

Supporting Information

Ion Pair-Directed Borylation of Aromatic Phosponium Salts

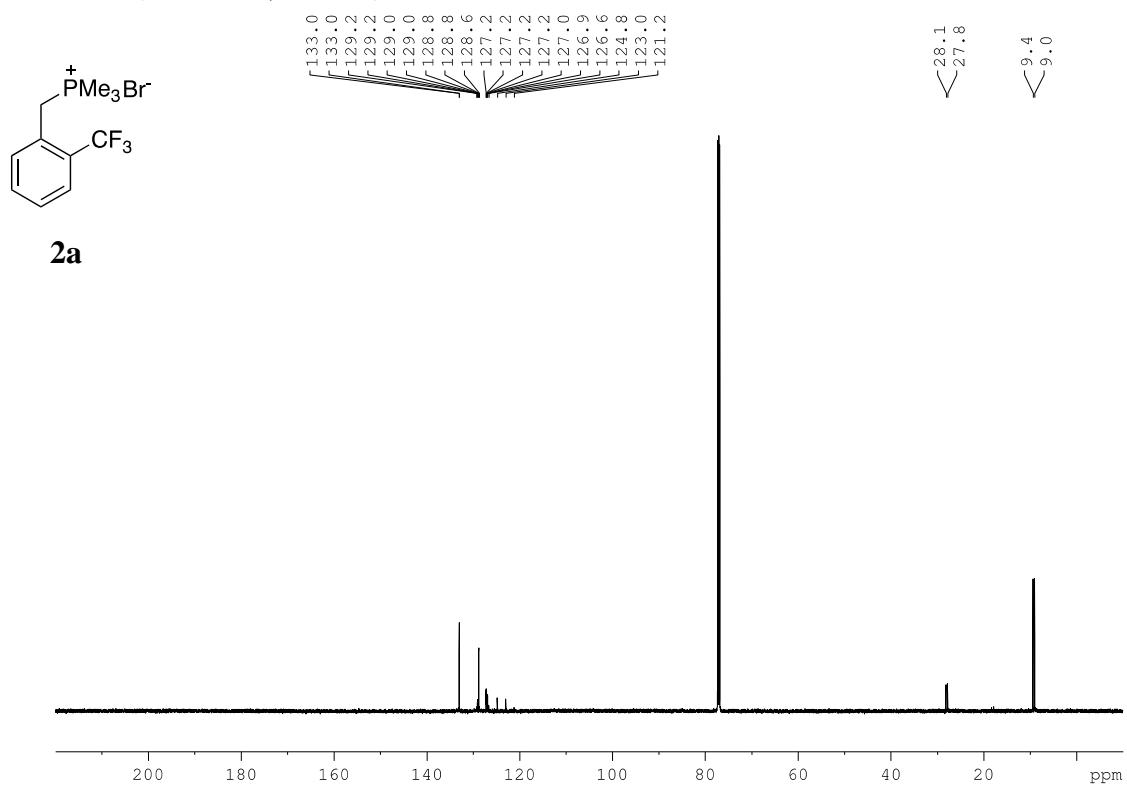
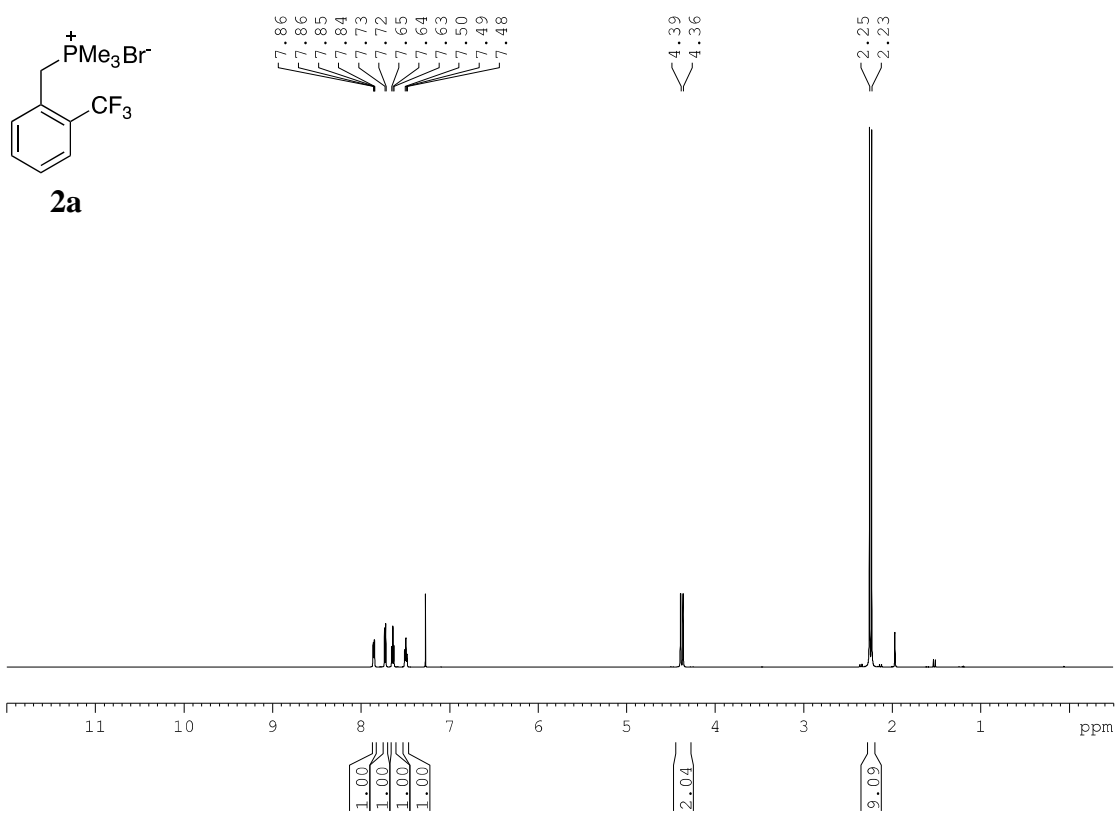
Bernadette Lee, Madalina T. Mihai, Violeta Stojalnikova and Robert J. Phipps*

Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge, CB2 1EW, UK.

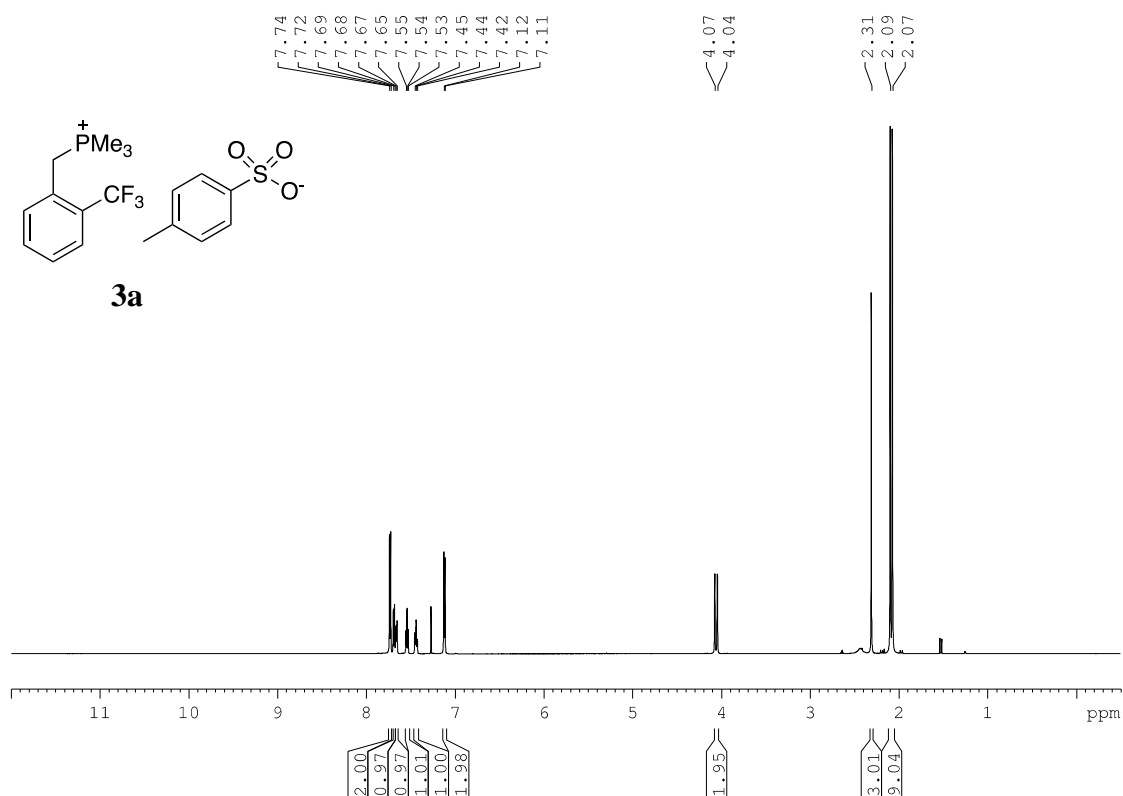
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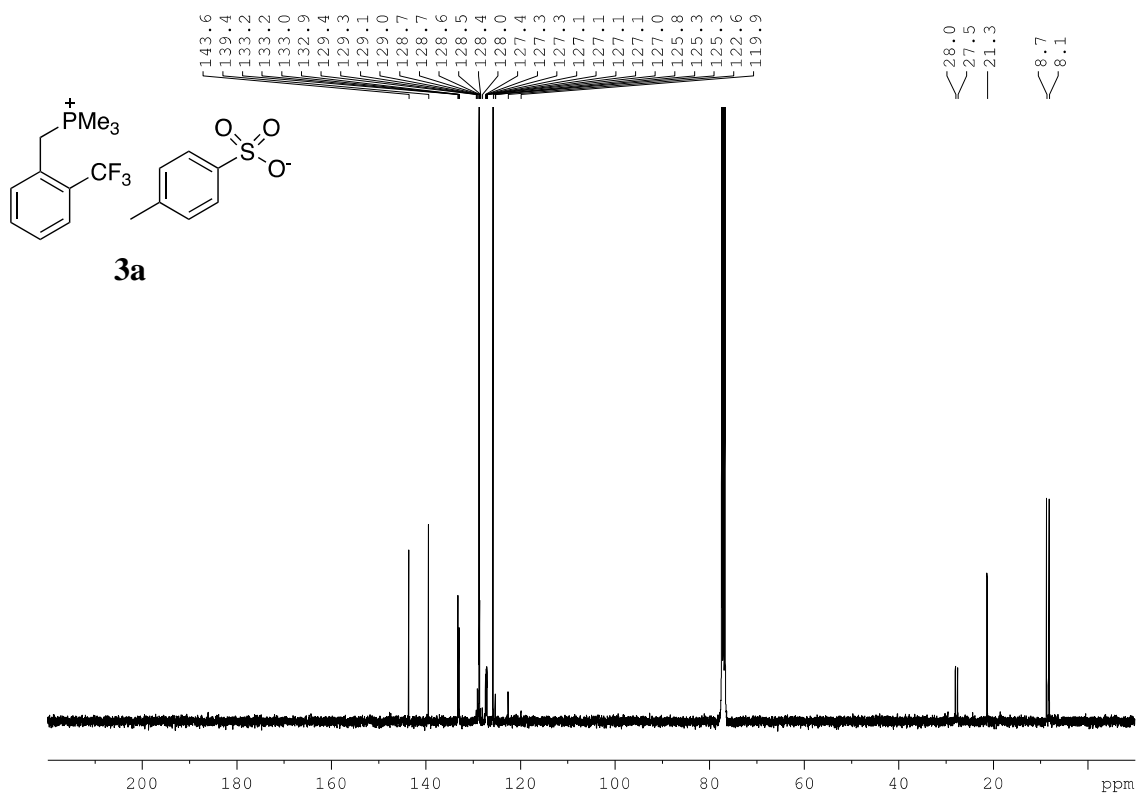
1.1 NMR data for substrates



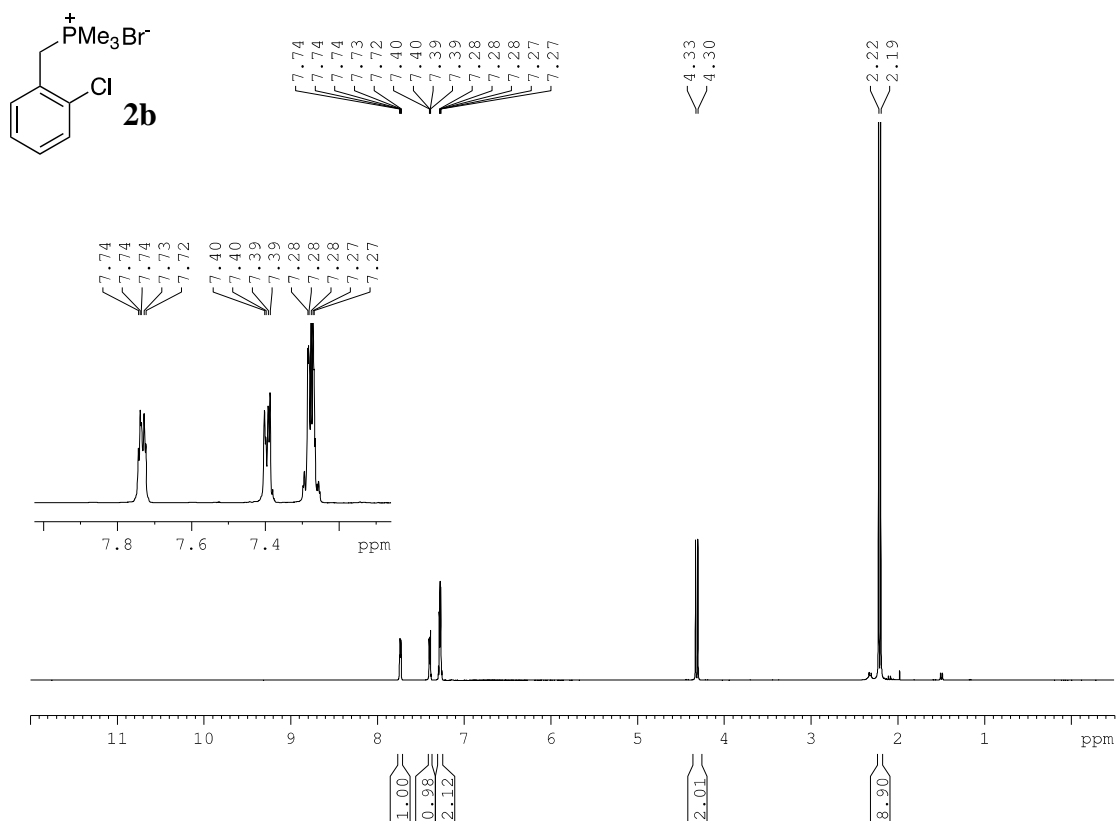
¹H NMR (600 MHz, CDCl₃)



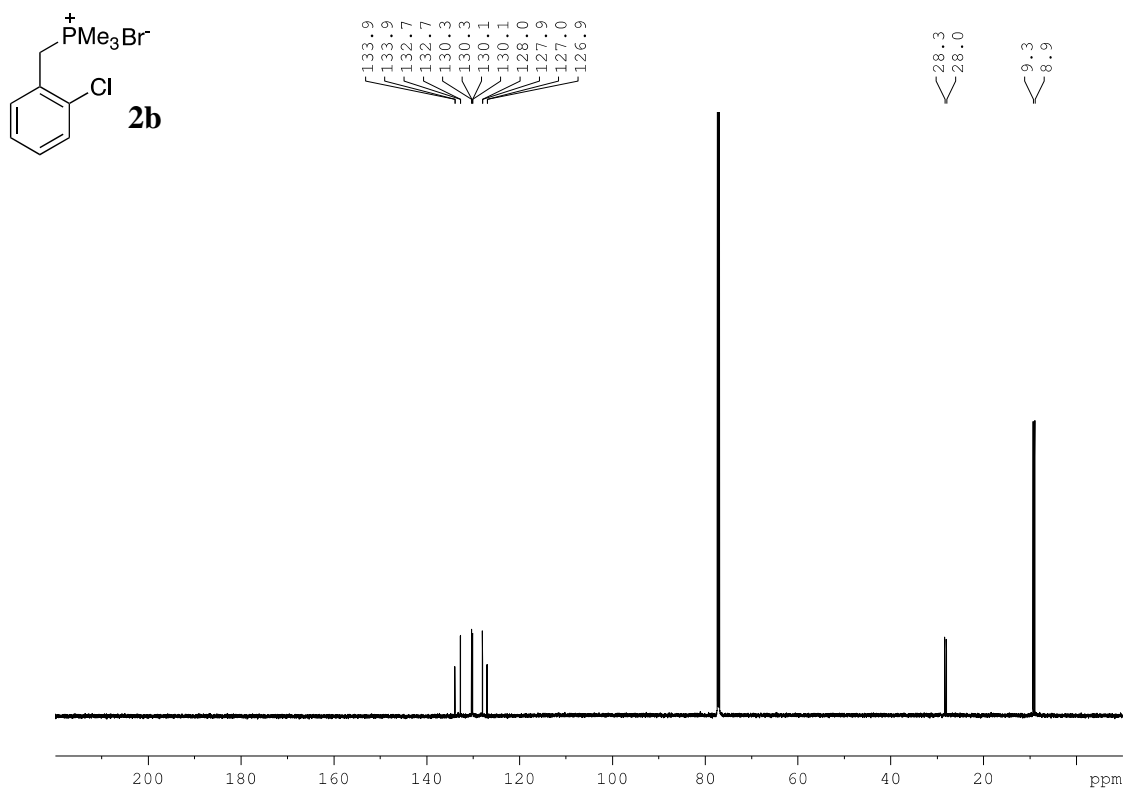
¹³C NMR (101 MHz, CDCl₃)



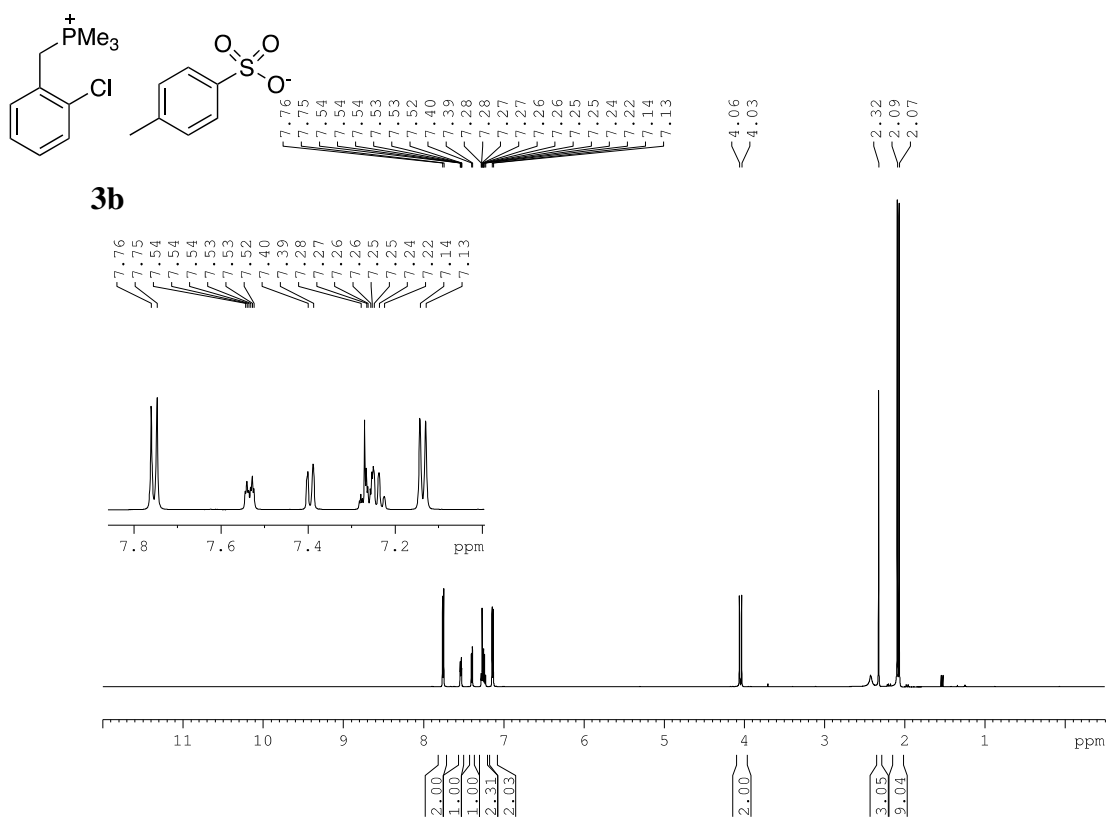
¹H NMR (600 MHz, CDCl₃)



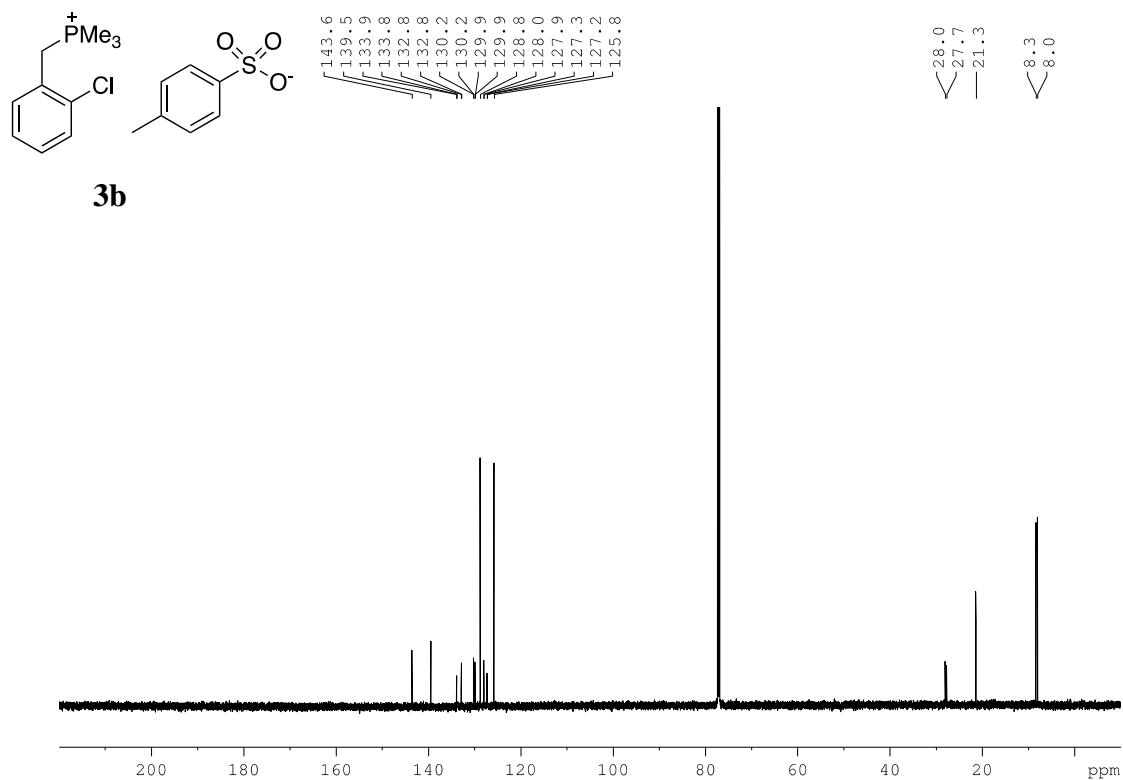
¹³C NMR (151 MHz, CDCl₃)



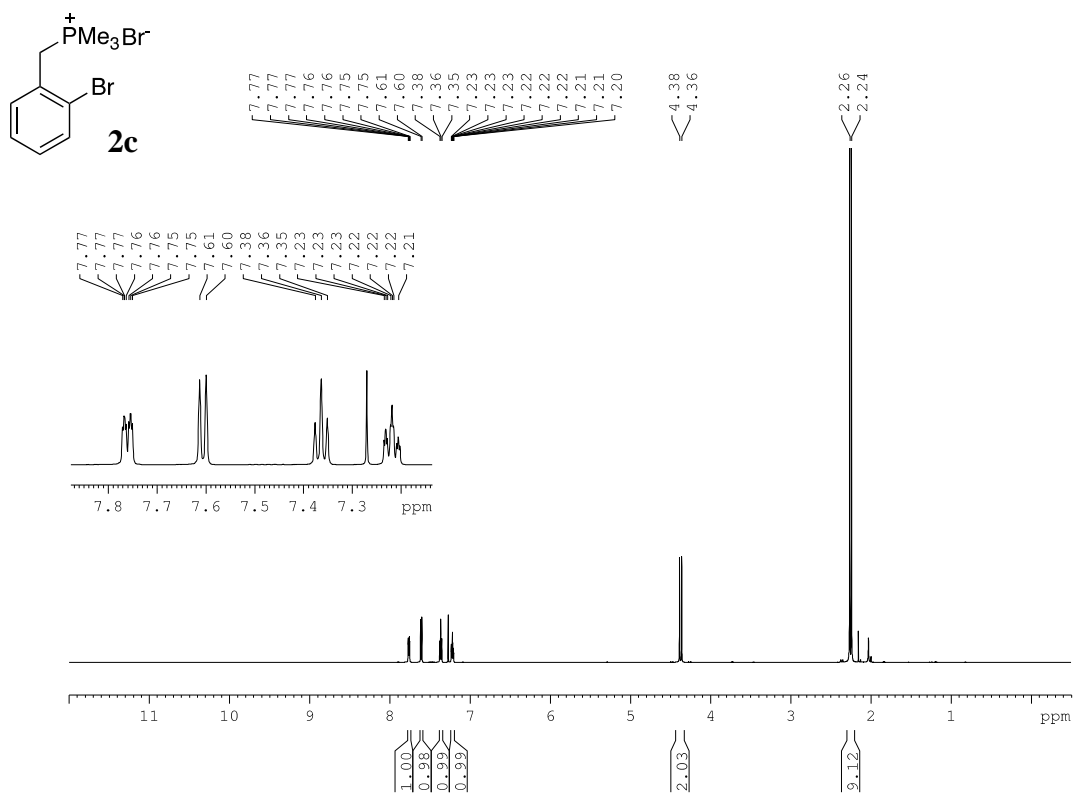
^1H NMR (600 MHz, CDCl_3)



