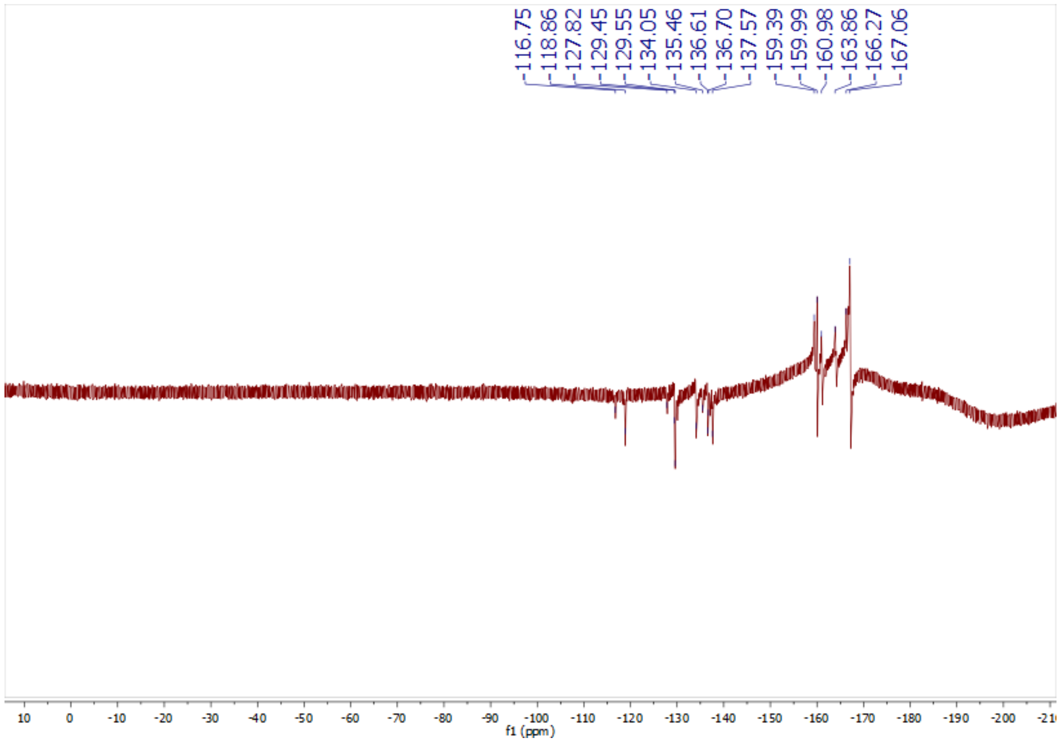
^{13}C NMR **Na[IMP-CO$_2$Me]** (CD_2Cl_2, 126 MHz)



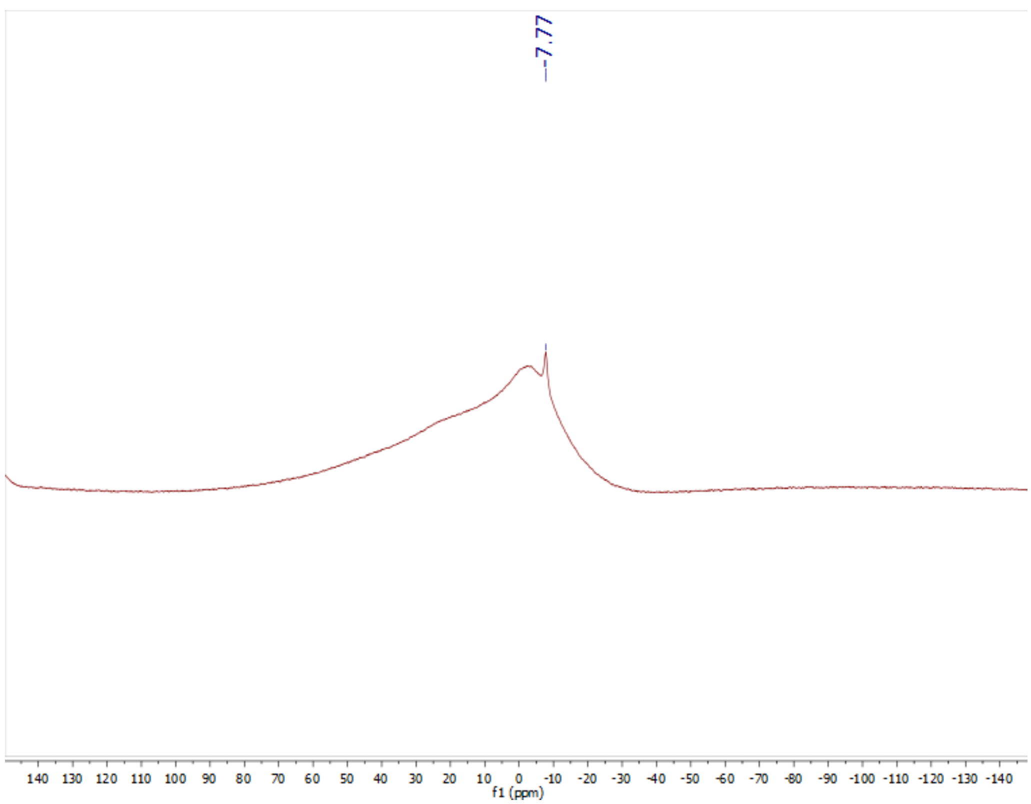
^{1}H NMR **Na[BIMP]** (CD_2Cl_2, 500 MHz)



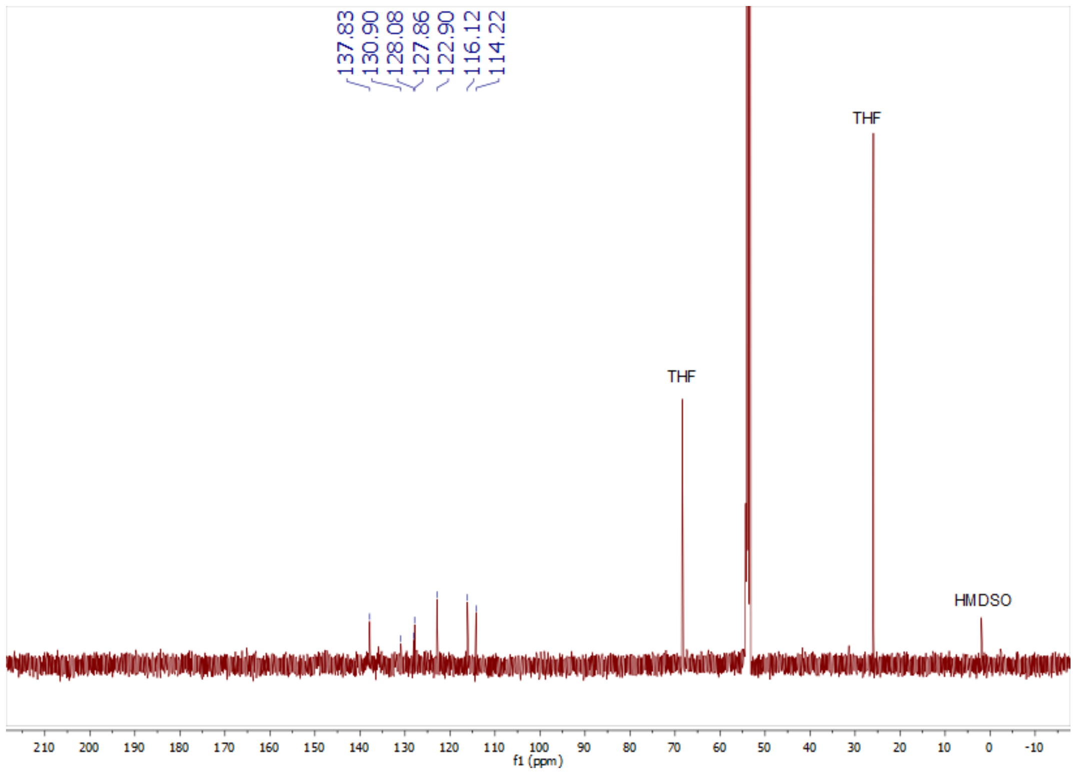
^{19}F NMR **Na[BIMP]** (CD_2Cl_2, 471 MHz)



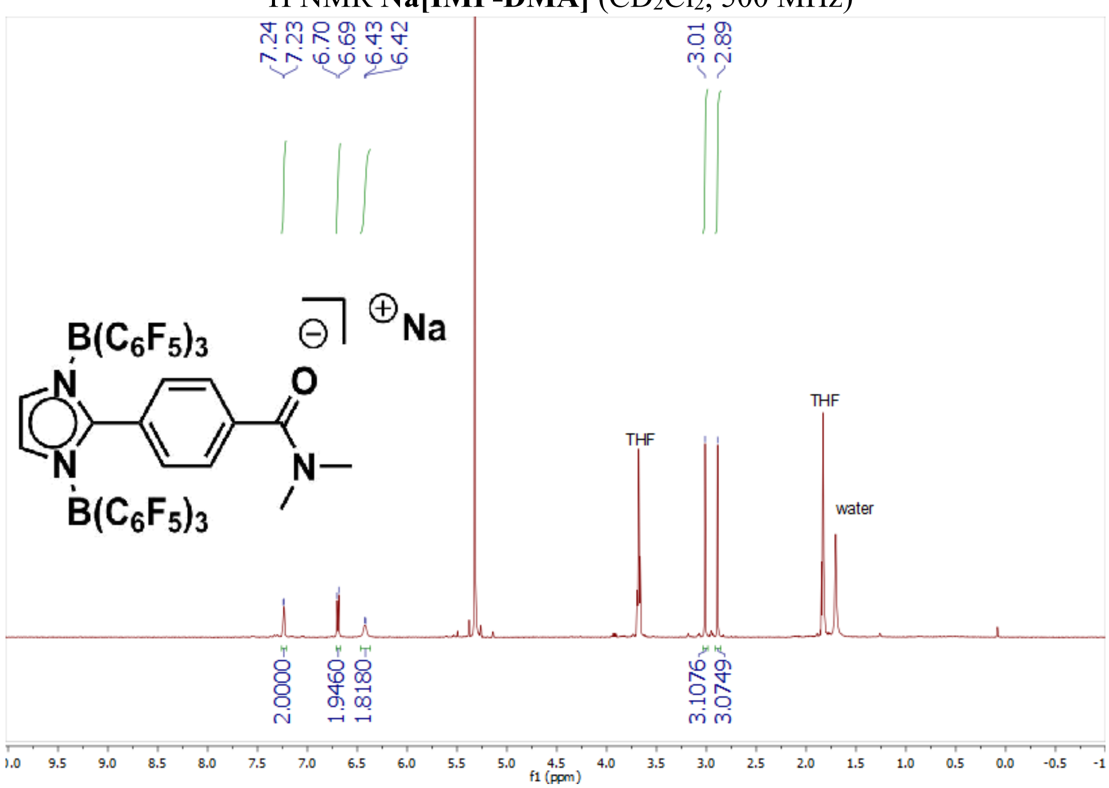
^{11}B NMR **Na[BIMP]** (CD_2Cl_2, 161 MHz)



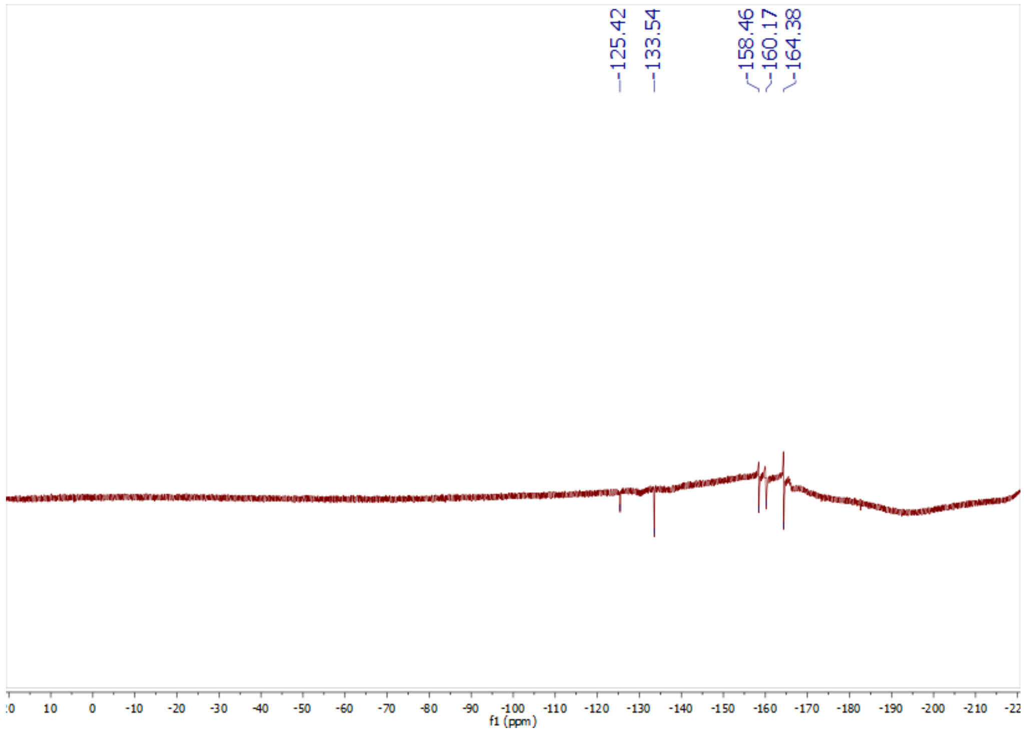
^{13}C NMR **Na[BIMP]** (CD_2Cl_2, 126 MHz)



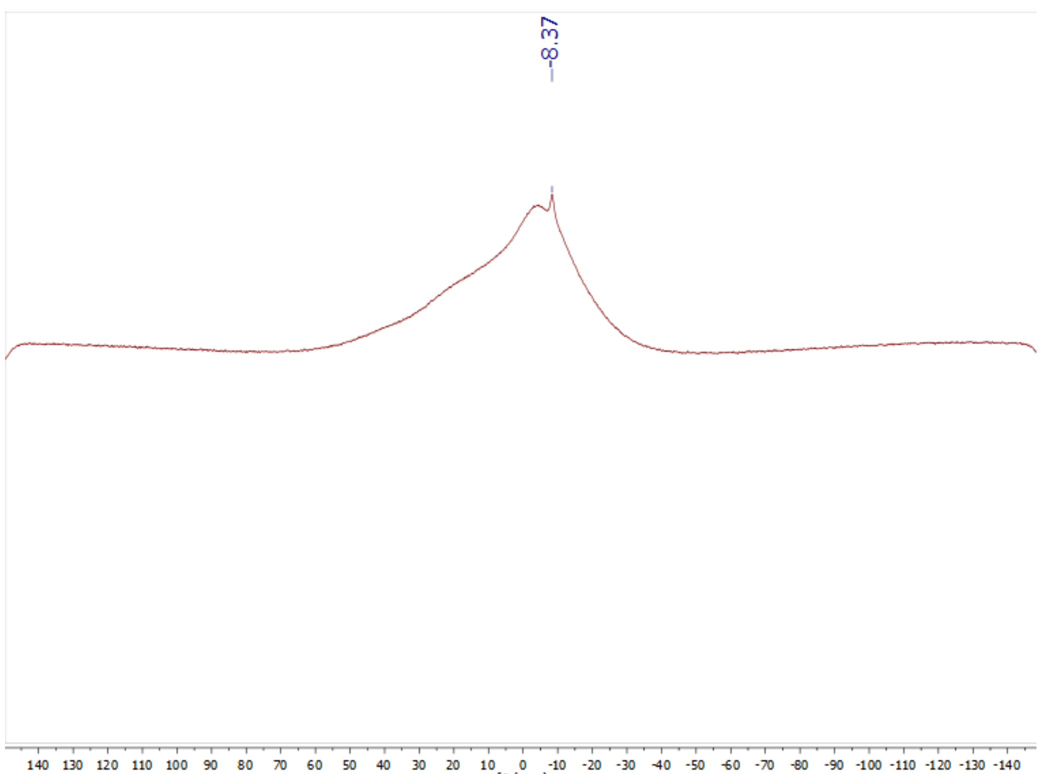
^{1}H NMR **Na[IMP-DMA]** (CD_2Cl_2, 500 MHz)



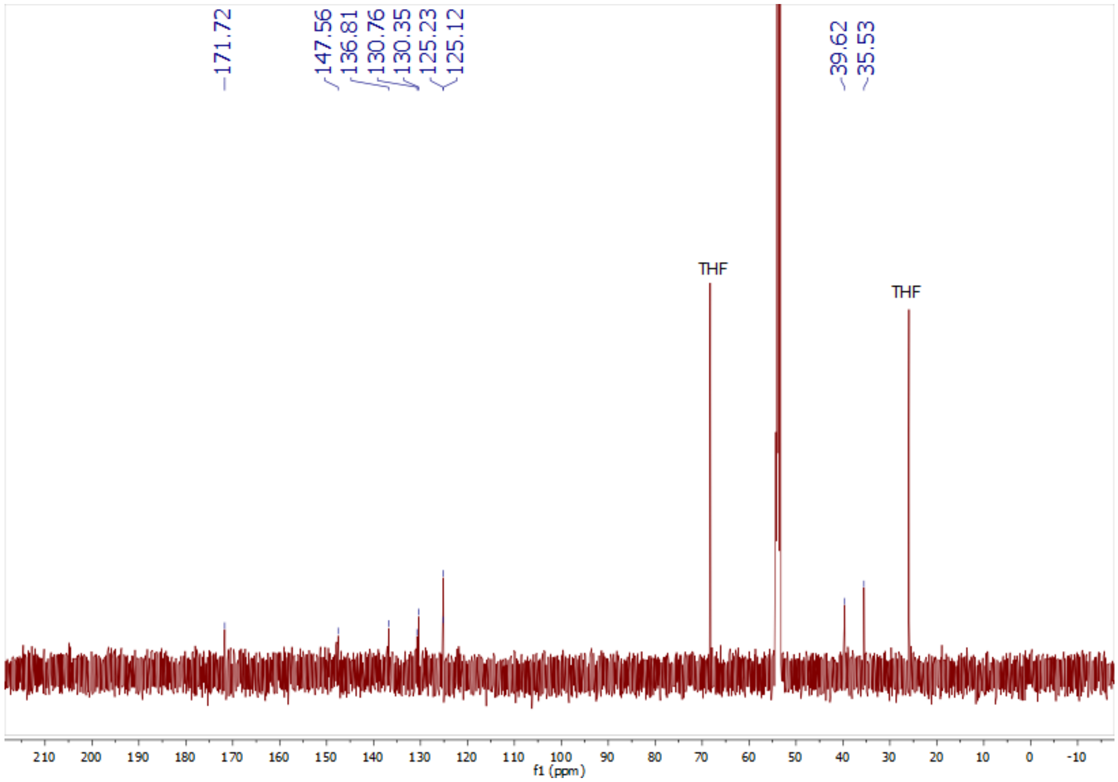
^{19}F NMR **Na[IMP-DMA]** (CD_2Cl_2, 471 MHz)



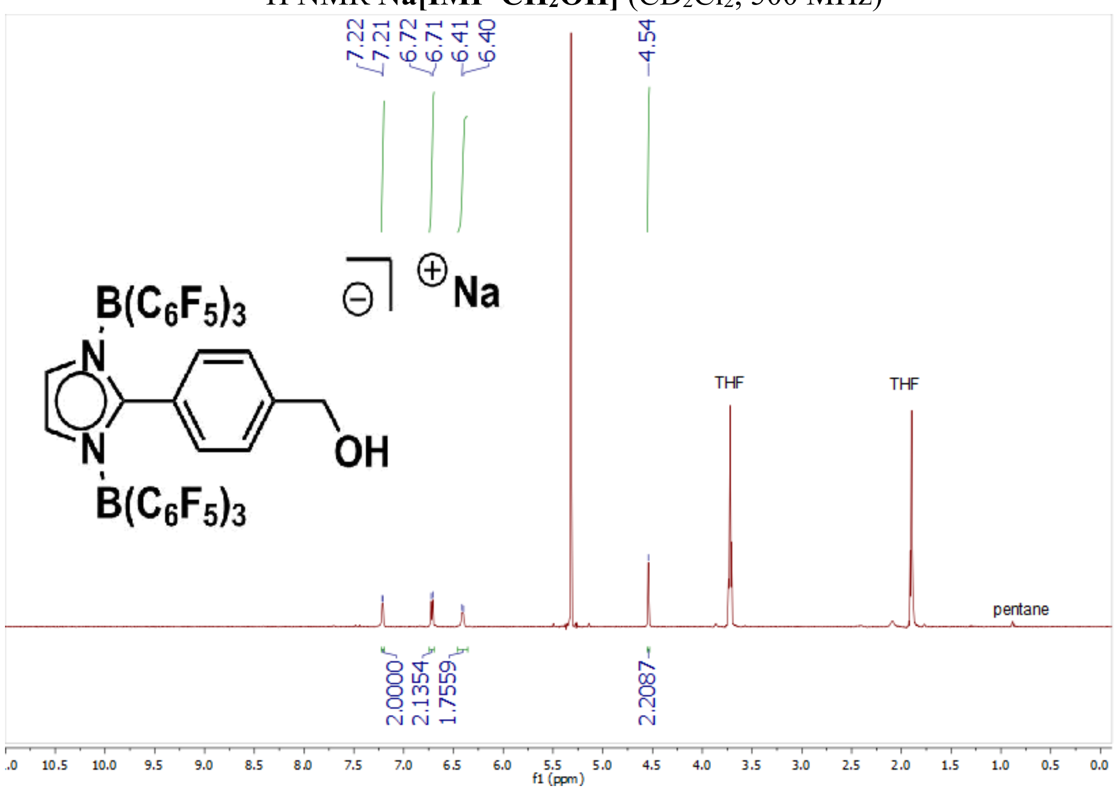
^{11}B NMR **Na[IMP-DMA]** (CD_2Cl_2, 161 MHz)



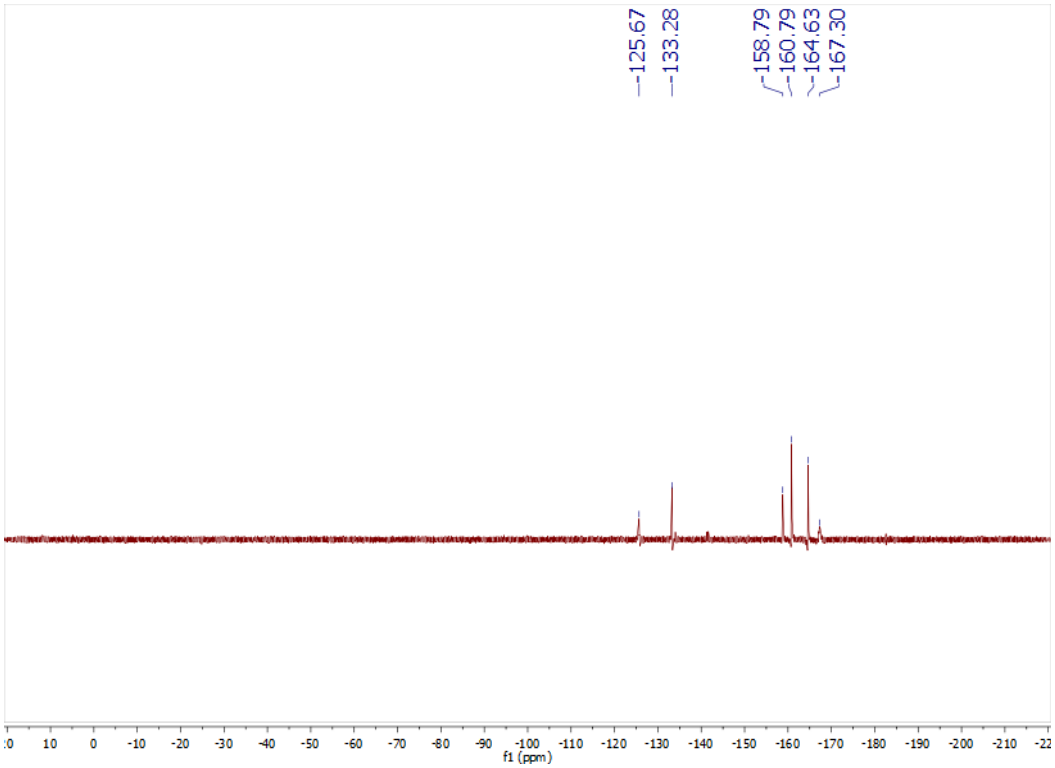
^{13}C NMR **Na[IMP-DMA]** (CD_2Cl_2, 126 MHz)



