

# Supporting information

## **Soft Heteroleptic N-Heterocyclic Carbene Palladium(II) Species For Efficient Catalytic Routes to Alkynones Via Carbonylative Sonogashira Coupling**

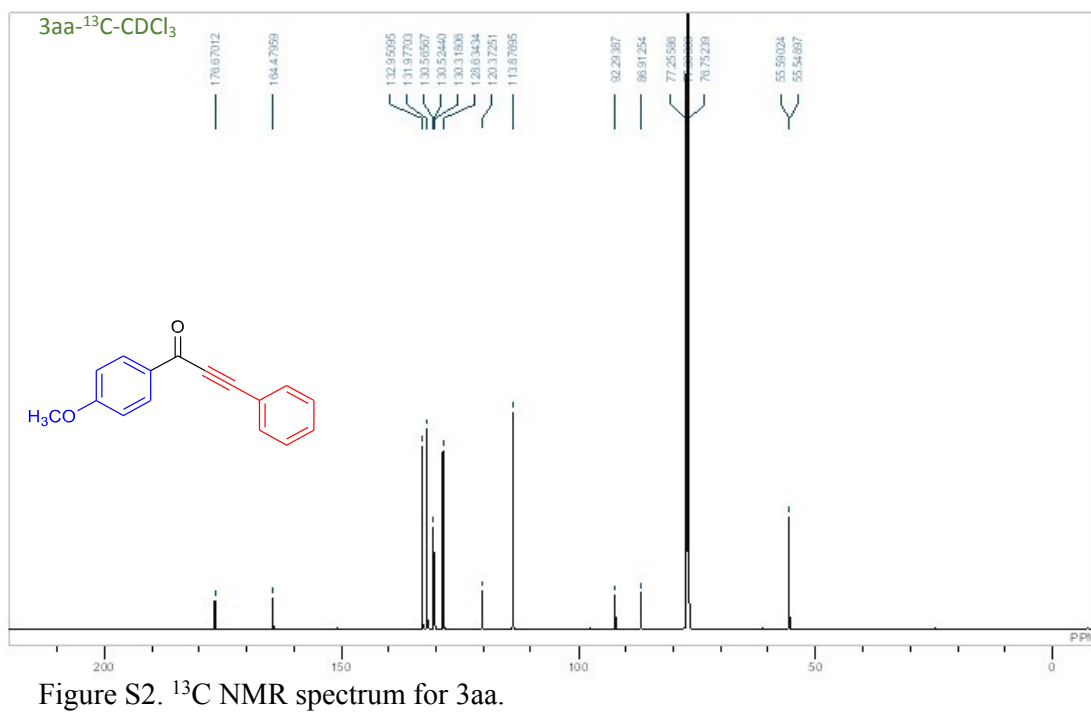
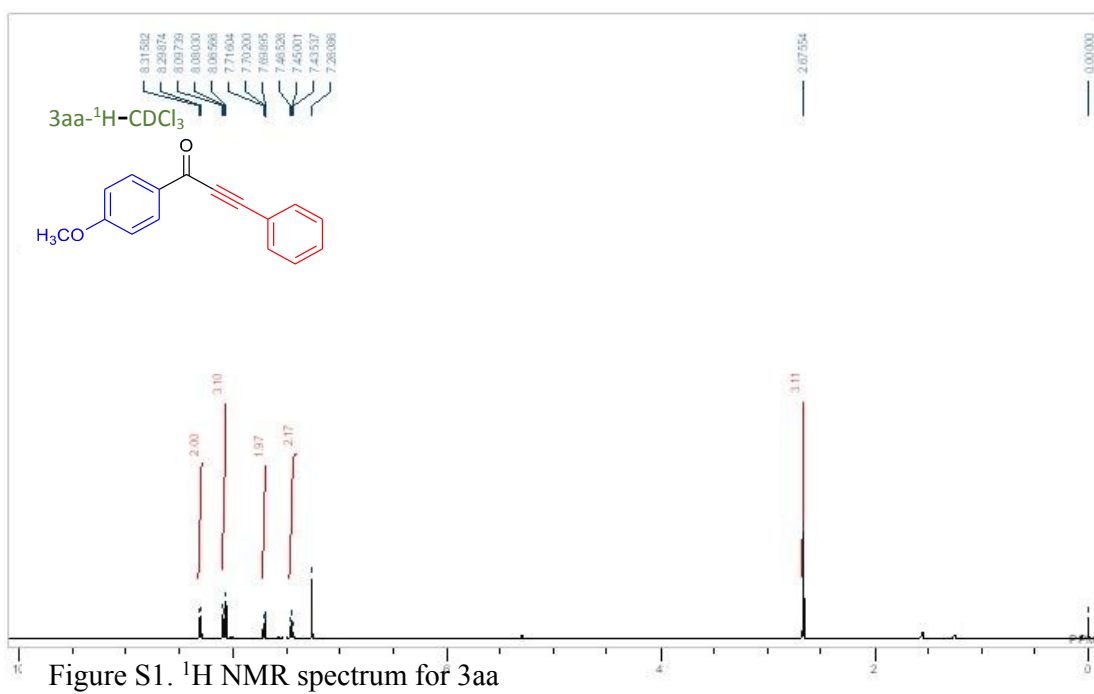
Waseem Mansour<sup>a</sup>, Rami Suleiman<sup>b</sup>, Mohammed Fettouhi<sup>a</sup>, Bassam El Ali<sup>a\*</sup>

*<sup>a</sup>Chemistry Department, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia*

*<sup>b</sup>Center of Research Excellence in Corrosion, King Fahd University of Petroleum & Minerals, Dhahran 31261, Saudi Arabia.*

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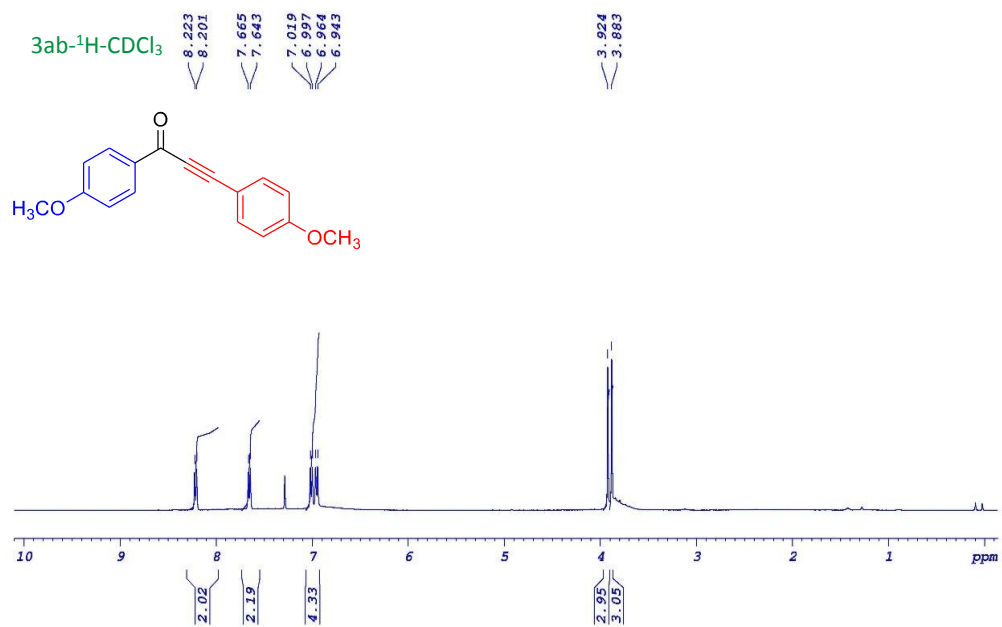