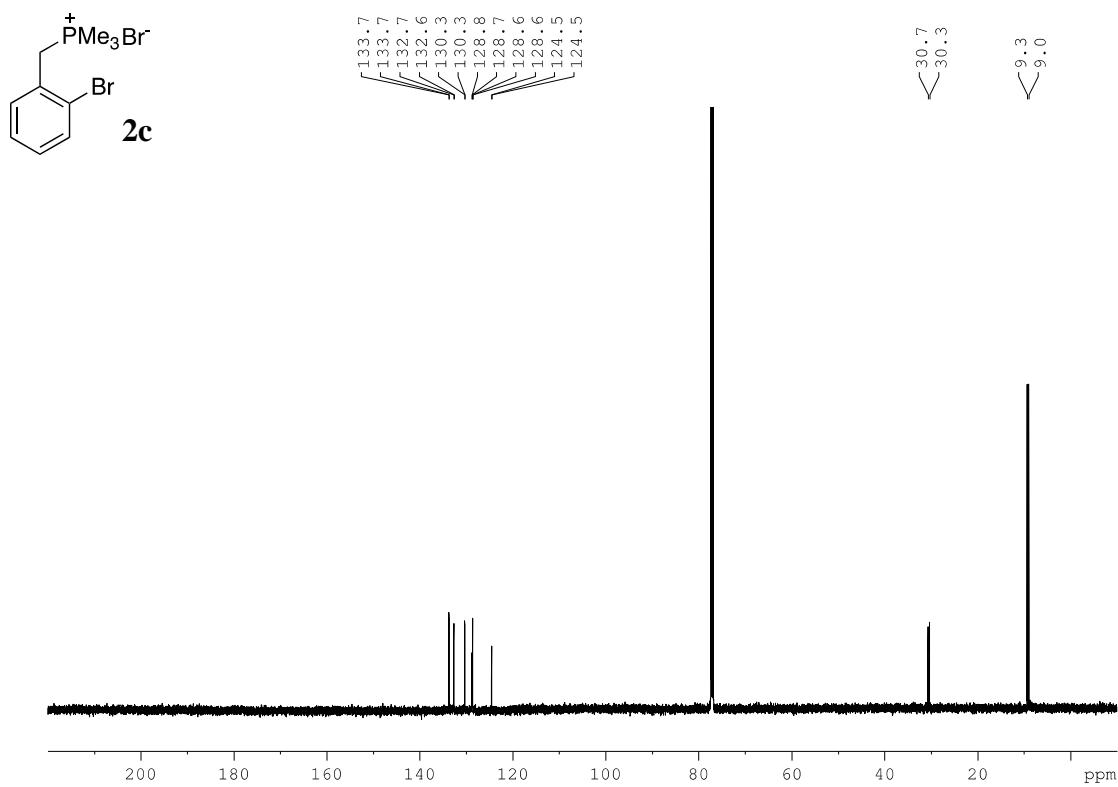
^{13}C NMR (151 MHz, CDCl_3)



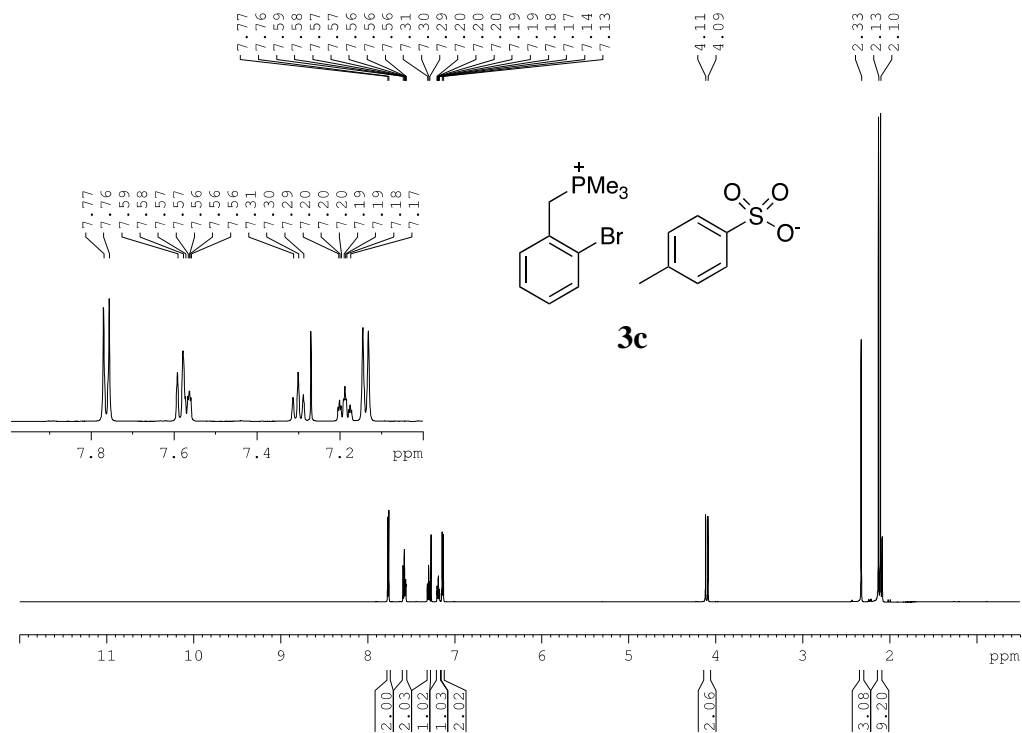
^1H NMR (600 MHz, CDCl_3)



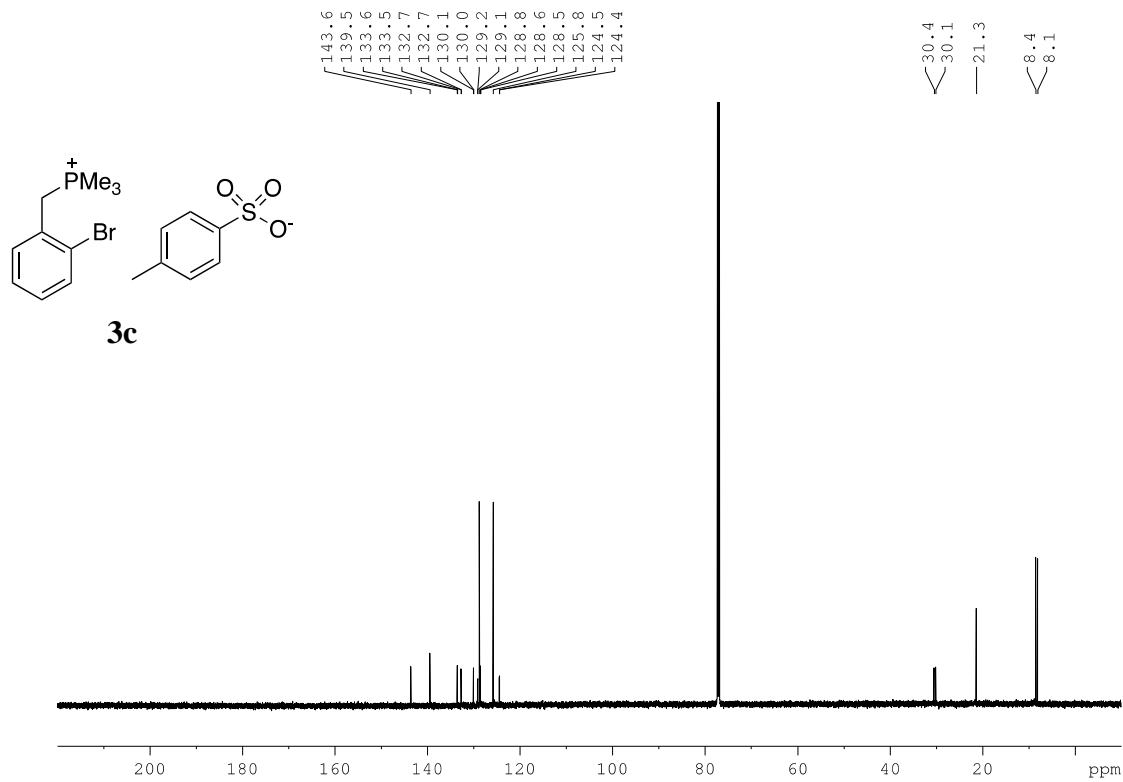
^{13}C NMR (151 MHz, CDCl_3)



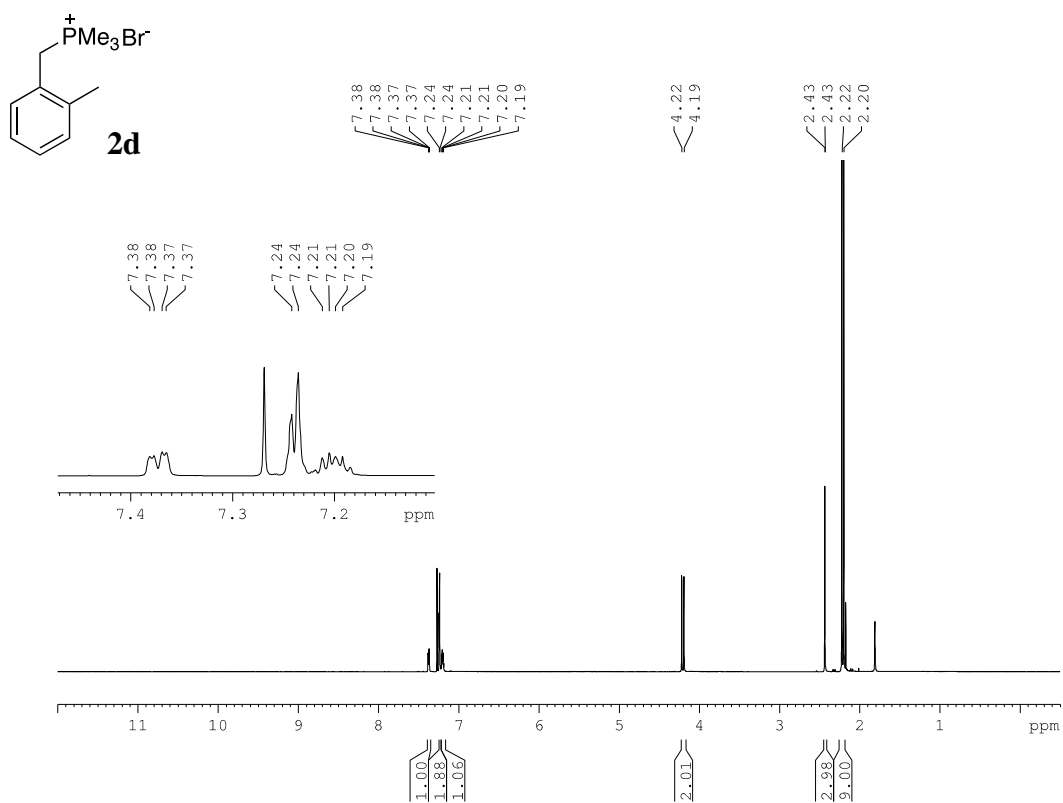
^1H NMR (600 MHz, CDCl_3)



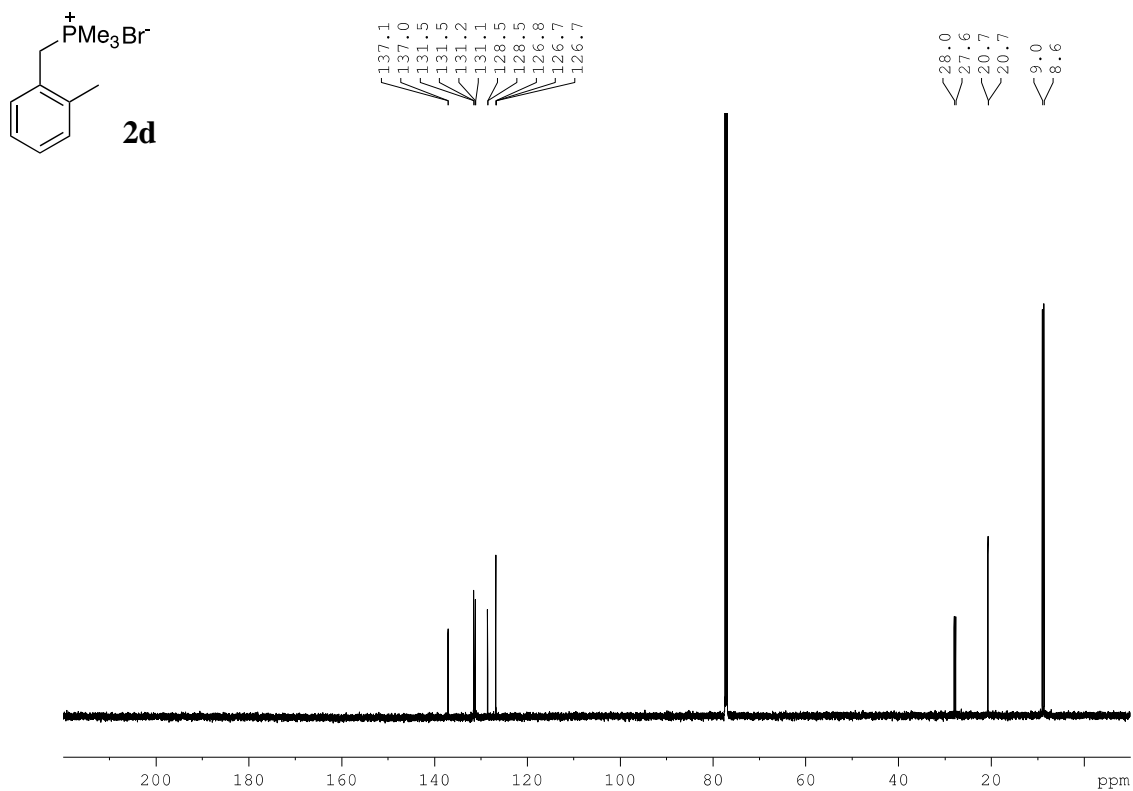
^{13}C NMR (151 MHz, CDCl_3)



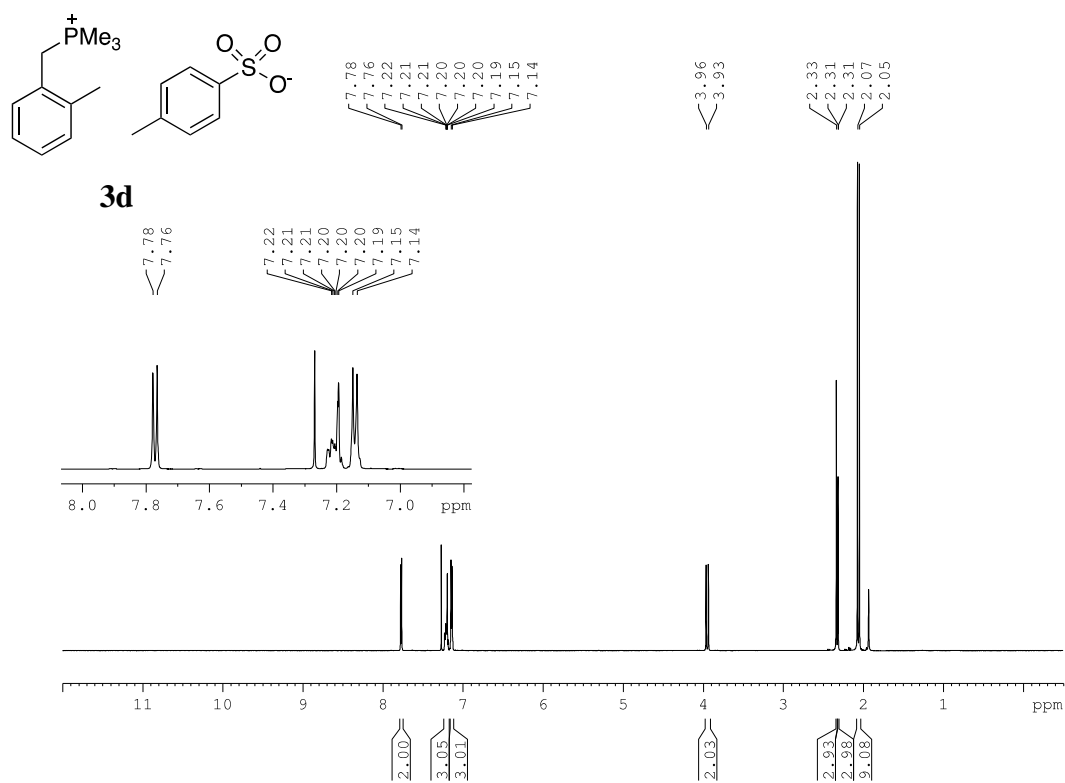
^1H NMR (600 MHz, CDCl_3)



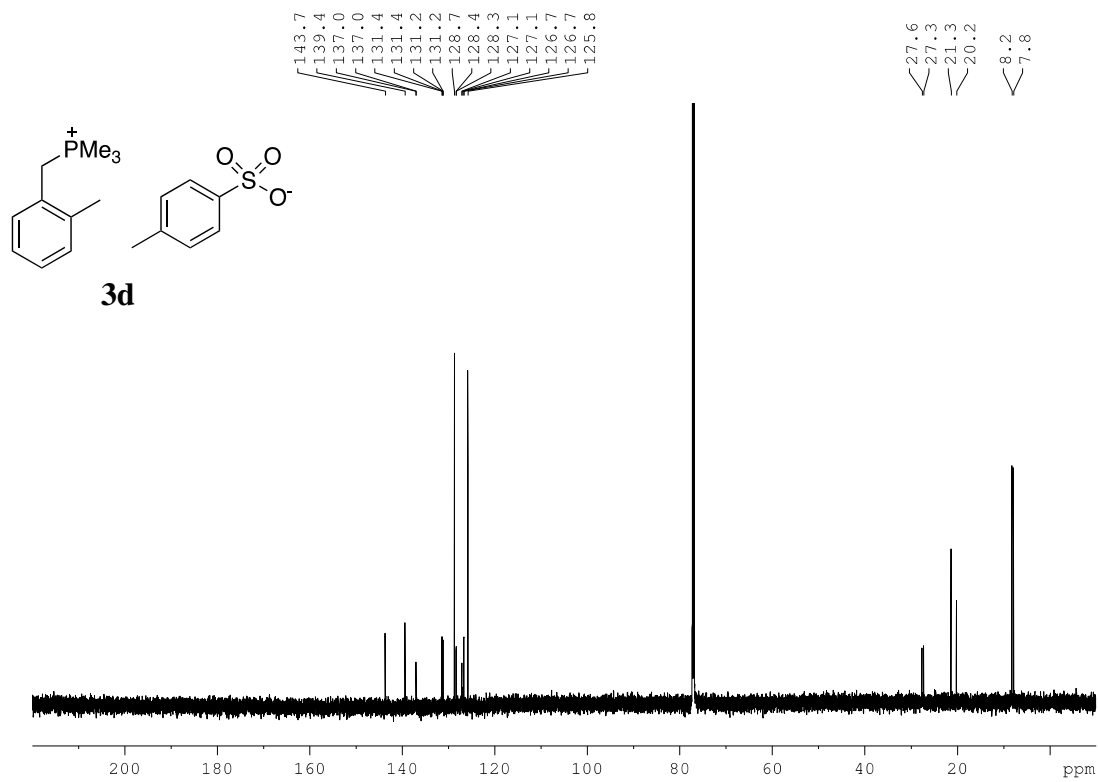
^{13}C NMR (151 MHz, CDCl_3)



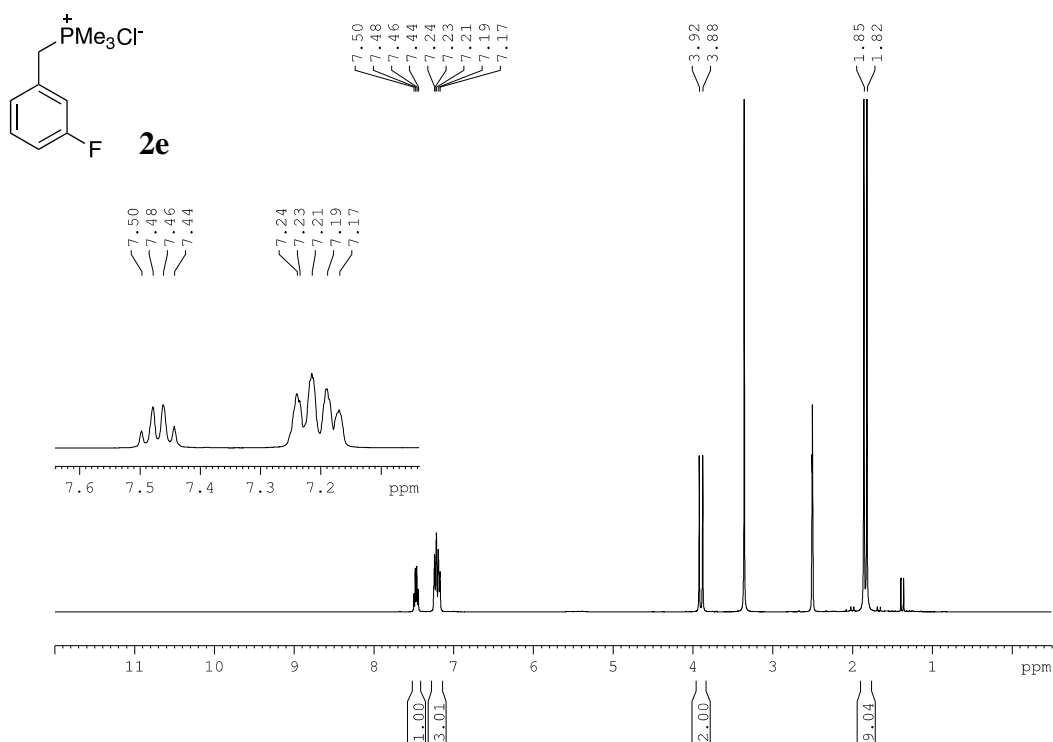
^1H NMR (600 MHz, CDCl_3)



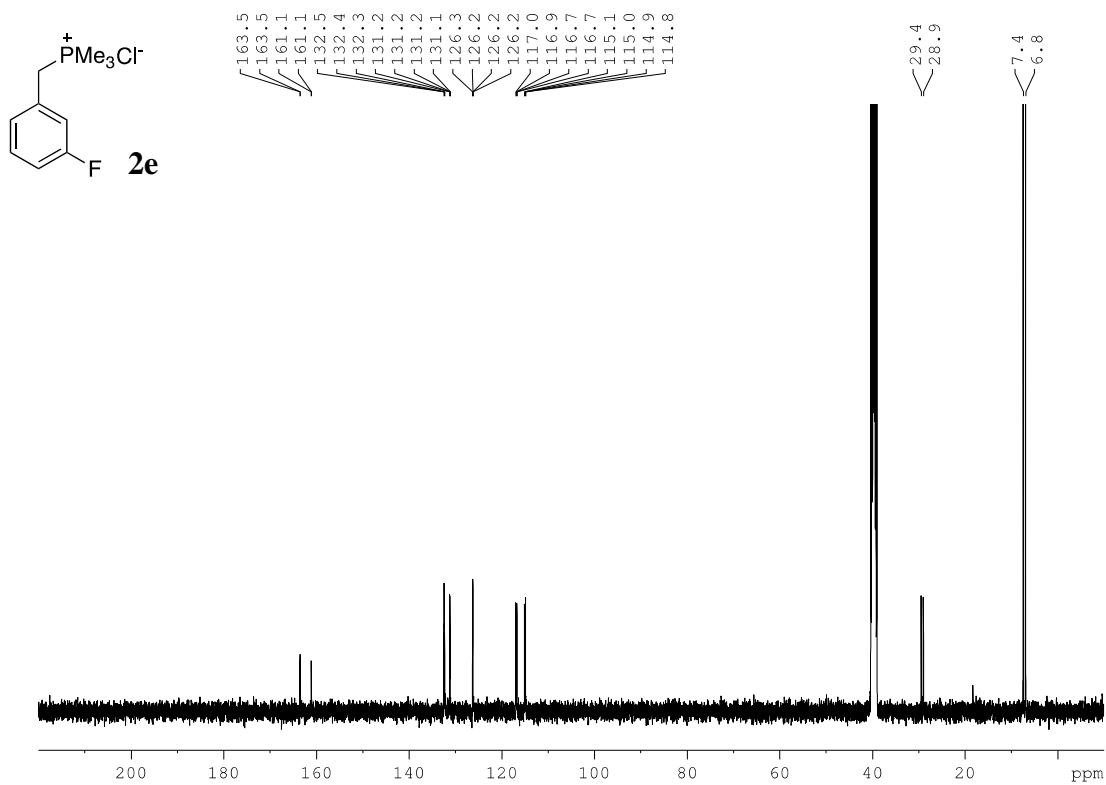
^{13}C NMR (151 MHz, CDCl_3)