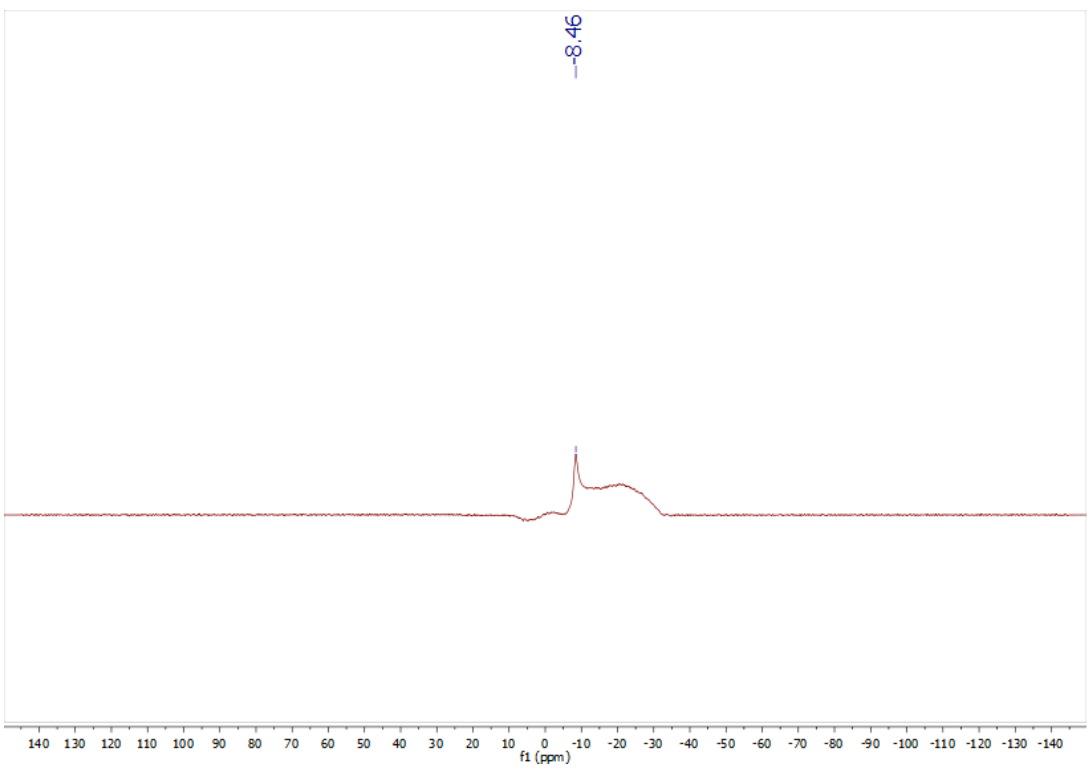
^{1}H NMR **Na[IMP-CH₂OH]** (CD_2Cl_2, 500 MHz)



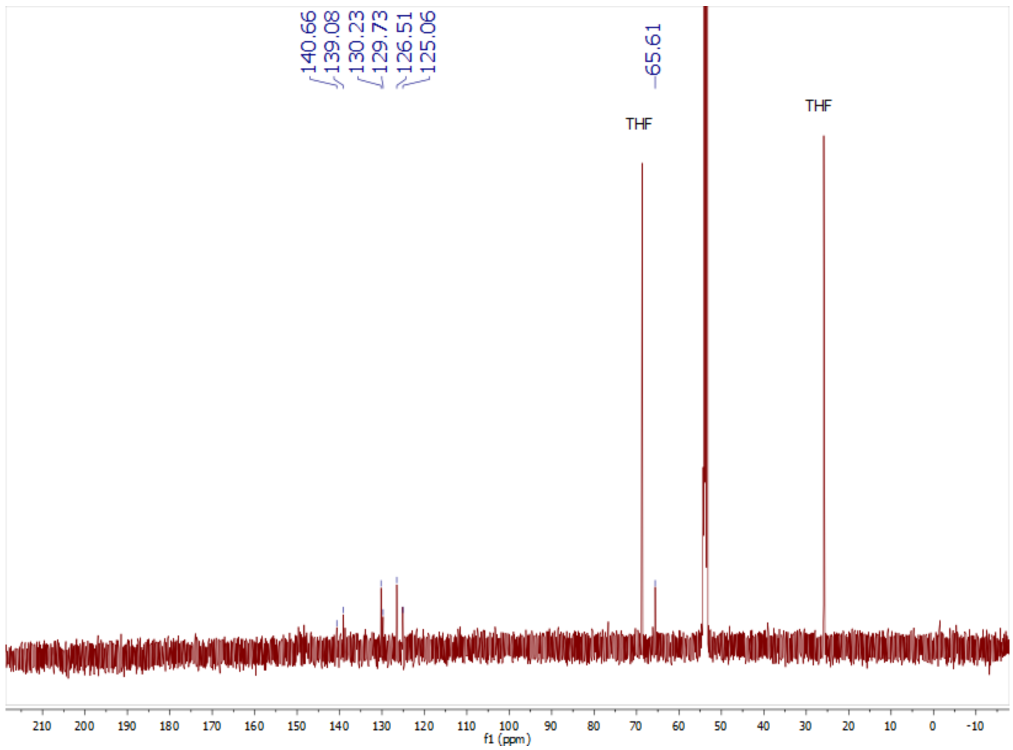
^{19}F NMR **Na[IMP-CH$_2$OH]** (CD_2Cl_2, 471 MHz)



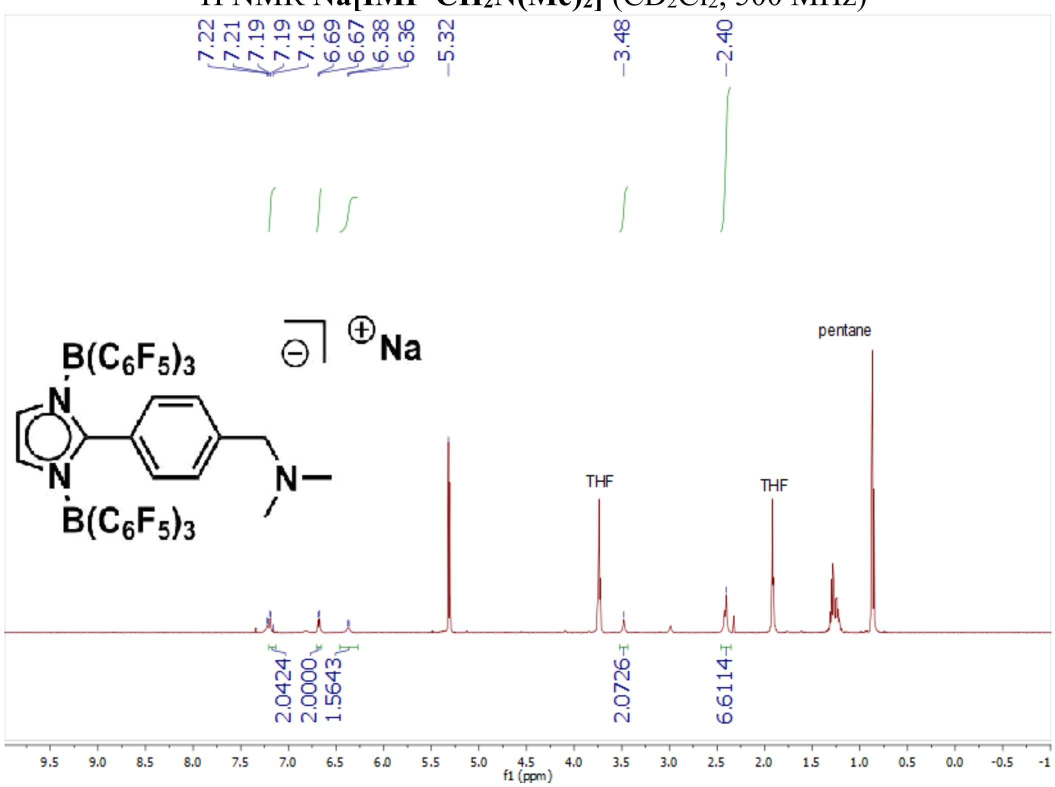
^{11}B NMR **Na[IMP-CH$_2$OH]** (CD_2Cl_2, 161 MHz)



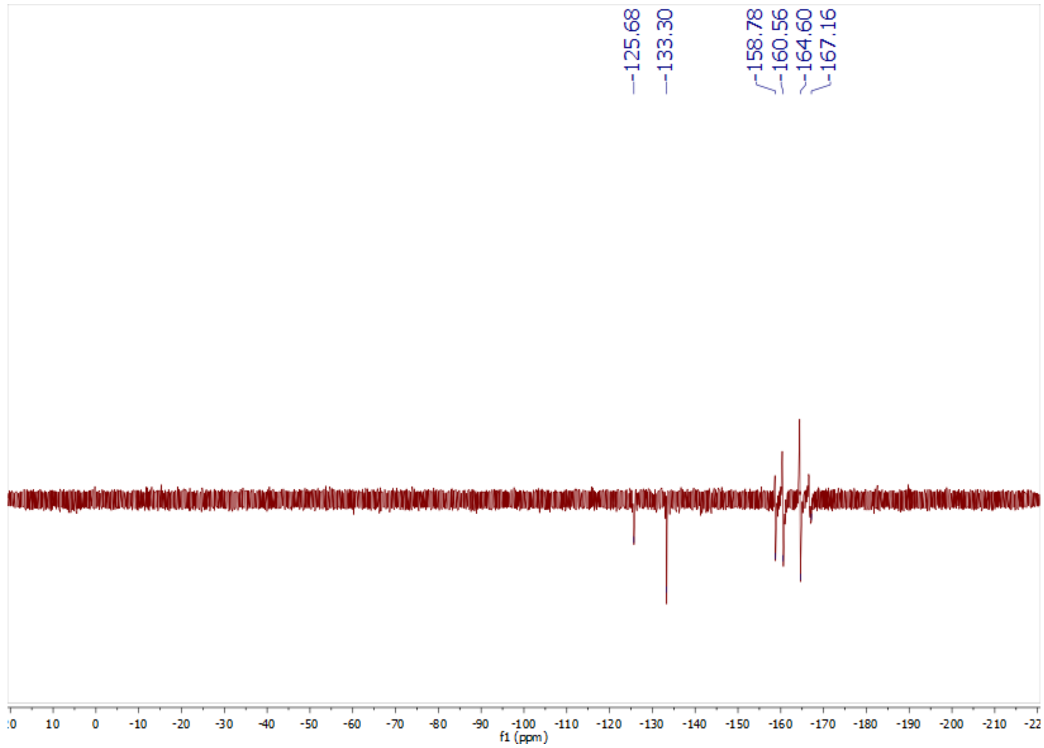
^{13}C NMR **Na[IMP-CH$_2$OH]** (CD$_2$Cl$_2$, 126 MHz)



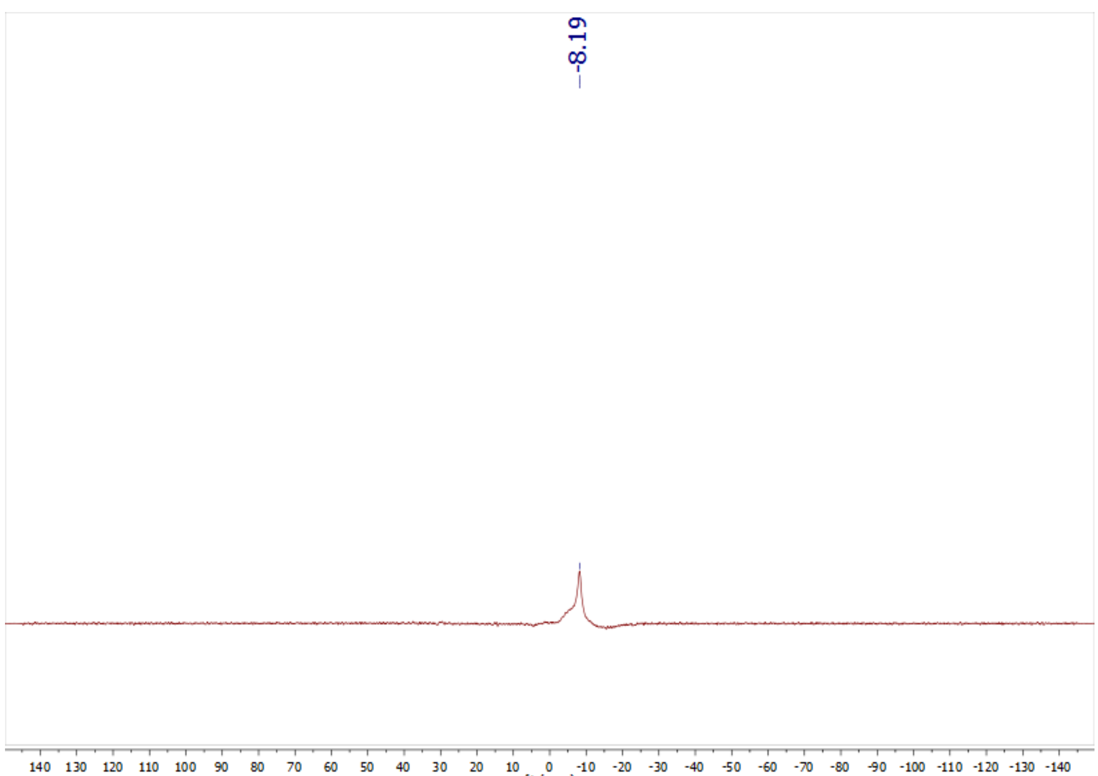
^{1}H NMR **Na[IMP-CH$_2$N(Me)$_2$]** (CD$_2$Cl$_2$, 500 MHz)



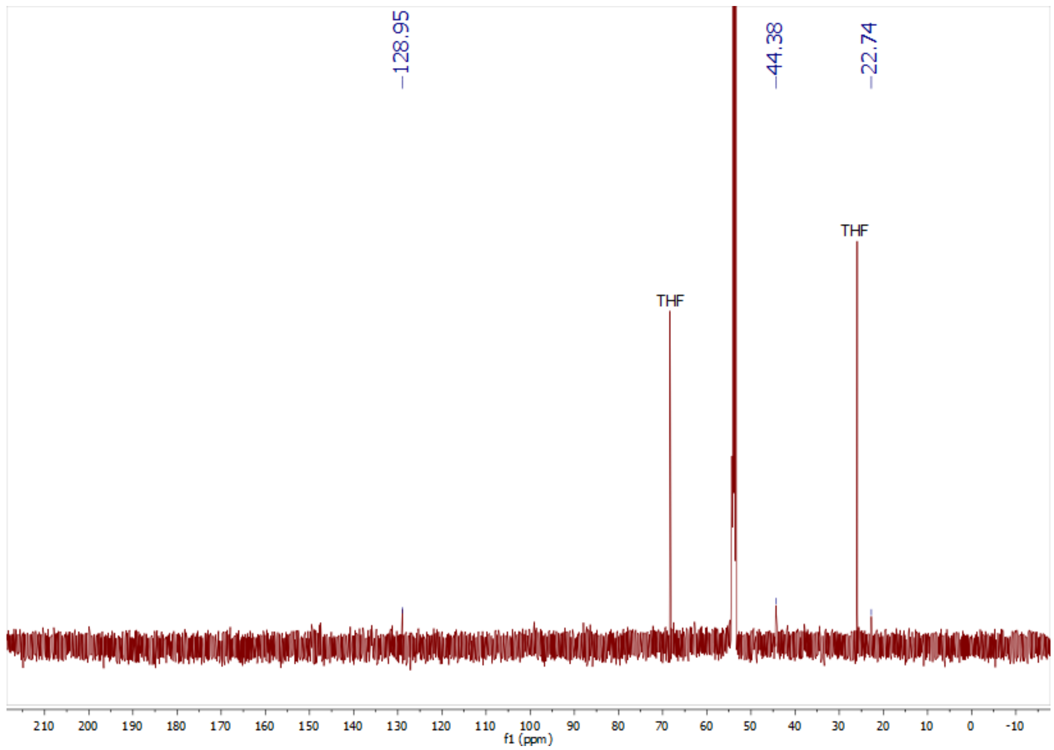
^{19}F NMR **Na[IMP-CH$_2$N(Me)$_2$]** (CD_2Cl_2, 471 MHz)



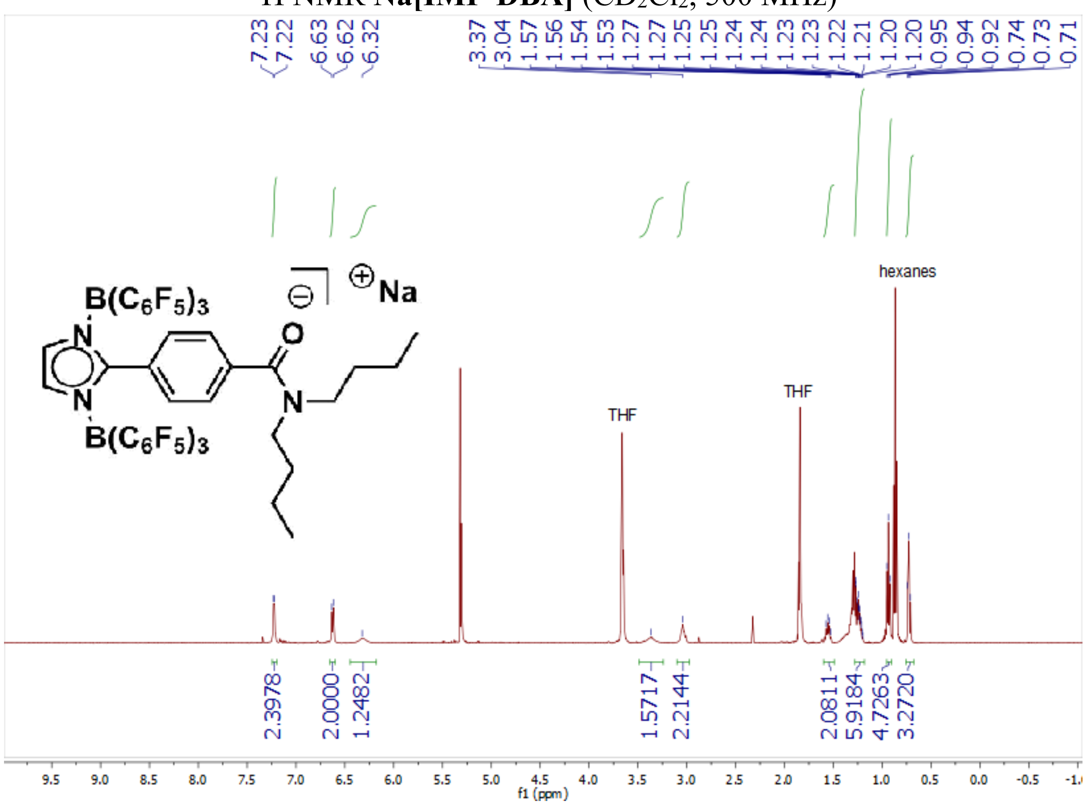
^{11}B NMR **Na[IMP-CH$_2$N(Me)$_2$]** (CD_2Cl_2, 161 MHz)



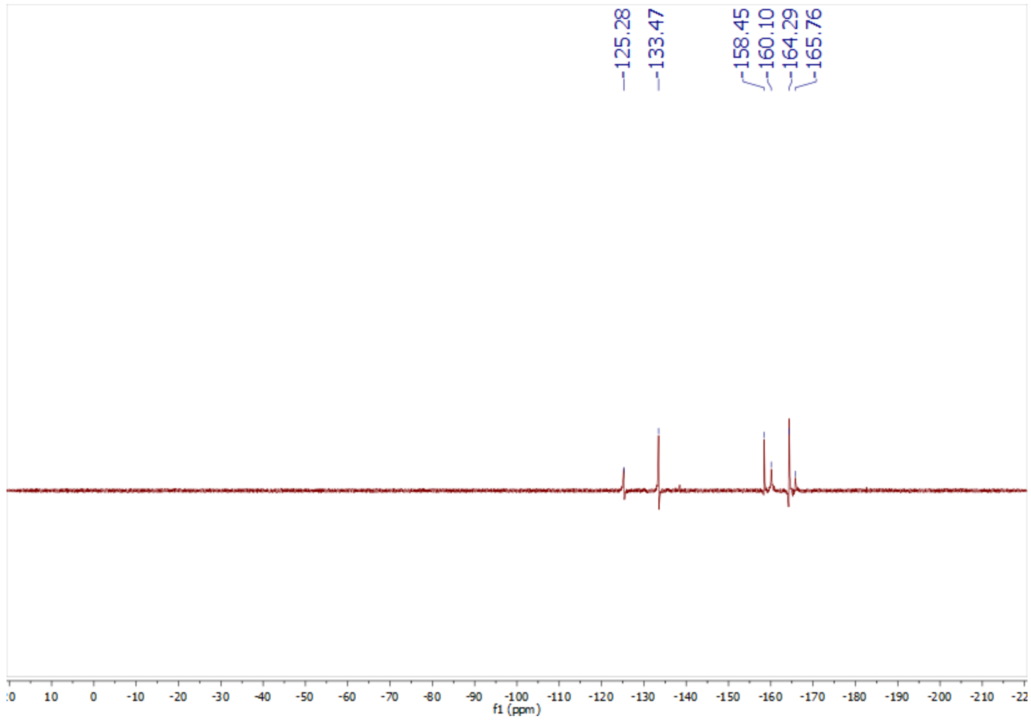
^{13}C NMR **Na[IMP-CH$_2$N(Me)$_2$]** (CD$_2$Cl$_2$, 126 MHz)



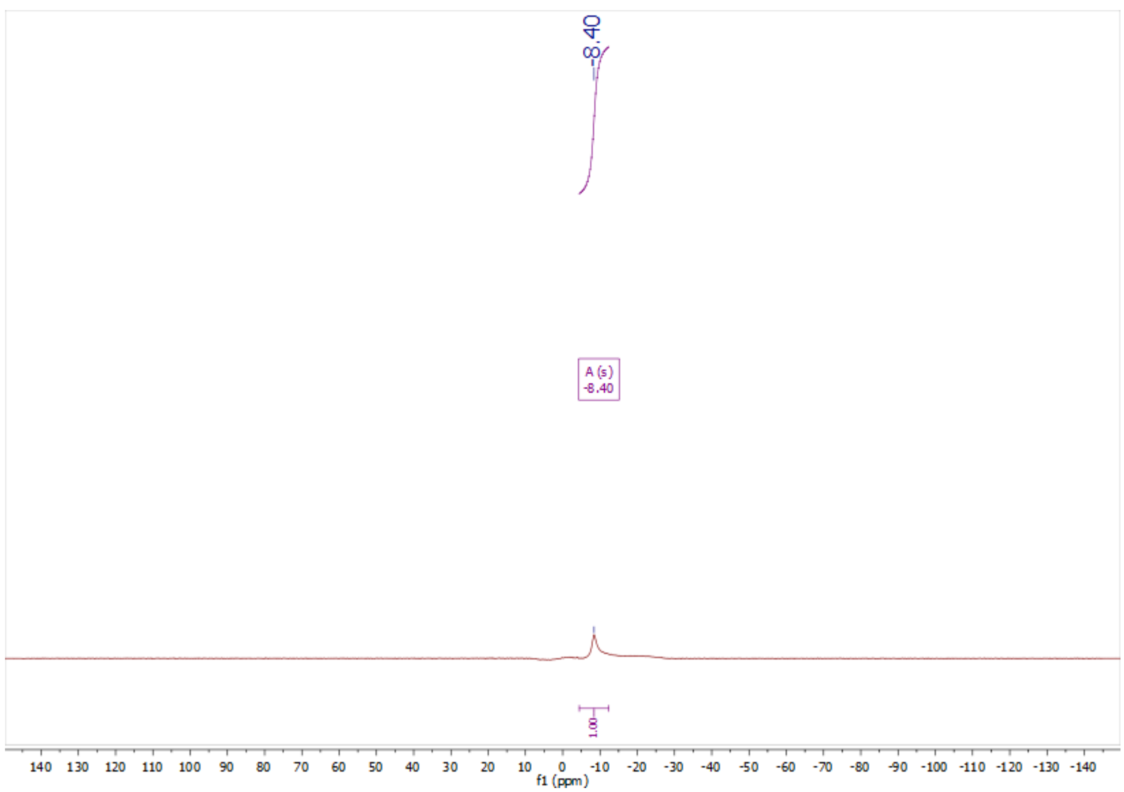
^{1}H NMR **Na[IMP-DBA]** (CD$_2$Cl$_2$, 500 MHz)