Figure S3. <sup>1</sup>H NMR spectrum for 3ab

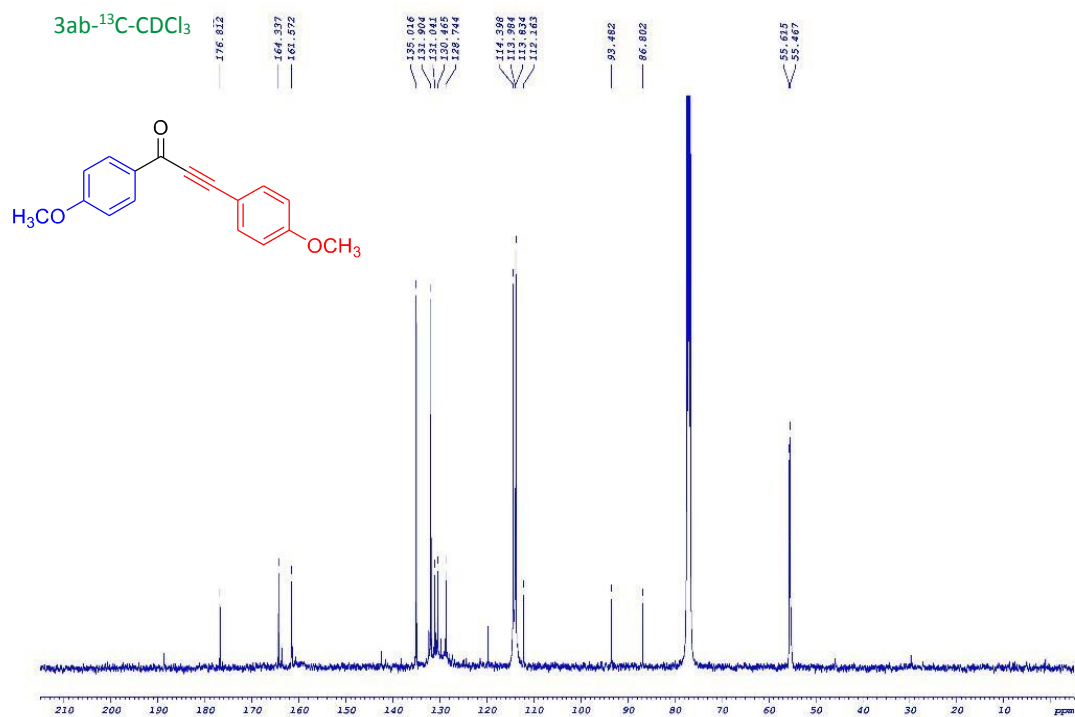


Figure S4. <sup>13</sup>C NMR spectrum for 3ab

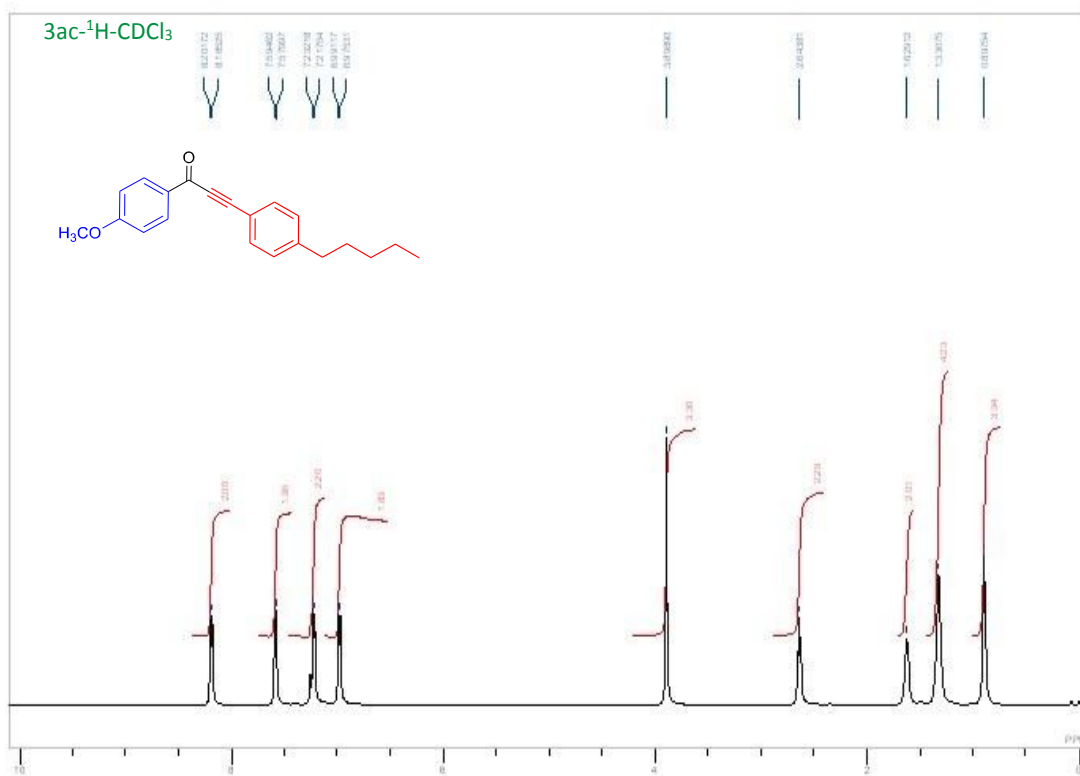


Figure S5. <sup>1</sup>H NMR spectrum for 3ac