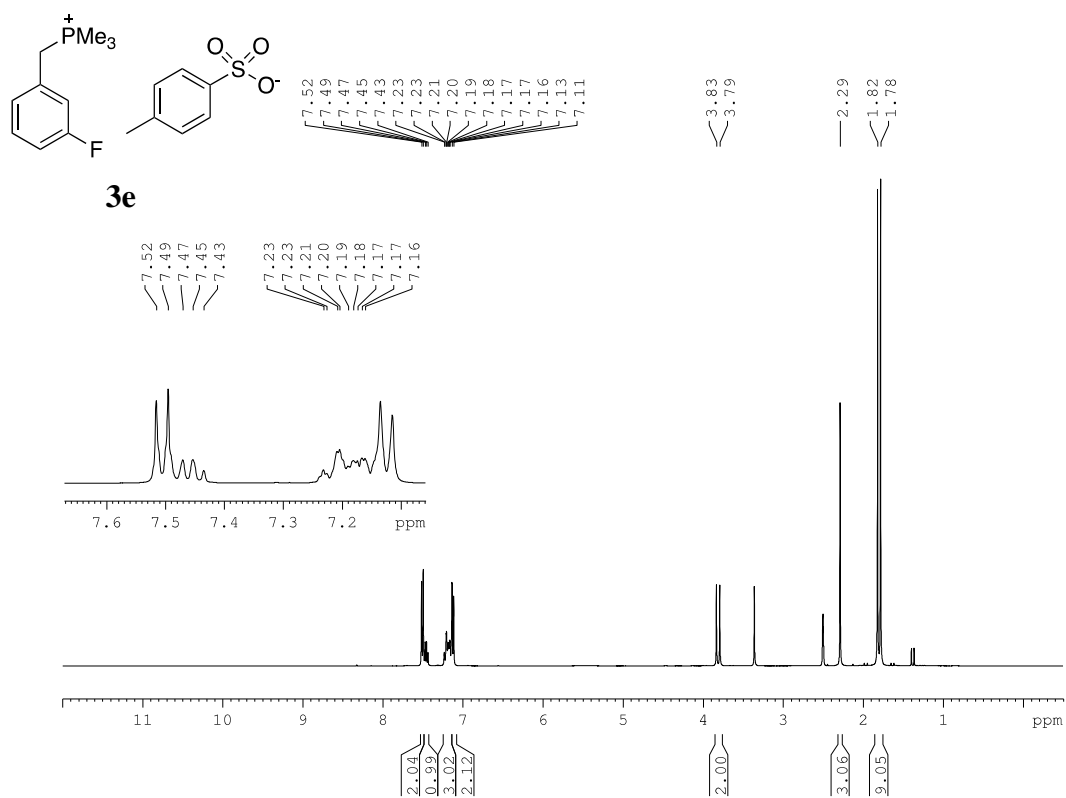
^1H NMR (400 MHz, DMSO-d_6)



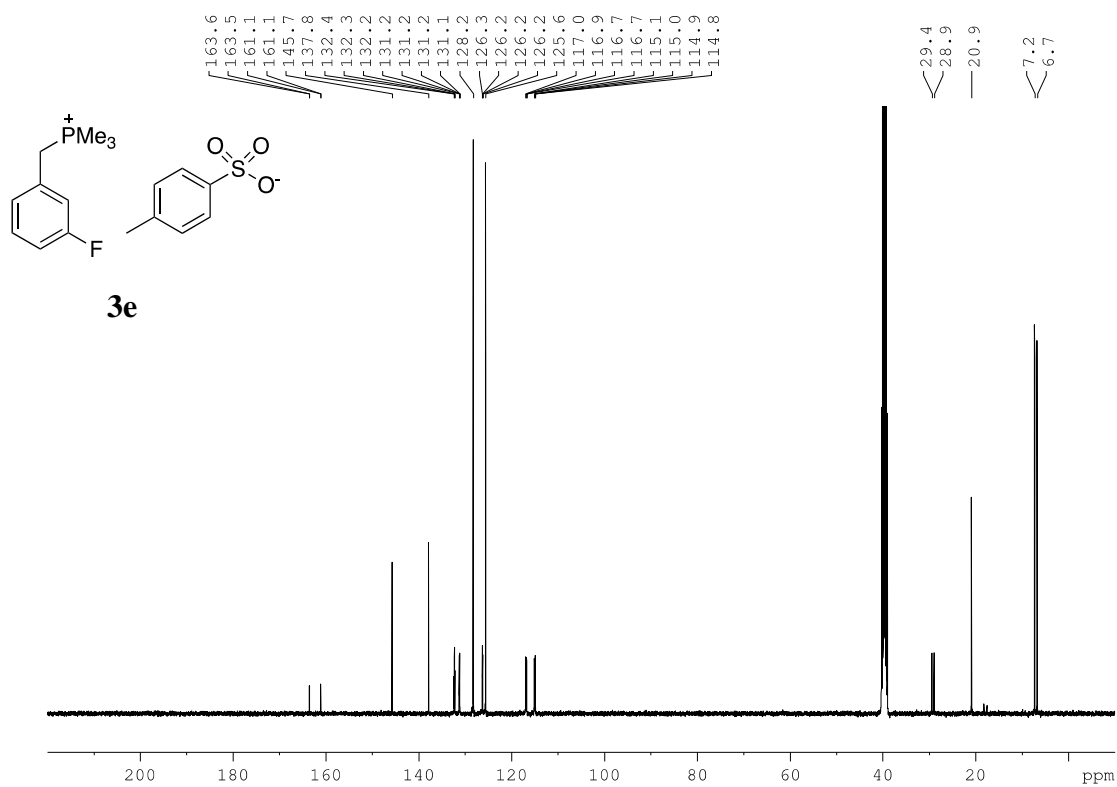
^{13}C NMR (101 MHz, DMSO-d_6)



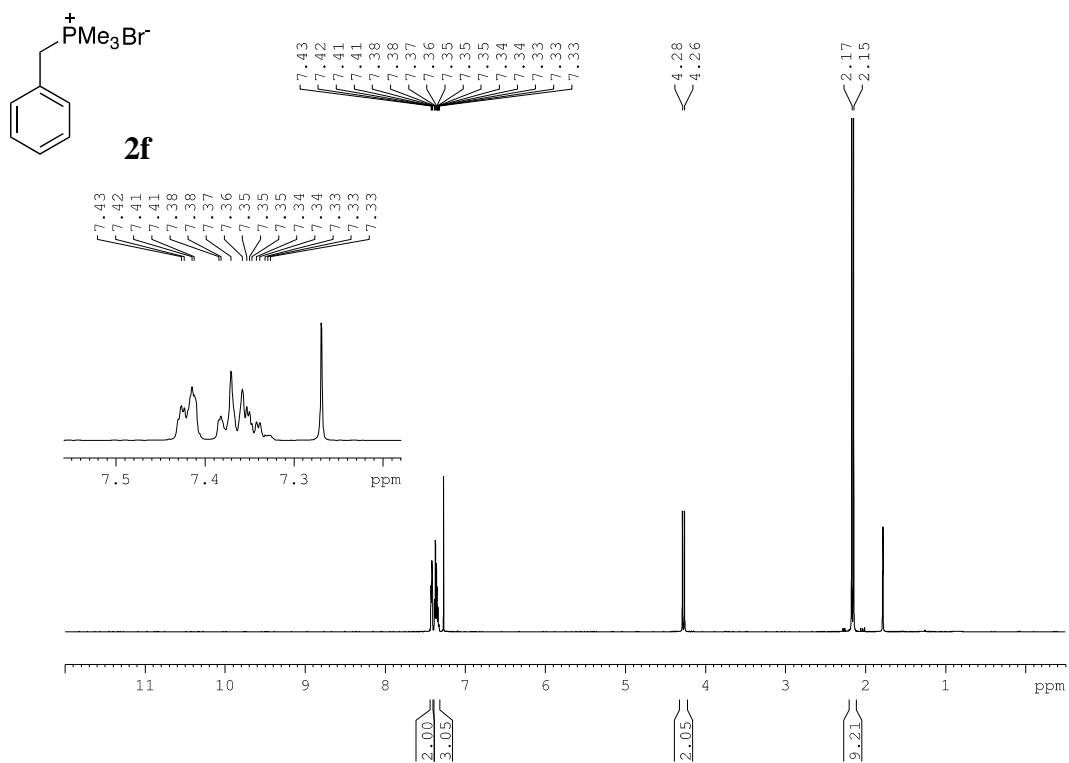
^1H NMR (400 MHz, DMSO-d_6)



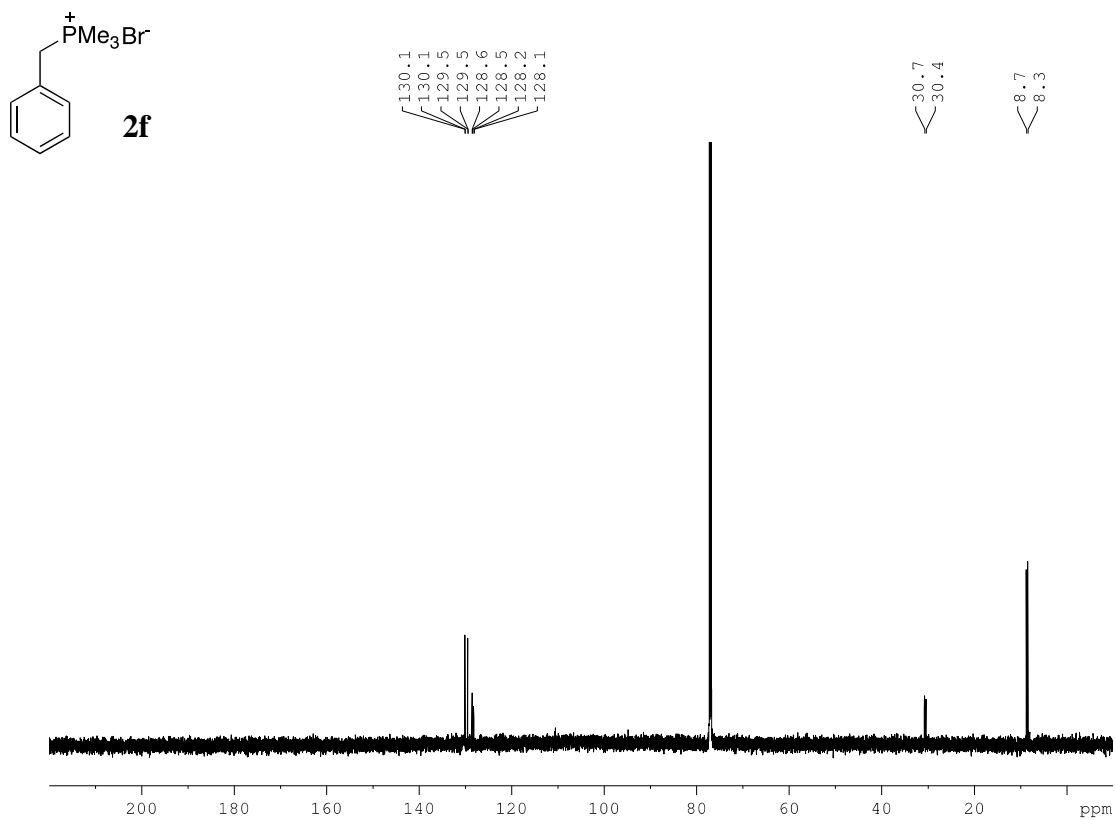
^{13}C NMR (101 MHz, DMSO-d_6)



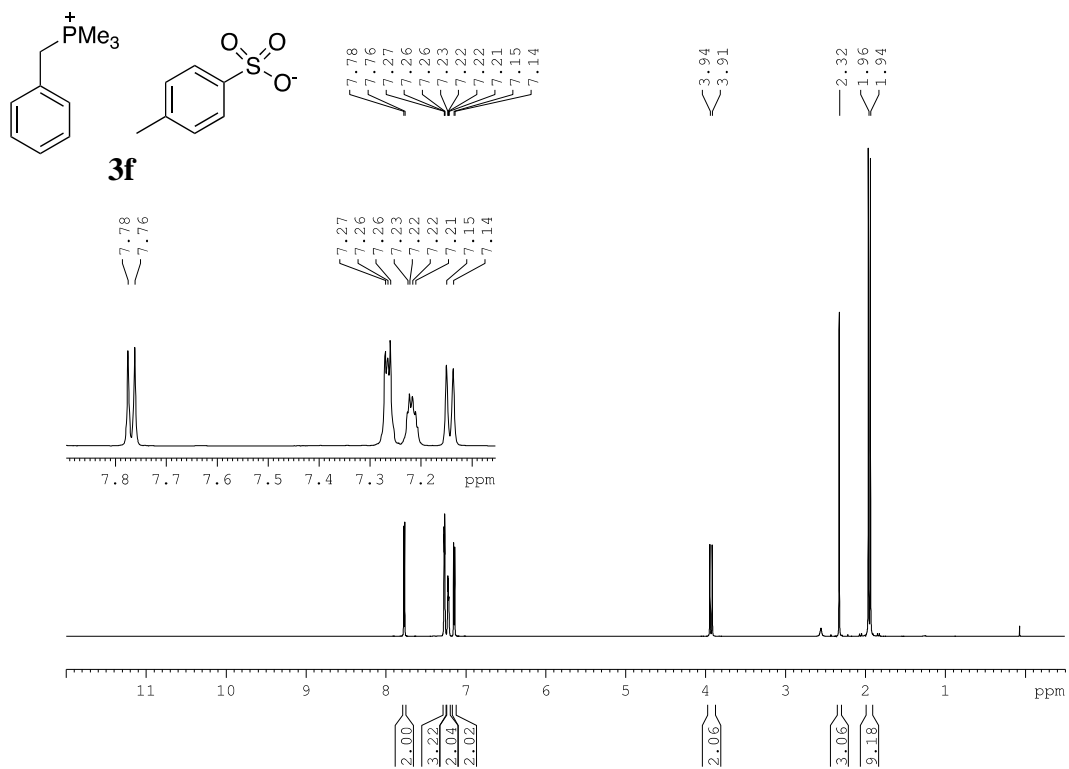
^1H NMR (600 MHz, CDCl_3)



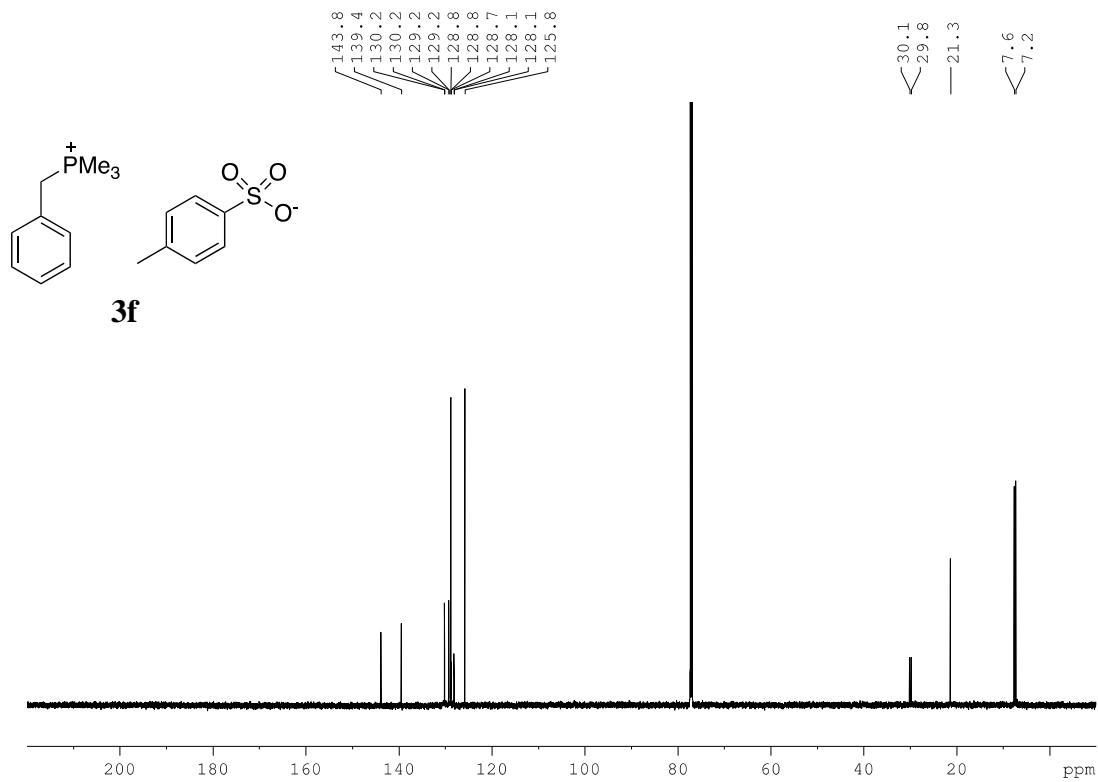
^{13}C NMR (151 MHz, CDCl_3)



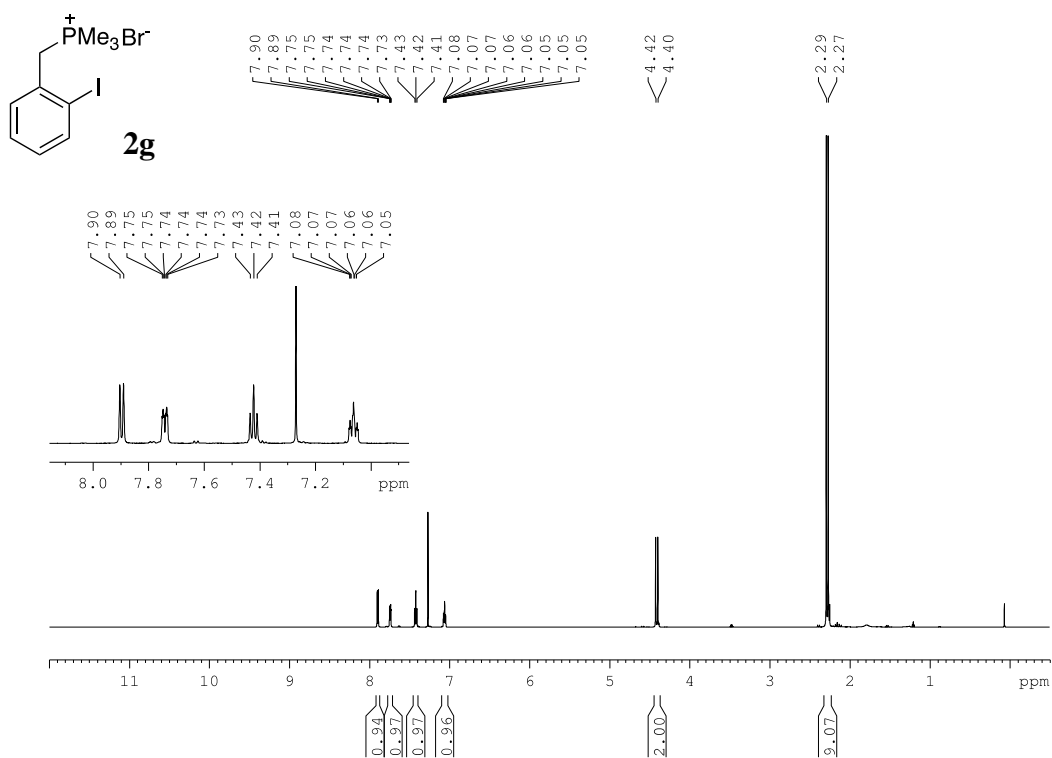
¹H NMR (600 MHz, CDCl₃)



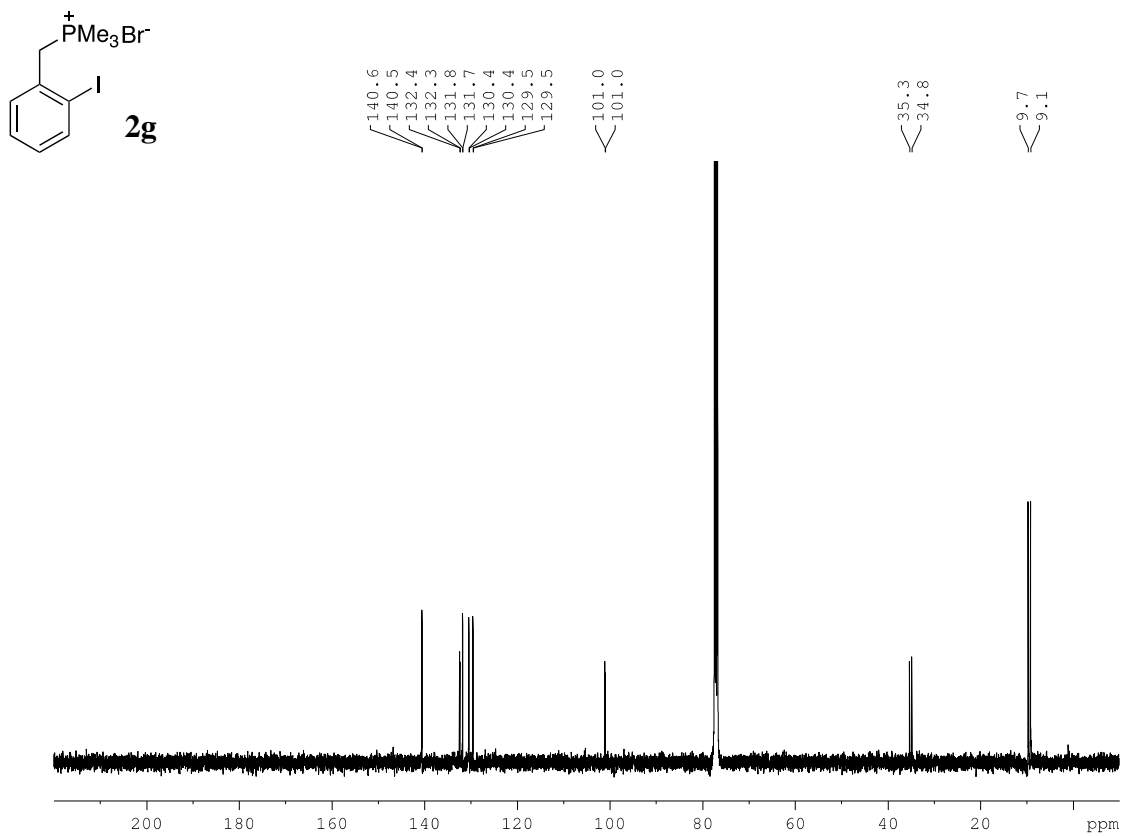
¹³C NMR (151 MHz, CDCl₃)



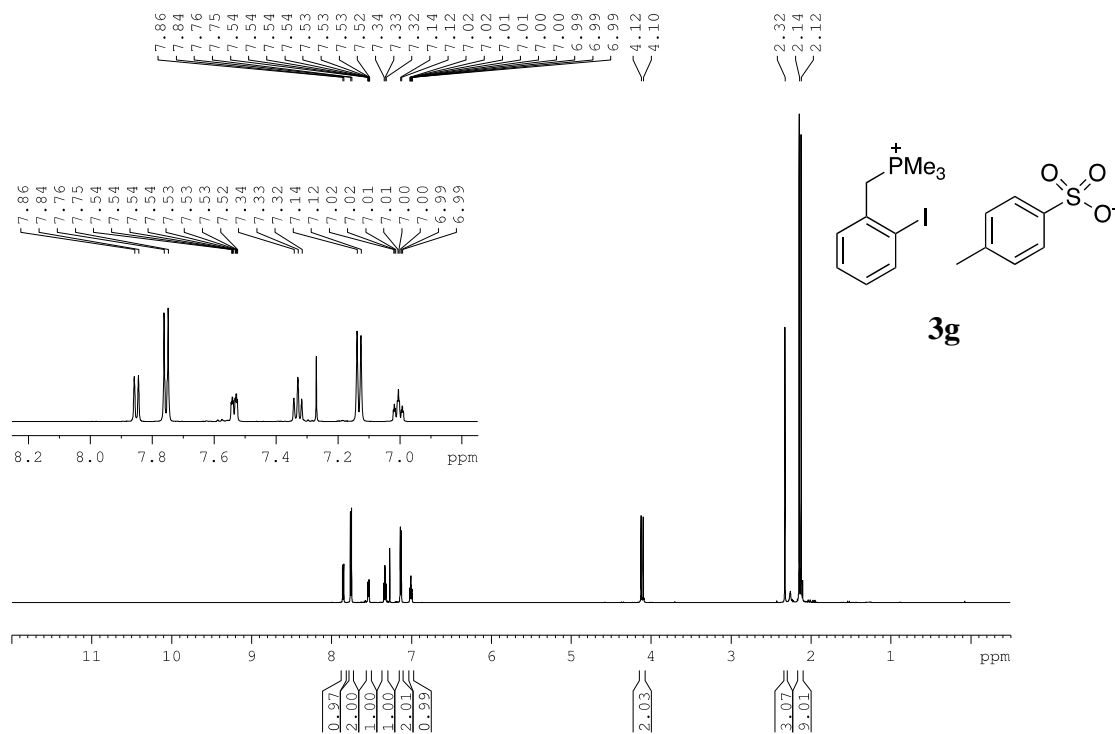
^1H NMR (600 MHz, CDCl_3)