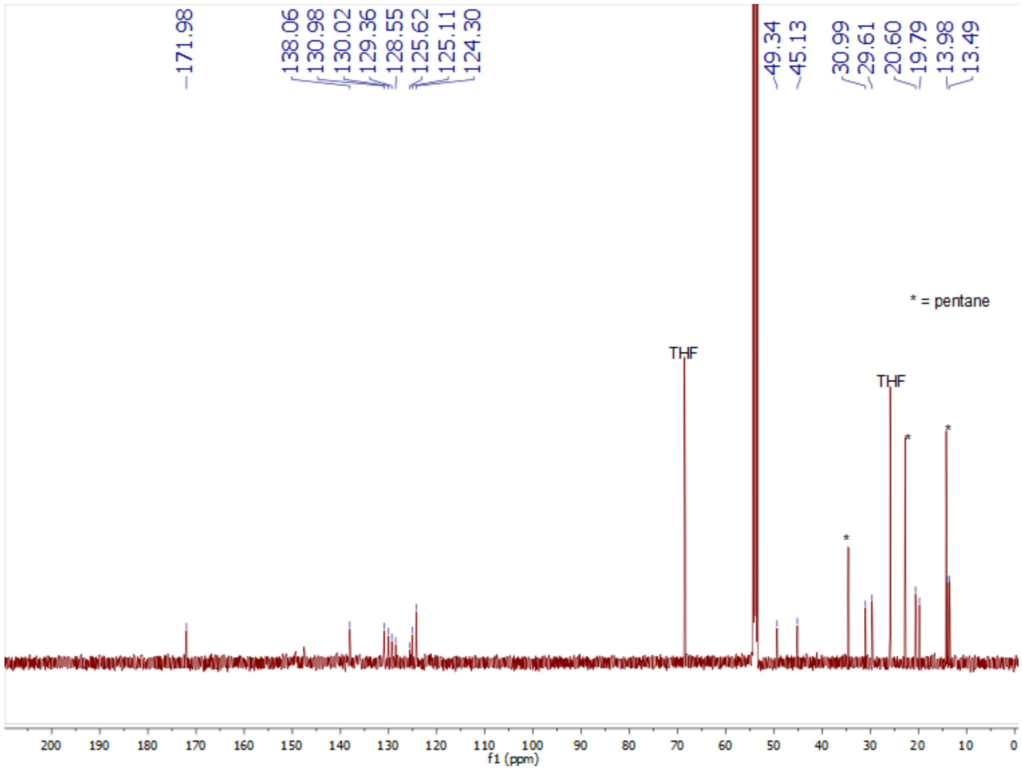
^{19}F NMR **Na[IMP-DBA]** (CD_2Cl_2, 471 MHz)



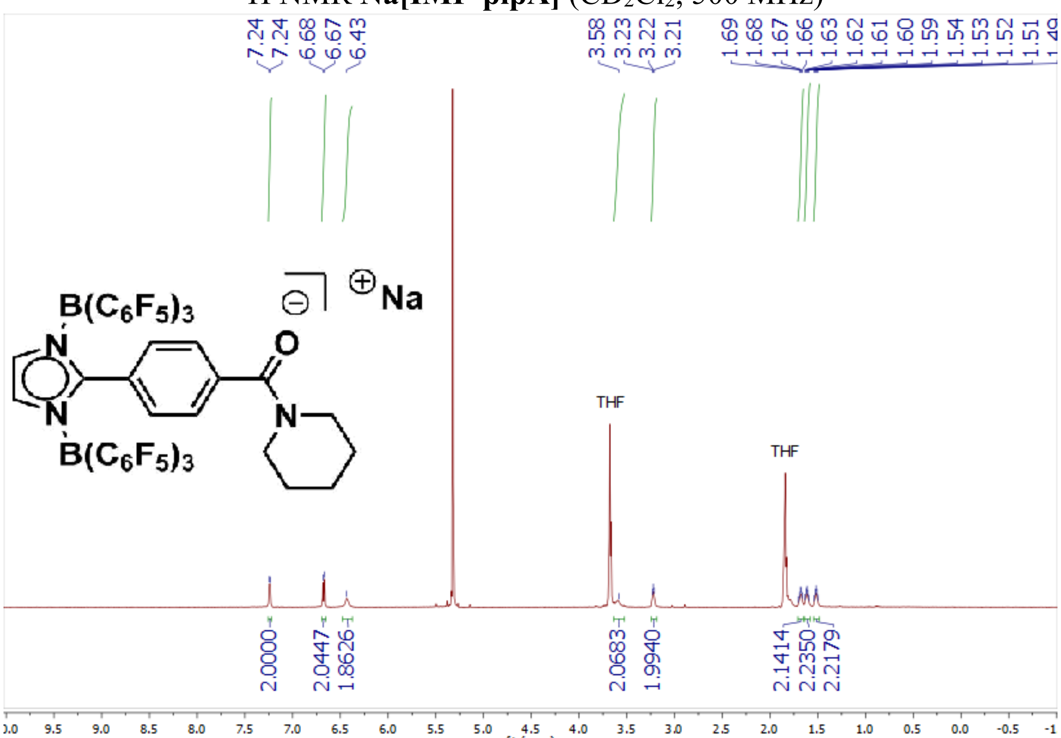
^{11}B NMR **Na[IMP-DBA]** (CD_2Cl_2, 161 MHz)



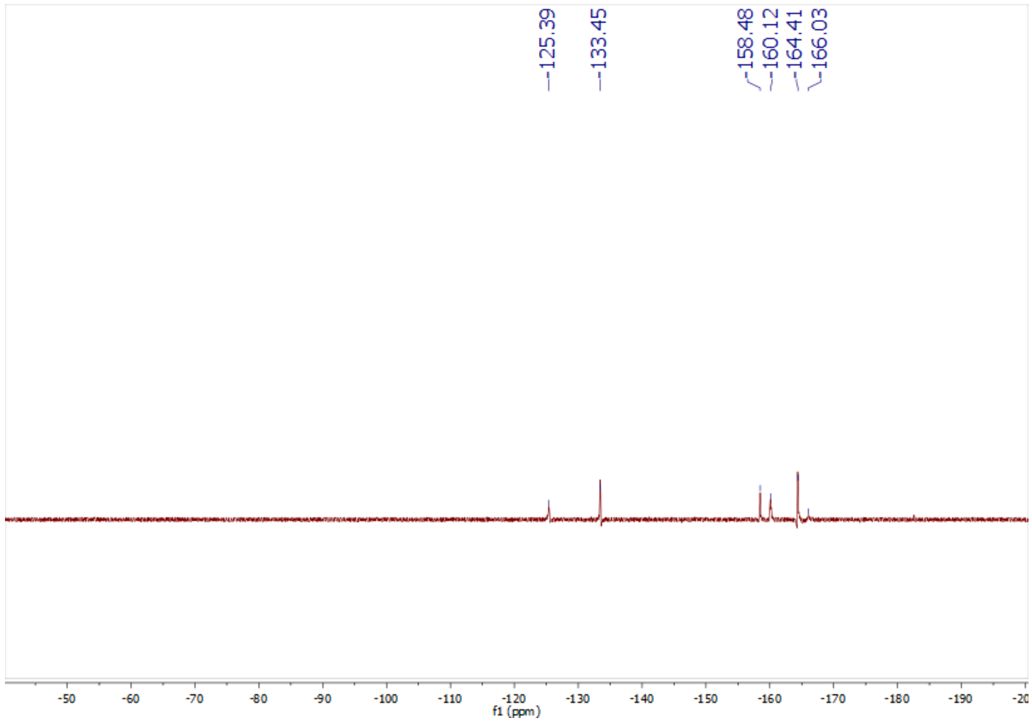
^{13}C NMR **Na[IMP-DBA]** (CD_2Cl_2, 126 MHz)



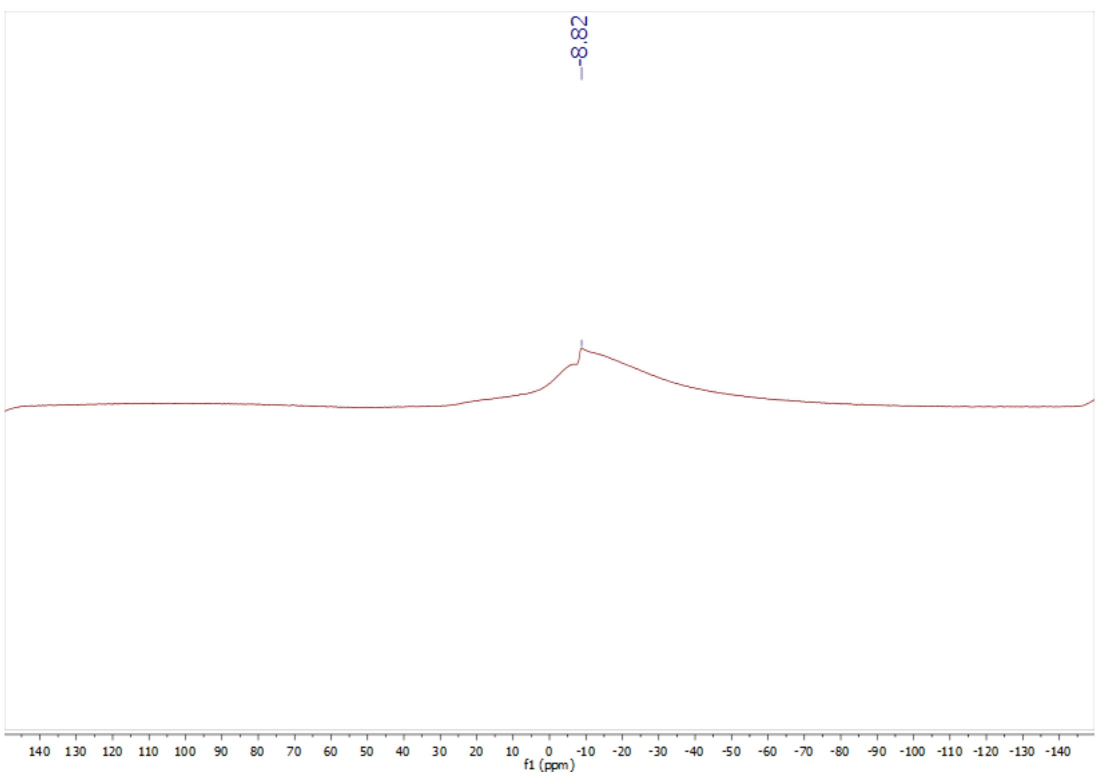
^{1}H NMR **Na[IMP-pipA]** (CD_2Cl_2, 500 MHz)



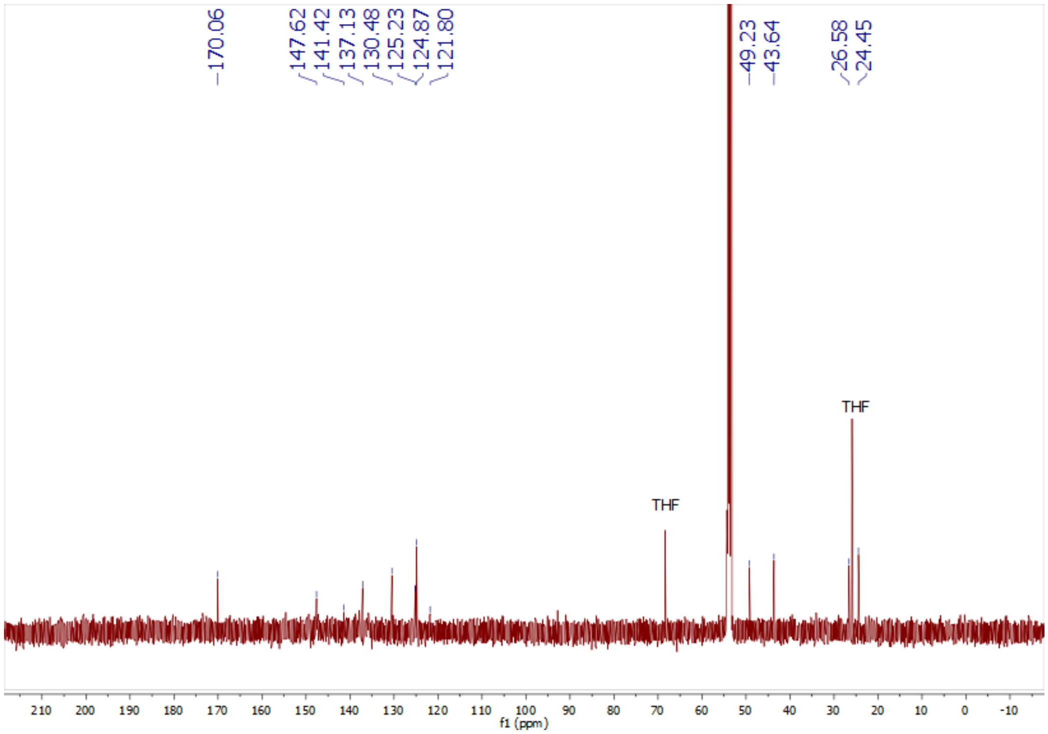
^{19}F NMR **Na[IMP-pipA]** (CD_2Cl_2, 471 MHz)



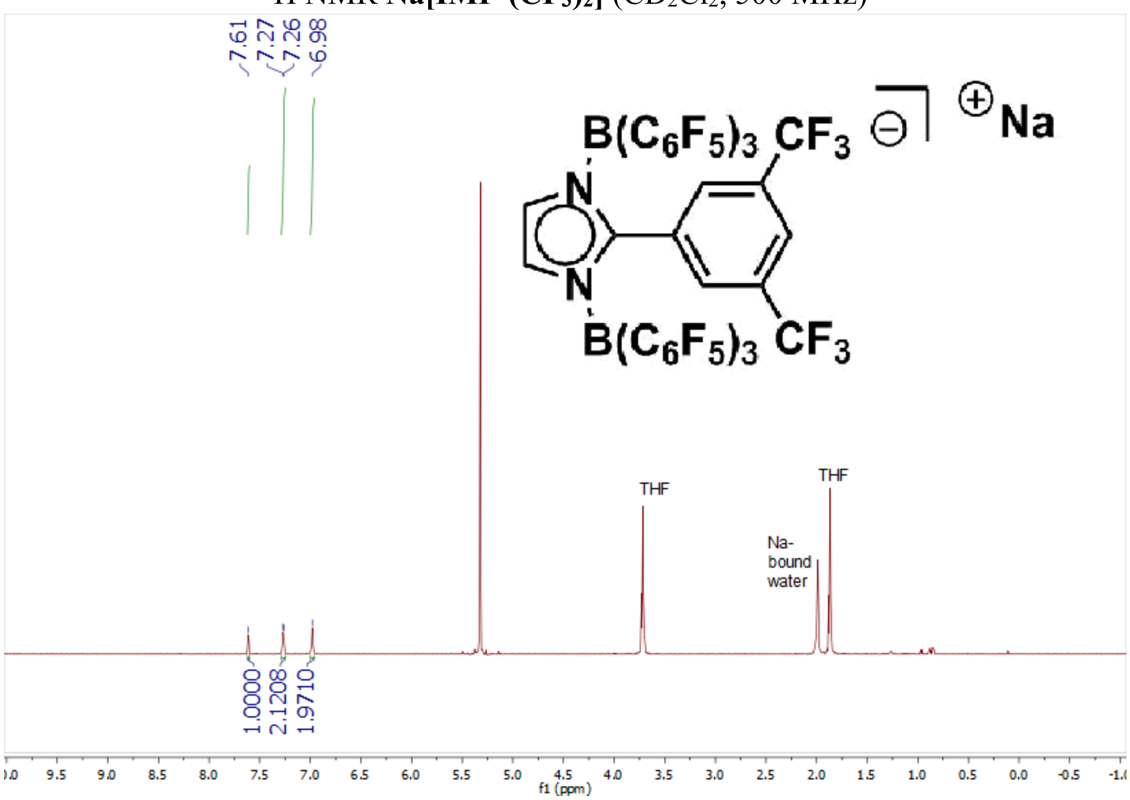
^{11}B NMR **Na[IMP-pipA]** (CD_2Cl_2, 161 MHz)



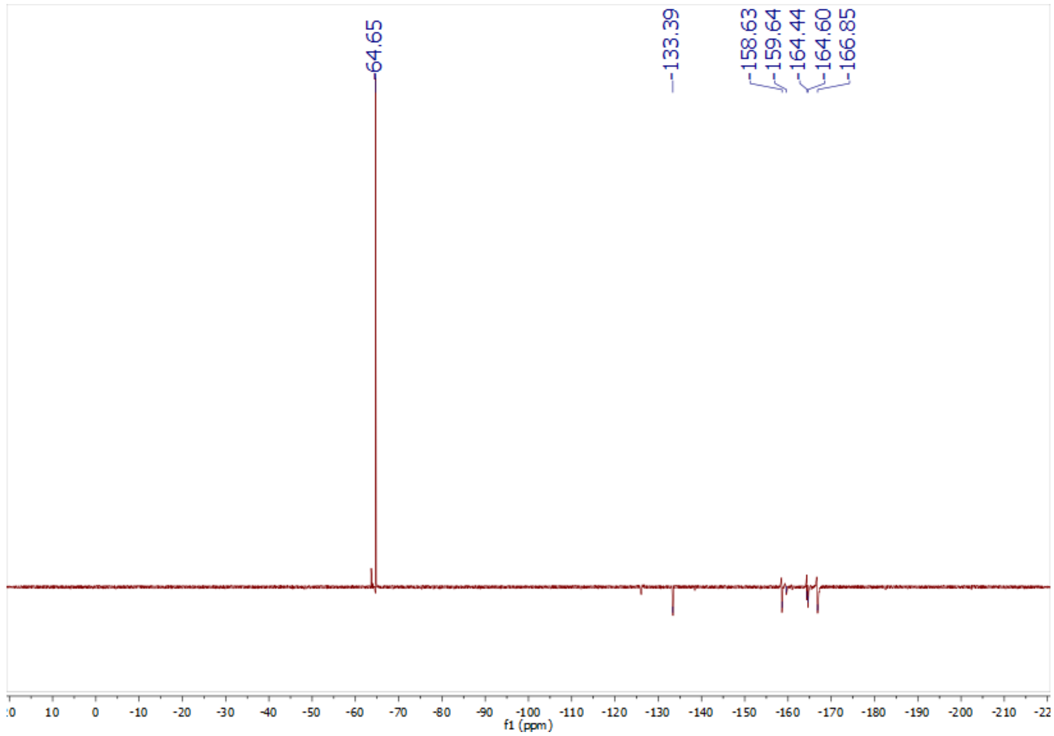
^{13}C NMR **Na[IMP-pipA]** (CD_2Cl_2, 126 MHz)



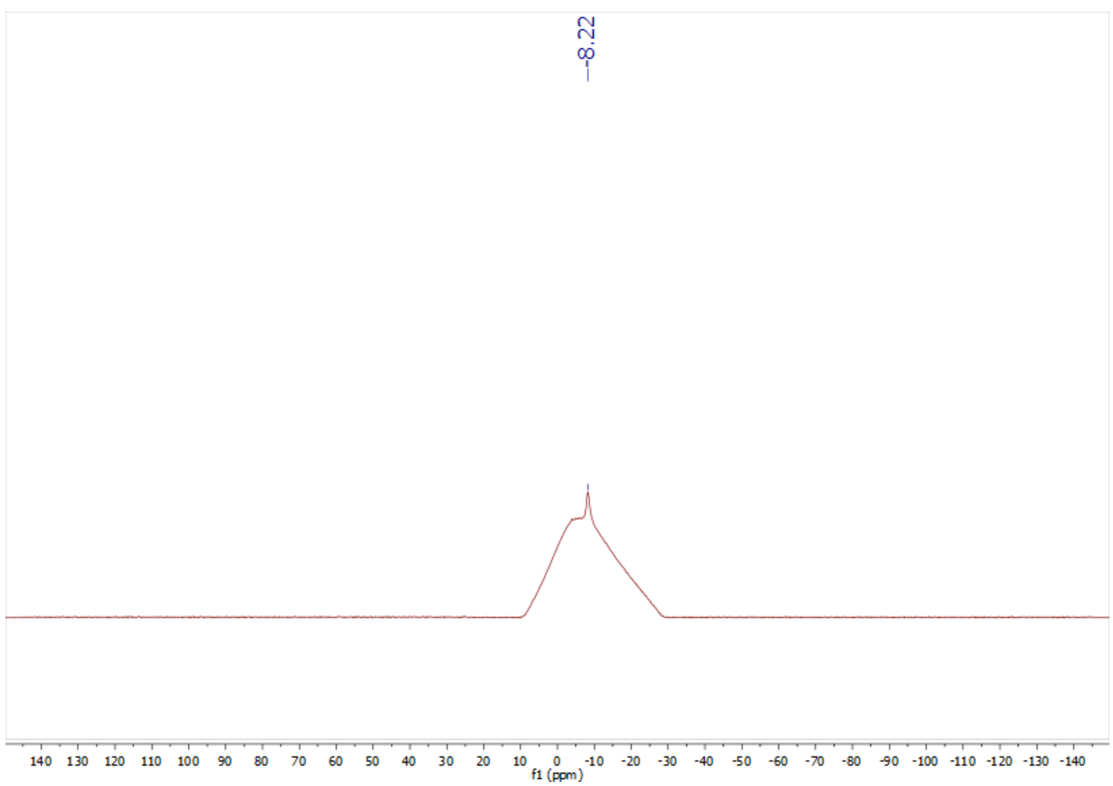
^{1}H NMR **Na[IMP-(CF$_3$)$_2$]** (CD_2Cl_2, 500 MHz)



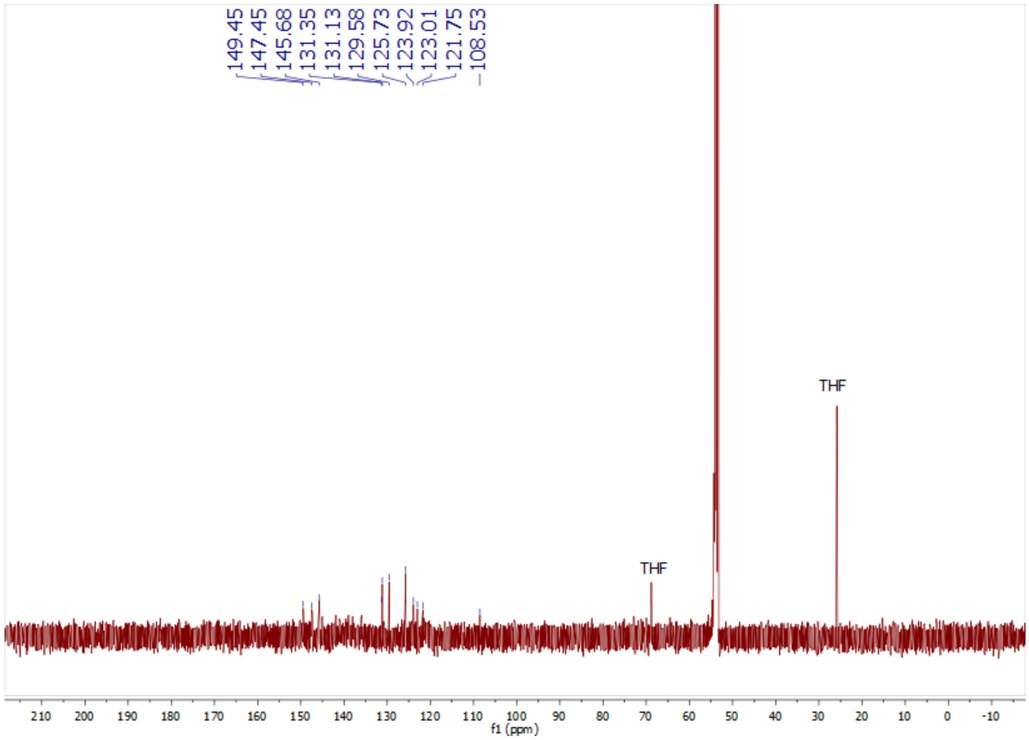
^{19}F NMR **Na[IMP-(CF$_3$)$_2$]** (CD_2Cl_2, 471 MHz)