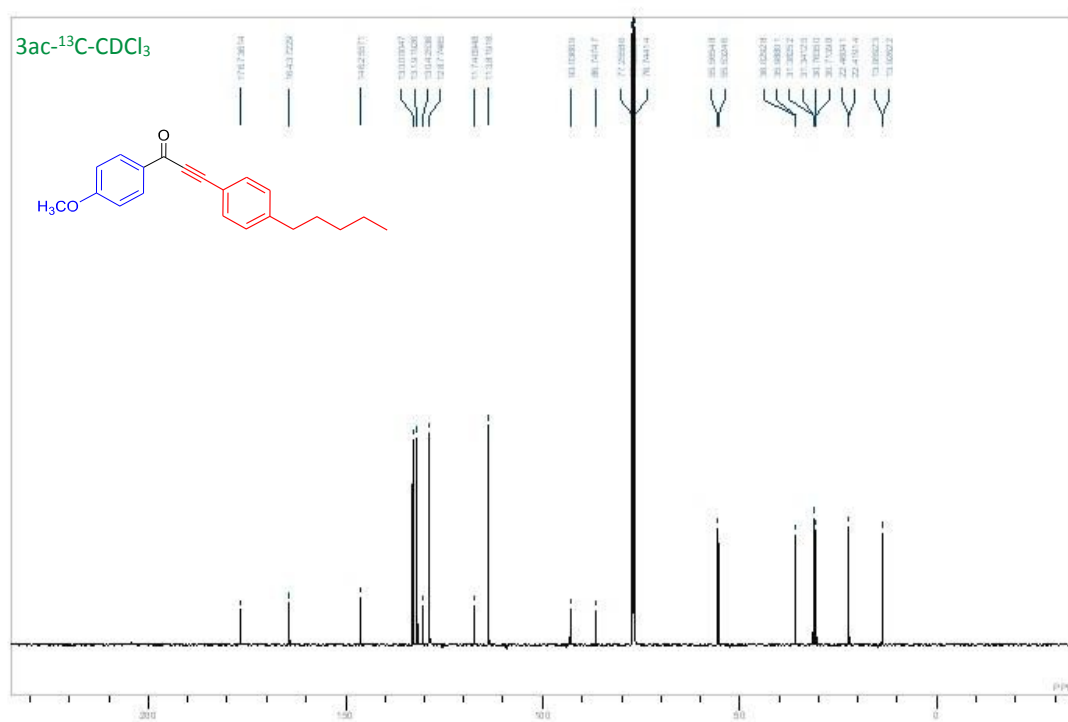


Figure S6. <sup>13</sup>C NMR spectrum for 3ac

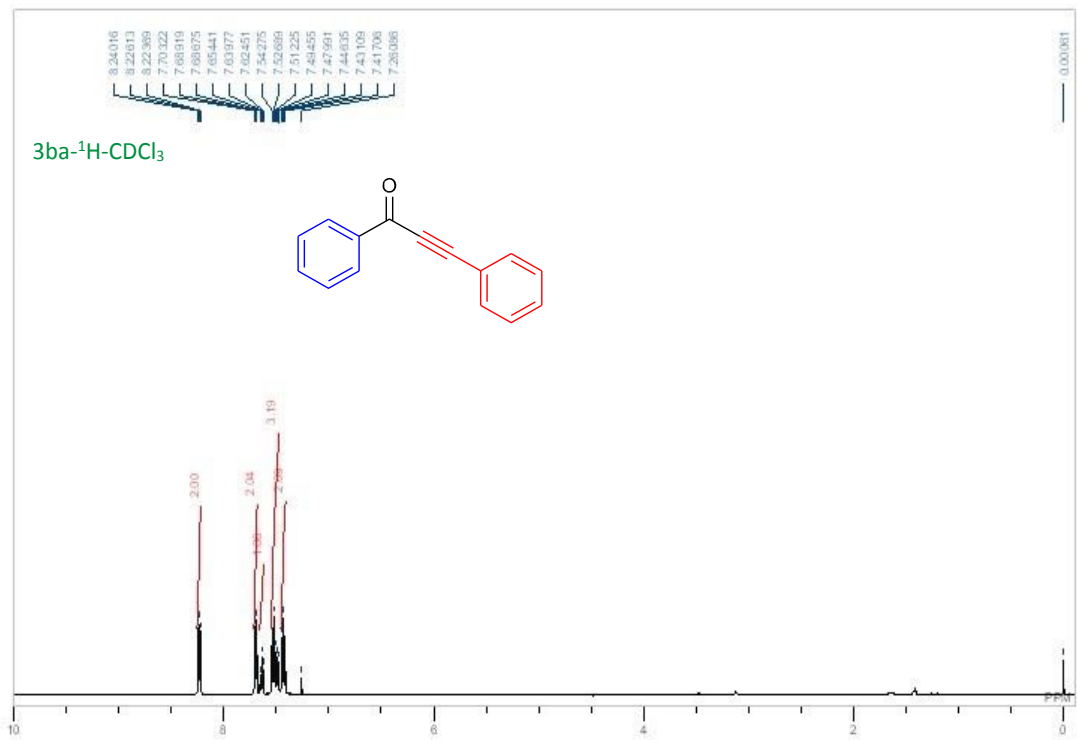


Figure S7. <sup>1</sup>H NMR spectrum for 3ba

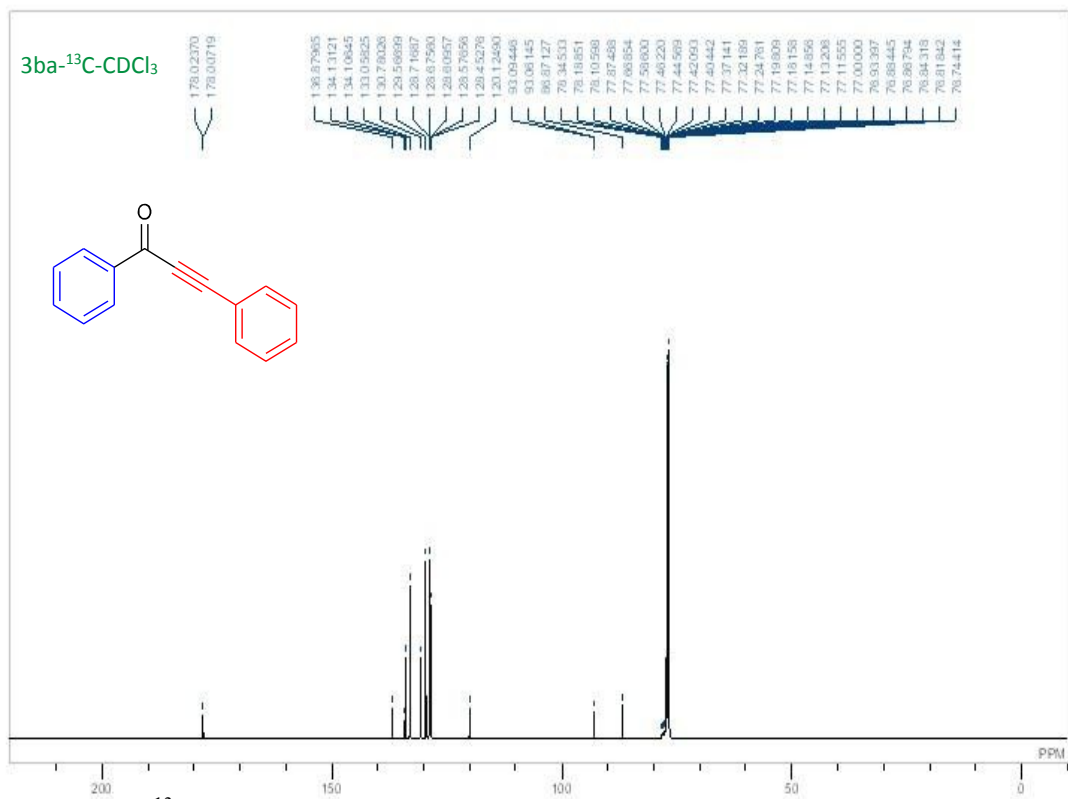