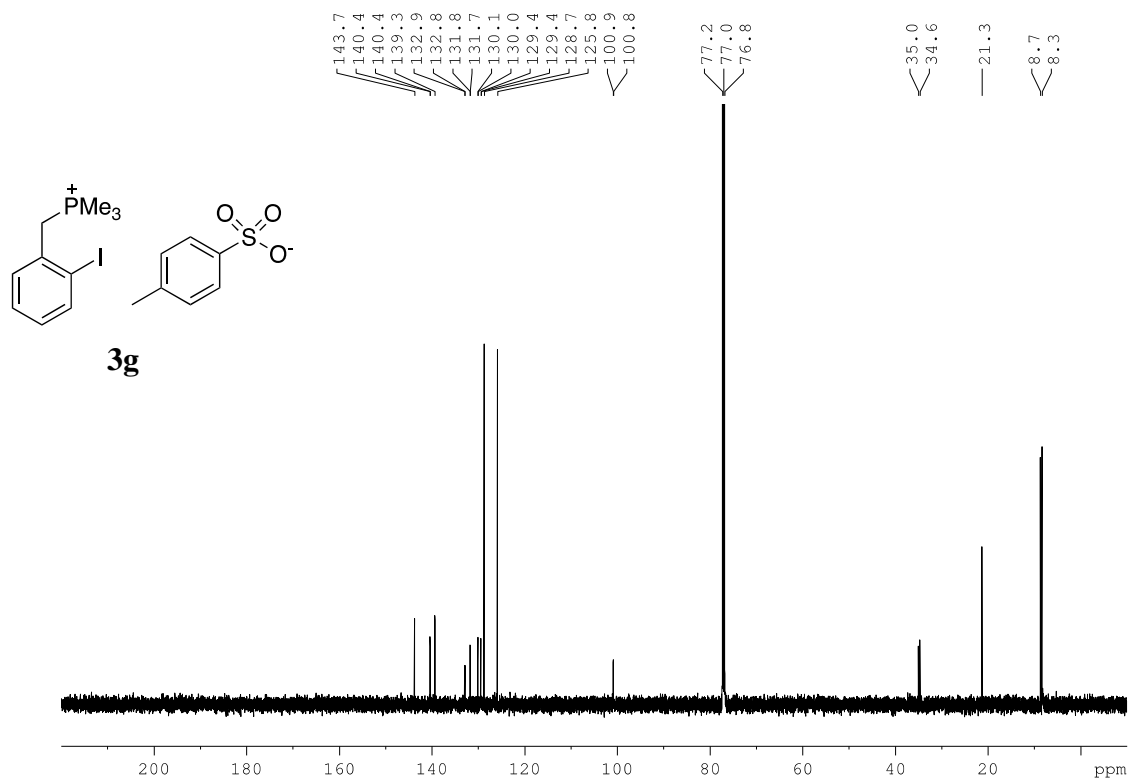
^{13}C NMR (101 MHz, CDCl_3)



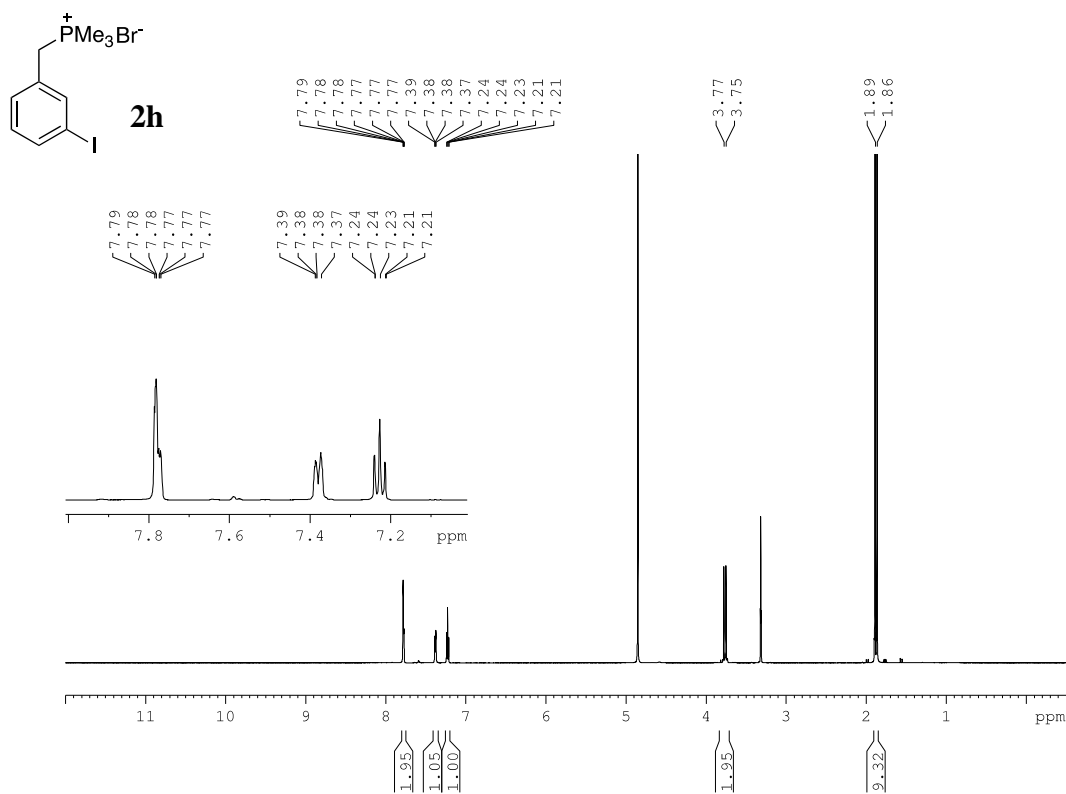
^1H NMR (600 MHz, CDCl_3)



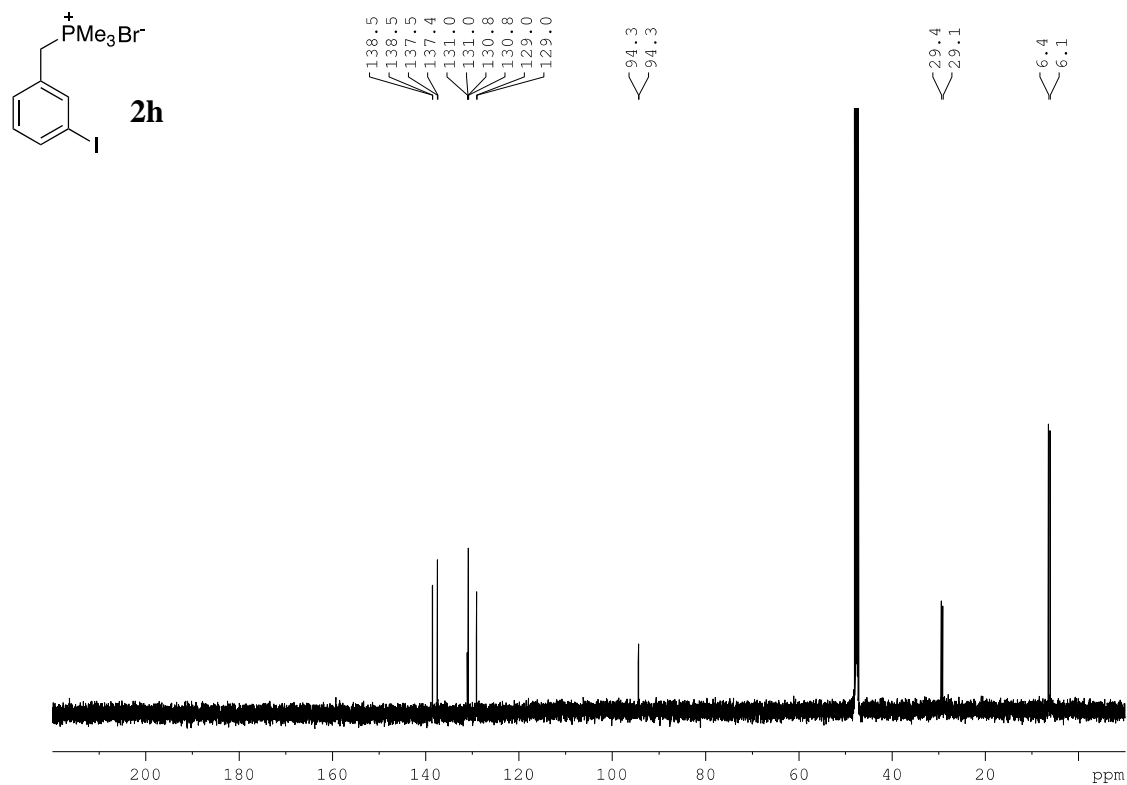
^{13}C NMR (151 MHz, CDCl_3)



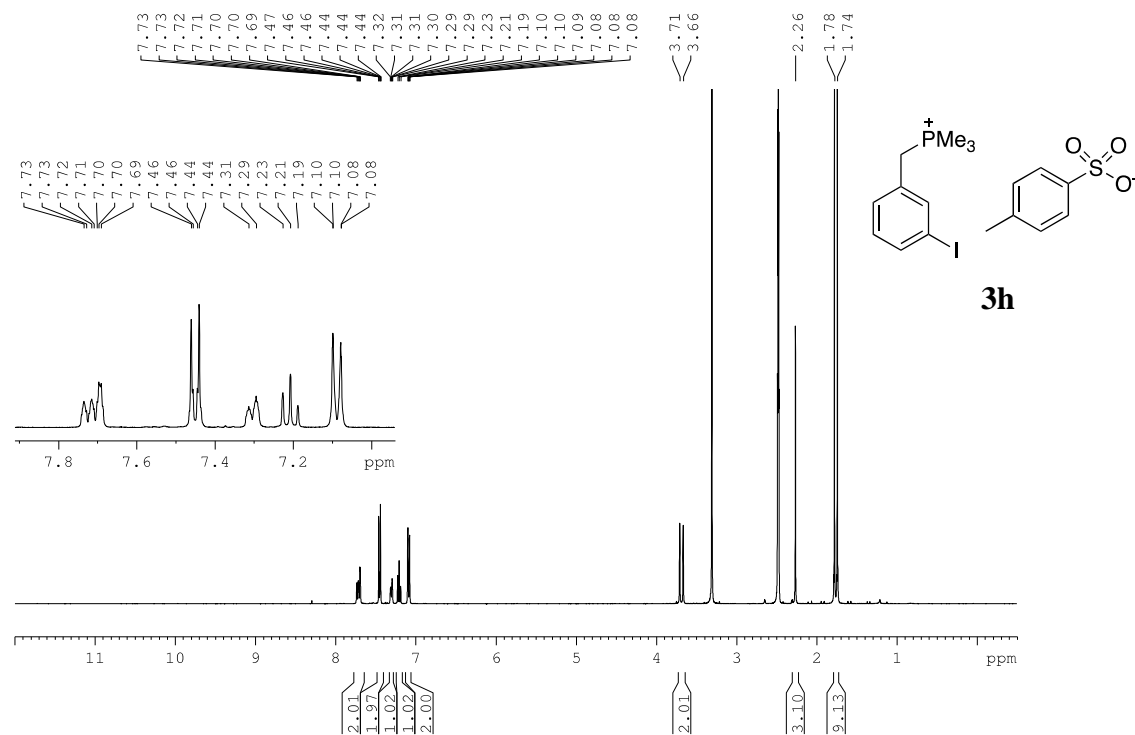
^1H NMR (600 MHz, CD_3OD)



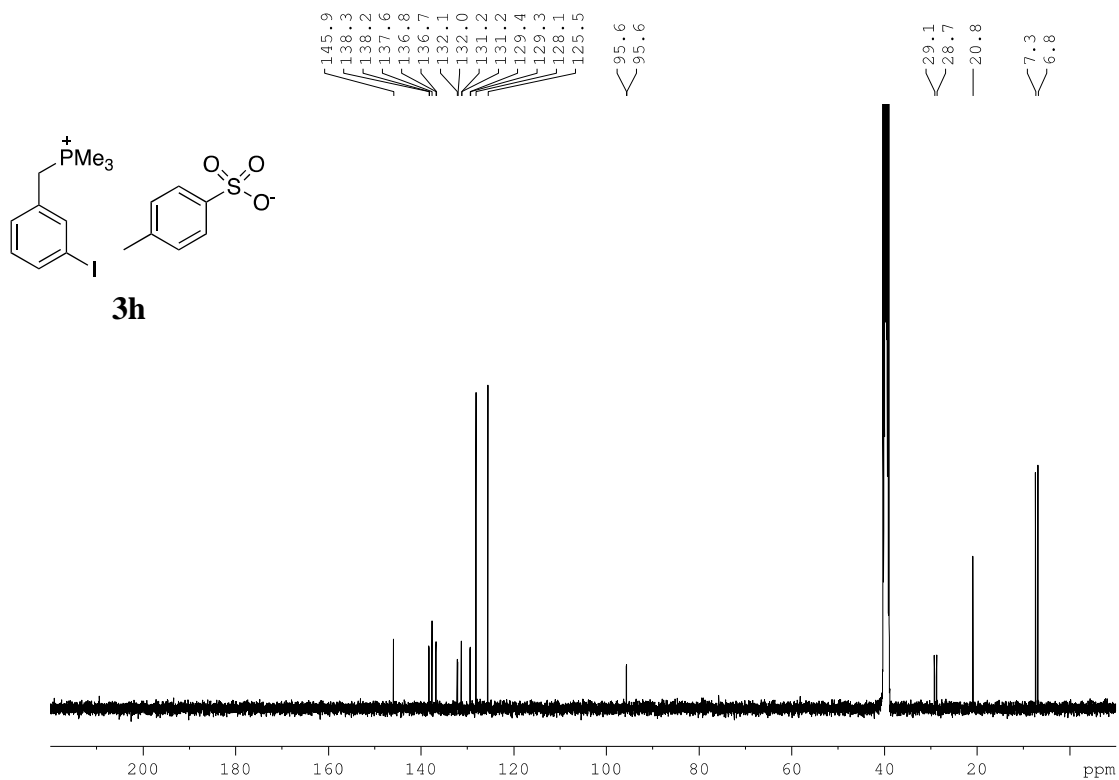
^{13}C NMR (151 MHz, CD_3OD)



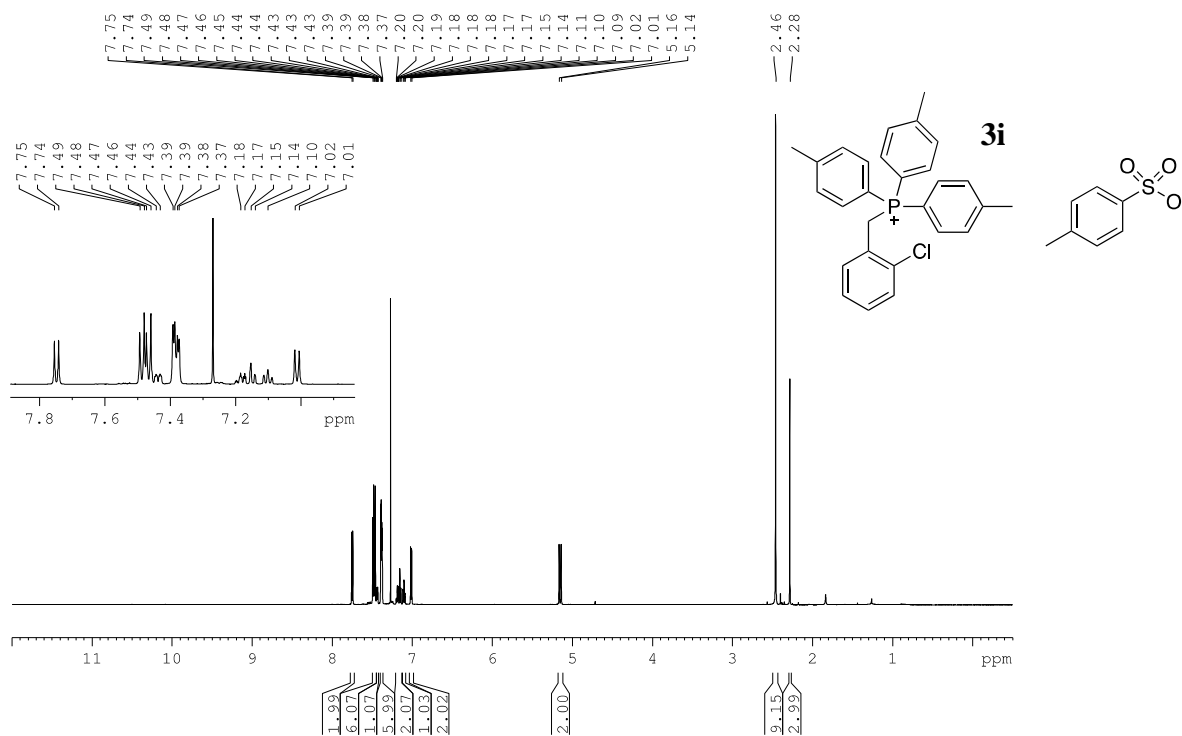
^1H NMR (400 MHz, DMSO-d_6)



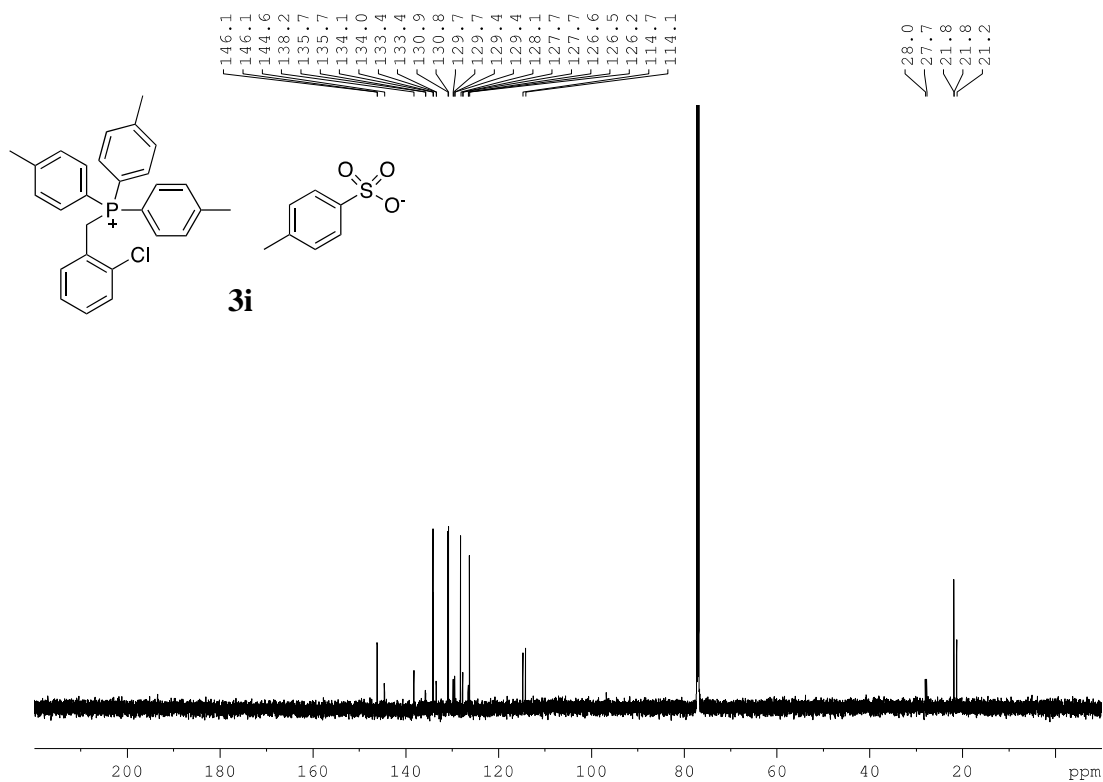
^{13}C NMR (101 MHz, DMSO-d_6)



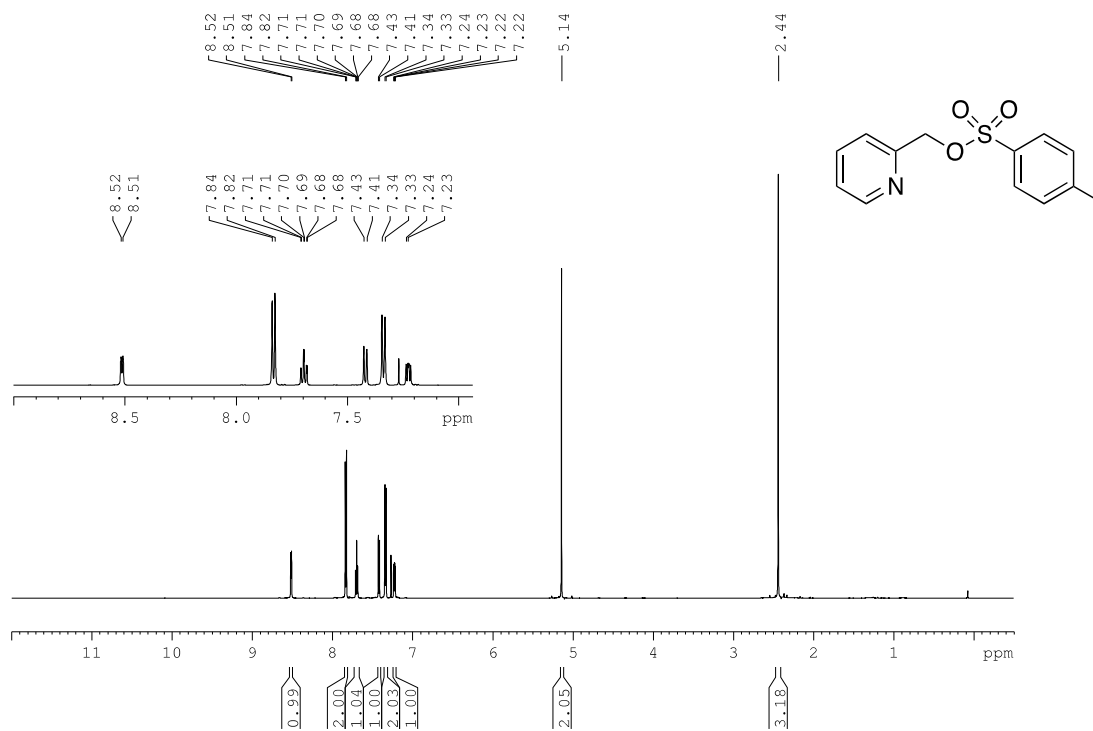
^1H NMR (600 MHz, CDCl_3)



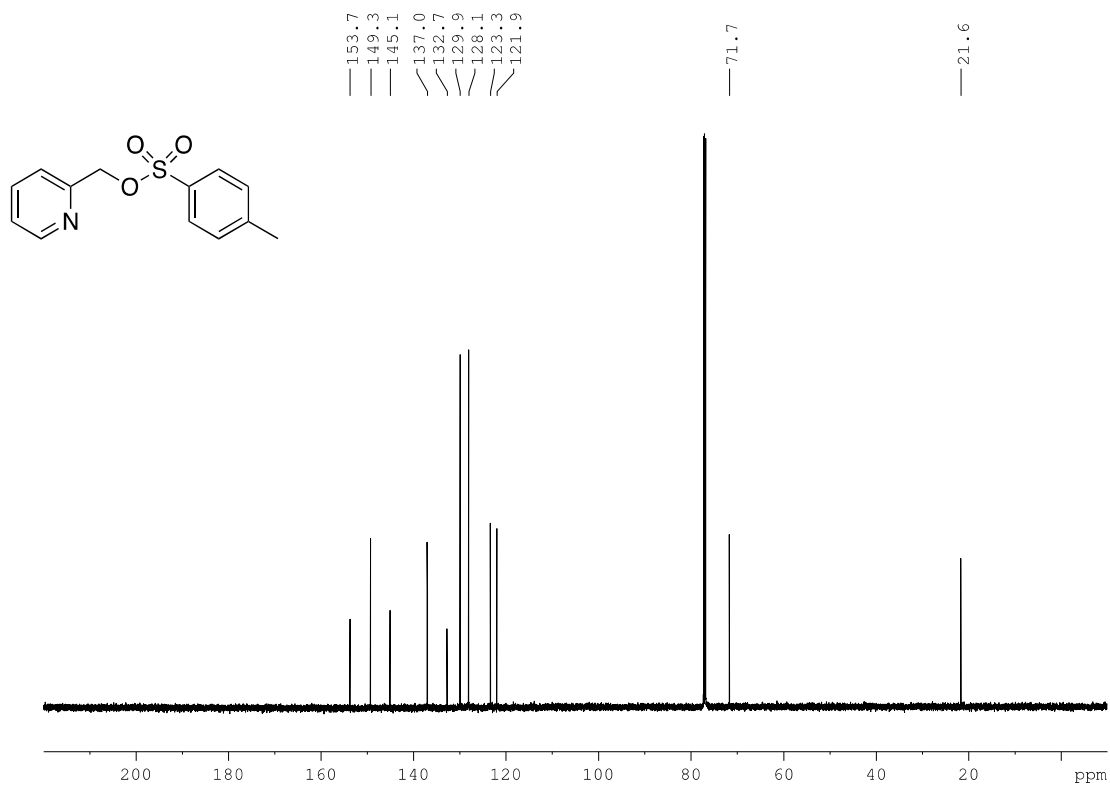
^{13}C NMR (151 MHz, CDCl_3)



¹H NMR (600 MHz, CDCl₃)