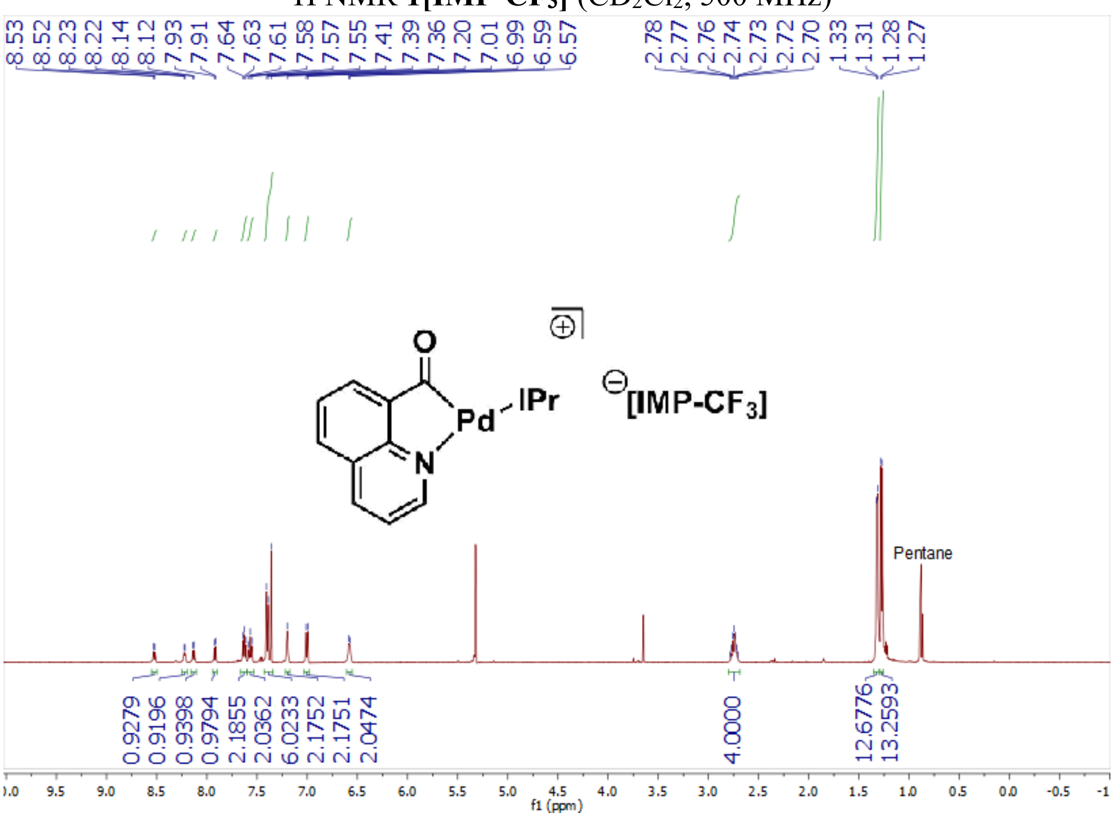
^{11}B NMR **Na[IMP-(CF$_3$)$_2$]** (CD_2Cl_2, 161 MHz)



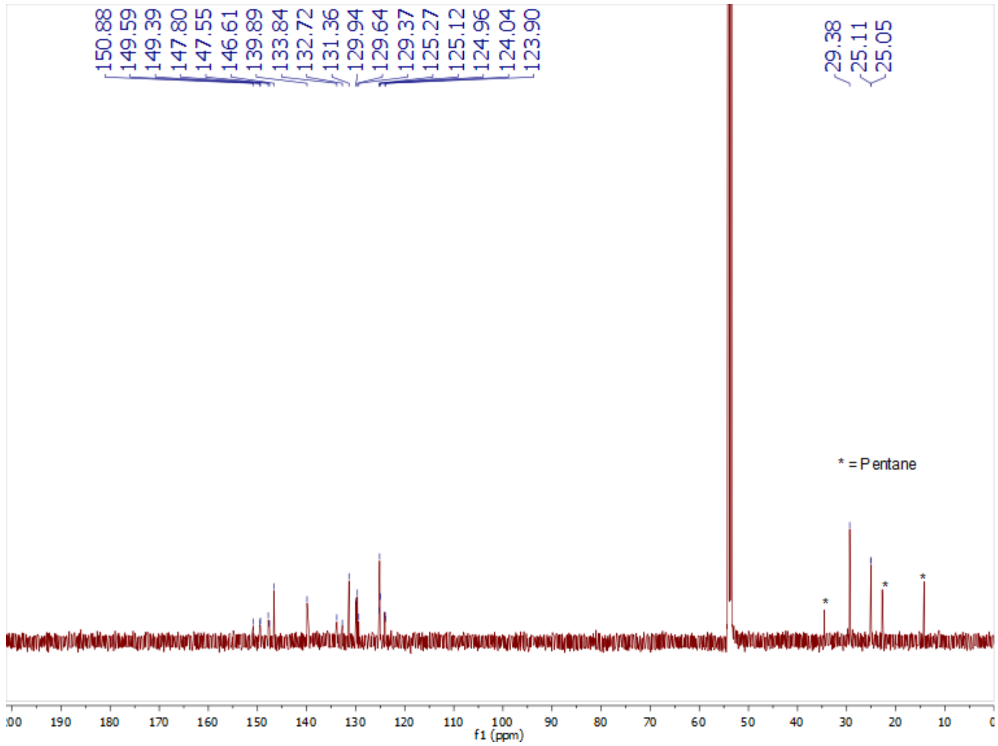
^{13}C NMR **Na[IMP-(CF$_3$)$_2$]** (CD_2Cl_2, 126 MHz)



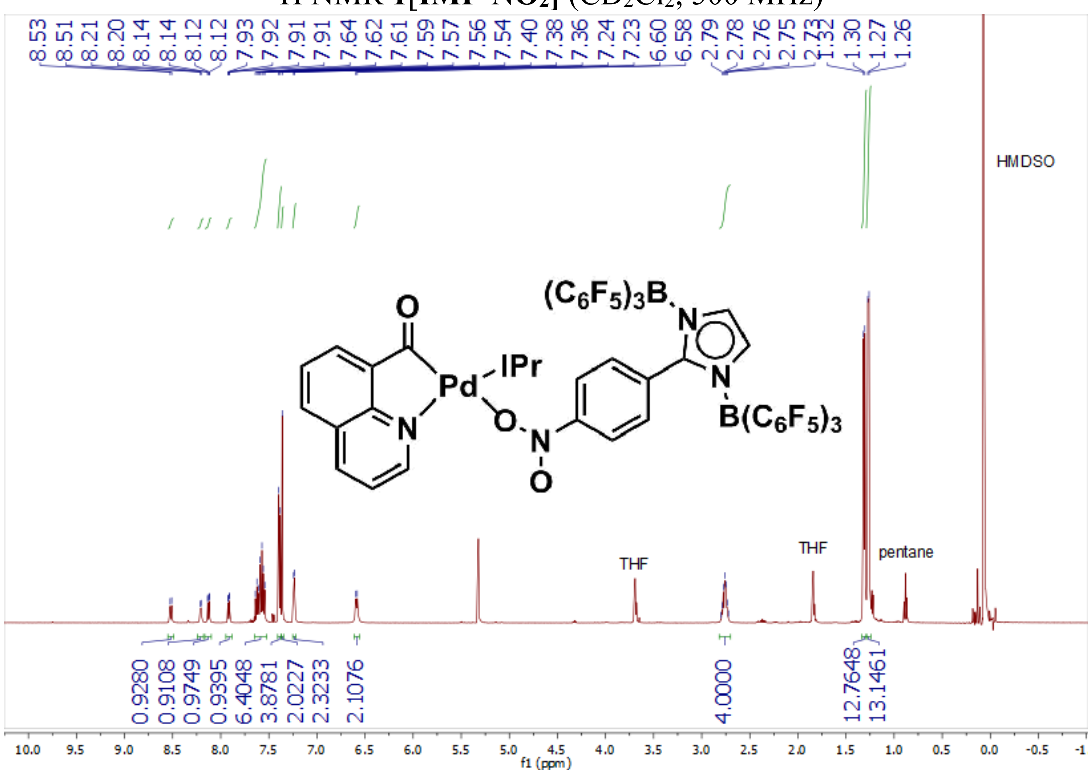
^{1}H NMR **1[IMP-CF$_3$]** (CD_2Cl_2, 500 MHz)



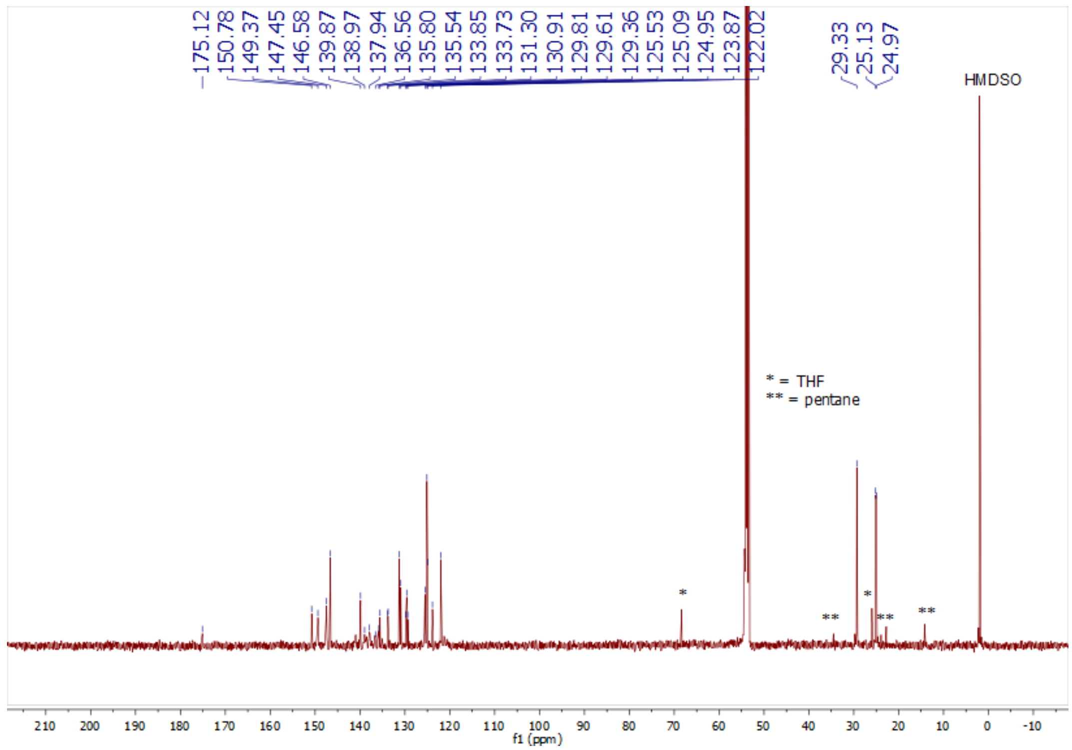
^{13}C NMR **1[IMP-CF$_3$]** (CD_2Cl_2, 126 MHz)



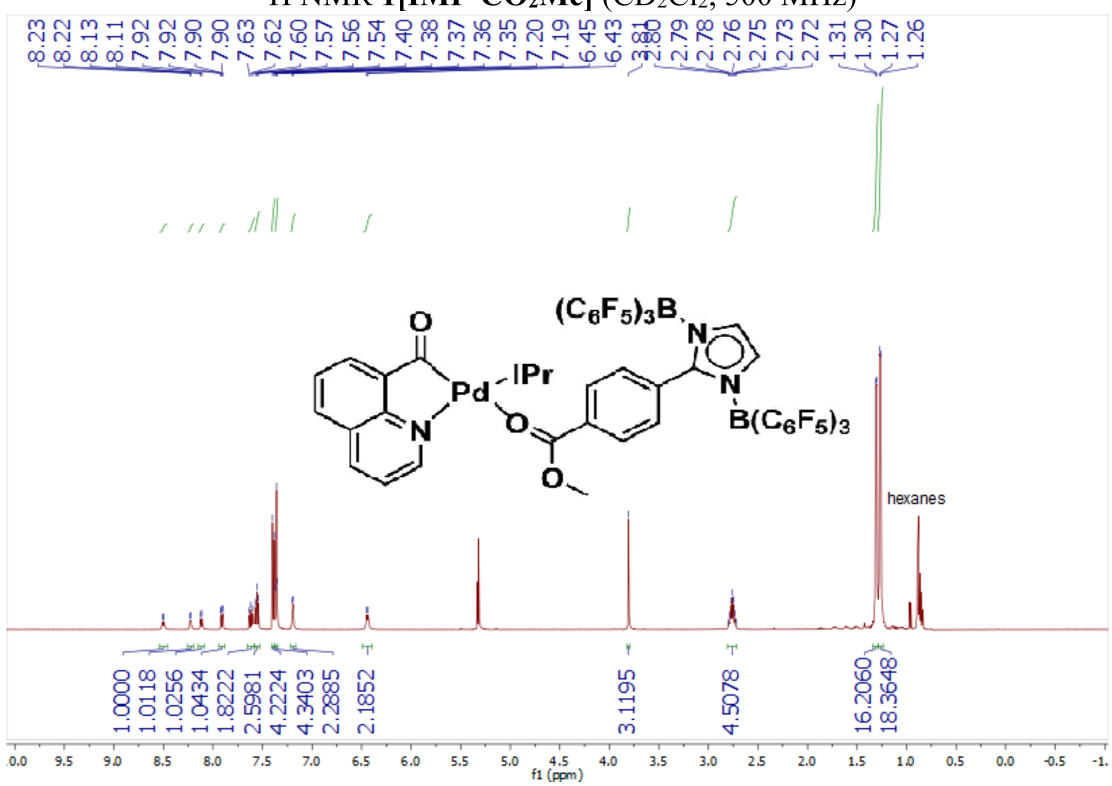
^{1}H NMR **1[IMP-NO$_2$]** (CD_2Cl_2, 500 MHz)



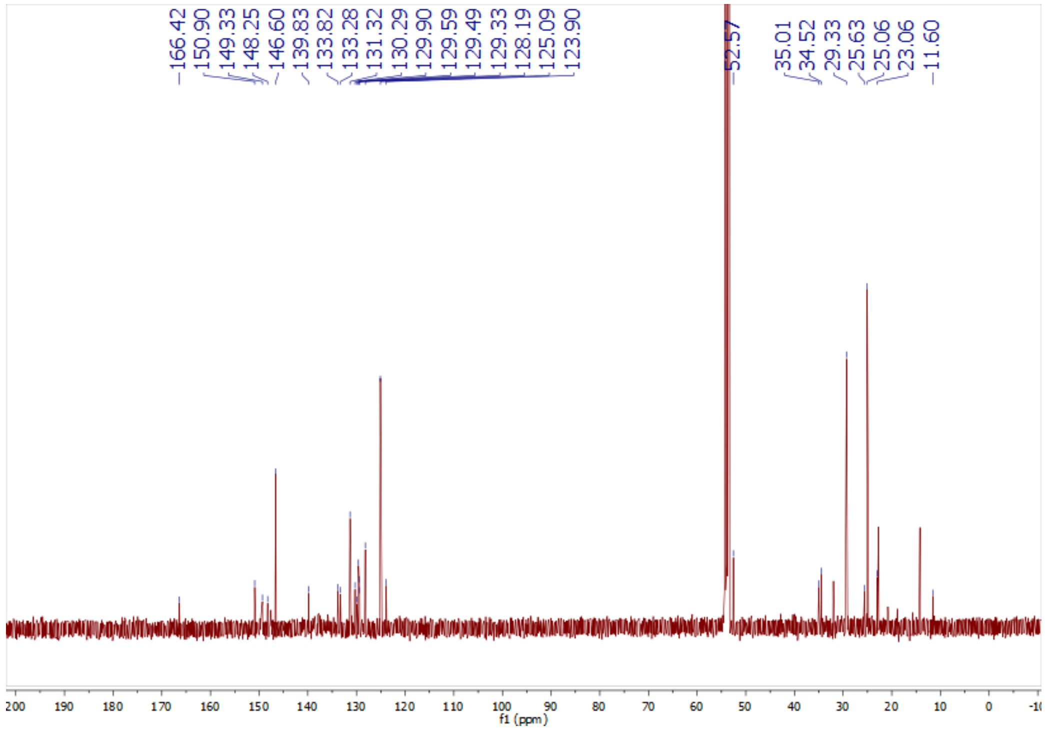
^{13}C NMR 1**[IMP-NO$_2$]** (CD_2Cl_2, 126 MHz)



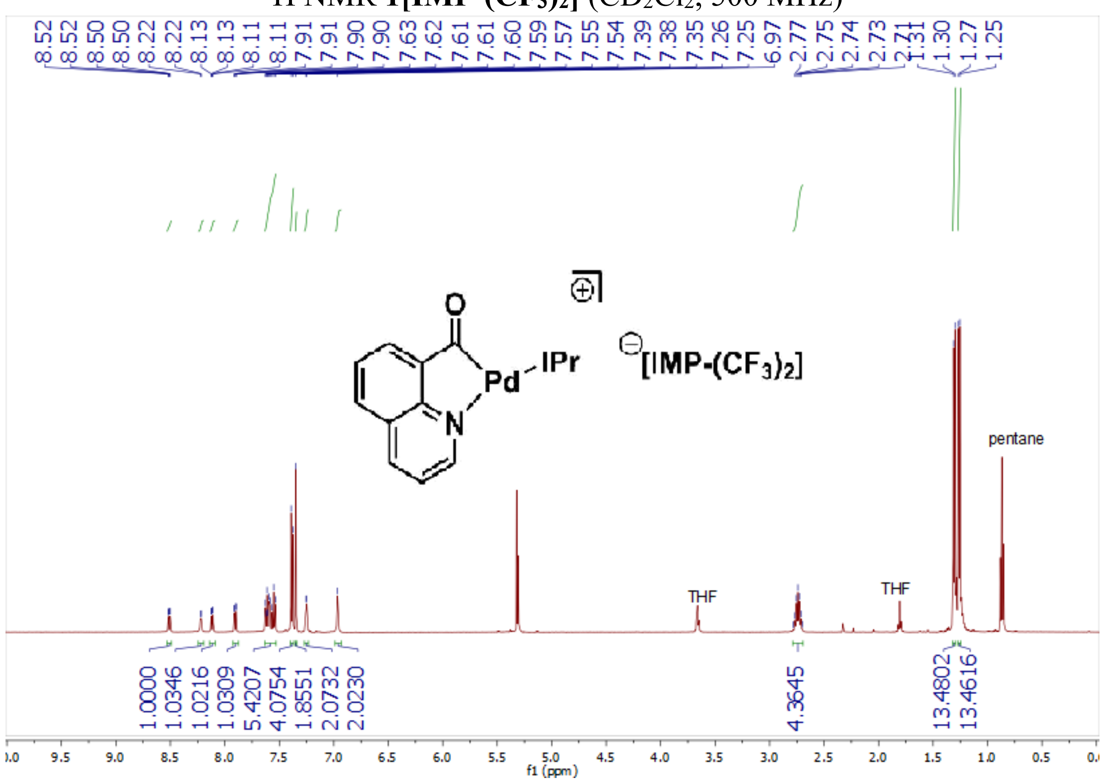
^{1}H NMR **1[IMP-CO$_2$Me]** (CD_2Cl_2, 500 MHz)



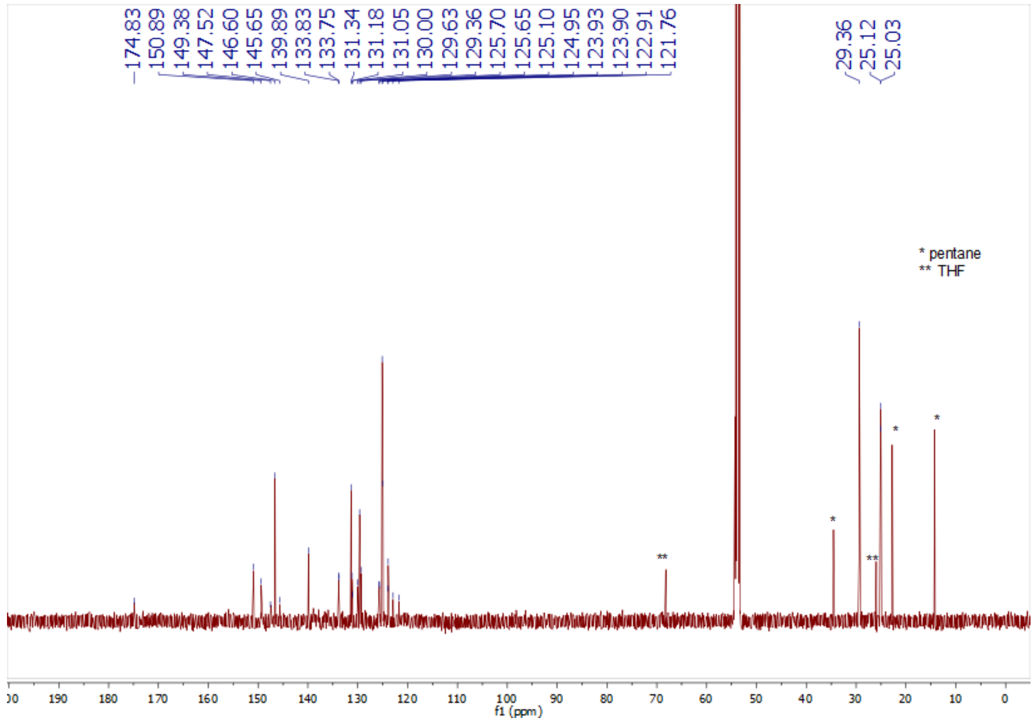
^{13}C NMR **1[IMP-CO_2Me]** (CD_2Cl_2, 126 MHz)



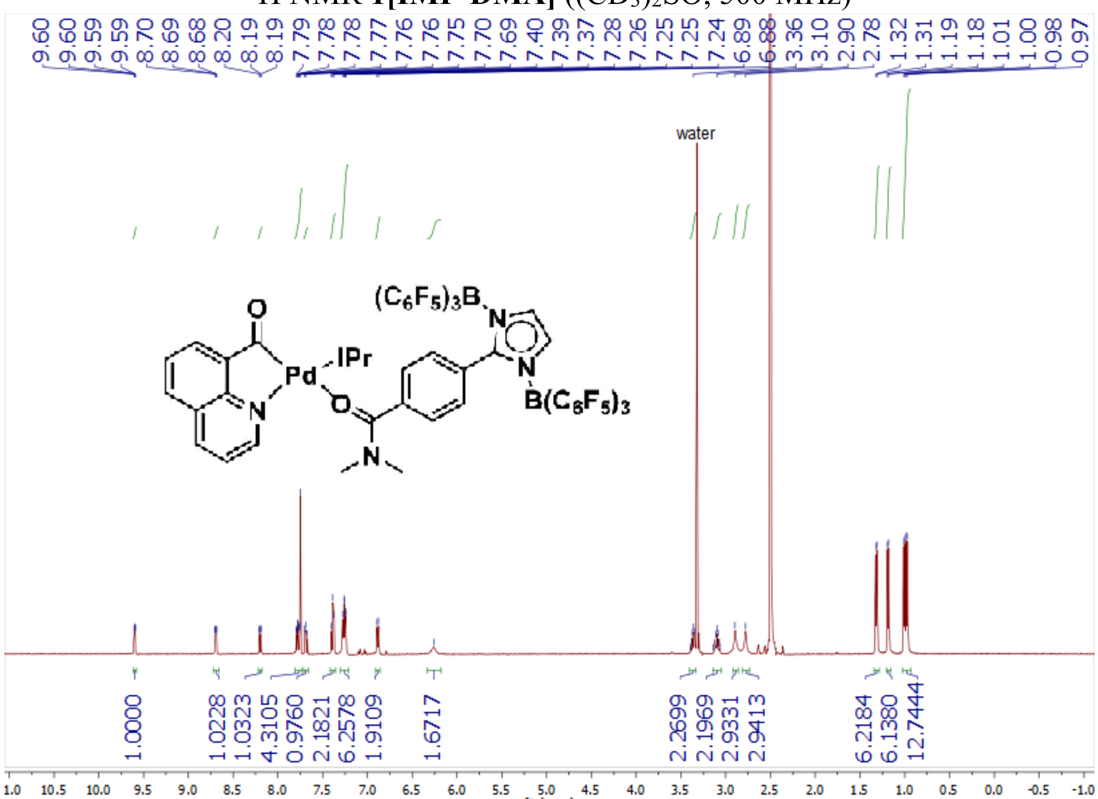
^{1}H NMR **1[IMP-$(CF_3)_2$]** (CD_2Cl_2, 500 MHz)