Figure S8. <sup>13</sup>C NMR spectrum for 3b

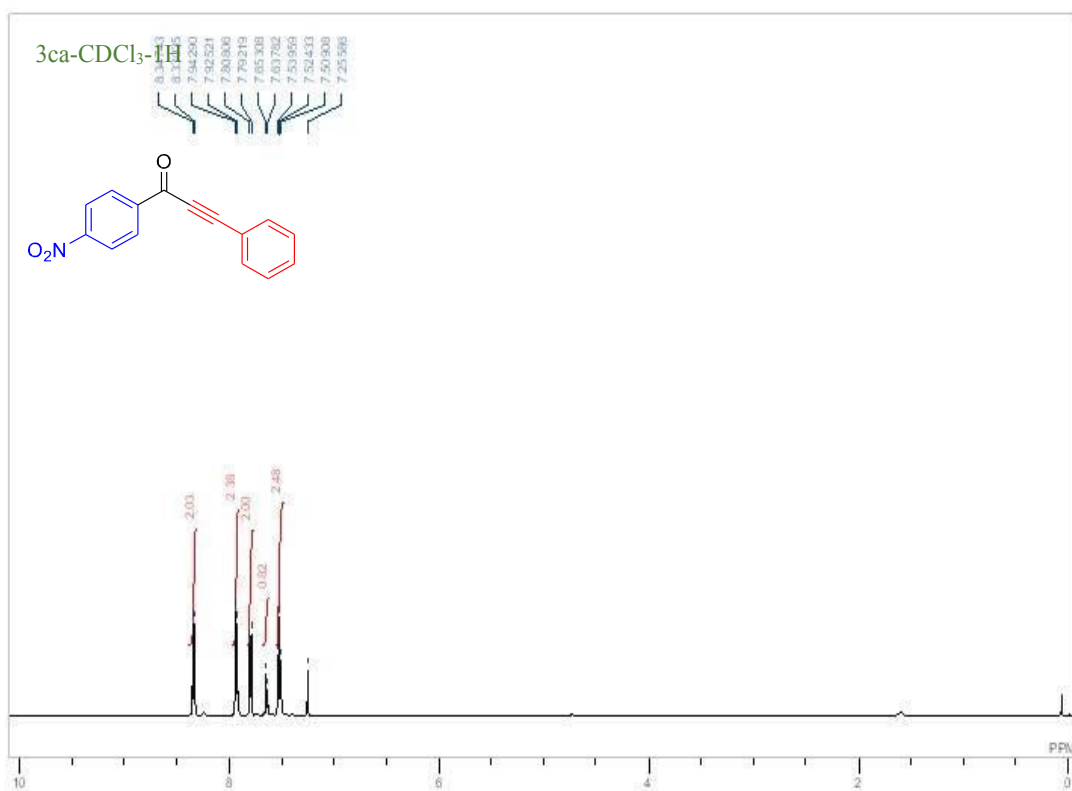


Figure S9. <sup>1</sup>H NMR spectrum for 3ca

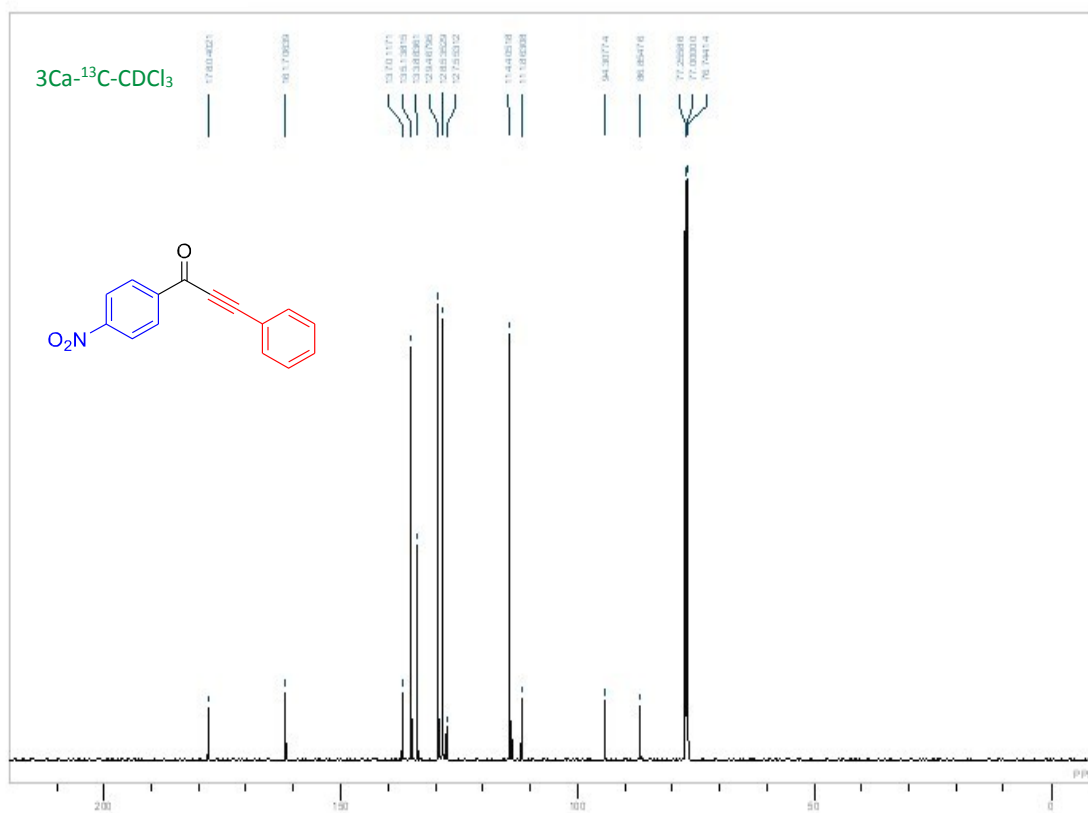