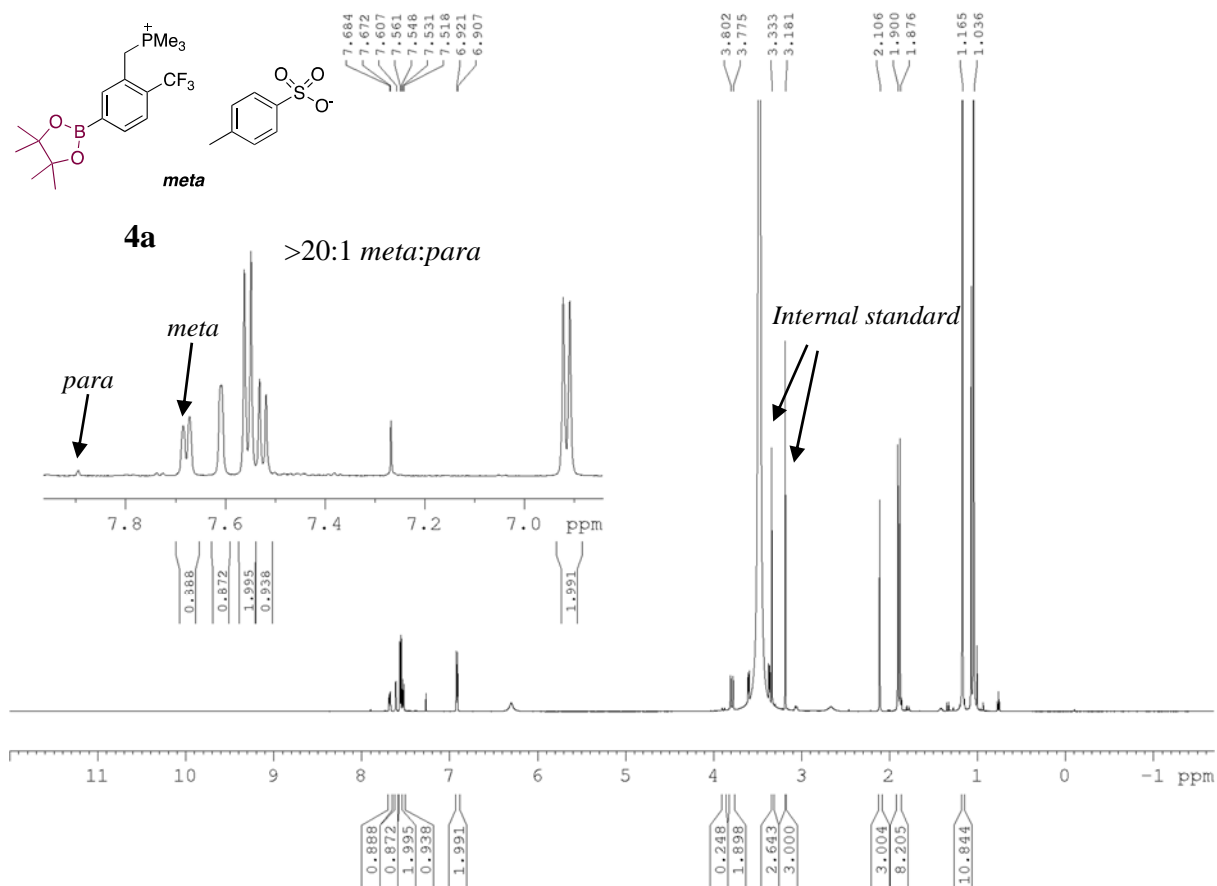


¹³C NMR (151 MHz, CDCl₃)

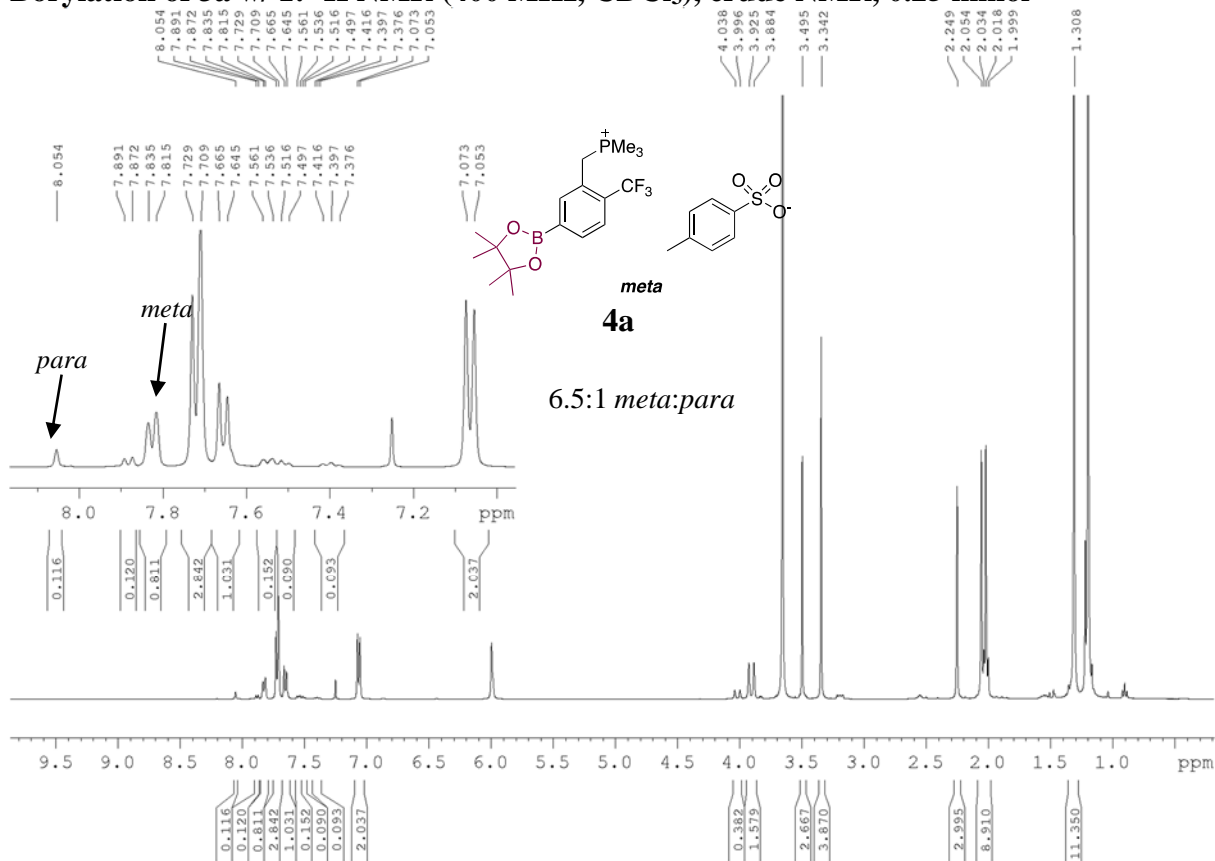


1.2 NMR data for borylation products

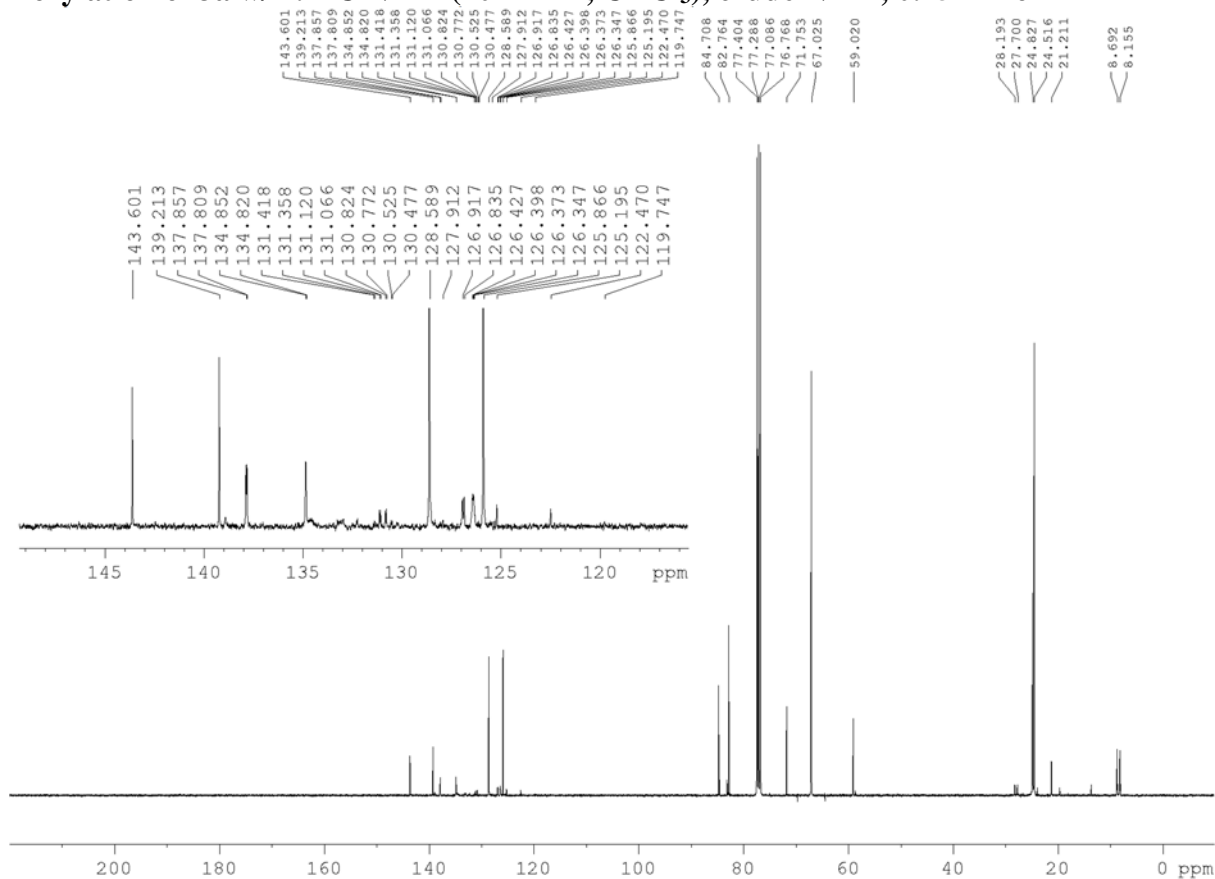
Borylation of 3a w/ 1: ^1H NMR (600 MHz, CDCl_3), crude NMR, 0.1 mmol



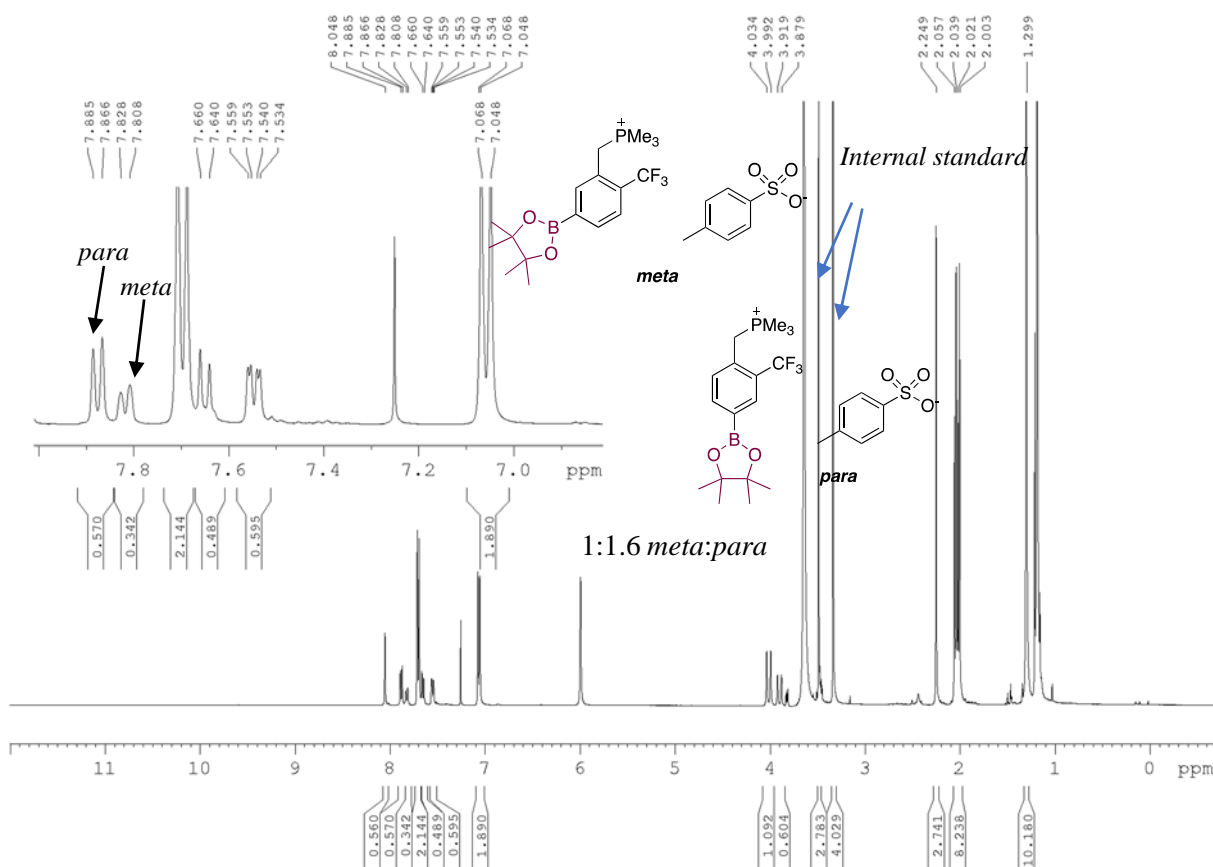
Borylation of 3a w/ 1: ^1H NMR (400 MHz, CDCl_3), crude NMR, 0.25 mmol



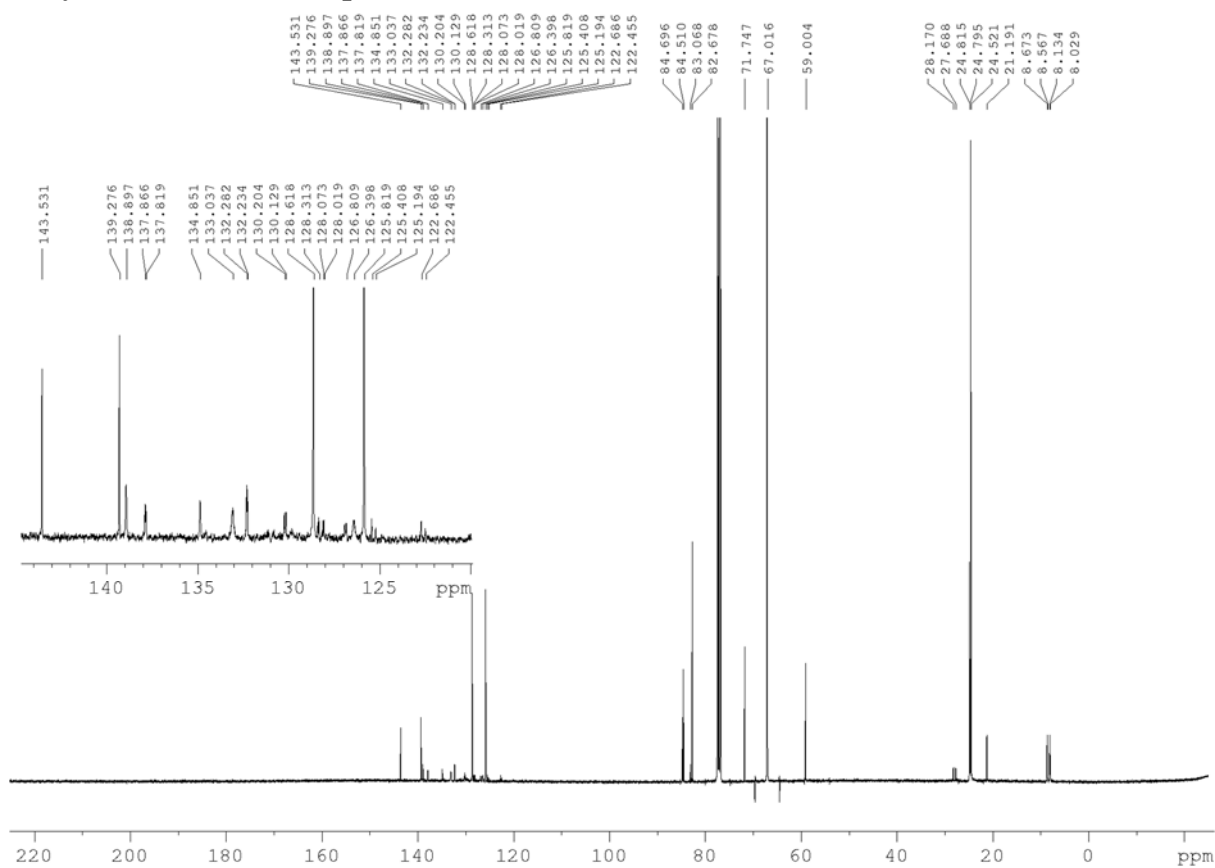
Borylation of 3a w/ 1: ^{13}C NMR (101 MHz, CDCl_3), crude NMR, 0.25 mmol



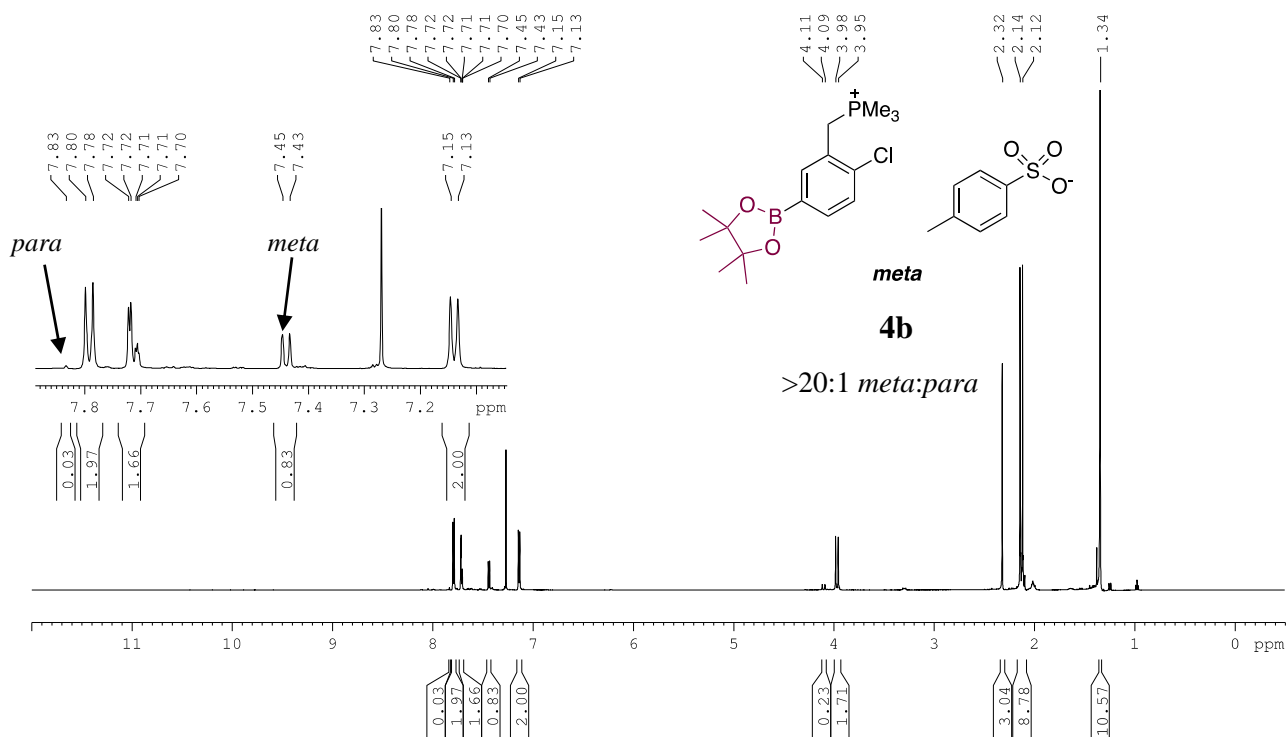
Borylation of 3a w/ tmphen: ^1H NMR (400 MHz, CDCl_3), crude NMR, 0.25 mmol



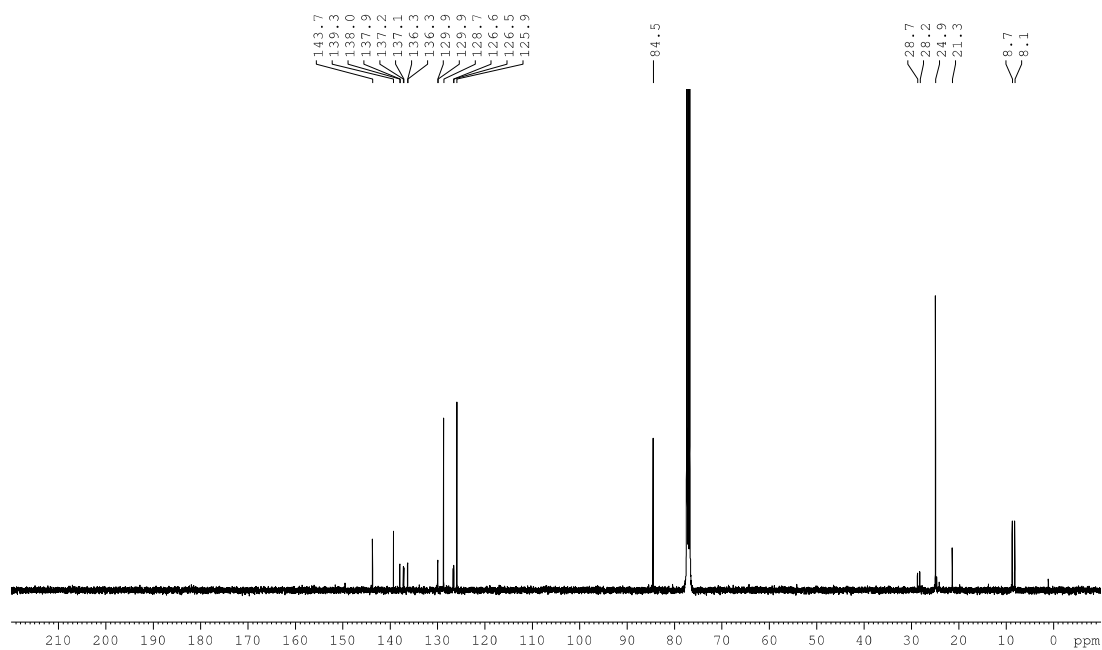
Borylation of 3a w/ tmphen: ^{13}C NMR (101 MHz, CDCl_3), crude NMR, 0.25 mmol



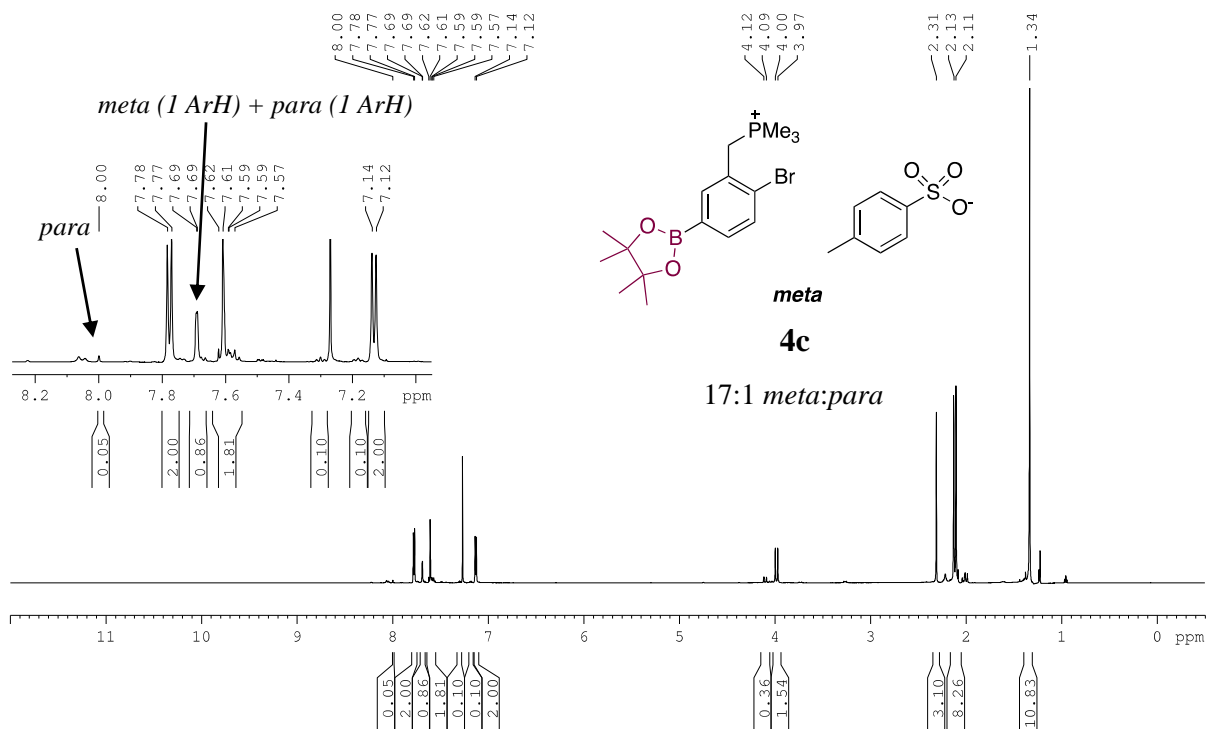
Borylation of 3b w/ 1: ^1H NMR (600 MHz, CDCl_3)