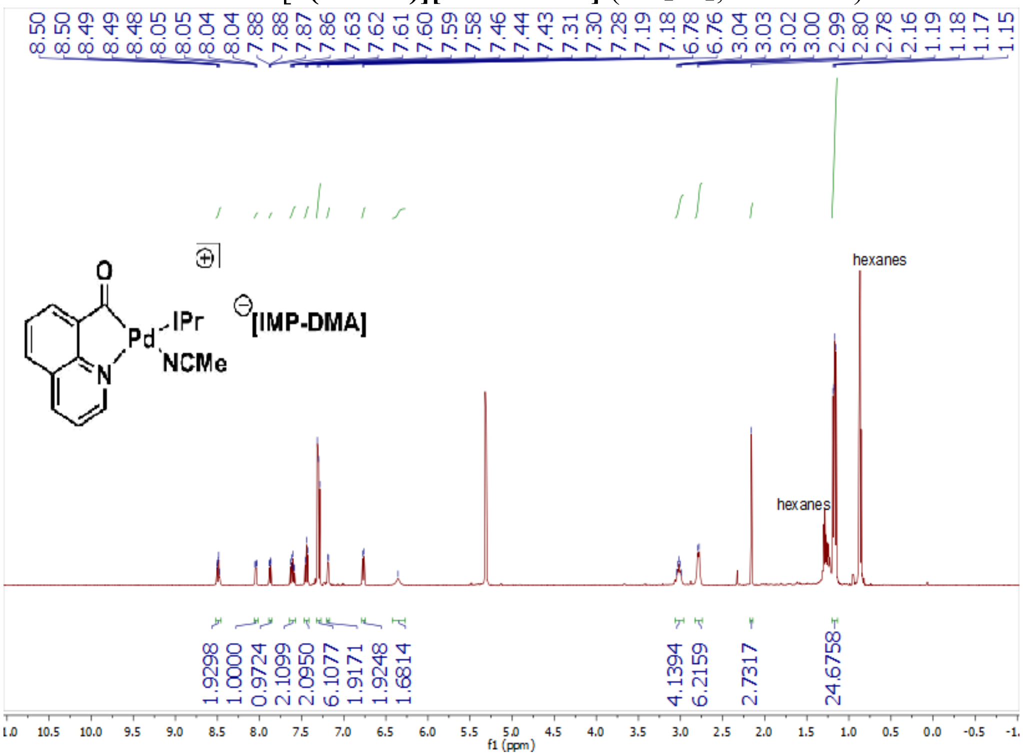
^{13}C NMR **1[IMP-(CF$_3$)$_2$]** (CD_2Cl_2, 126 MHz)



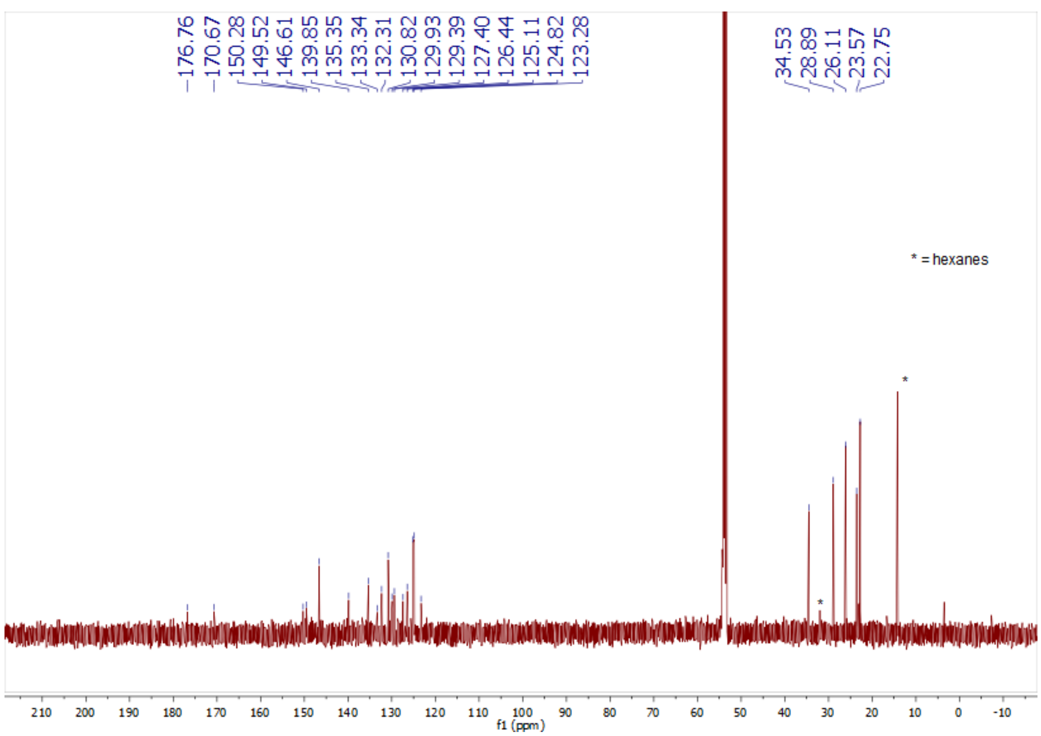
^{1}H NMR **1[IMP-DMA]** ((CD_3)$_2$SO, 500 MHz)



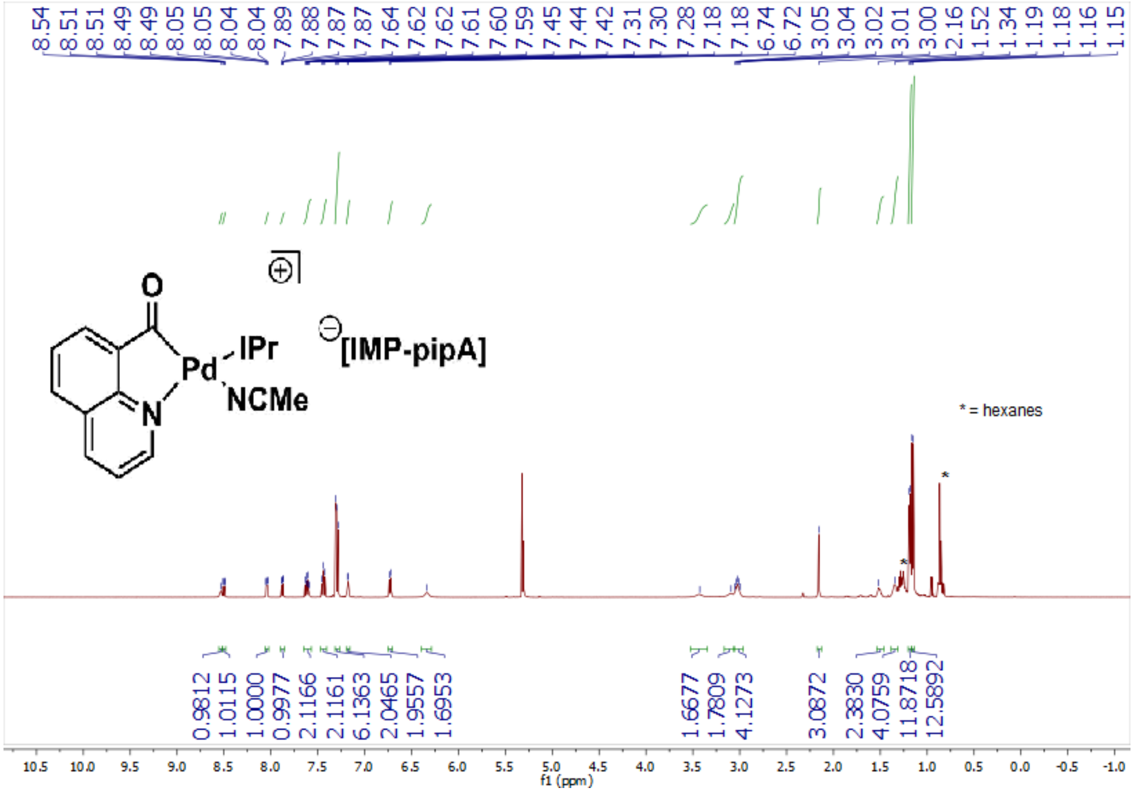
^{1}H NMR [**1(MeCN)][IMP-DMA]** (CD_2Cl_2, 500 MHz)



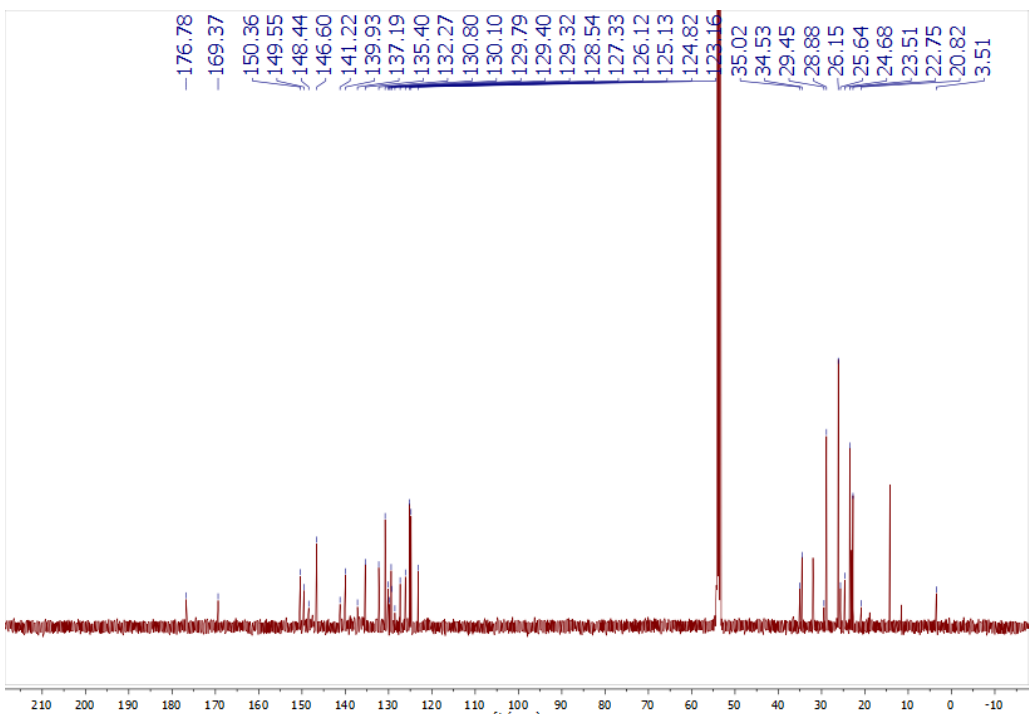
^{13}C NMR [**1(MeCN)][IMP-DMA]** (CD_2Cl_2, 126 MHz)



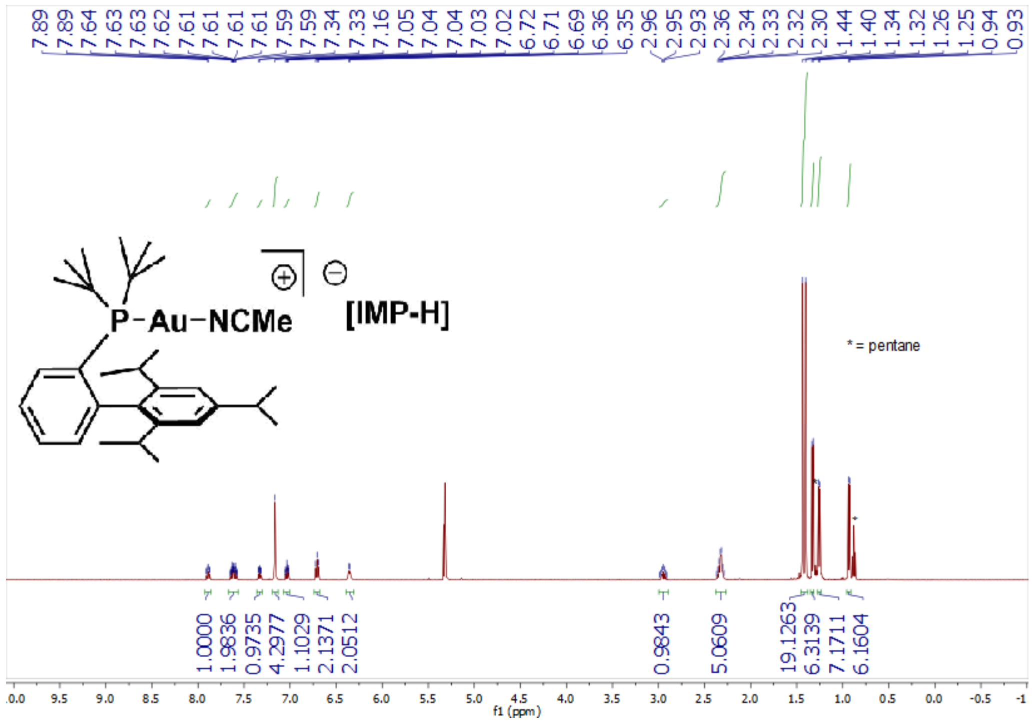
^{1}H NMR [**1(MeCN)][IMP-pipA]** (CD_2Cl_2, 500 MHz)



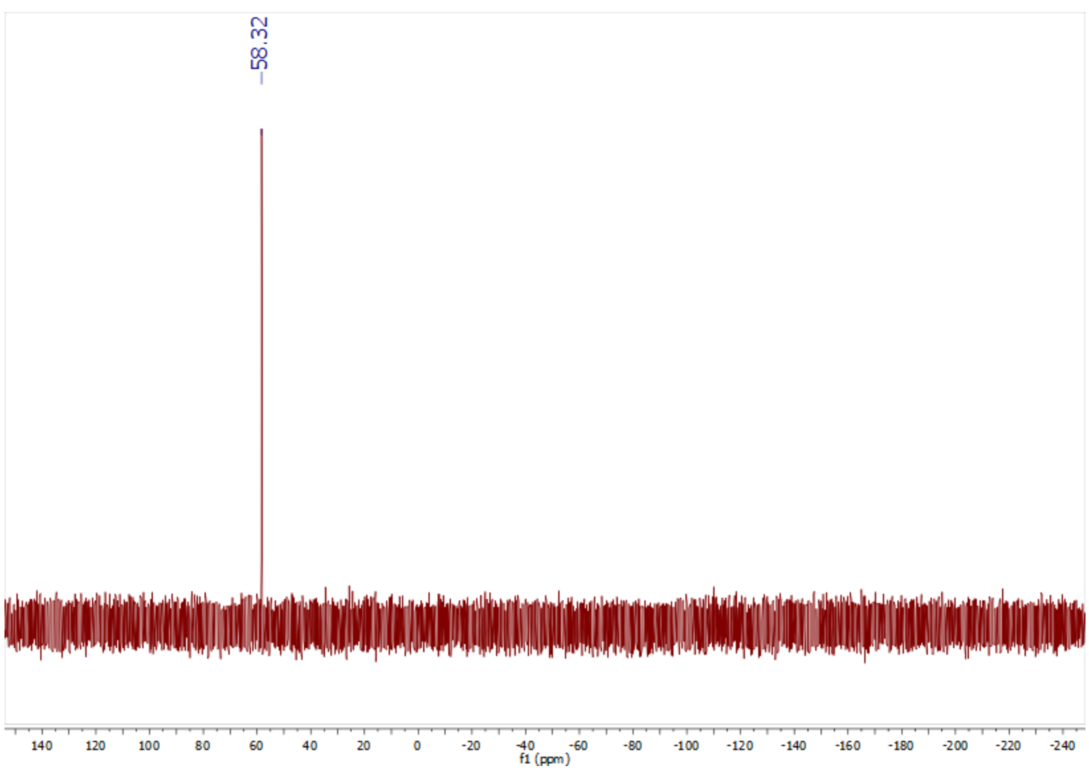
^{13}C NMR [**1(MeCN)][IMP-pipA]** (CD_2Cl_2, 126 MHz)



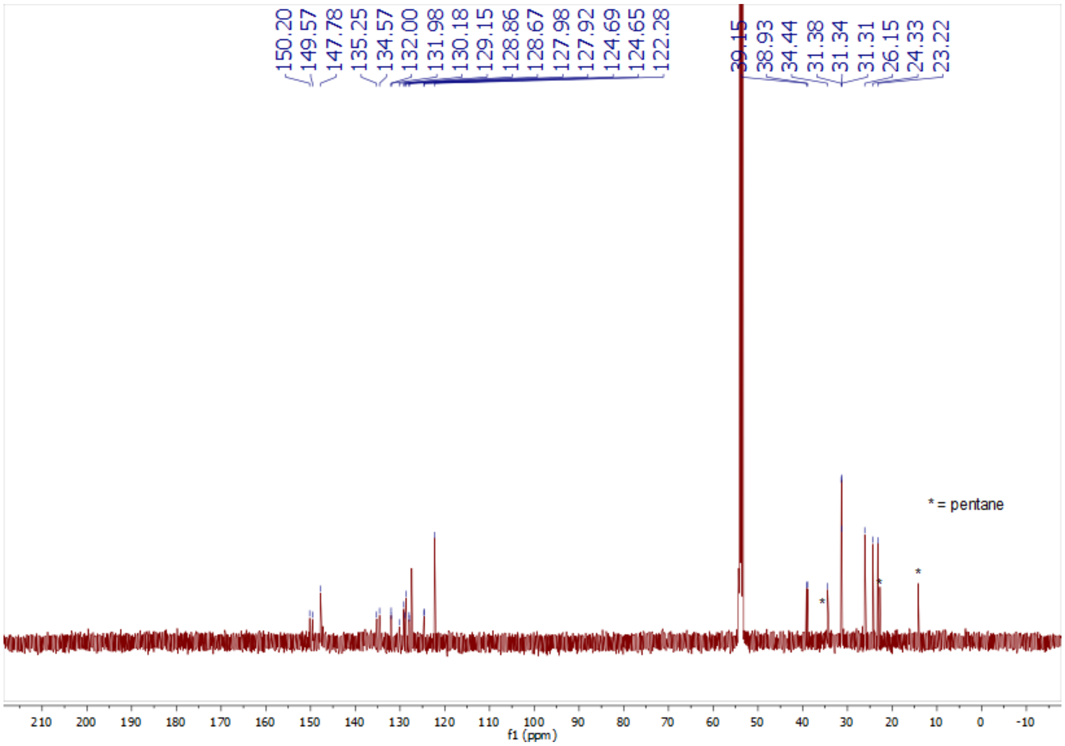
^{1}H NMR **2[IMP-H]** (CD_2Cl_2, 500 MHz)



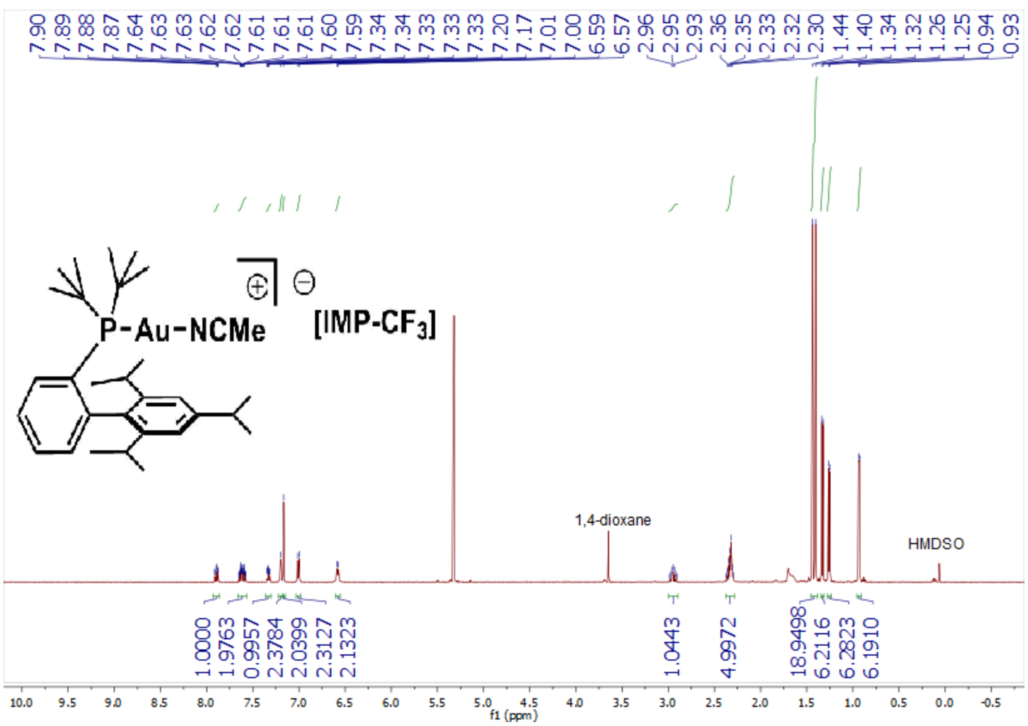
^{31}P NMR **2[IMP-H]** (CD_2Cl_2, 203 MHz)



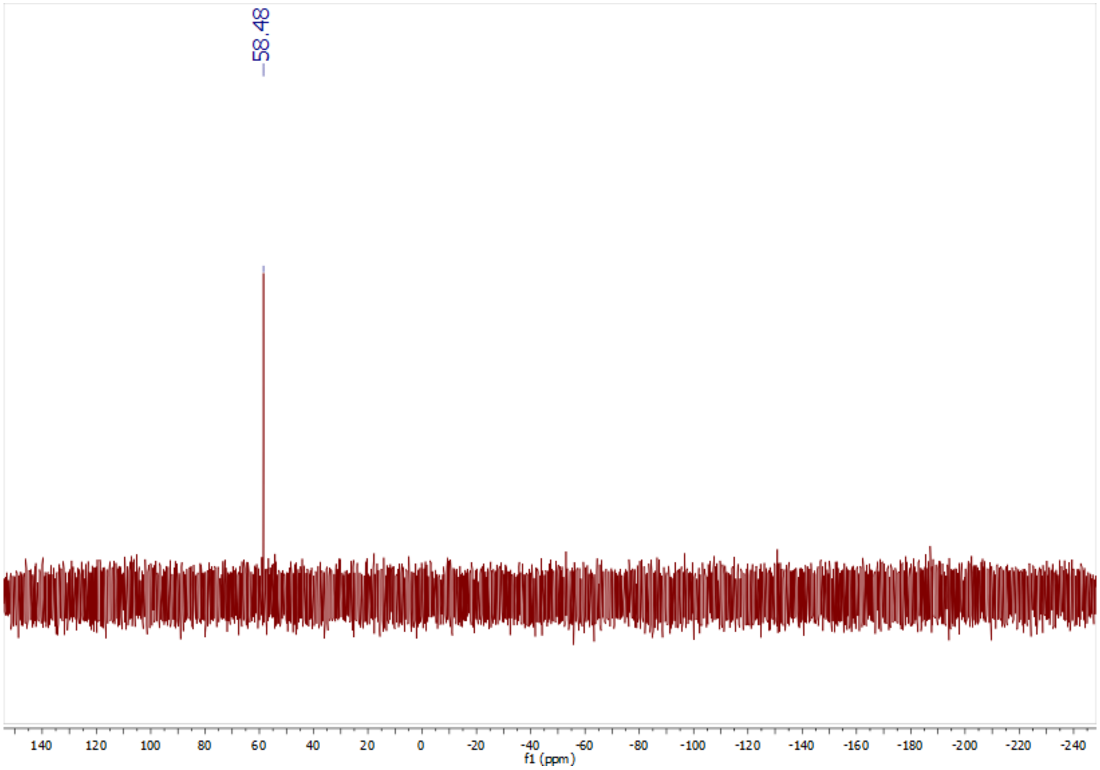
^{13}C NMR **2[IMP-H]** (CD_2Cl_2, 126 MHz)