Figure S10. <sup>13</sup>C NMR spectrum for 3Ca

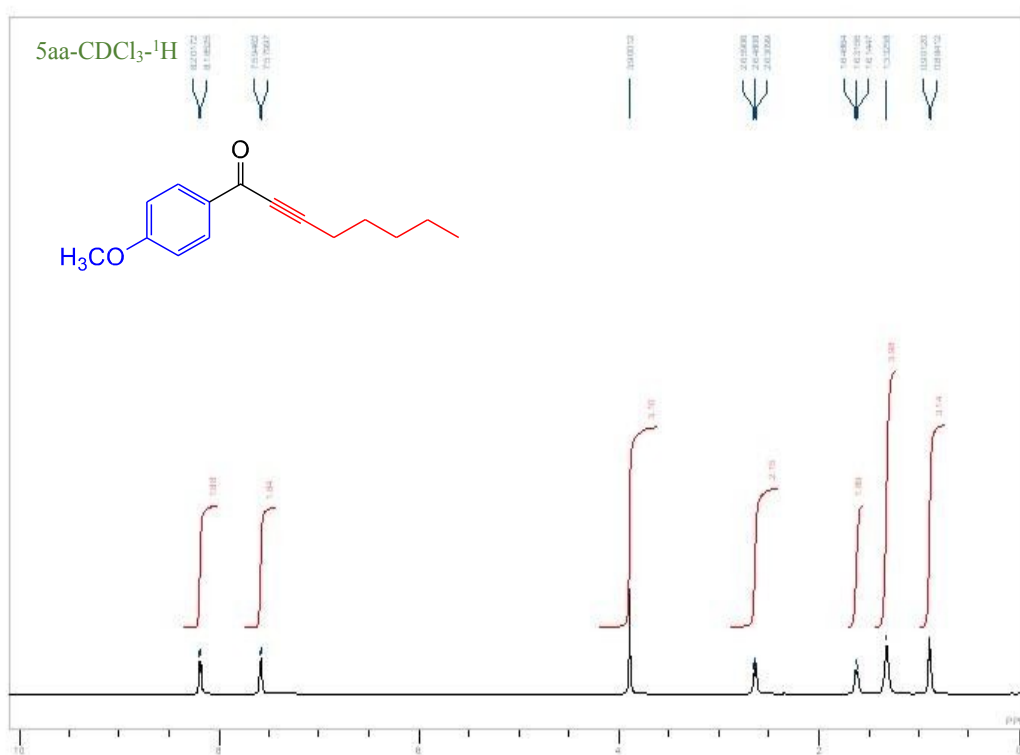


Figure S11. <sup>1</sup>H NMR spectrum for 5aa

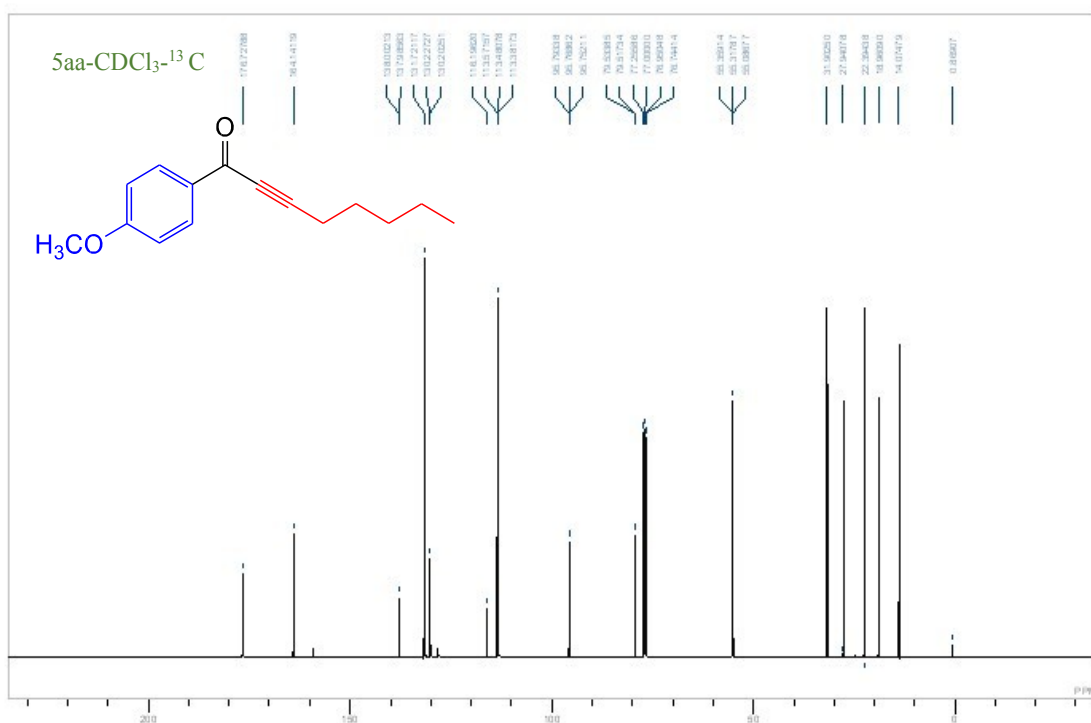


Figure S12. <sup>13</sup>C NMR spectrum for 5aa