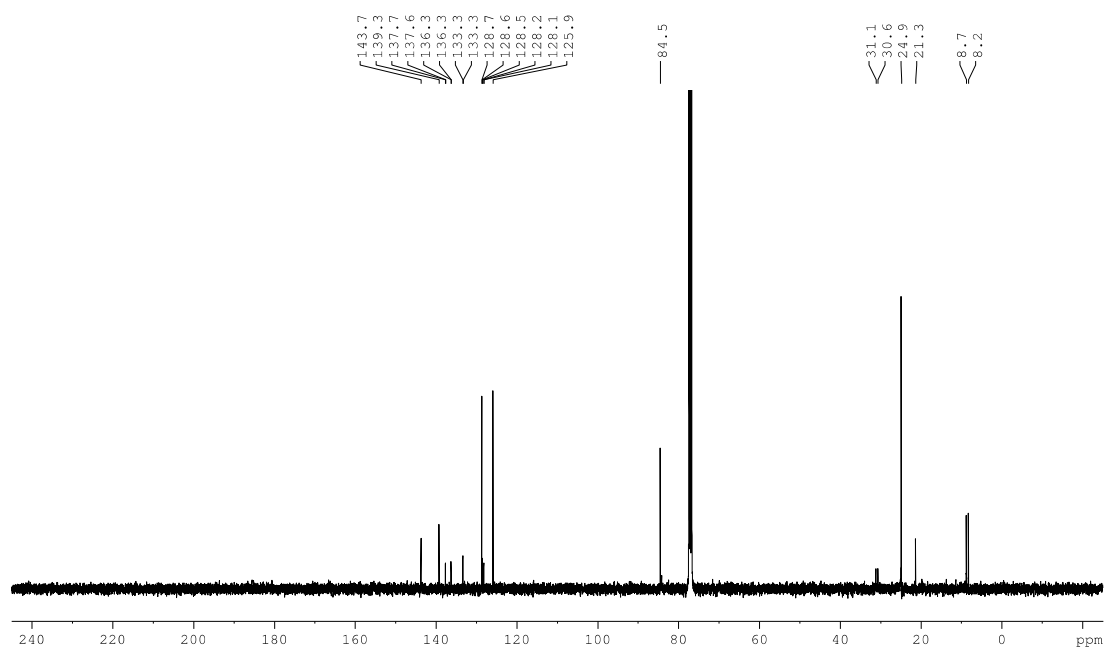
Borylation of 3b w/ 1: ^{13}C NMR (101 MHz, CDCl_3)



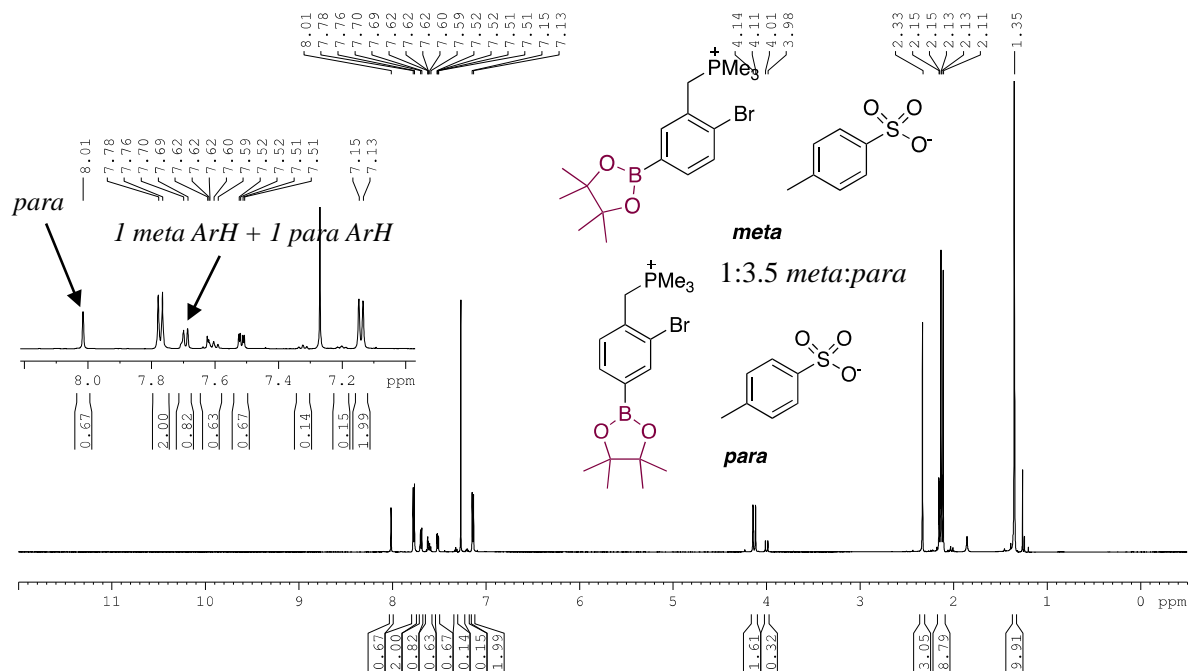
Borylation of 3c w/ 1: ¹H NMR (600 MHz, CDCl₃)



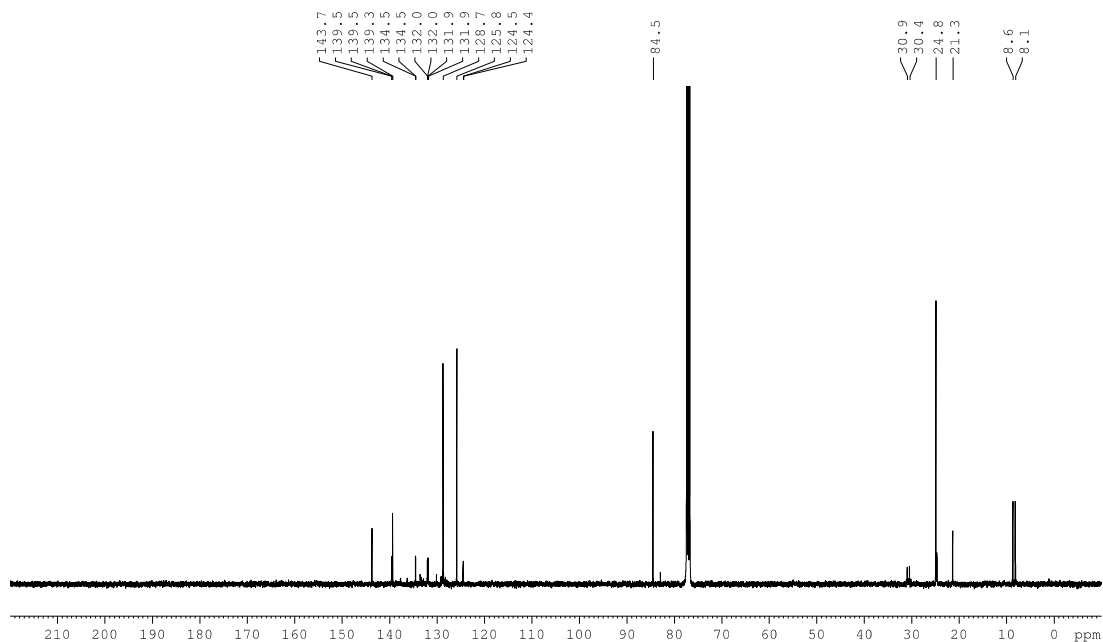
Borylation of 3c w/ 1: ¹³C NMR (101 MHz, CDCl₃)



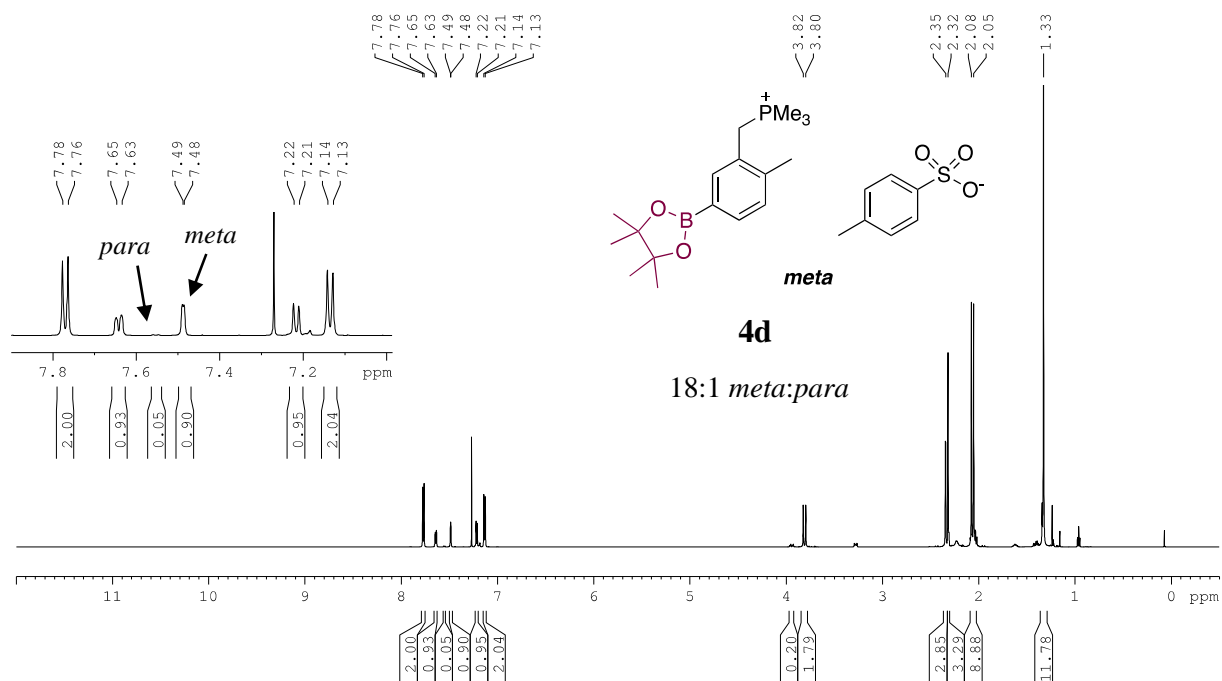
Borylation of 3c w/ tmphen: ^1H NMR (600 MHz, CDCl_3)



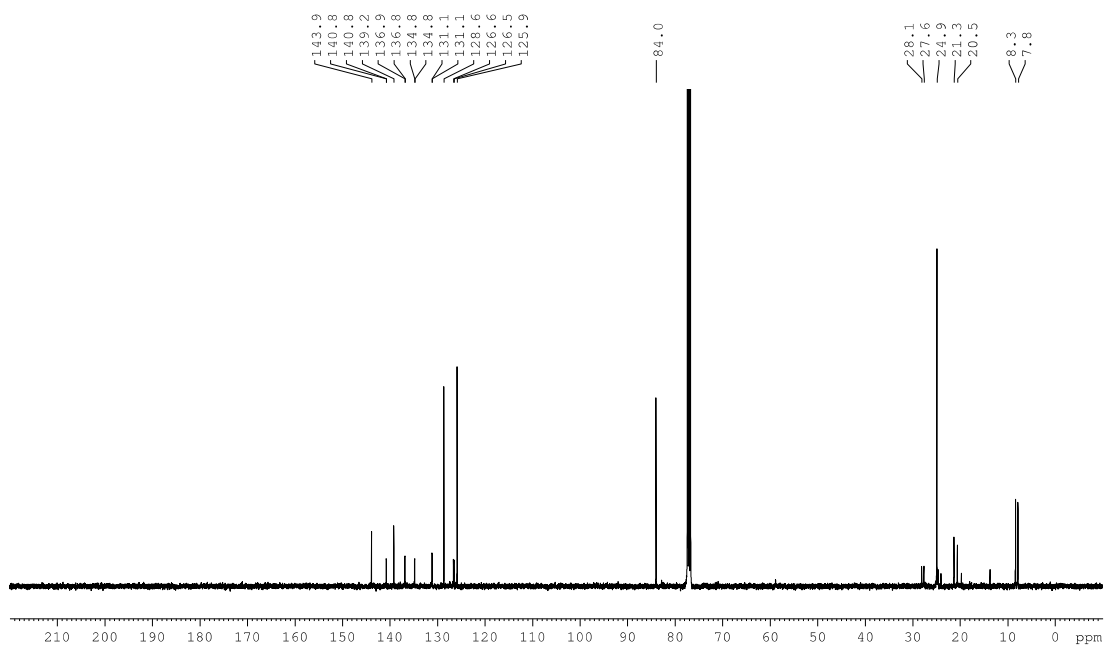
Borylation of 3c w/ tmphen: ^{13}C NMR (101 MHz, CDCl_3)



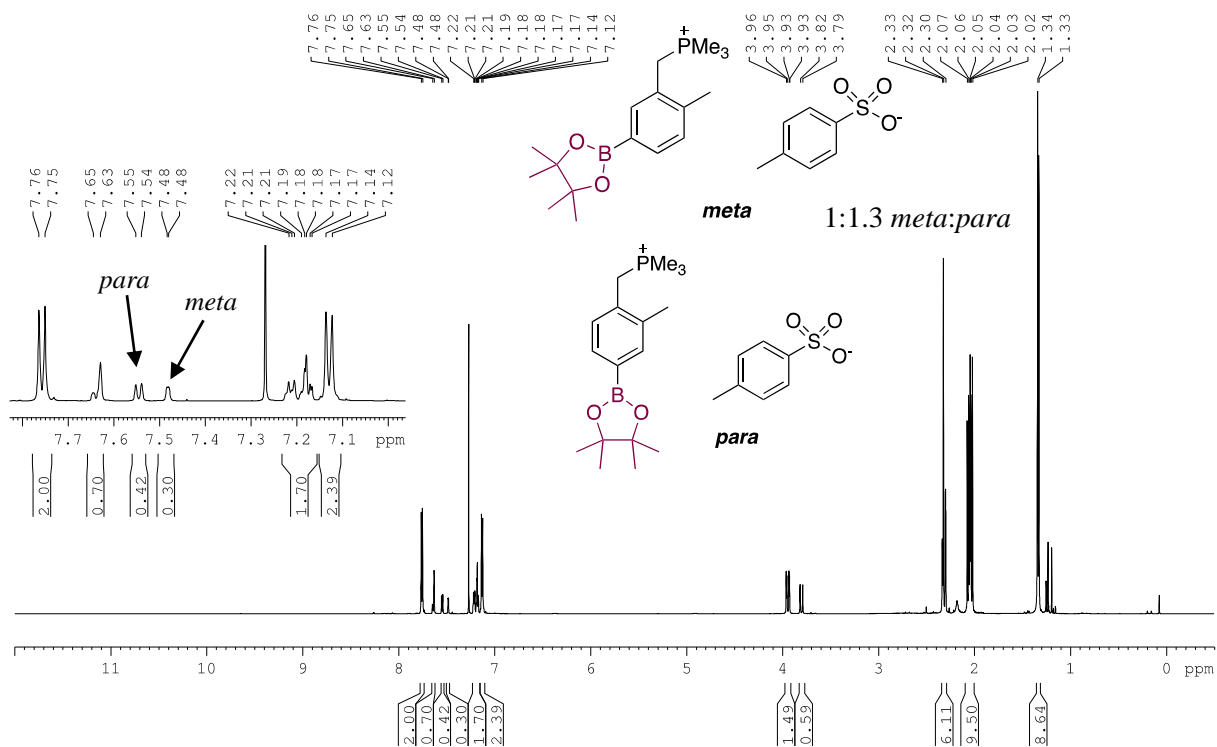
Borylation of 3d w/ 1: ^1H NMR (600 MHz, CDCl_3)



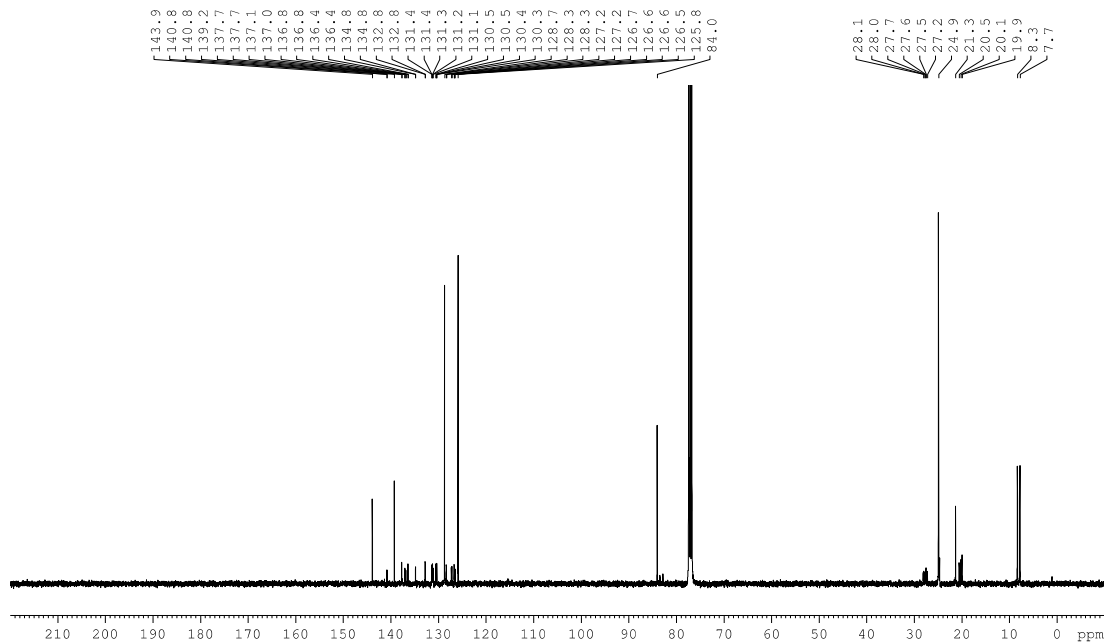
Borylation of 3d w/ 1: ^{13}C NMR (101 MHz, CDCl_3)



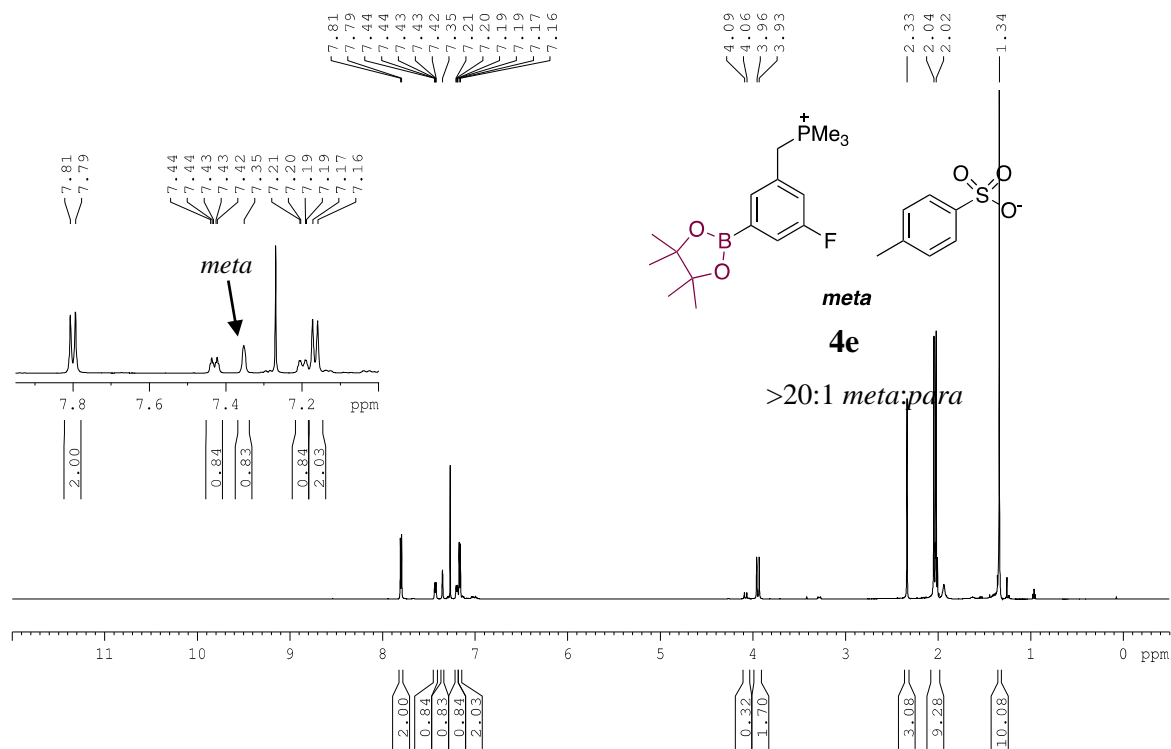
Borylation of 3d w/ tmphen: ^1H NMR (600 MHz, CDCl_3)



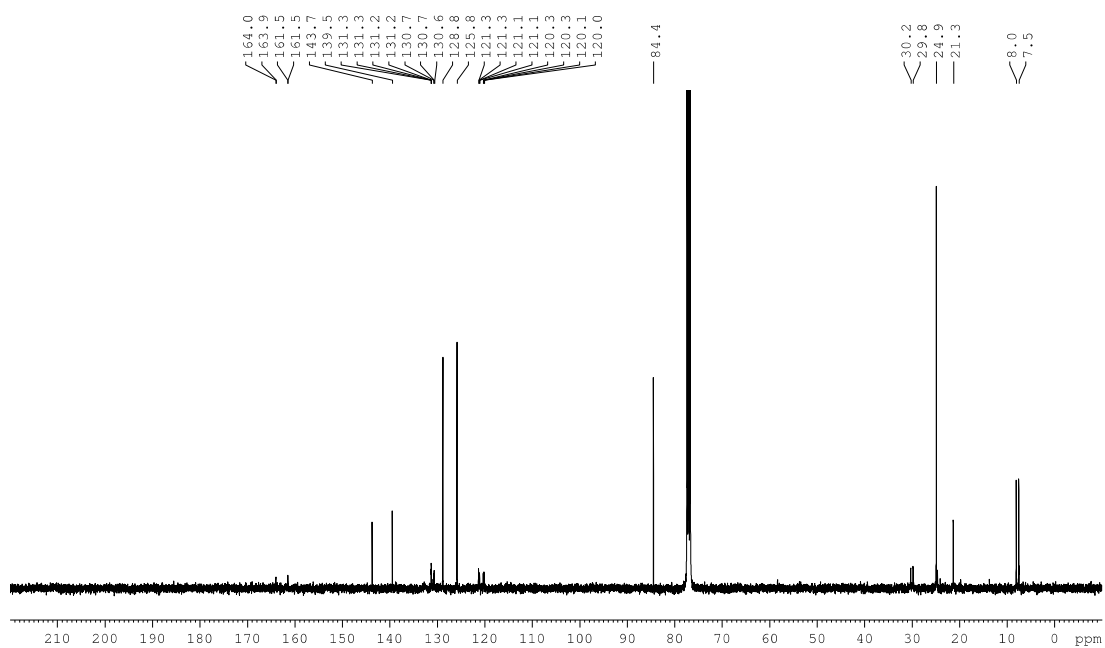
Borylation of 3d w/ tmphen: ^{13}C NMR (101 MHz, CDCl_3)



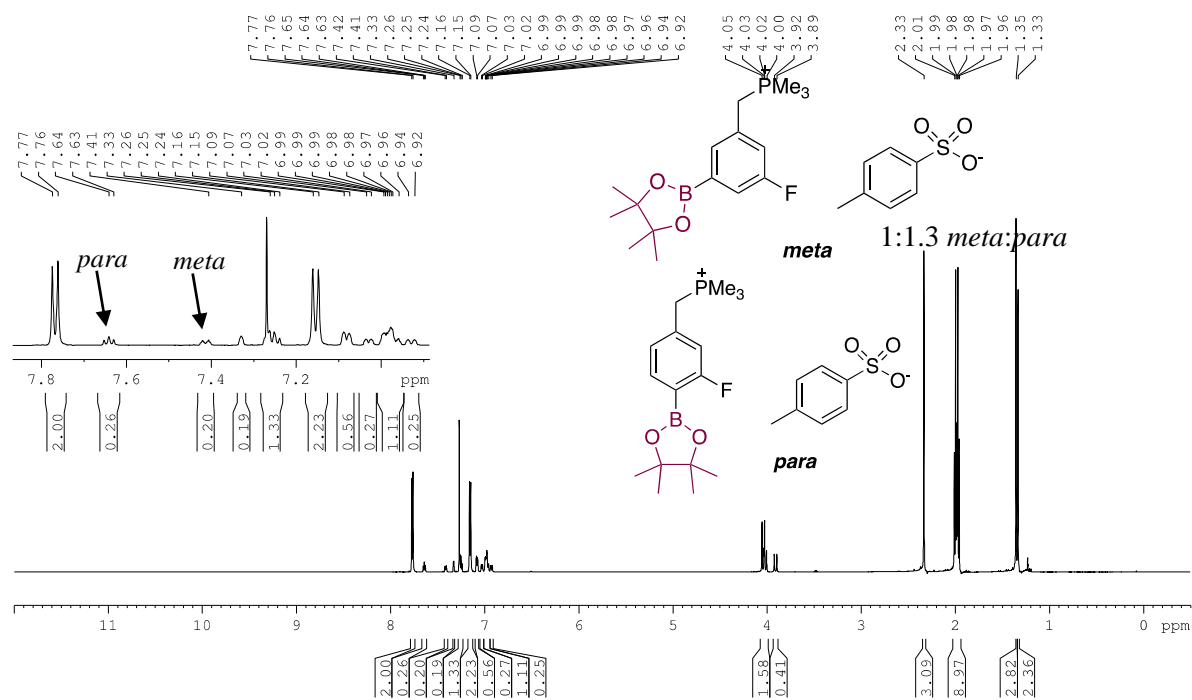
Borylation of 3e w/ 1: ¹H NMR (600 MHz, CDCl₃)