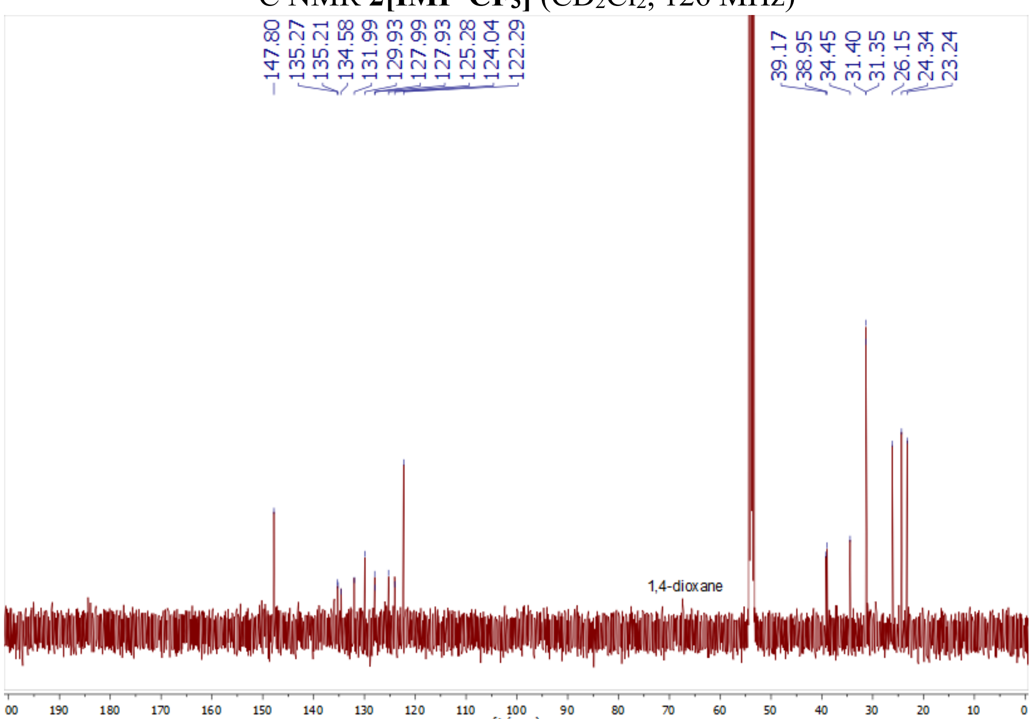
^{1}H NMR **2[IMP-CF$_3$]** (CD_2Cl_2, 500 MHz)



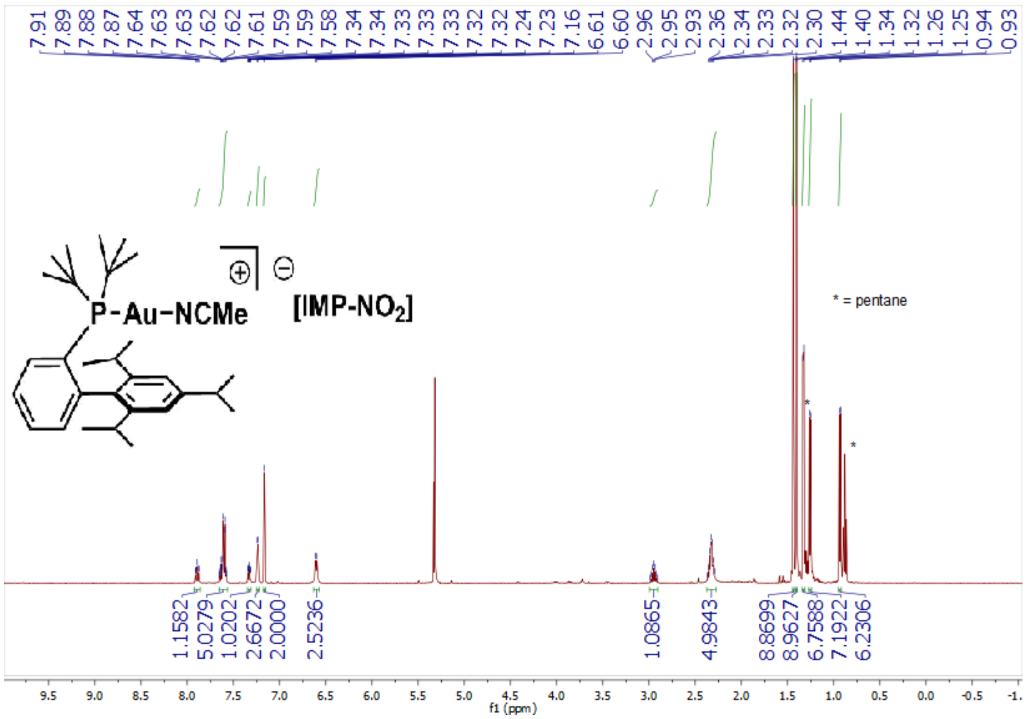
^{31}P NMR **2[IMP-CF$_3$]** (CD_2Cl_2, 203 MHz)



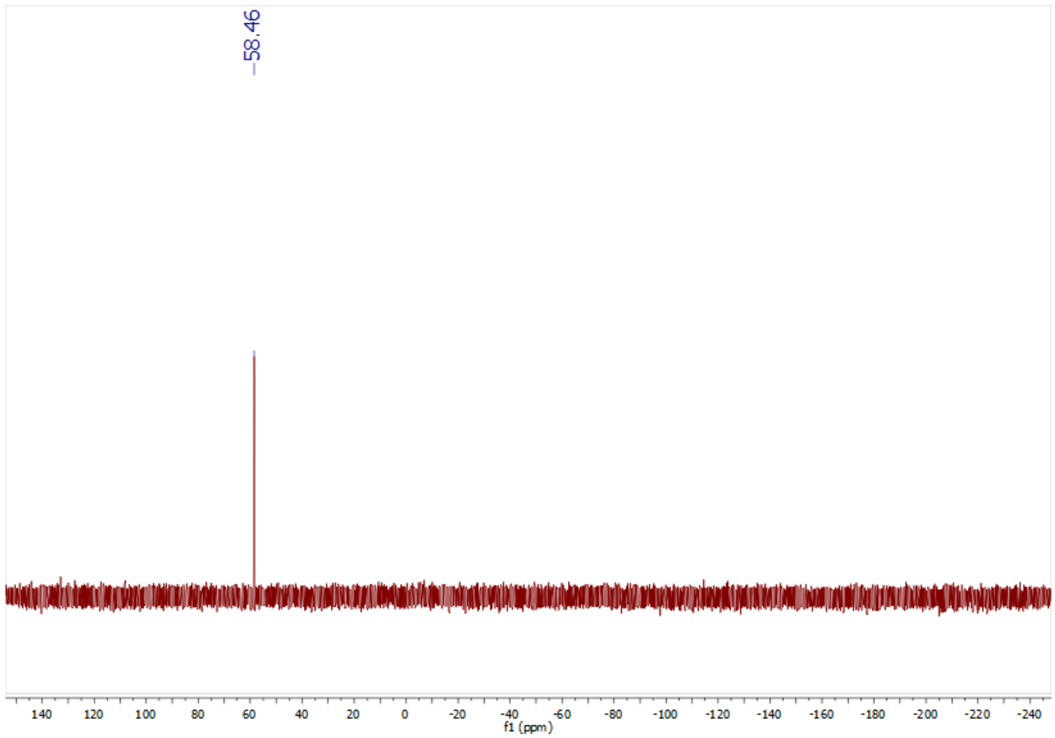
^{13}C NMR **2[IMP-CF$_3$]** (CD_2Cl_2, 126 MHz)



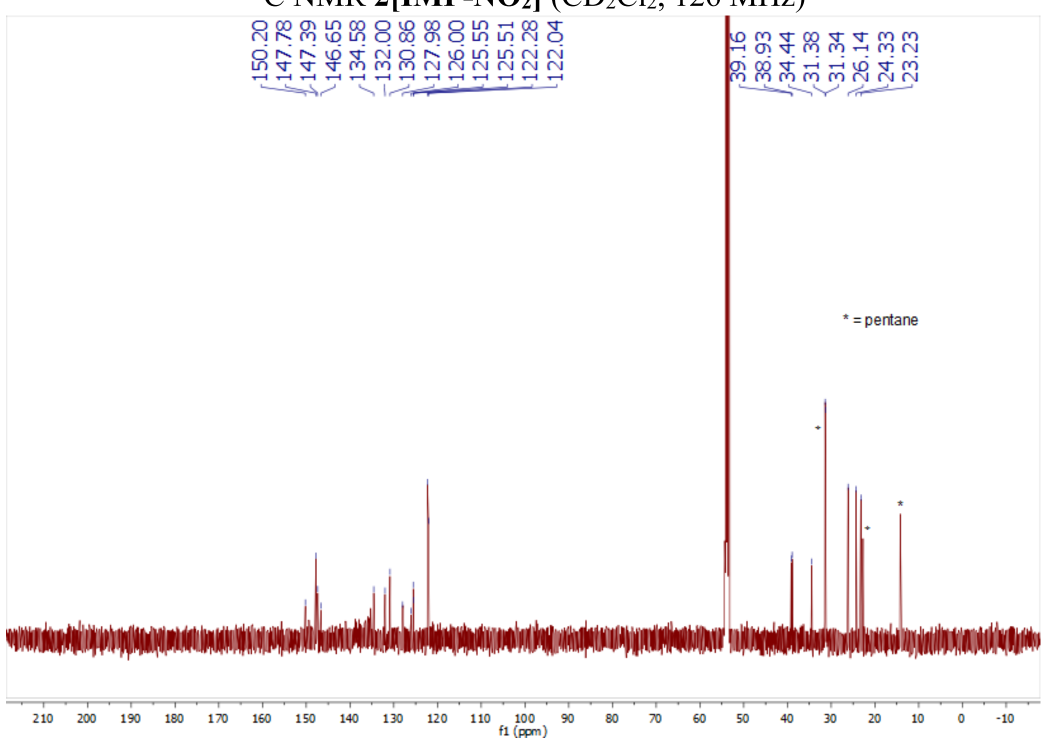
^{1}H NMR **2[IMP-NO$_2$]** (CD_2Cl_2, 500 MHz)



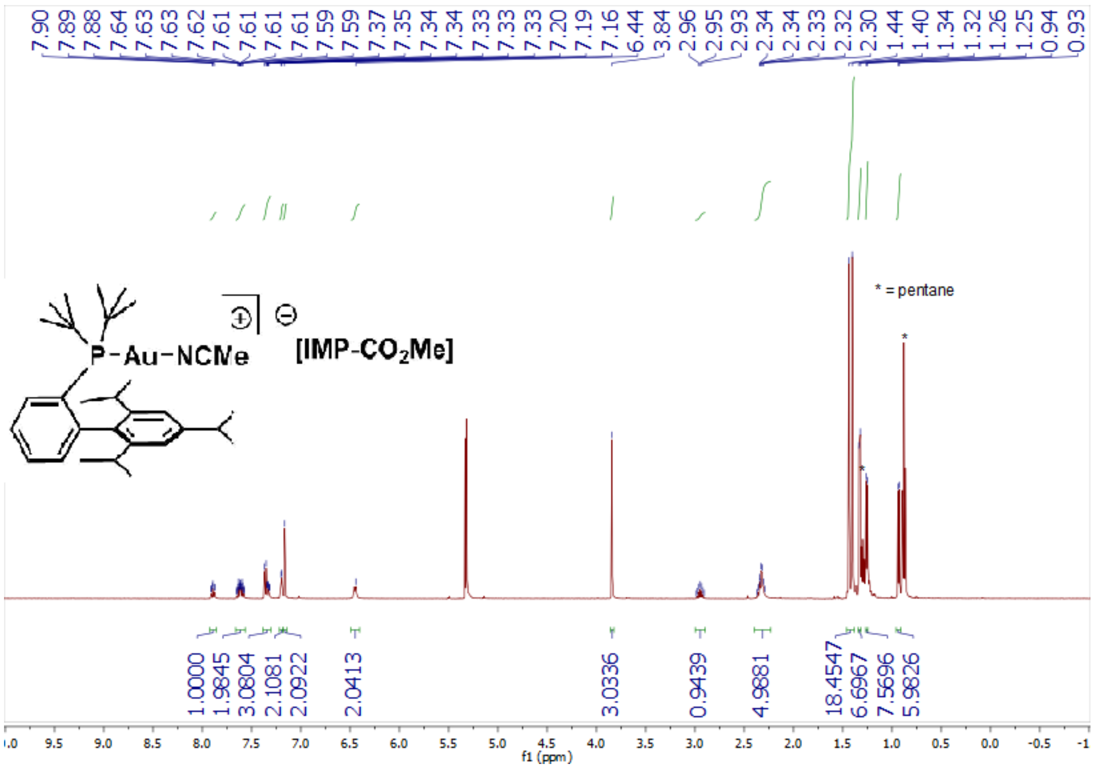
^{31}P NMR **2[IMP-NO$_2$]** (CD_2Cl_2, 203 MHz)



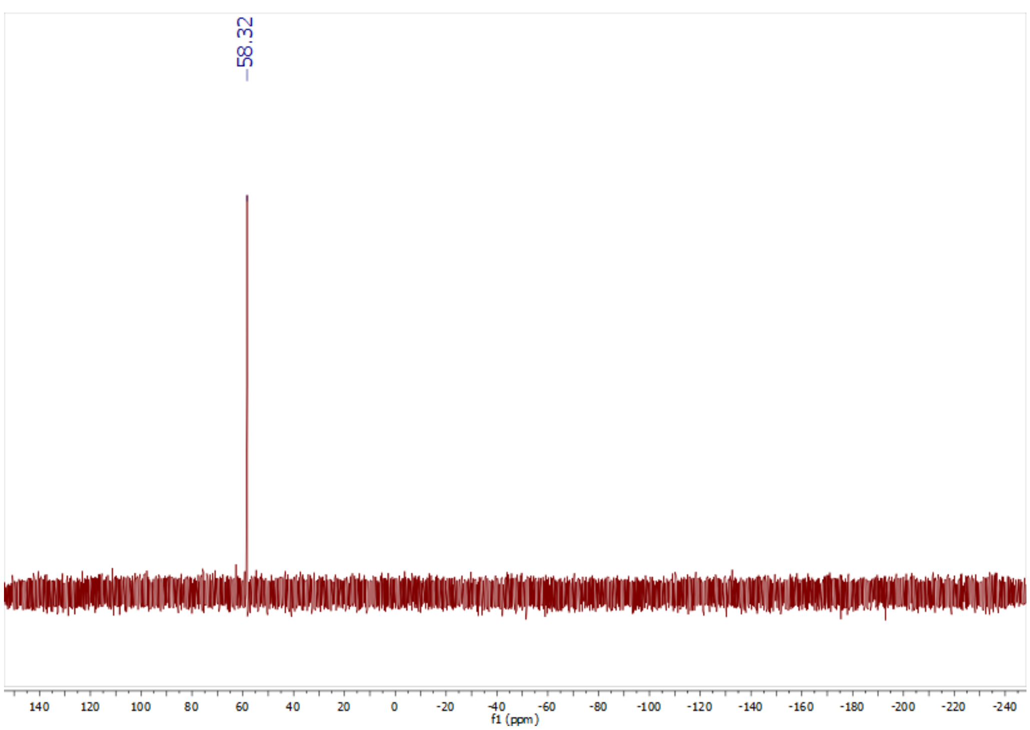
^{13}C NMR **2[IMP-NO$_2$]** (CD_2Cl_2, 126 MHz)



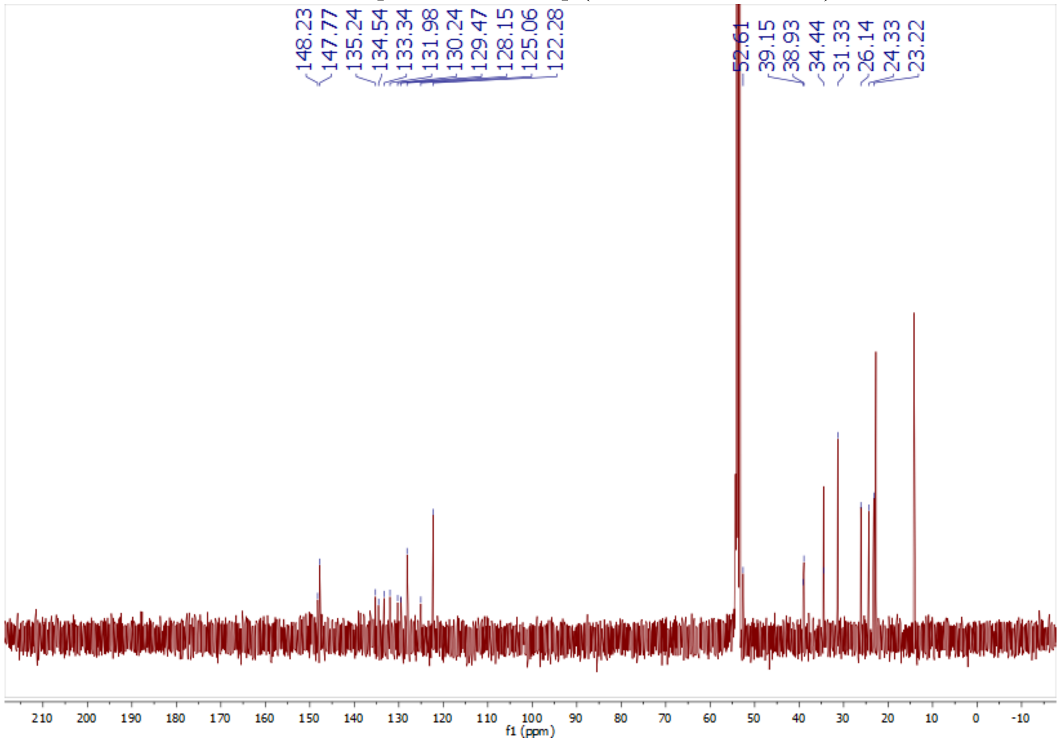
^{1}H NMR **2[IMP-CO$_2$Me]** (CD_2Cl_2, 500 MHz)



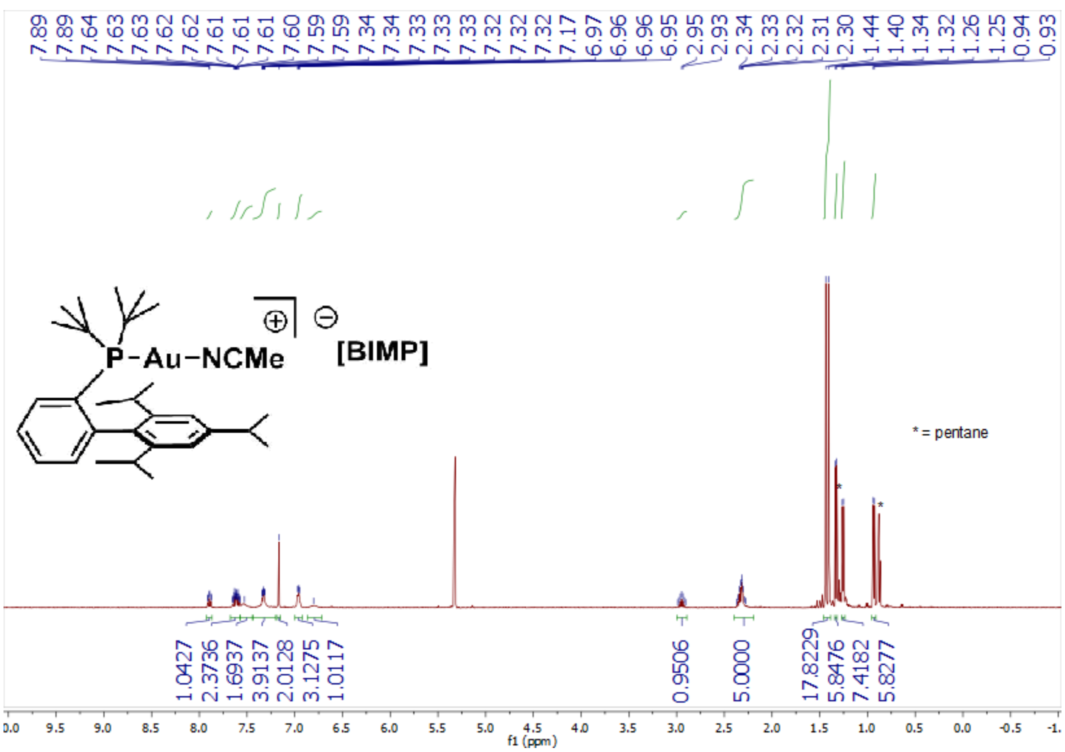
^{31}P NMR **2[IMP-CO$_2$Me]** (CD_2Cl_2, 203 MHz)



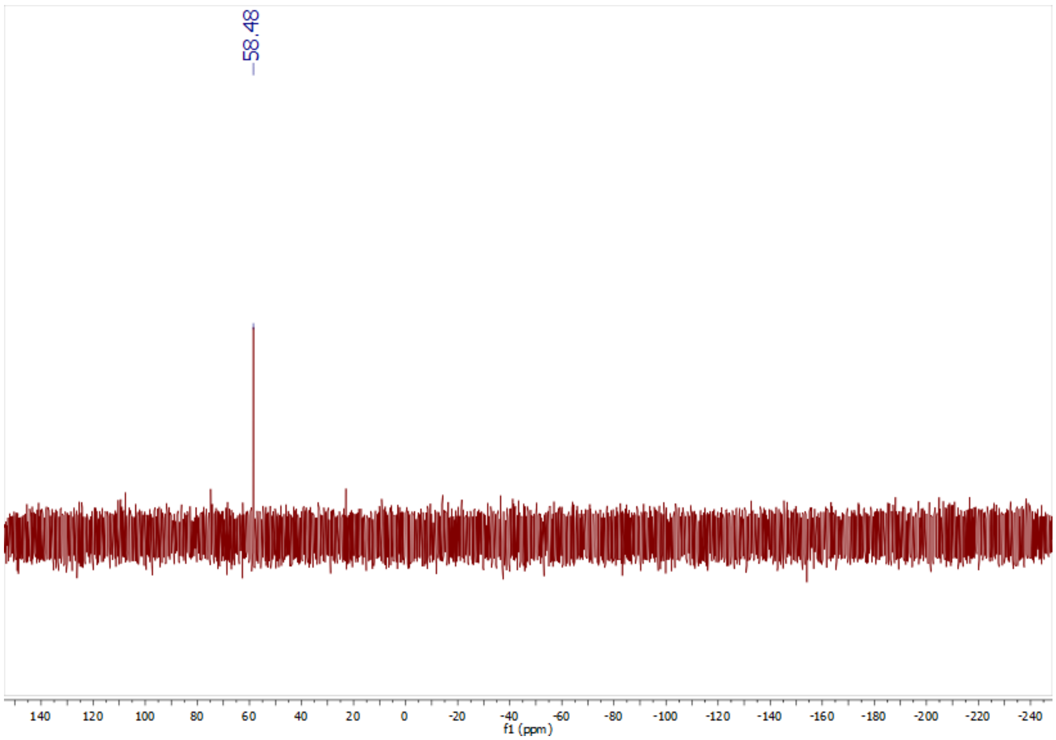
^{13}C NMR **2[IMP-CO$_2$Me]** (CD_2Cl_2, 126 MHz)



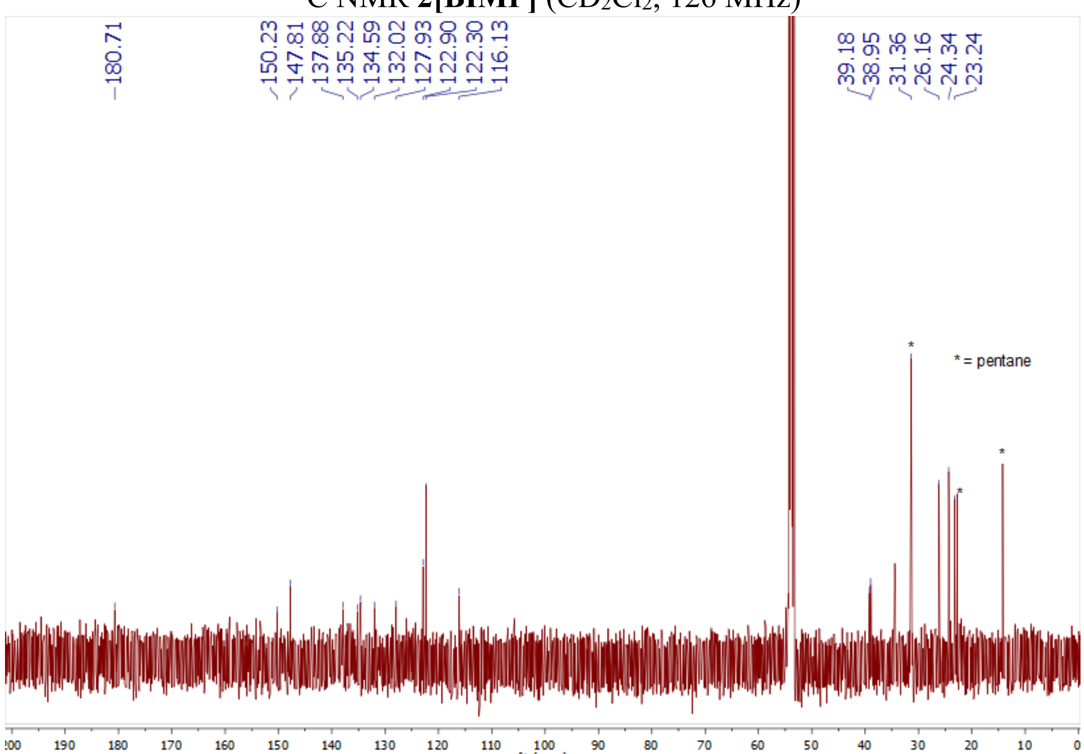
^{1}H NMR **2[BIMP]** (CD_2Cl_2, 500 MHz)