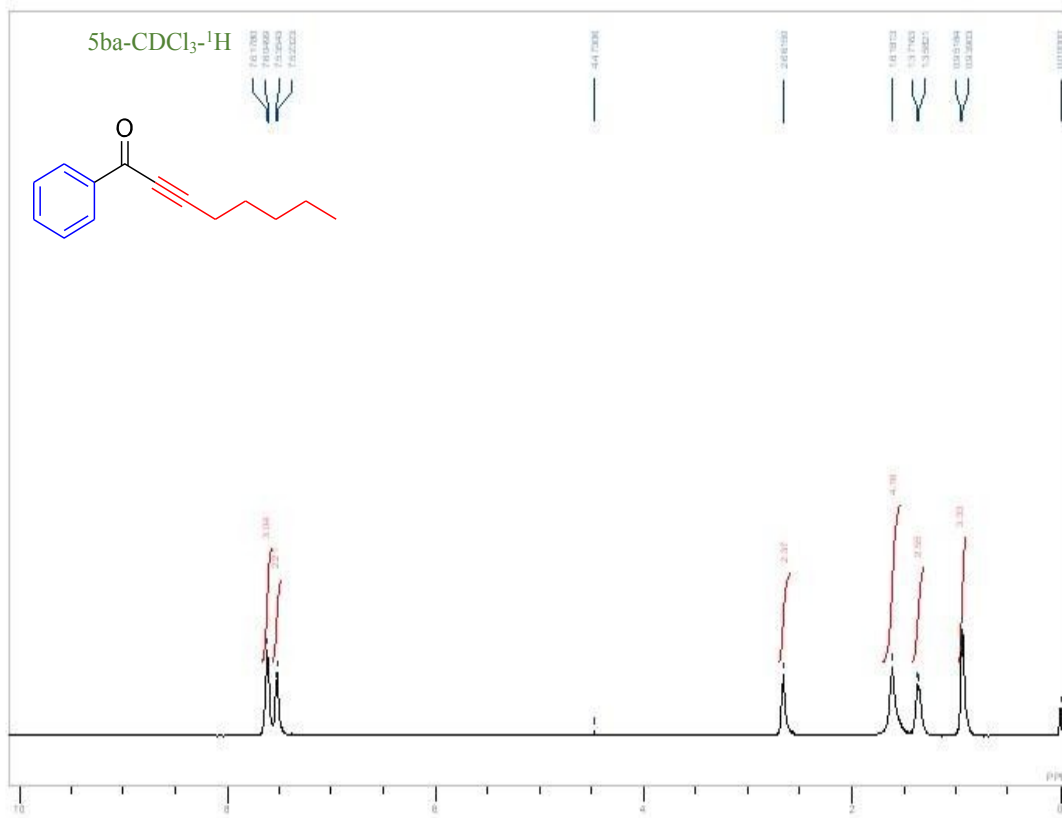


Figure S13. <sup>1</sup>H NMR spectrum for 5ba

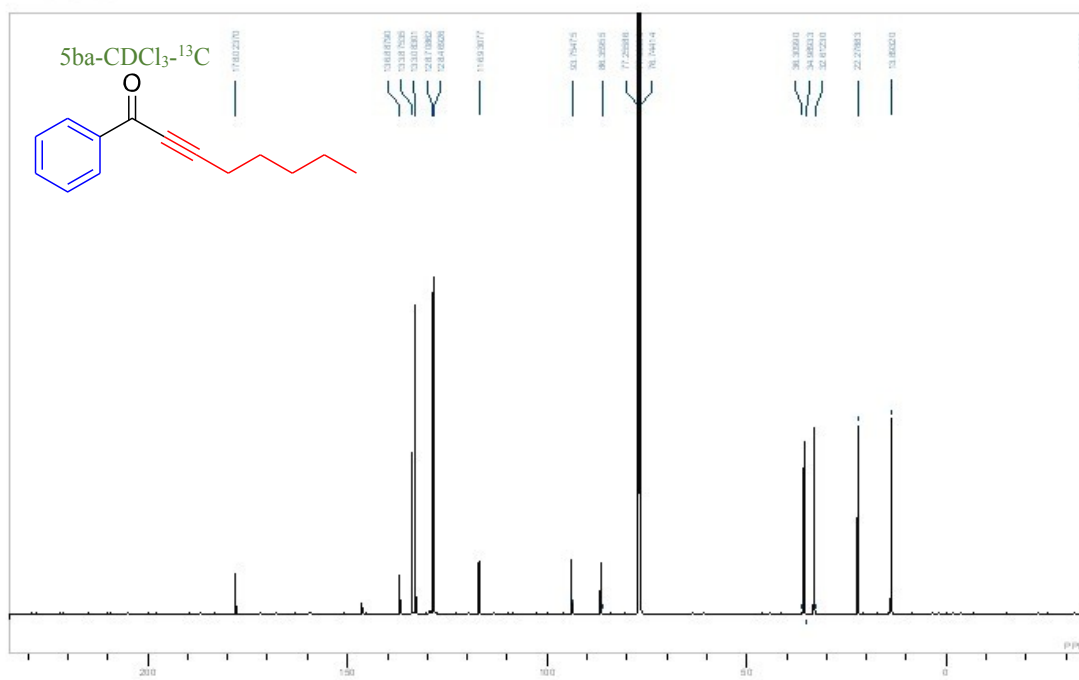
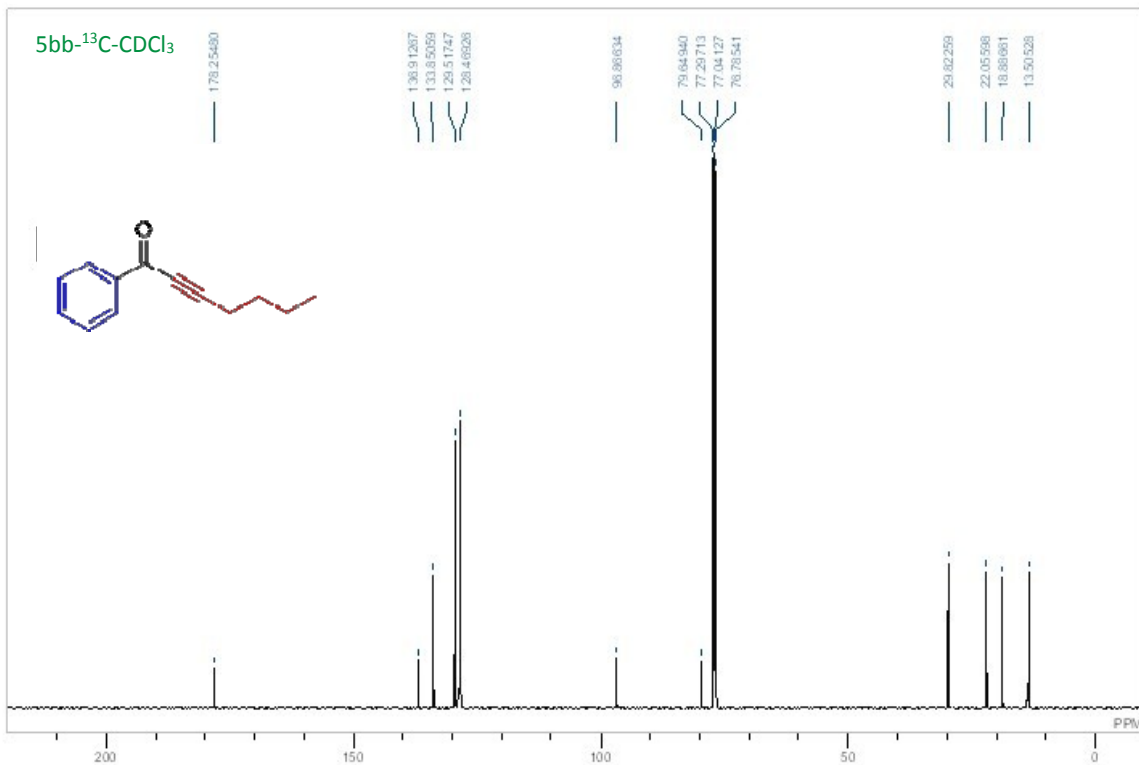
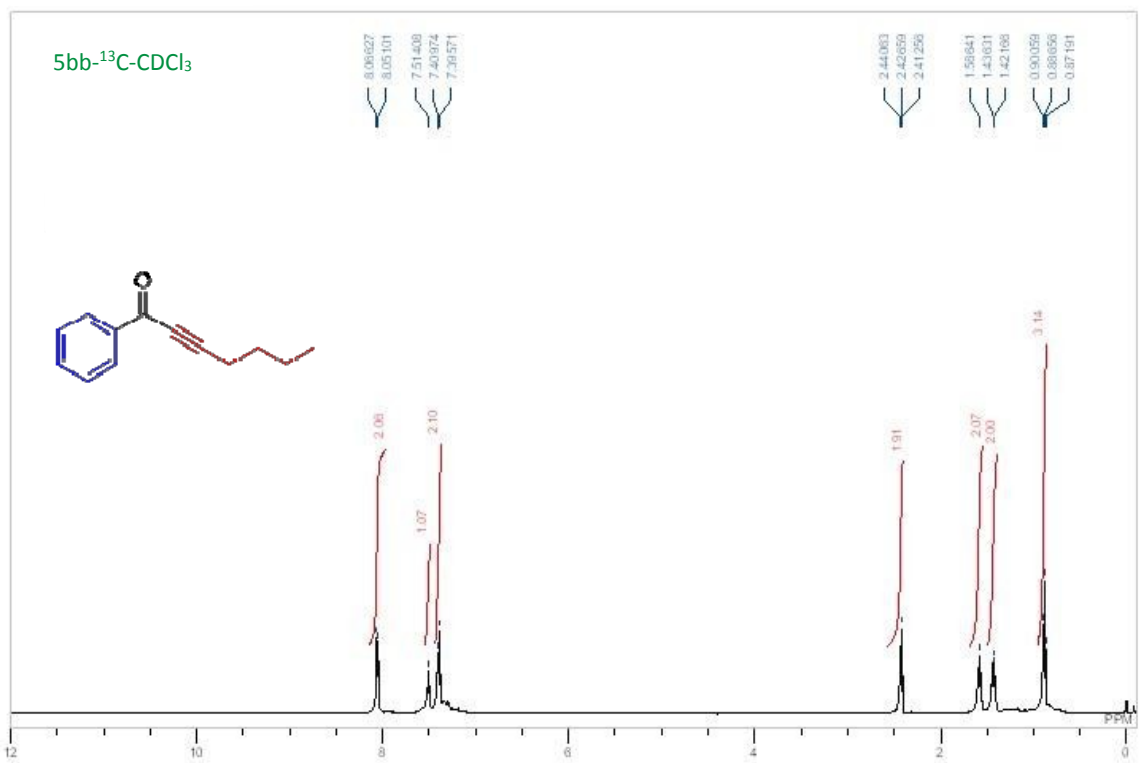