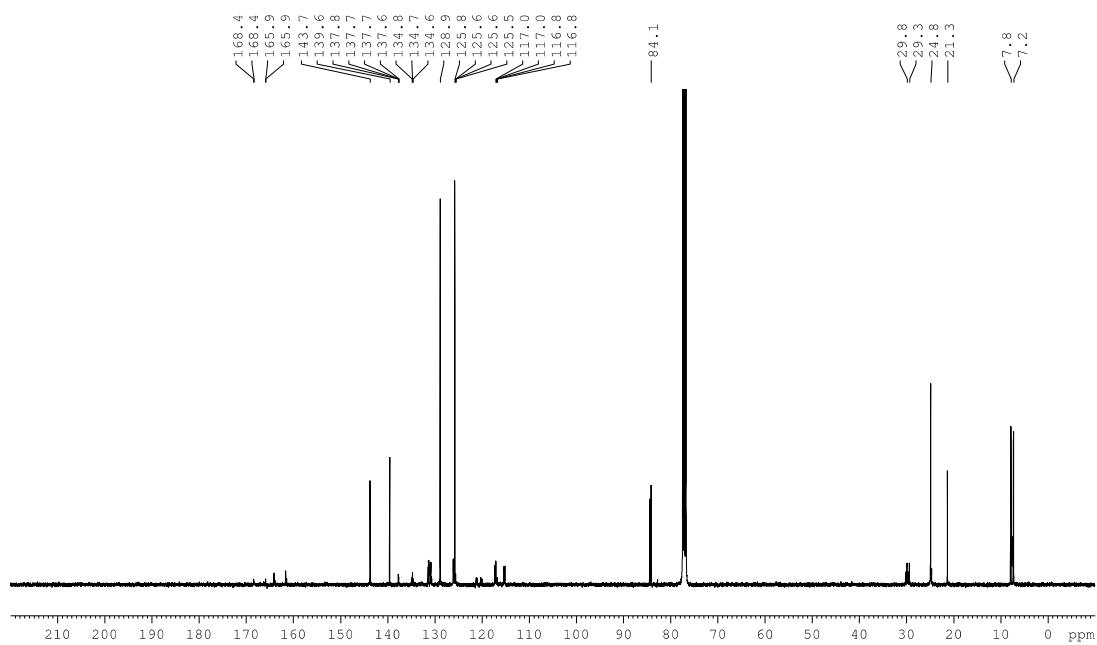
Borylation of 3e w/ 1: ¹³C NMR (101 MHz, CDCl₃)



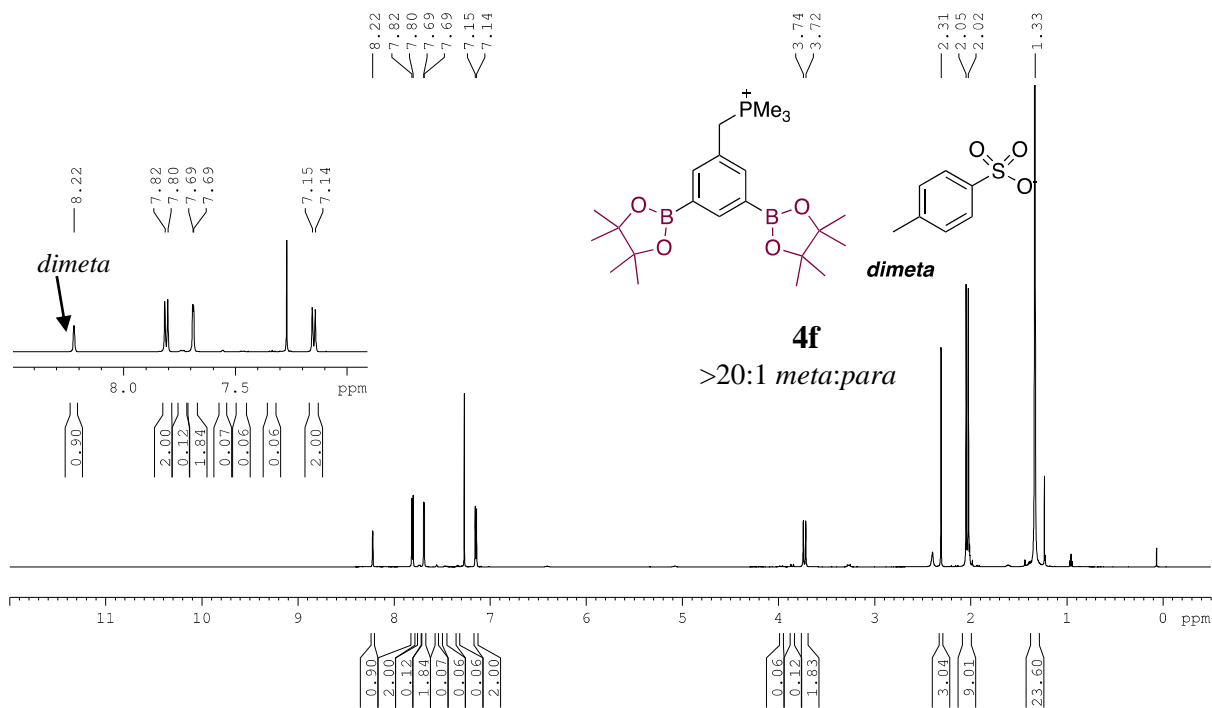
Borylation of 3e w/ tmphen: ^1H NMR (600 MHz, CDCl_3)



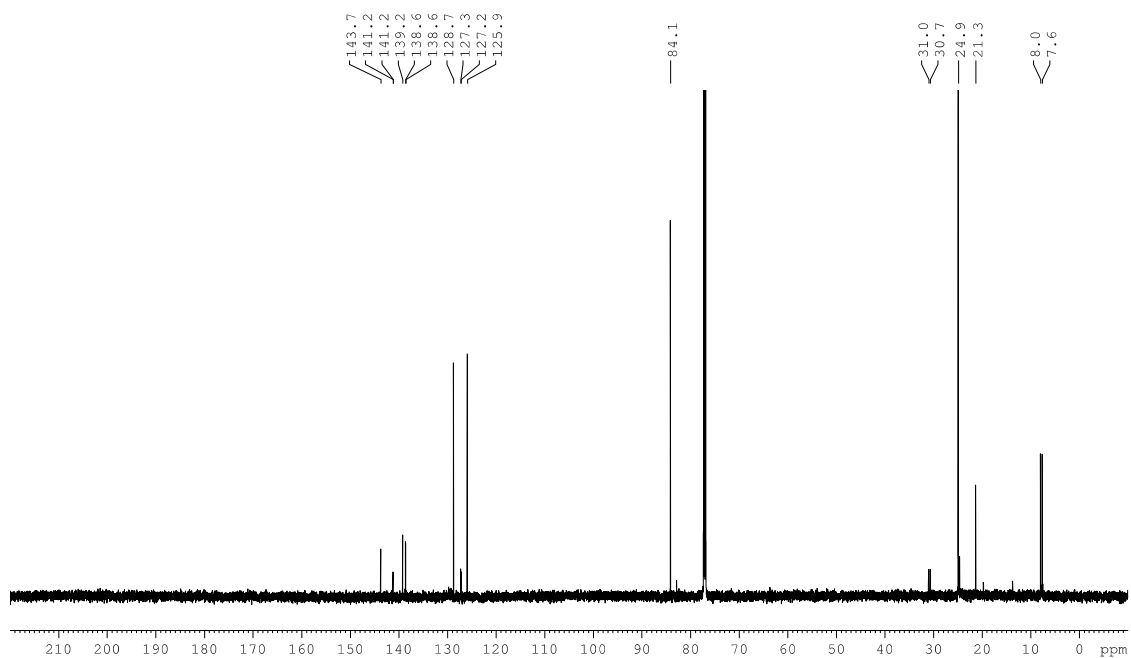
Borylation of 3e w/ tmphen: ^{13}C NMR (101 MHz, CDCl_3)



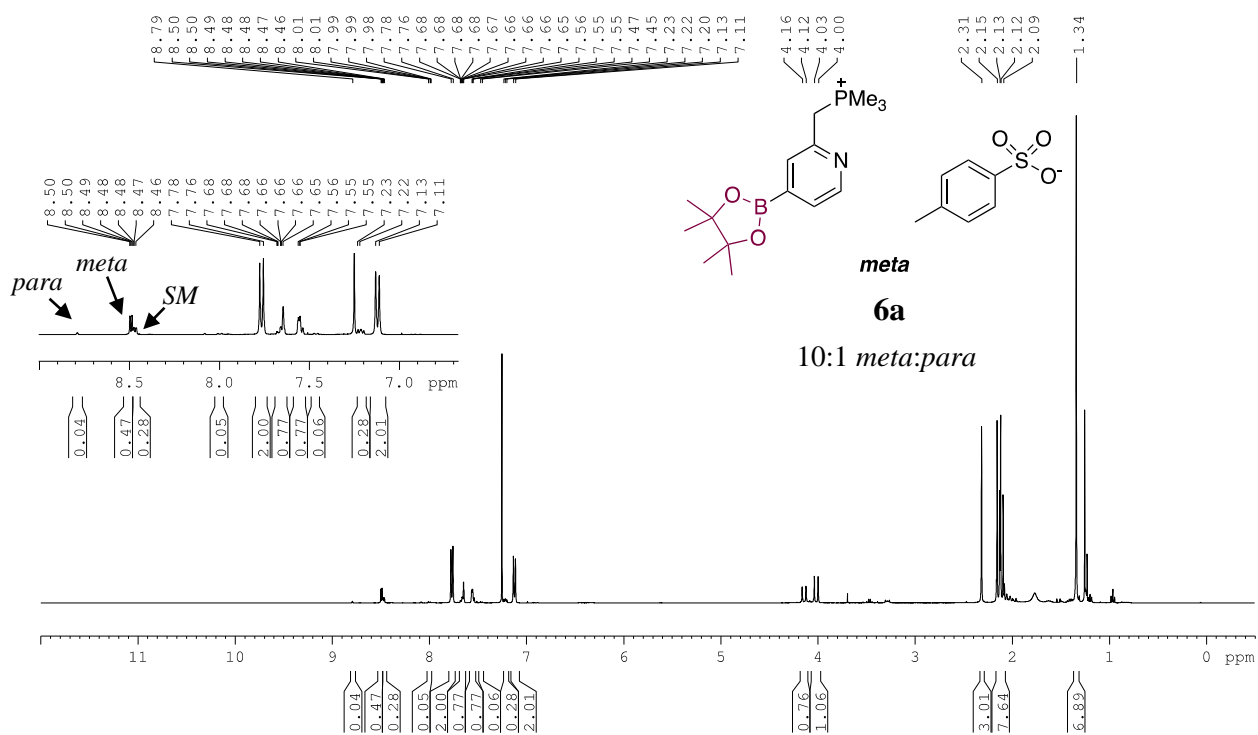
Borylation of 3f w/ 1: ^1H NMR (600 MHz, CDCl_3)



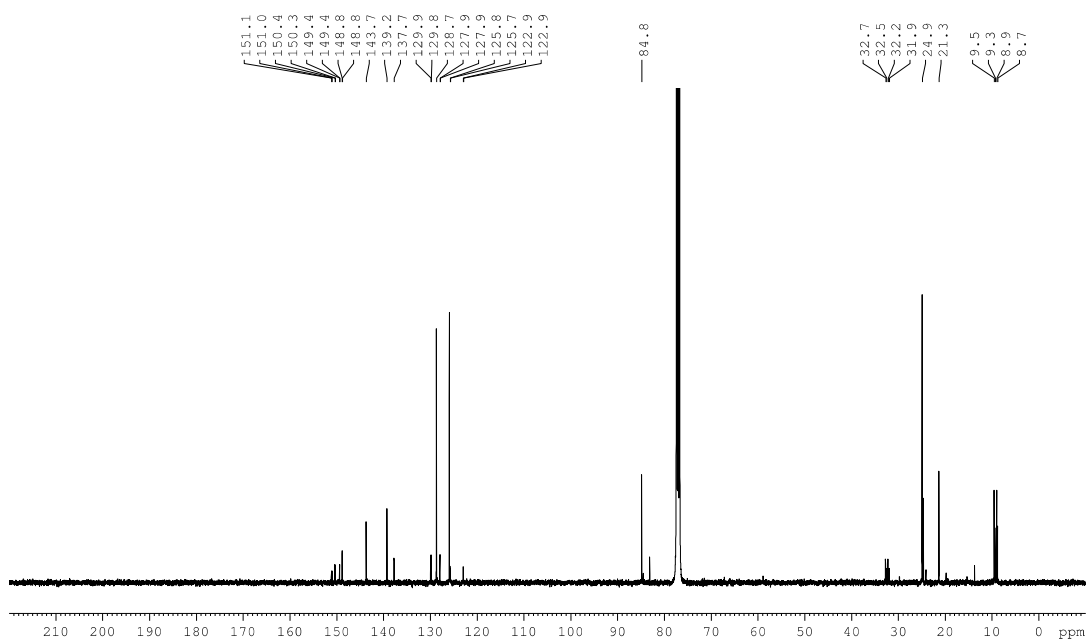
Borylation of 3f w/ 1: ^{13}C NMR (151 MHz, CDCl_3)



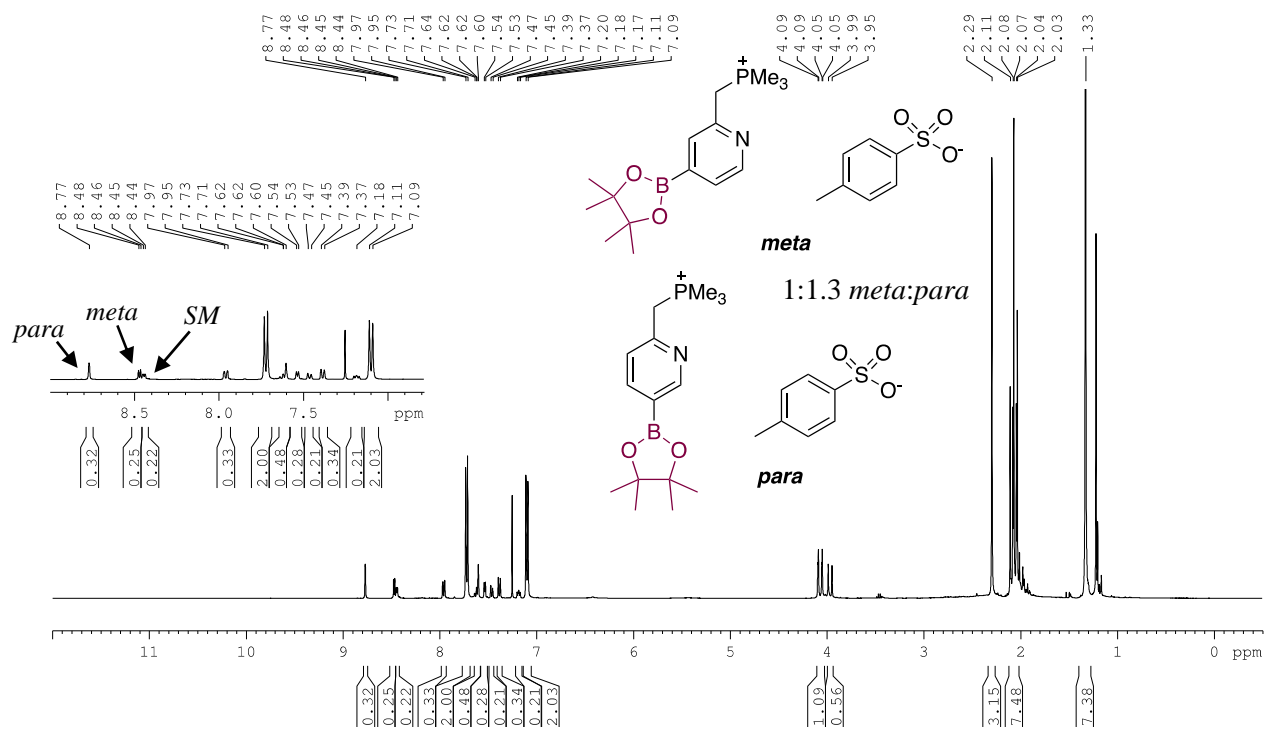
Borylation of 5a w/ 1: ¹H NMR (400 MHz, CDCl₃)



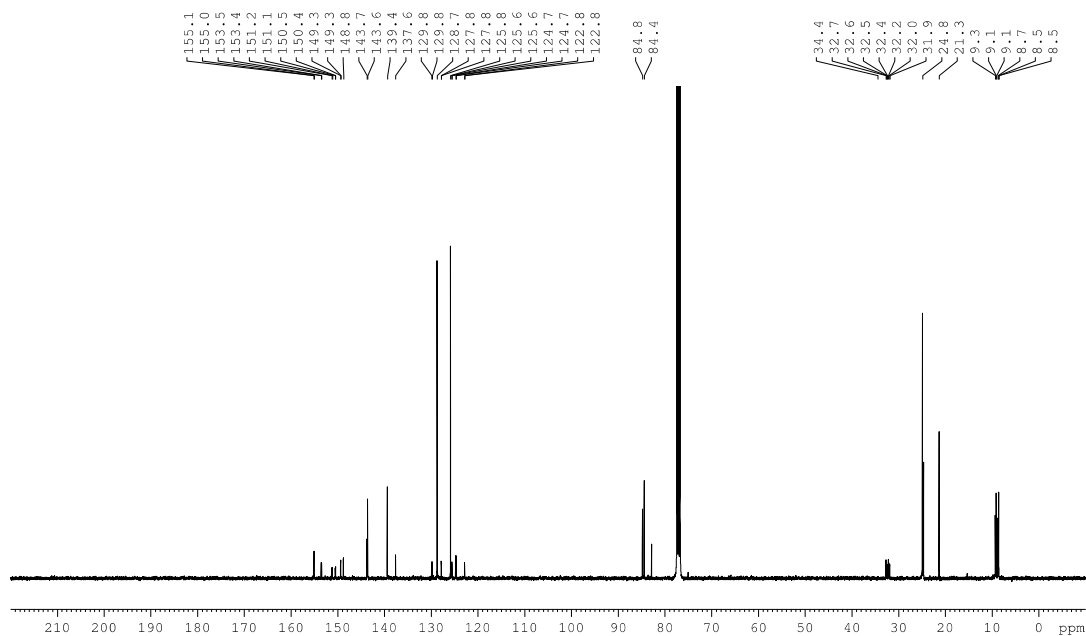
Borylation of 5a w/ 1: ¹³C NMR (101 MHz, CDCl₃)



Borylation of 5a w/ tmphen: ^1H NMR (400 MHz, CDCl_3)

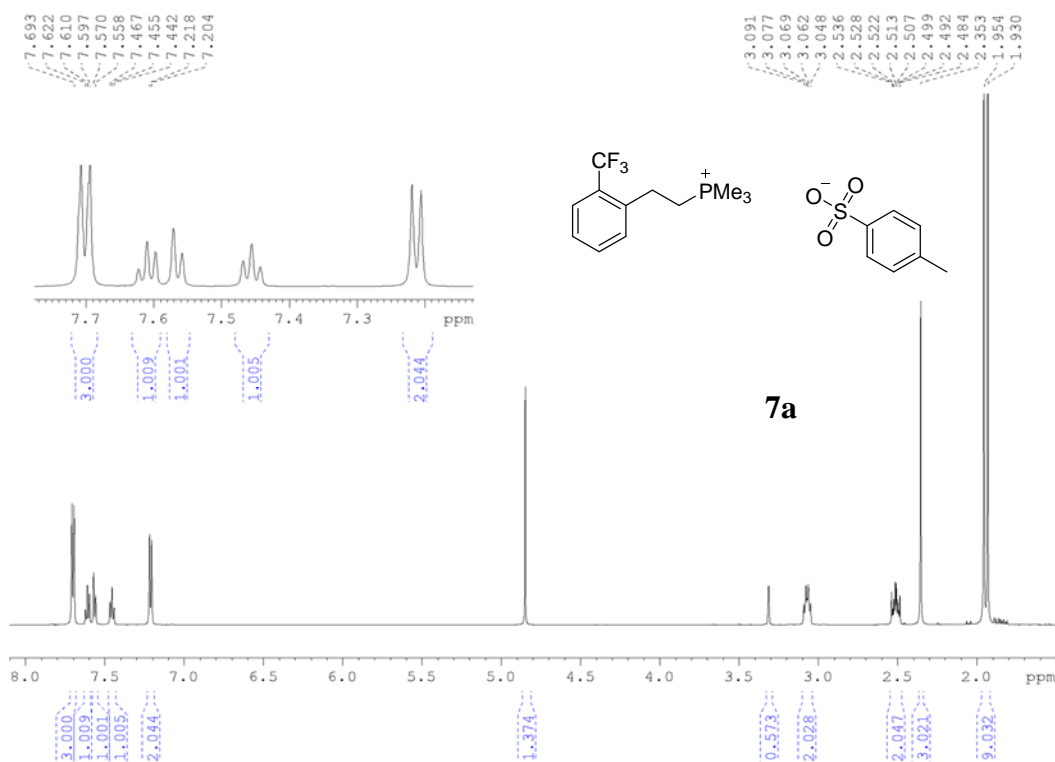


Borylation of 5a w/ tmphen: ^{13}C NMR (101 MHz, CDCl_3)

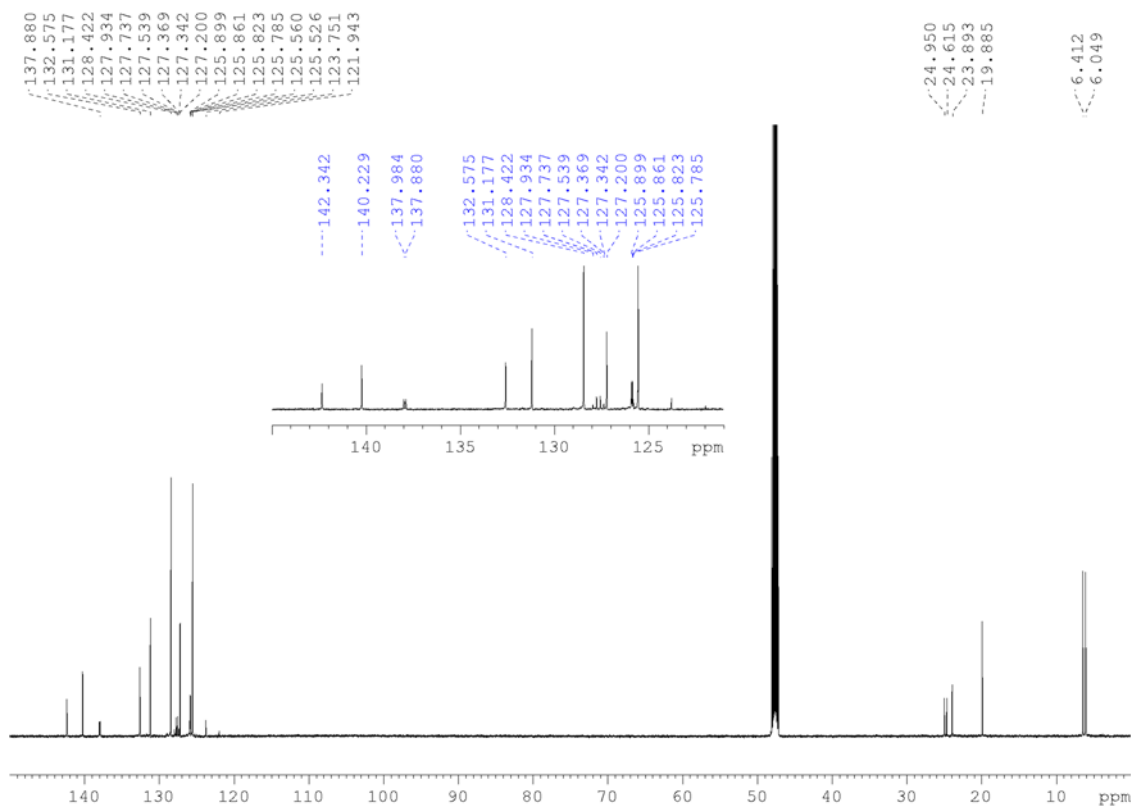


1.3 NMR data for Scheme 4

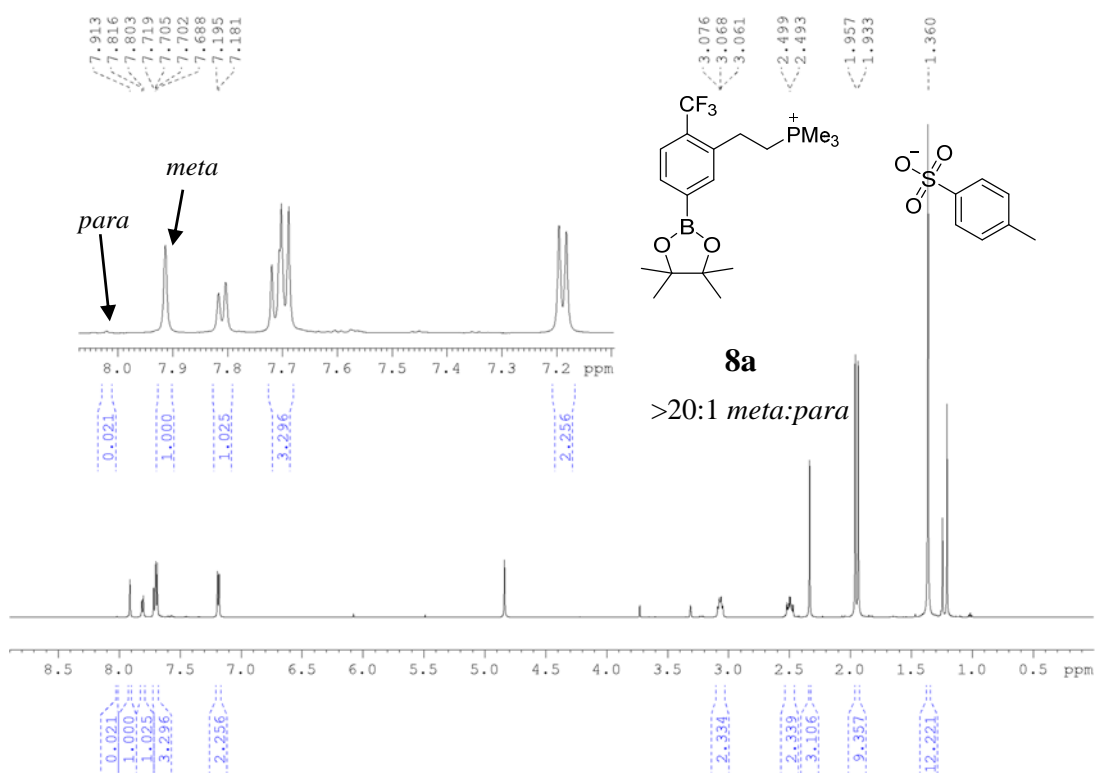
^1H NMR (600 MHz, $\text{MeOD-}d_4$)