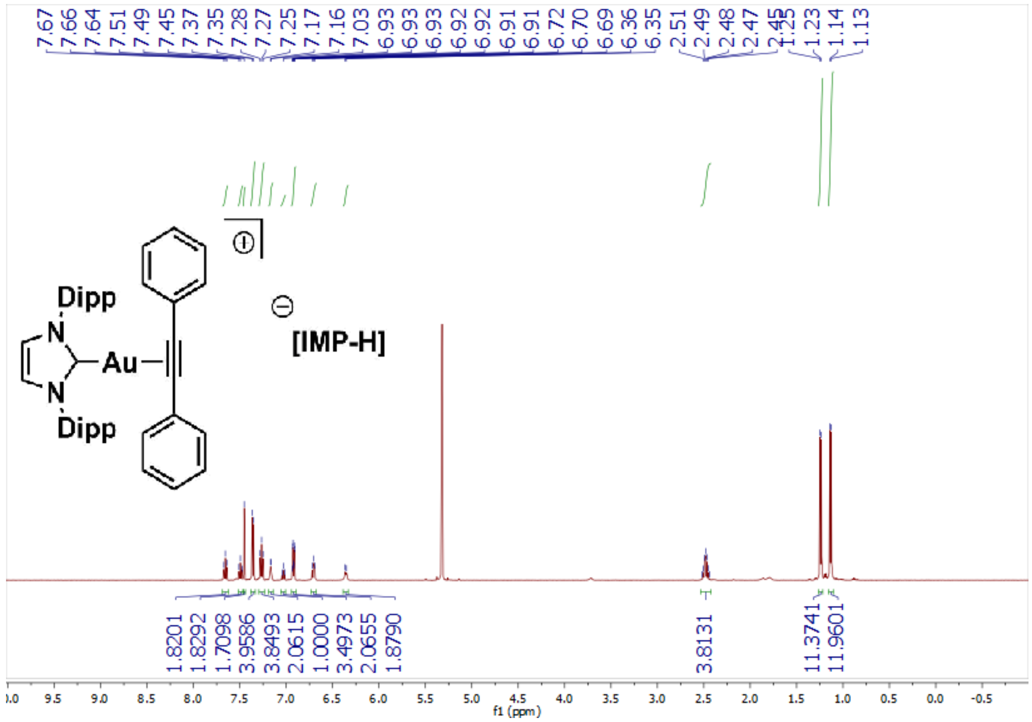
^{31}P NMR **2[BIMP]** (CD_2Cl_2, 203 MHz)



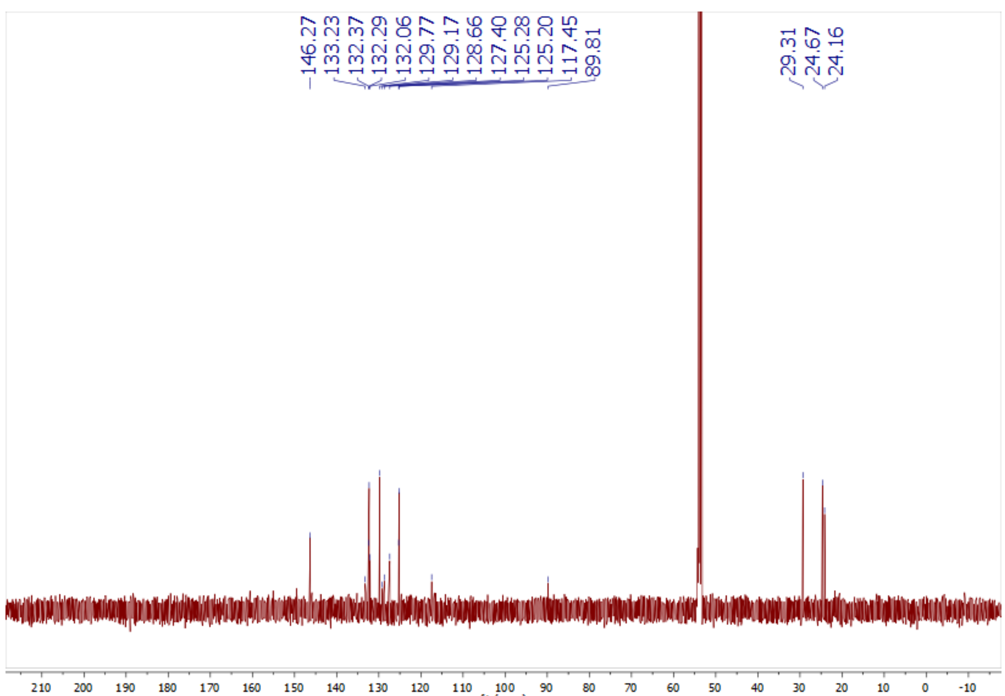
^{13}C NMR **2[BIMP]** (CD_2Cl_2, 126 MHz)



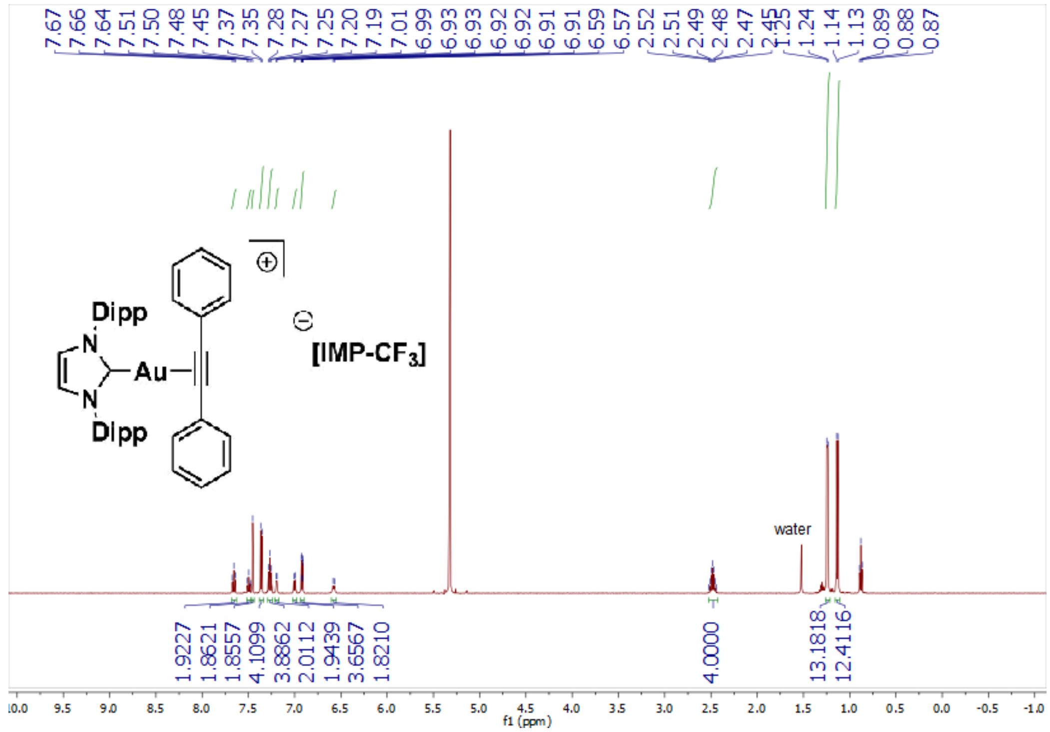
^1H NMR **3[IMP-H]** (CD_2Cl_2, 500 MHz)



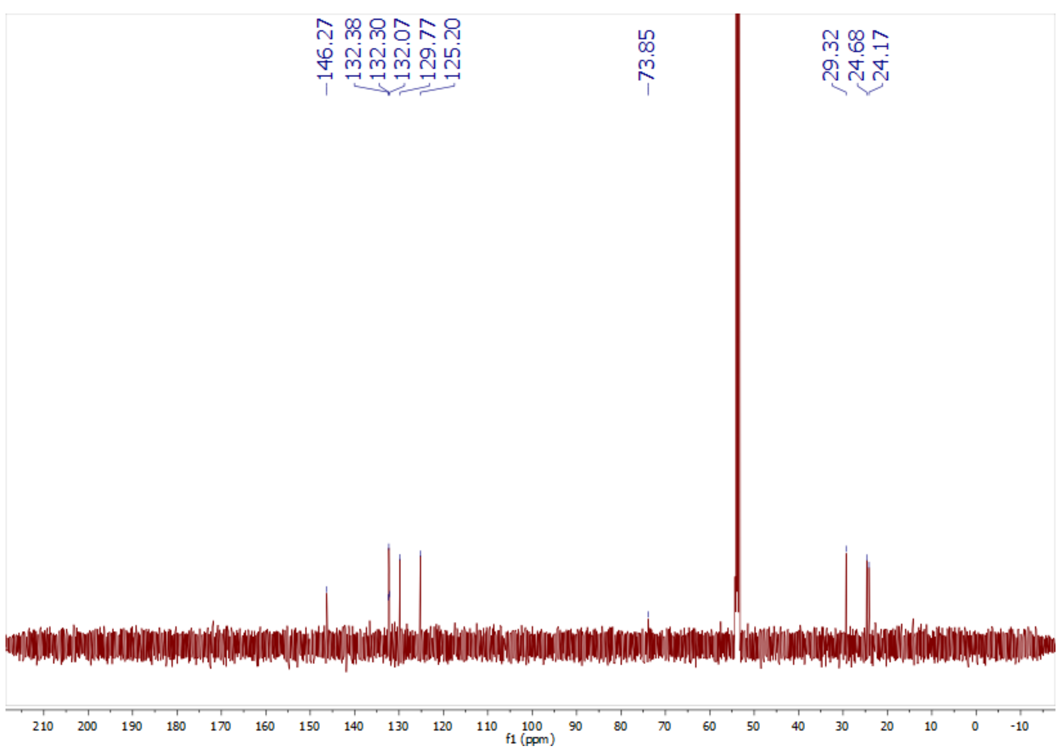
^{13}C NMR **3[IMP-H]** (CD_2Cl_2, 126 MHz)



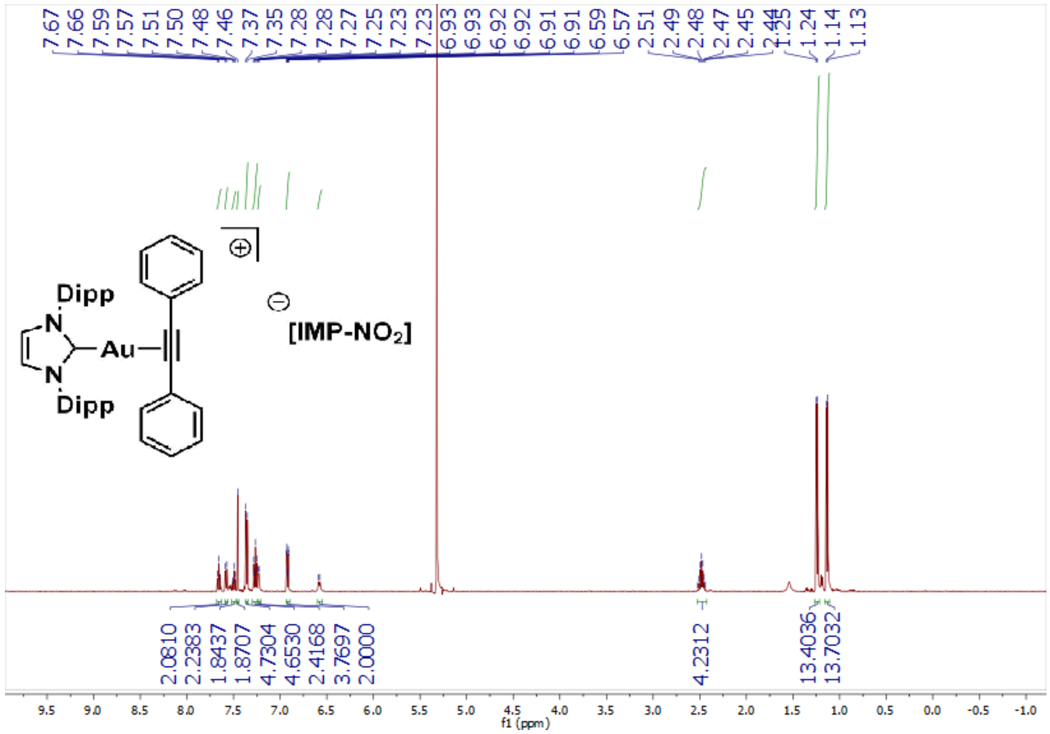
^1H NMR **3[IMP-CF$_3$]** (CD_2Cl_2, 500 MHz)



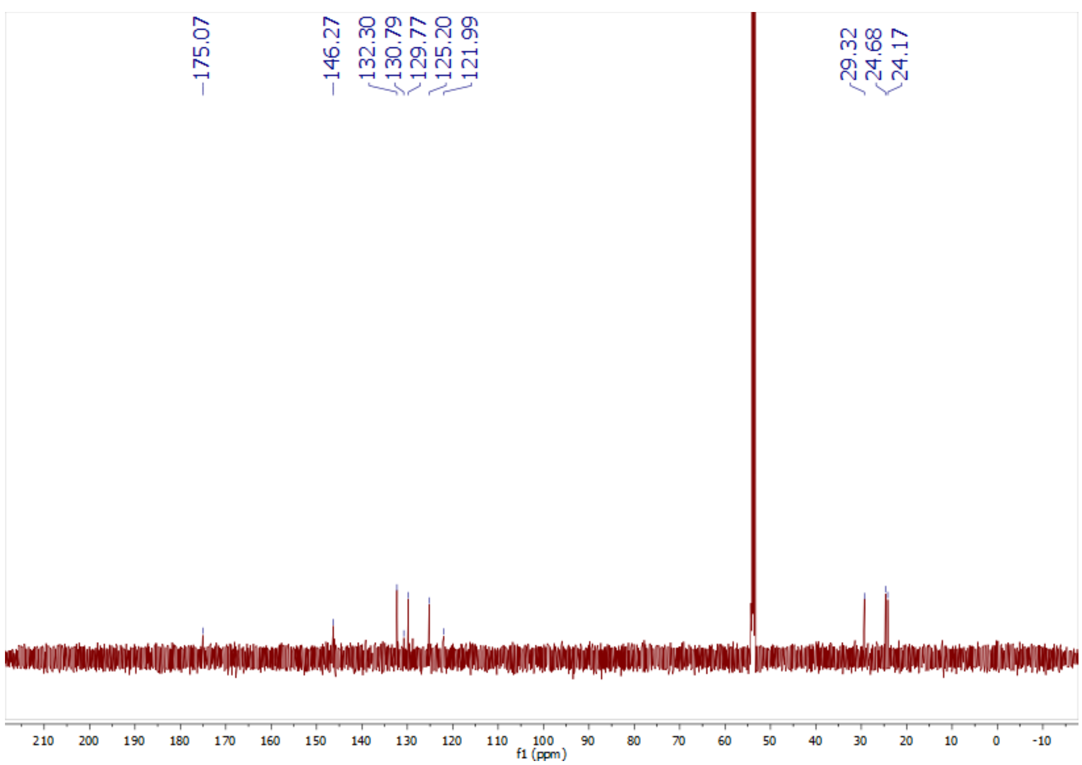
^{13}C NMR **3[IMP-CF$_3$]** (CD_2Cl_2, 126 MHz)



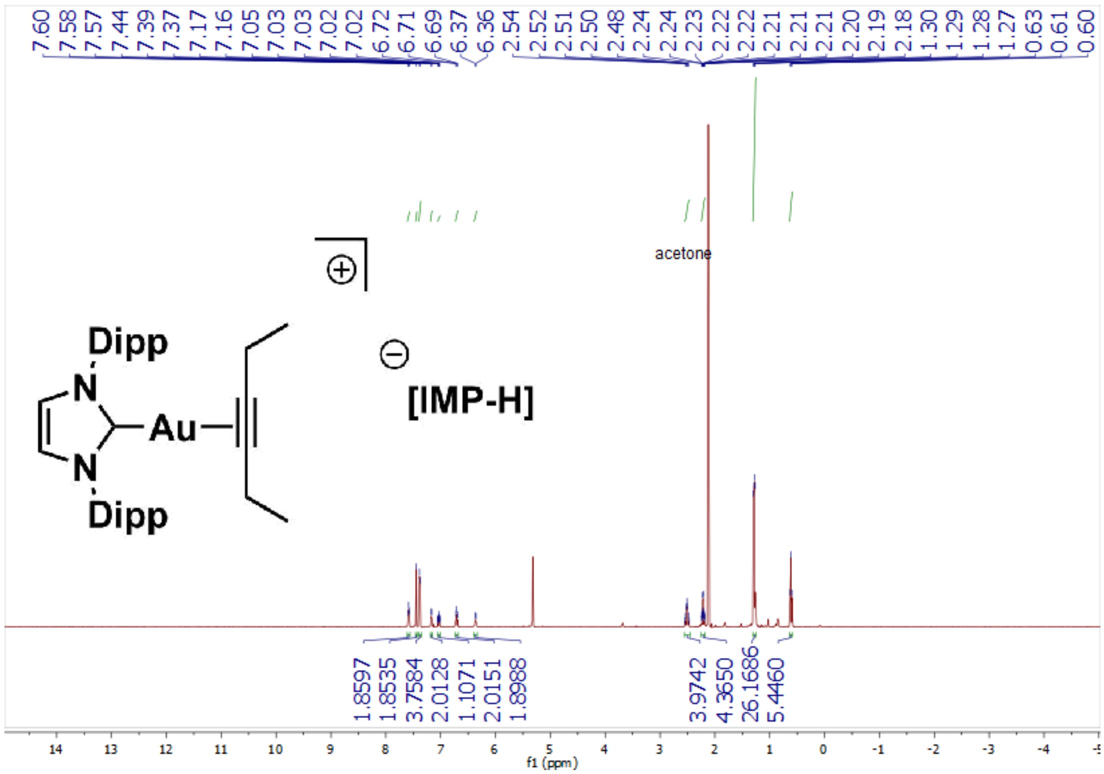
[1]H NMR **3[IMP-NO$_2$]** (CD_2Cl_2, 500 MHz)



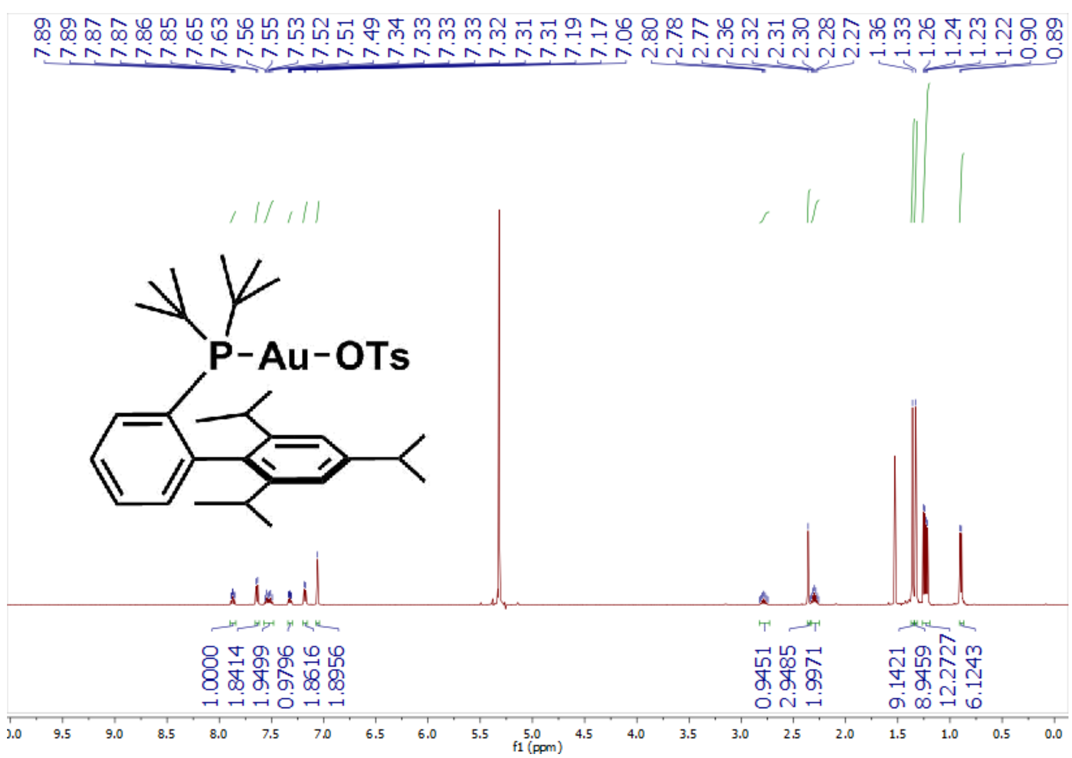
[13]C NMR **3[IMP-NO$_2$]** (CD_2Cl_2, 126 MHz)



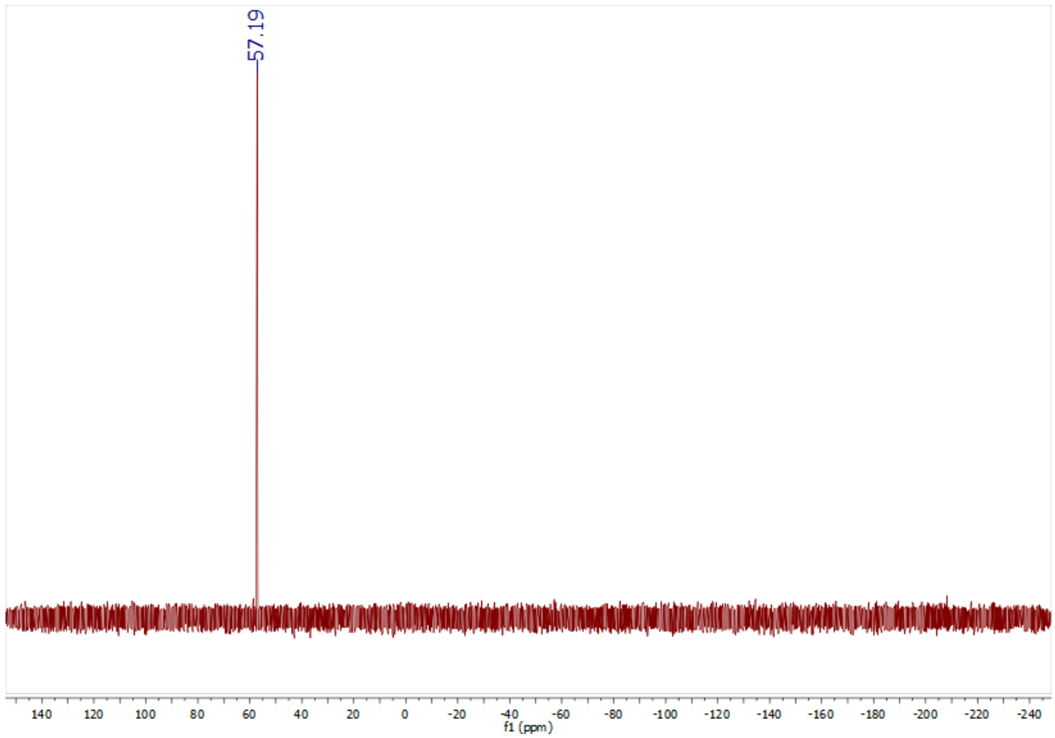
^{1}H NMR **4[IMP-H]** (CD_2Cl_2, 500 MHz)