Figure S14. <sup>13</sup>C NMR spectrum for 5ba



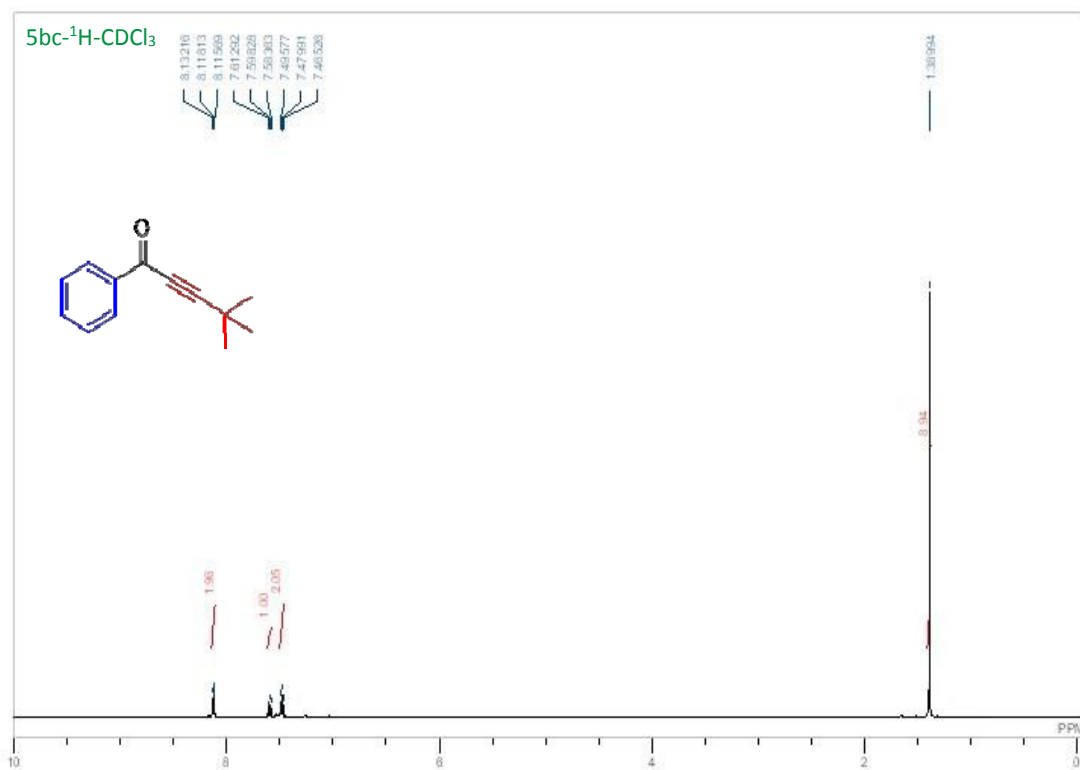


Figure S17. <sup>1</sup>H NMR spectrum for 5bc

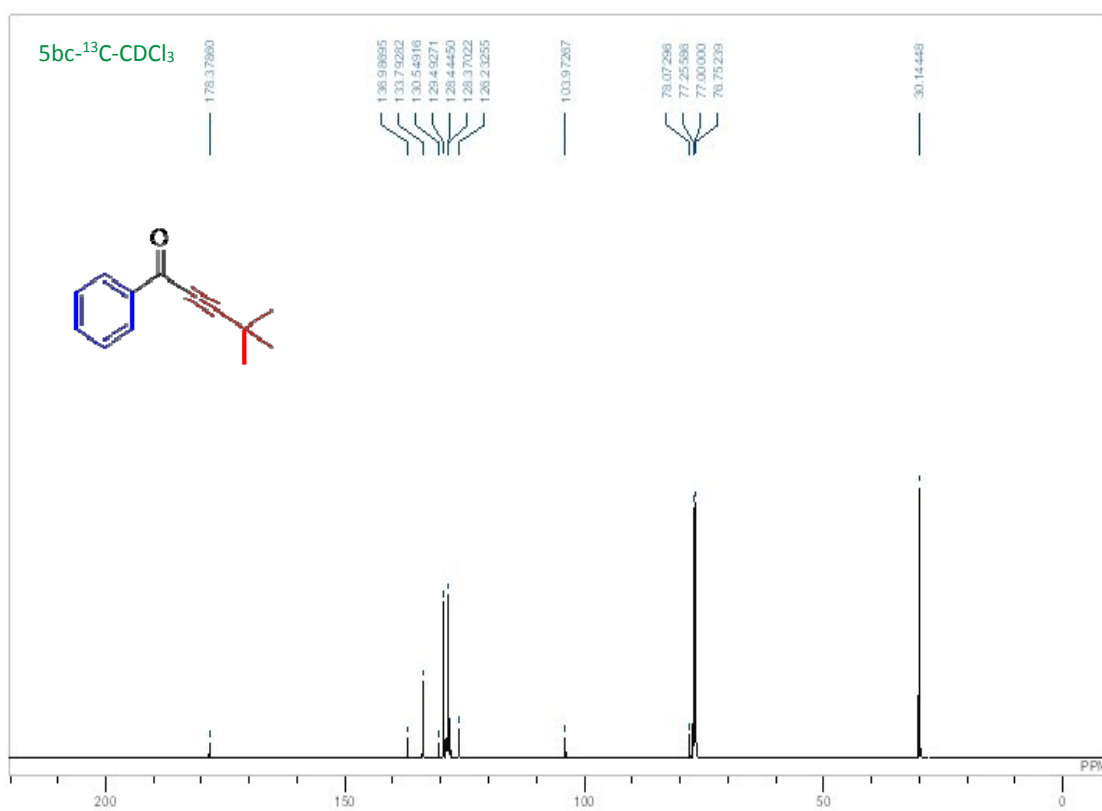