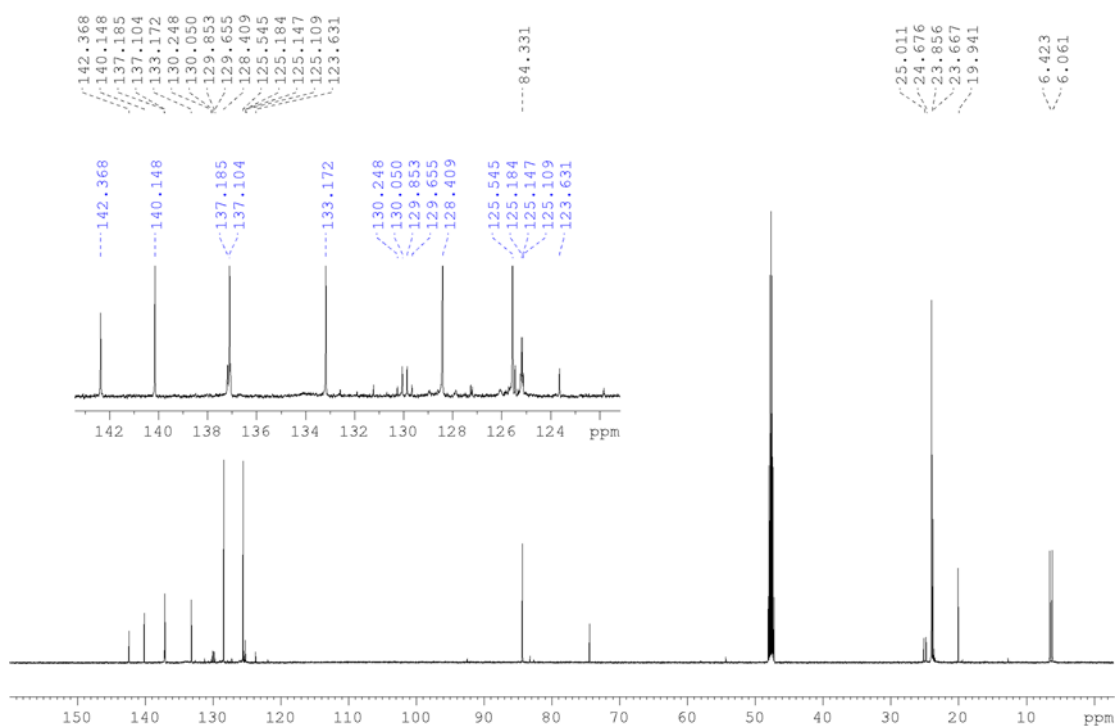
^{13}C NMR (151 MHz, $\text{MeOD-}d_4$)



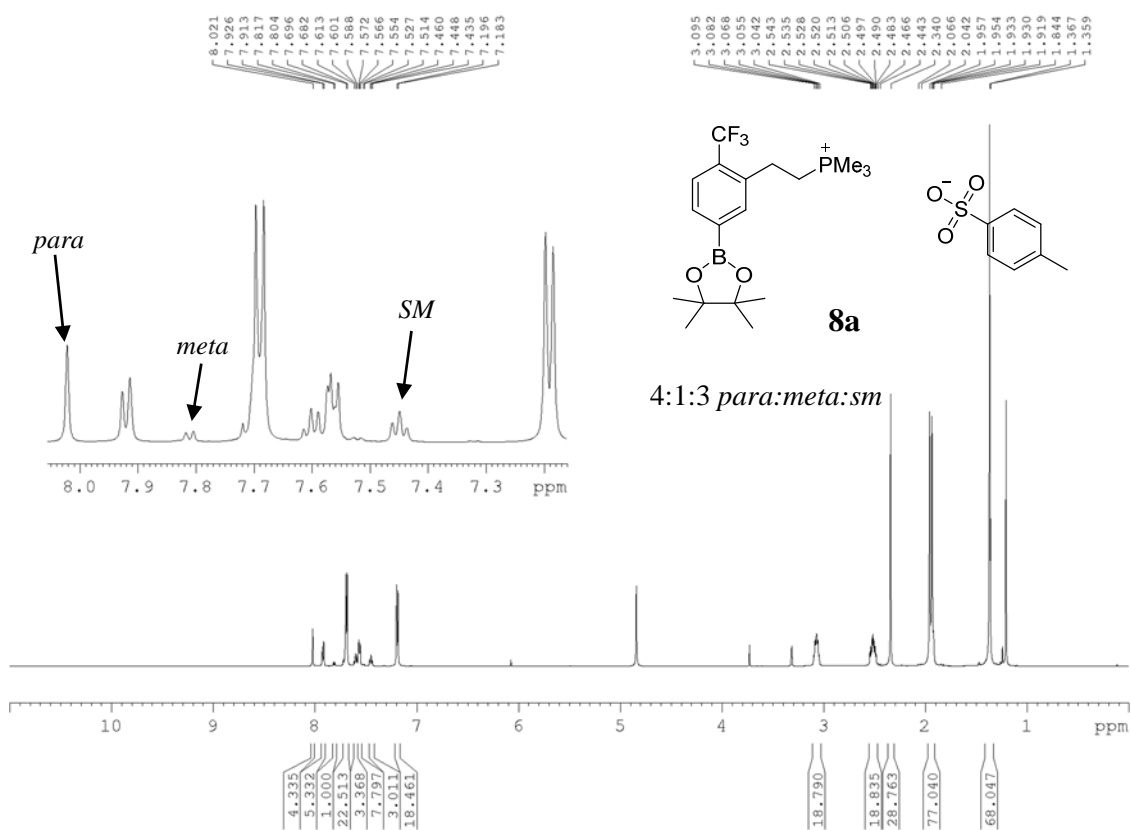
^1H NMR (600 MHz, $\text{MeOD-}d_4$) – Borylation with ligand 1



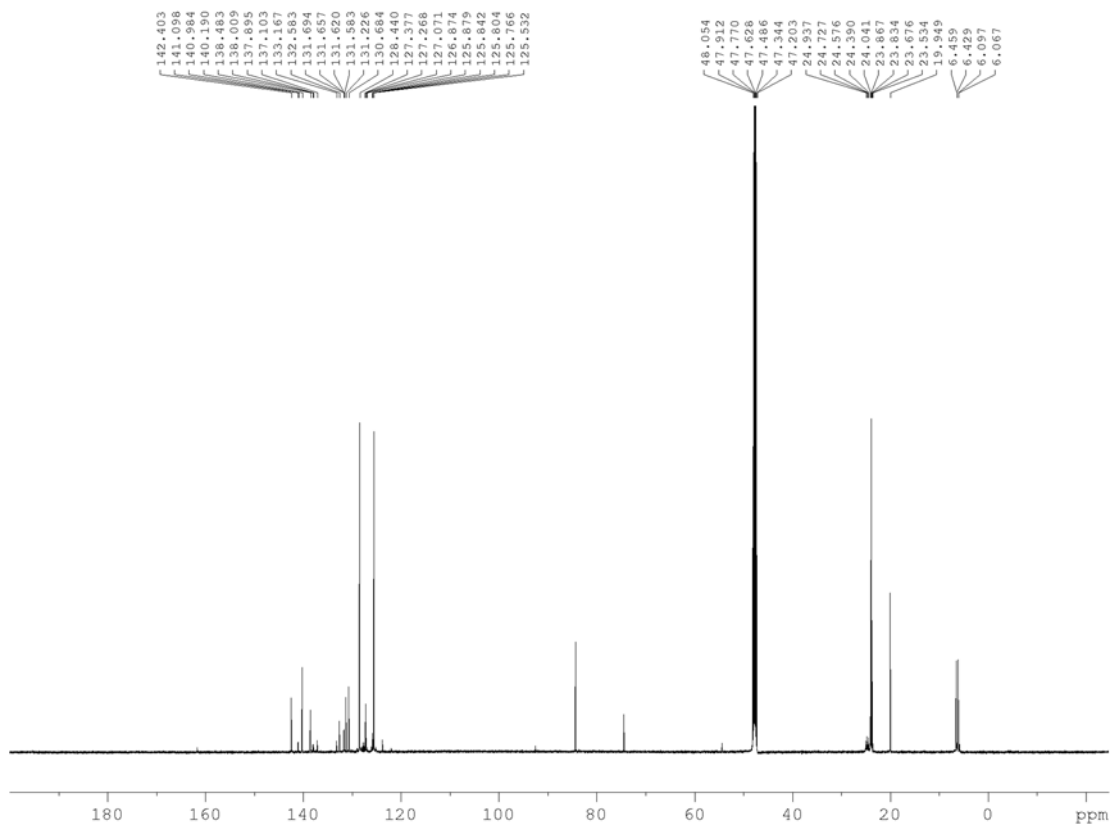
^{13}C NMR (151 MHz, $\text{MeOD-}d_4$) – Borylation with ligand 1



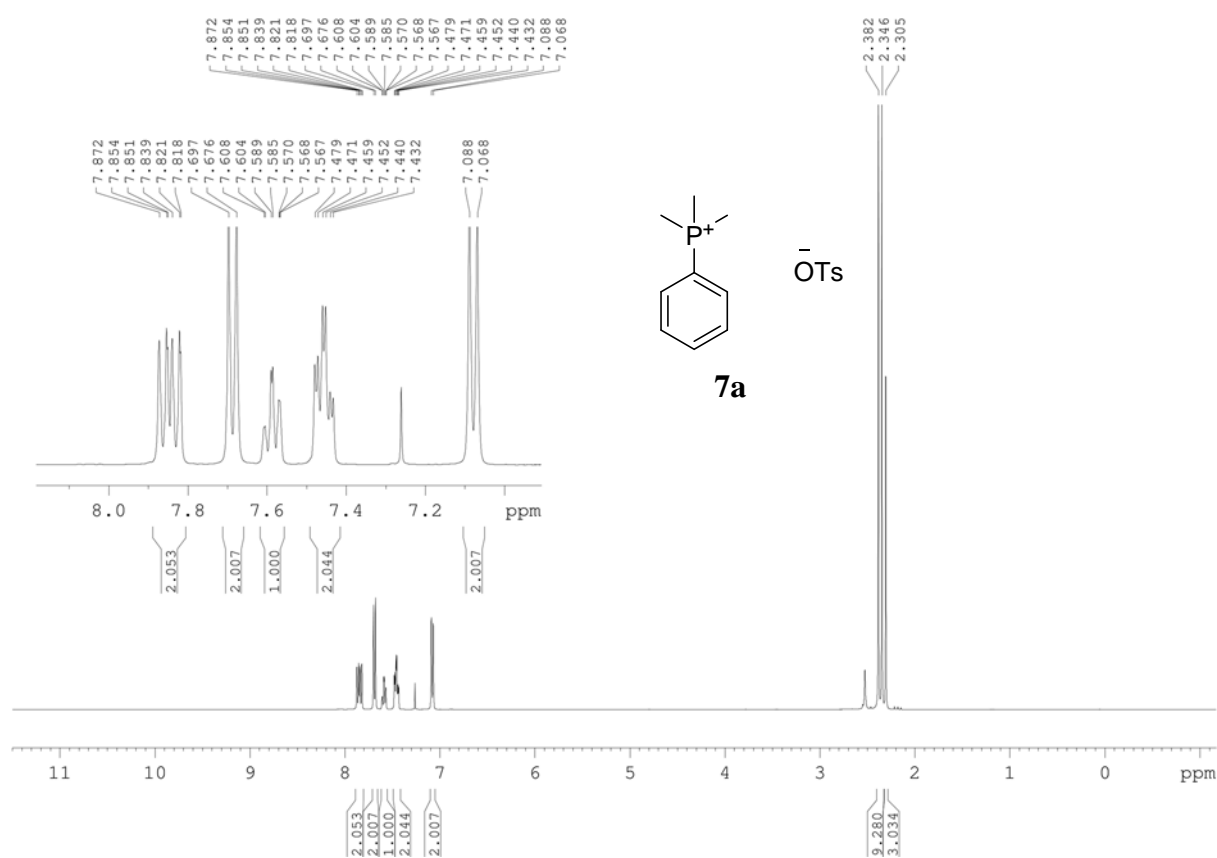
¹H NMR (600 MHz, MeOD-*d*₄) – Borylation with tmphen – triturated sample



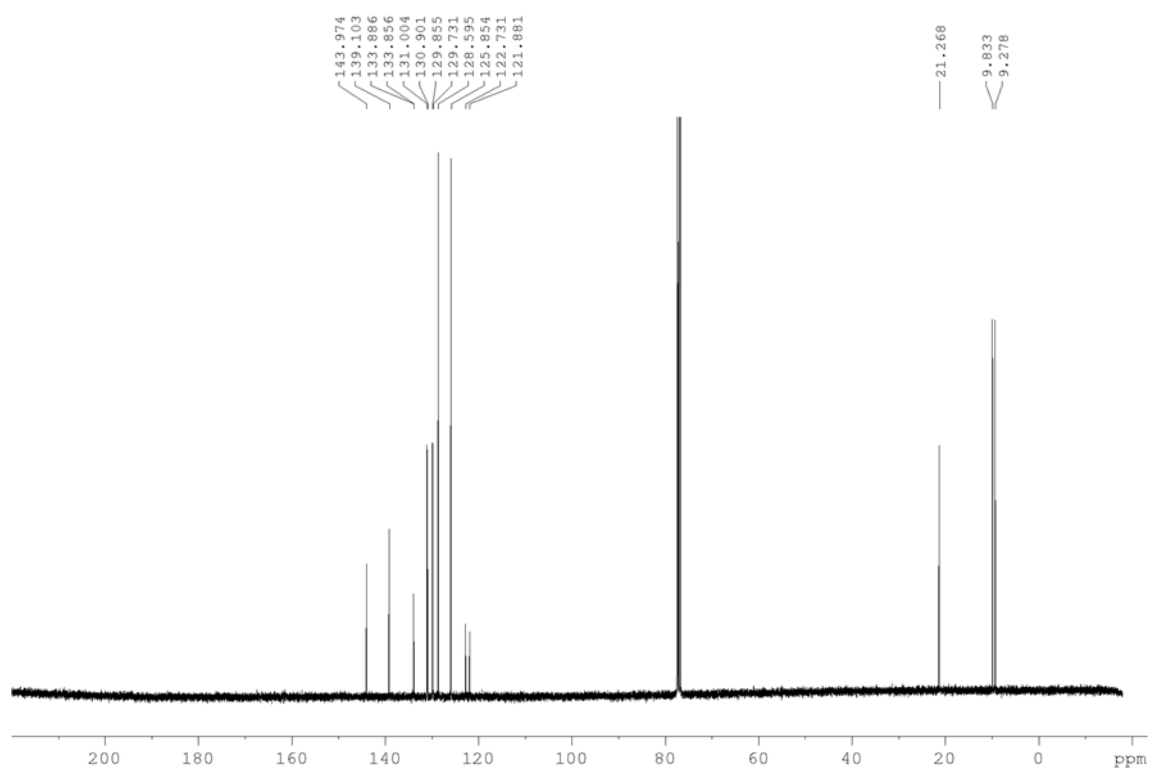
¹³C NMR (151 MHz, MeOD-*d*₄) – Borylation with tmphen – triturated sample



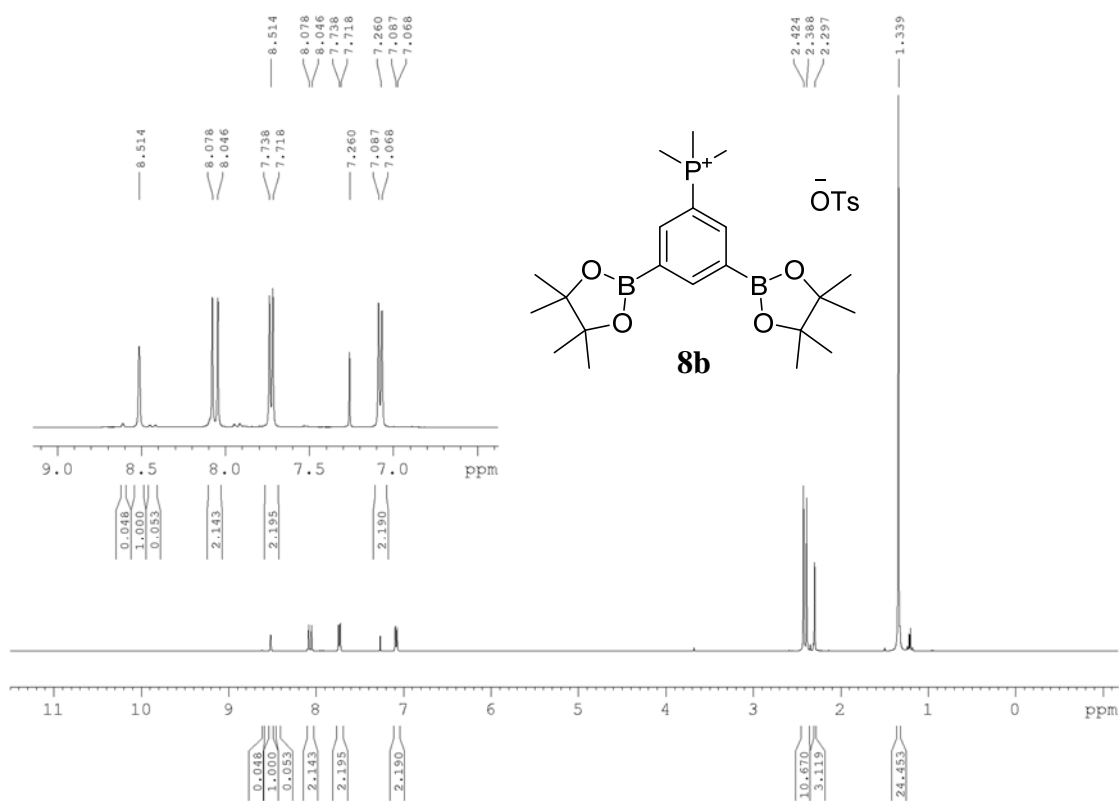
¹H NMR (400 MHz, CDCl₃) – 7b



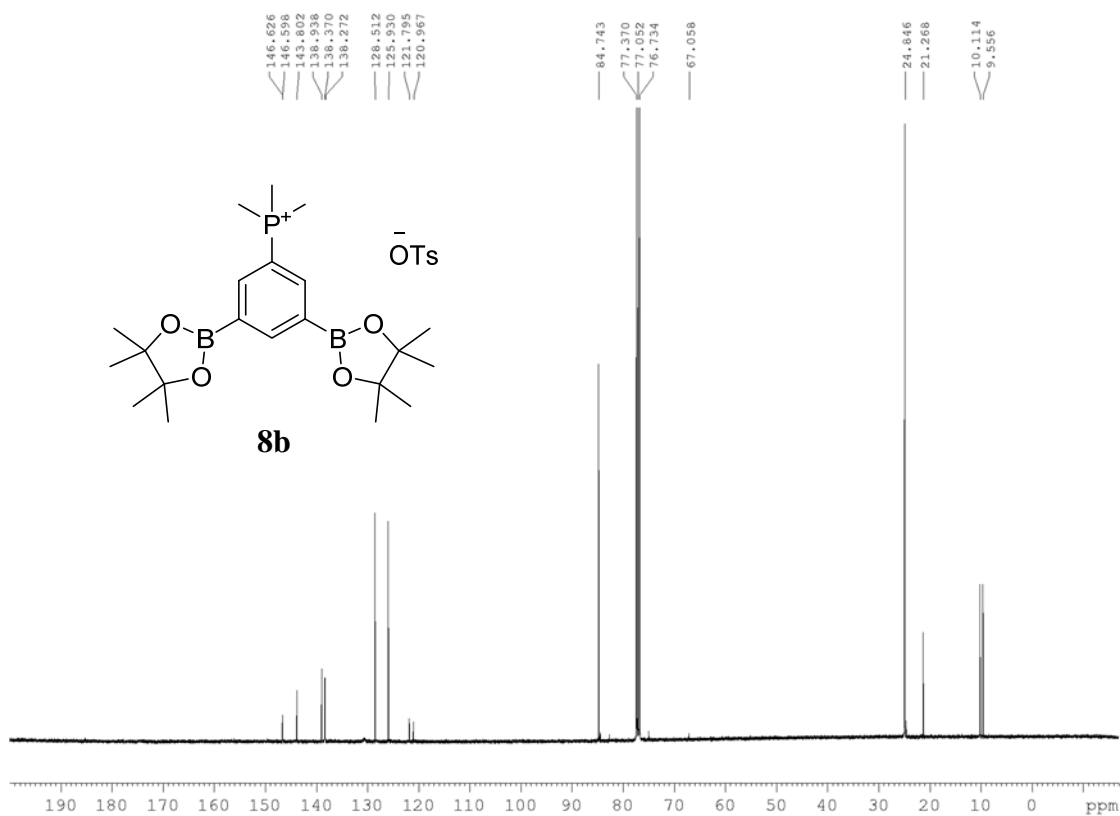
¹³C NMR (101 MHz, CDCl₃) – 7b



¹H NMR (400 MHz, CDCl₃) – Borylation with ligand 1

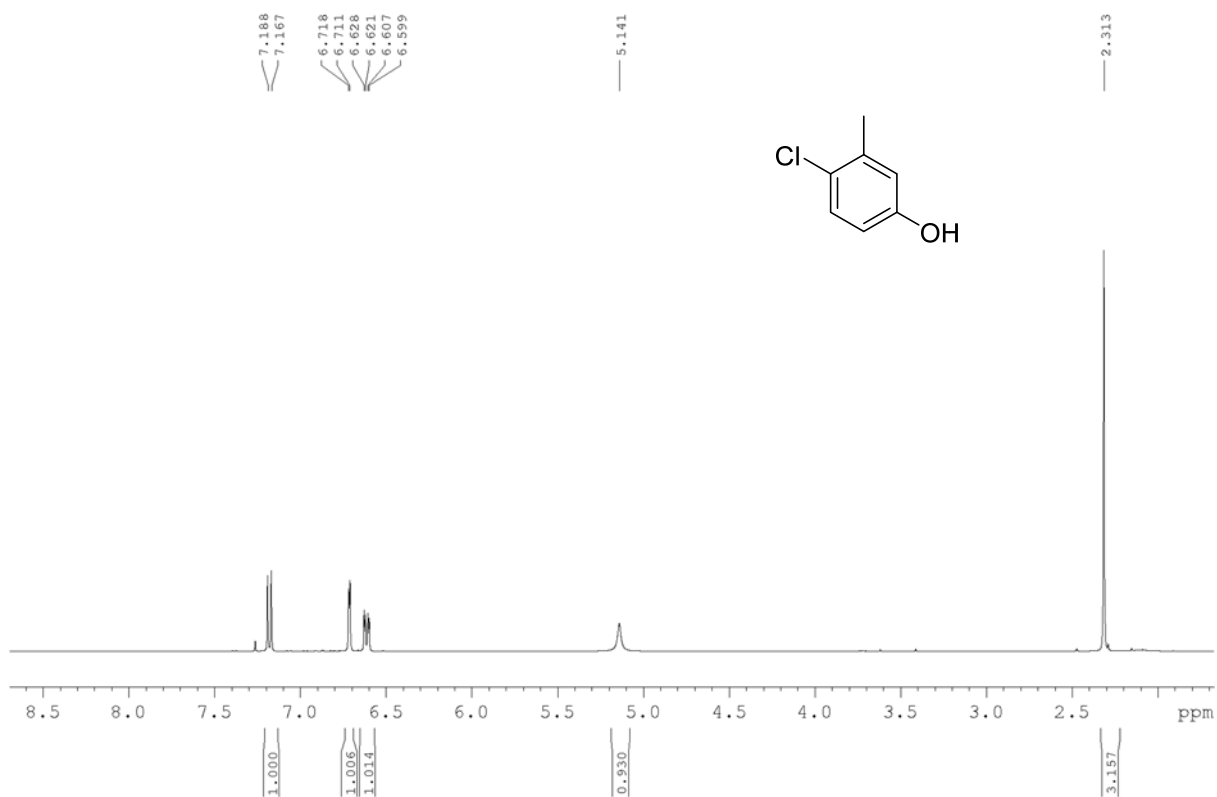


¹³C NMR (101 MHz, CDCl₃) – Borylation with ligand 1



1.4 NMR data for Scheme 5

^1H NMR (400 MHz, CDCl_3) – 4-Chloro-3-methylphenol (9)



^{13}C NMR (101 MHz, CDCl_3) – 4-Chloro-3-methylphenol (9)