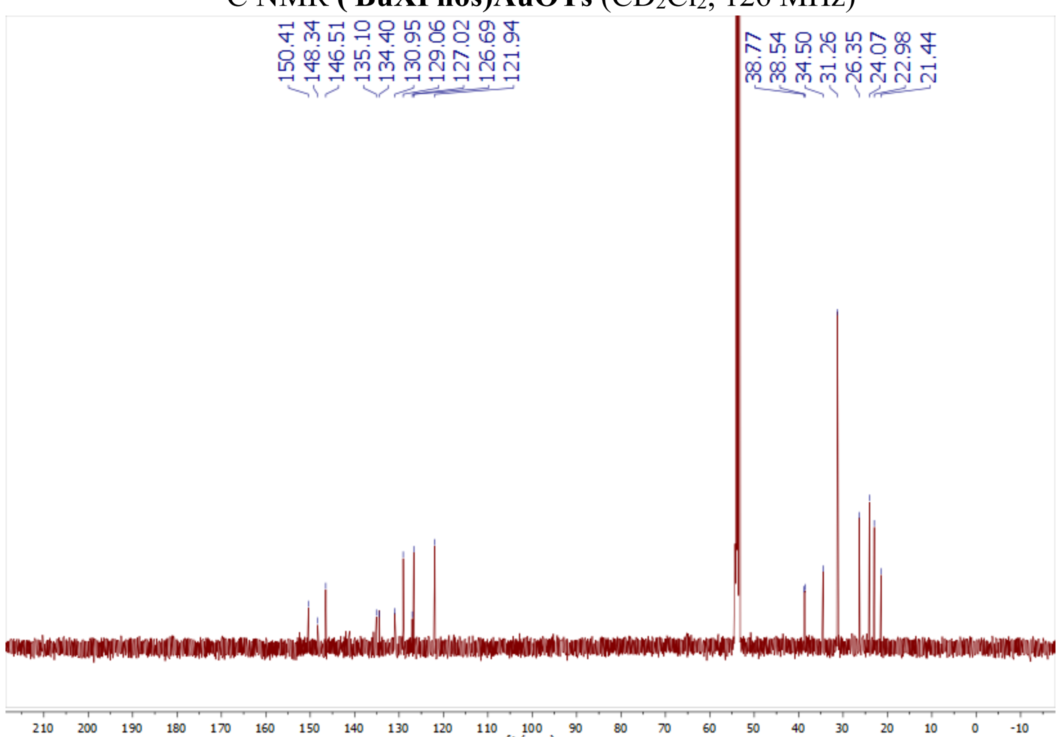
^{1}H NMR **(^{t}BuXPhos)AuOTs** (CD_2Cl_2, 500 MHz)



^{31}P NMR **(^{t}BuXPhos)AuOTs** (CD_2Cl_2, 203 MHz)

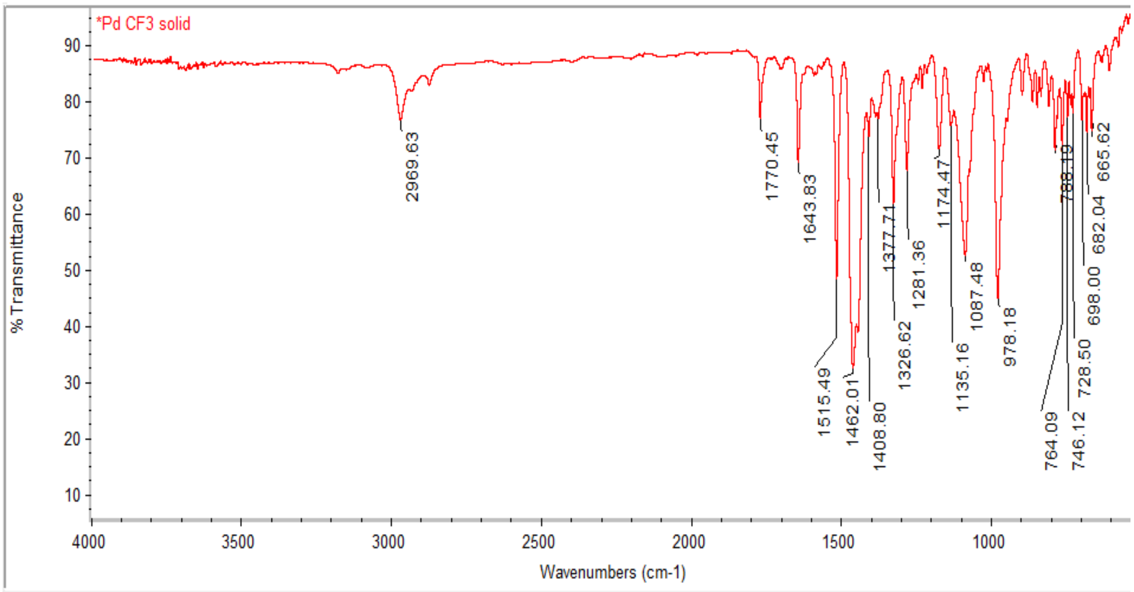


^{13}C NMR **(^{t}BuXPhos)AuOTs** (CD_2Cl_2, 126 MHz)

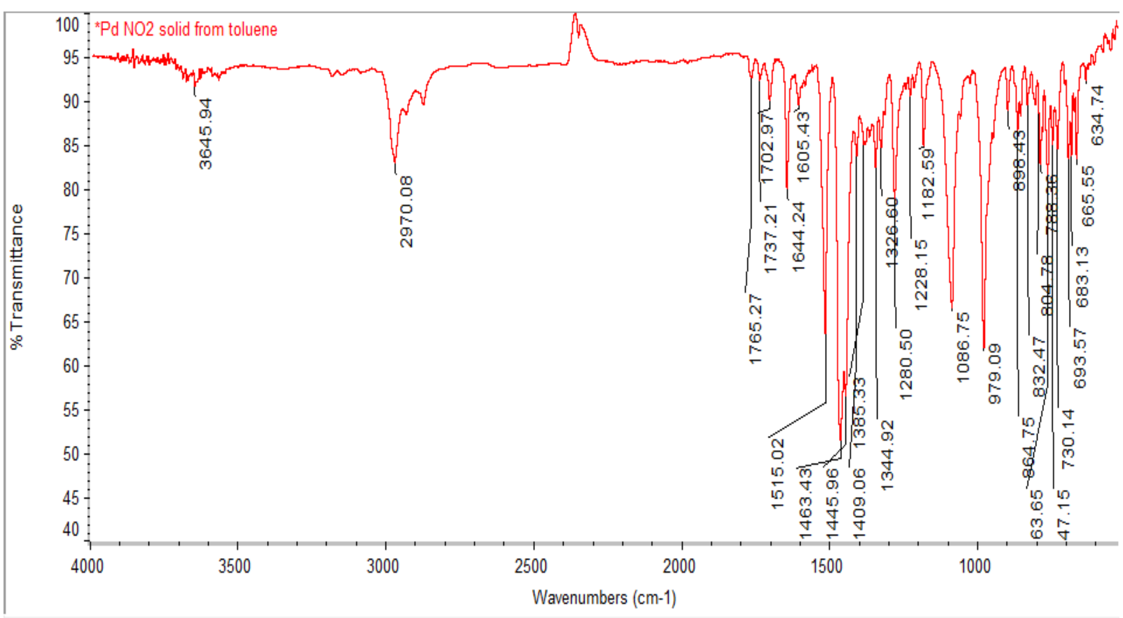


II. Solid-State IR Spectra

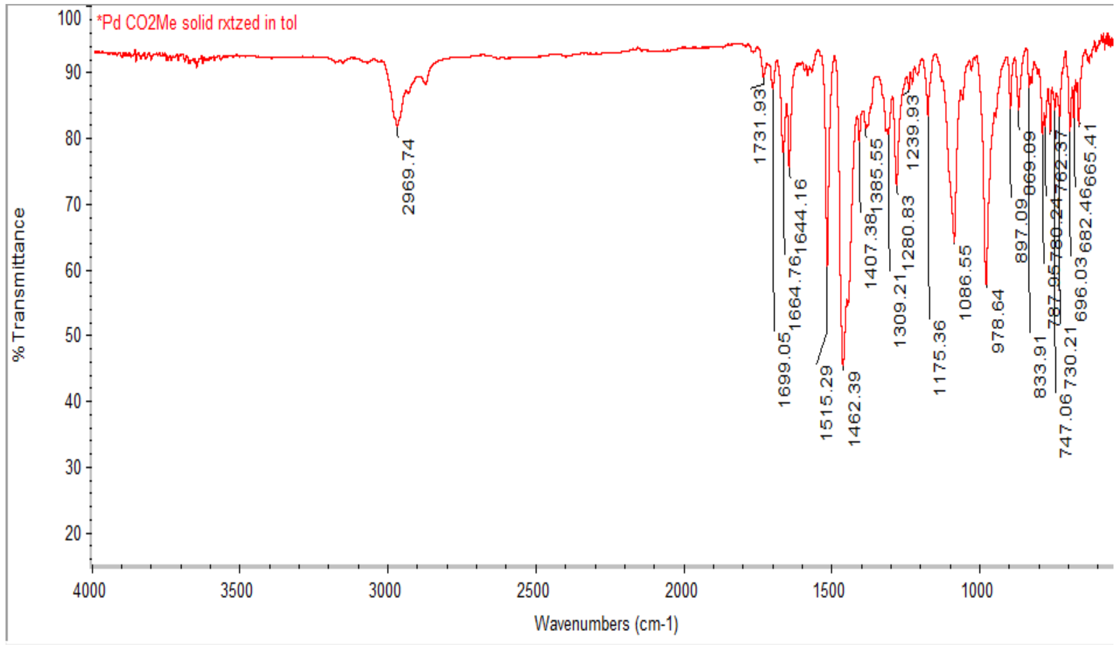
ATR-FTIR 1[IMP-CF$_3$]



ATR-FTIR 1[IMP-NO$_2$]

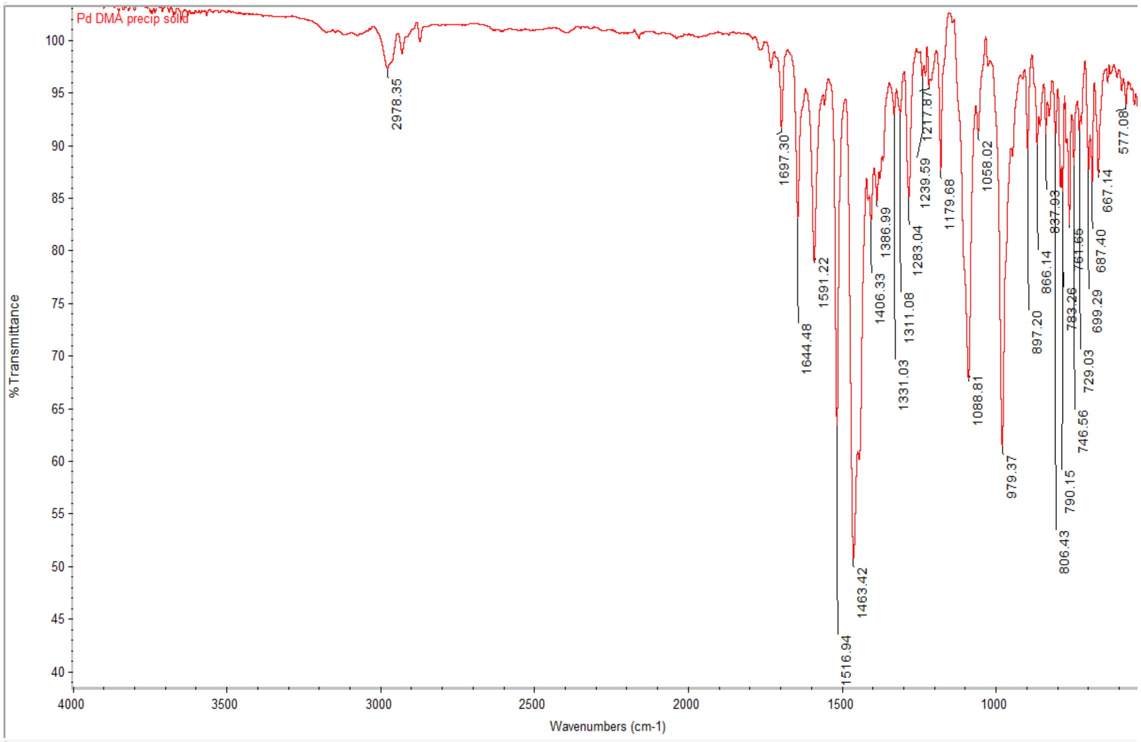


ATR-FTIR 1[IMP-CO_2Me]

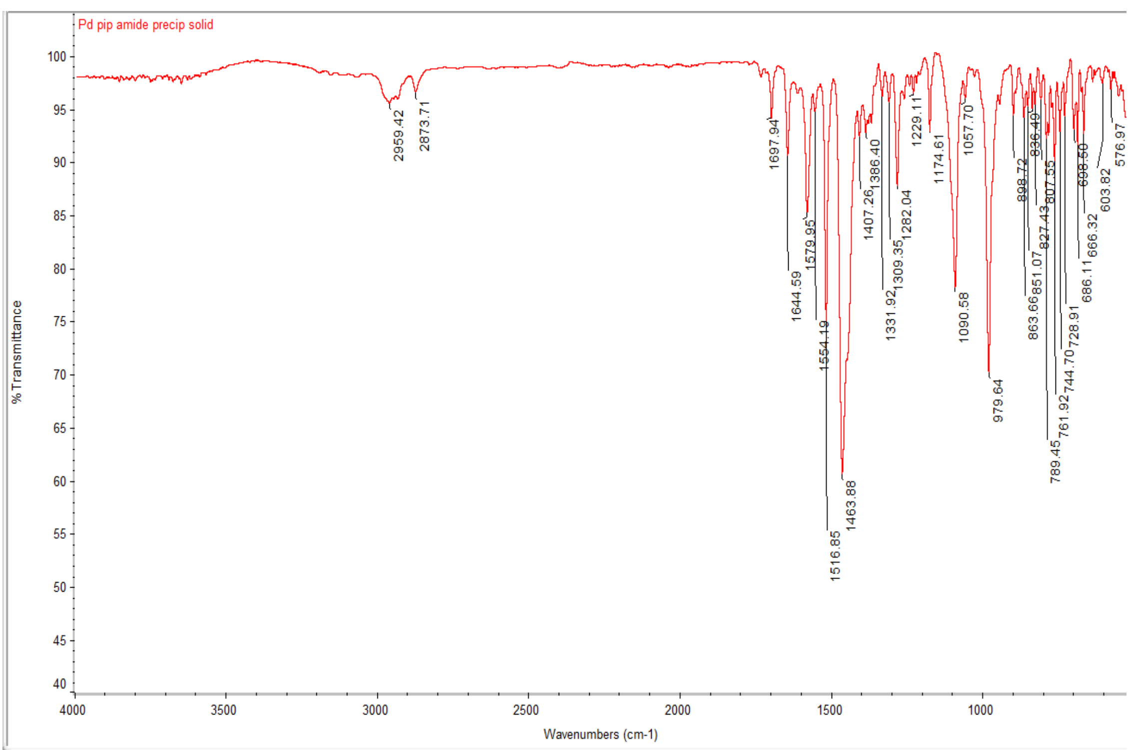


ATR-FTIR 1[IMP-$(CF_3)_2$]

ATR-FTIR 1[IMP-DMA]



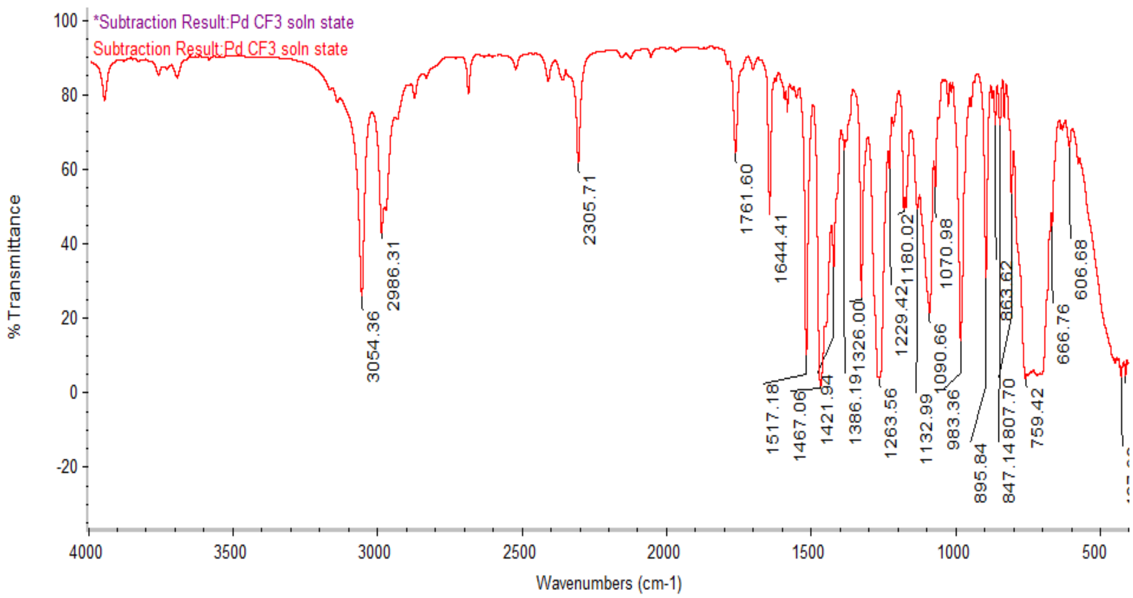
ATR-FTIR 1[IMP-pipA]



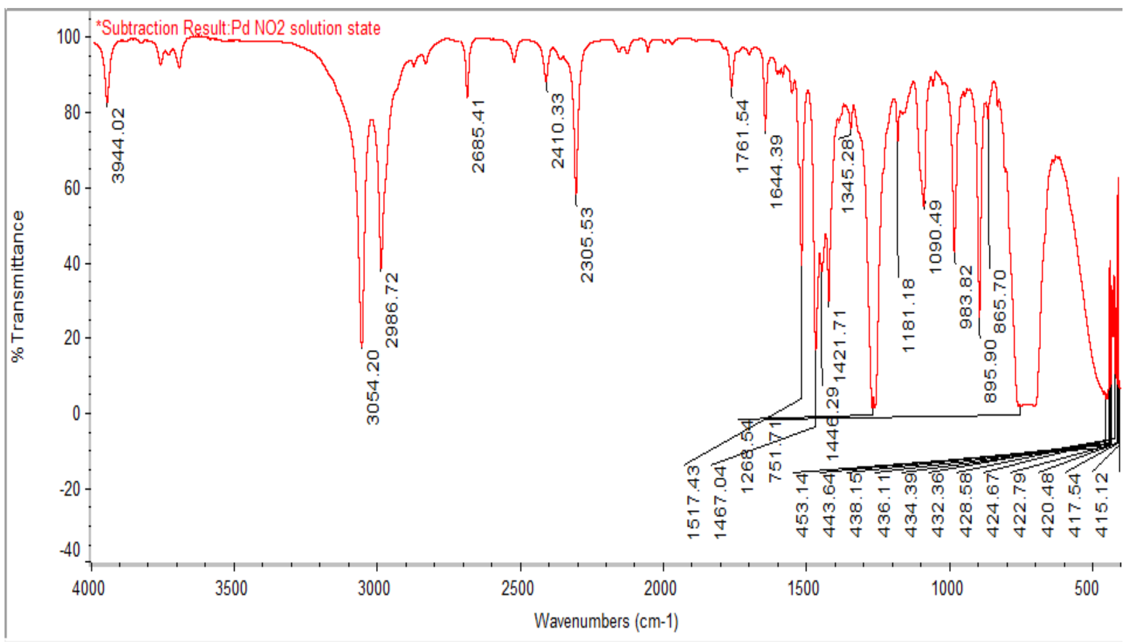
III. Solution-State IR

All solutions were prepared in an inert atmosphere glovebox as 10mM solutions in methylene chloride and injected into NaCl-window solution cells.

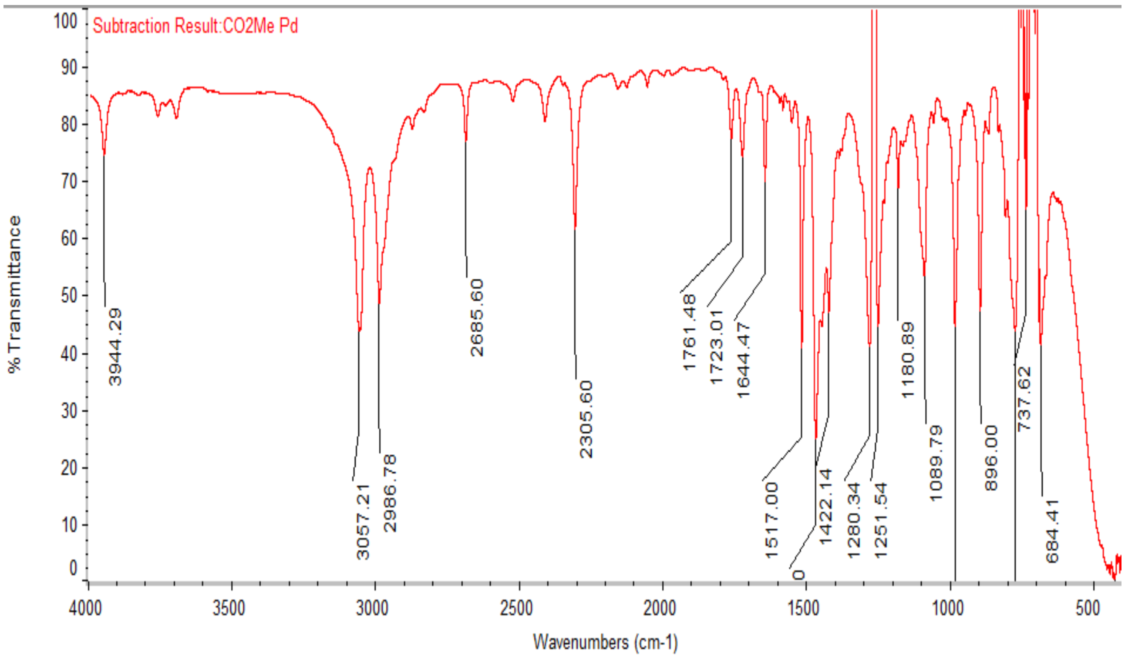
Solution-State 1[IMP-CF_3]



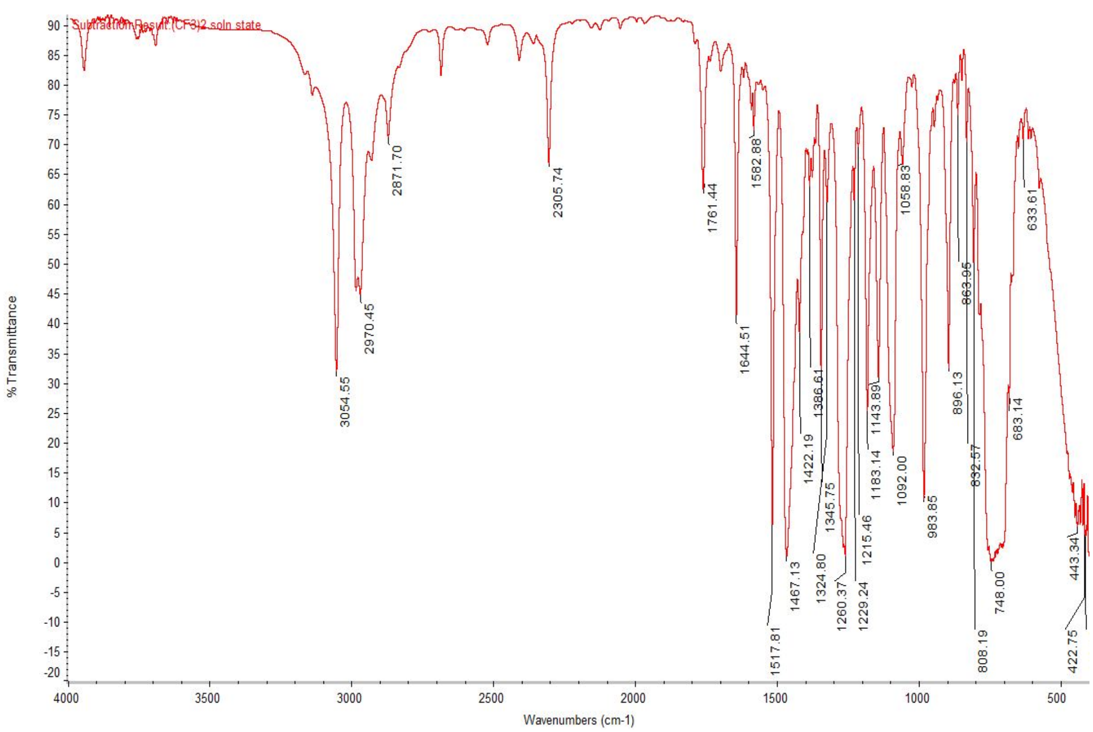
Solution-State 1[IMP-NO_2]



Solution-State 1[IMP-CO_2Me]



Solution-State 1[IMP-$(CF_3)_2$]



IV. References

(1) Fulmer, G. R.; Miller, A. J. M.; Sherden, N. H.; Gottlieb, H. E.; Nudelman, A.; Stoltz, B. M.; Bercaw, J. E.; Goldberg, K. I. *Organometallics* **2010**, *29*, 2176–2179.