Figure S18. <sup>13</sup>C NMR spectrum for 5bc



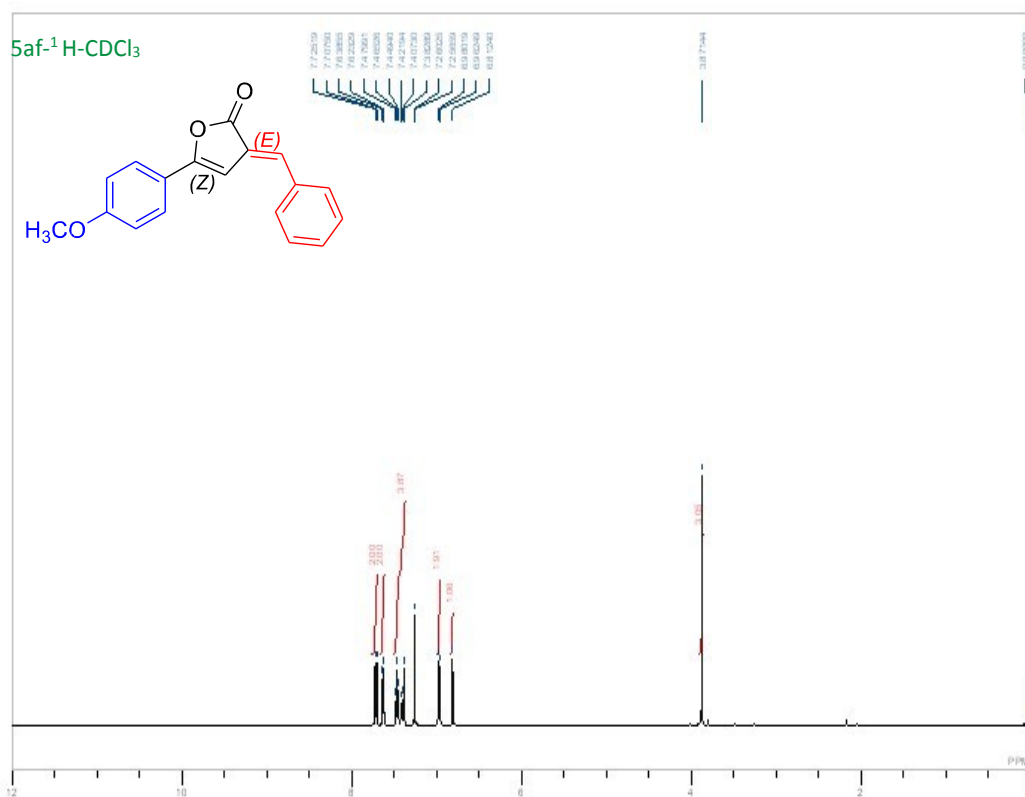


Figure S21. <sup>1</sup>H NMR spectrum for 5af

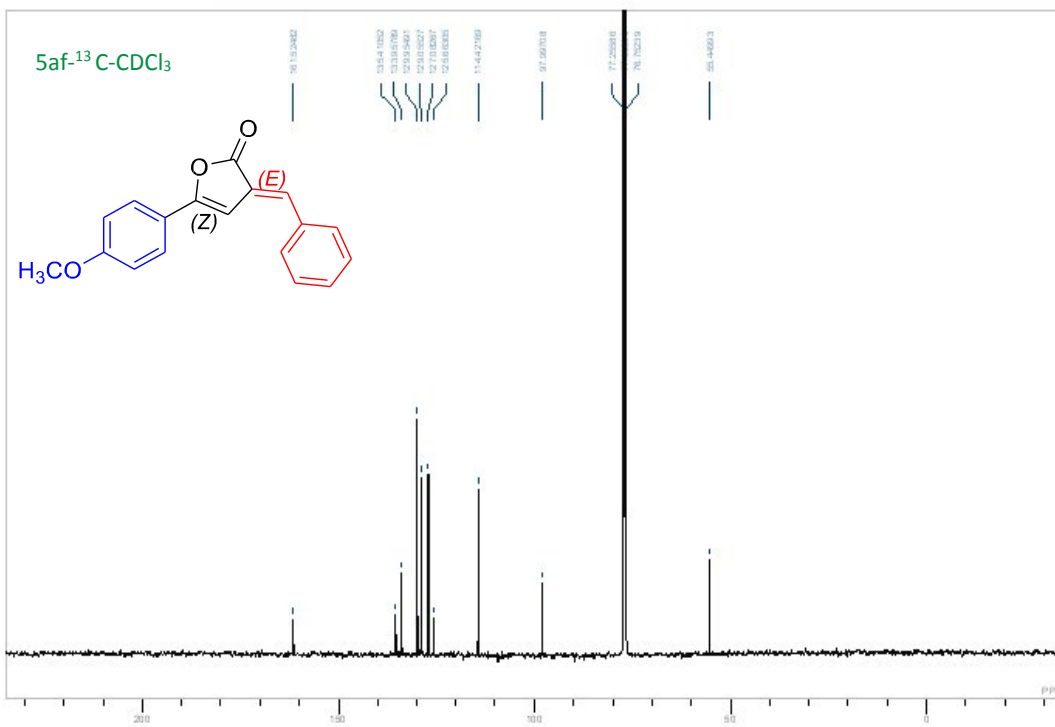


Figure S22. <sup>13</sup>C NMR spectrum for 5af

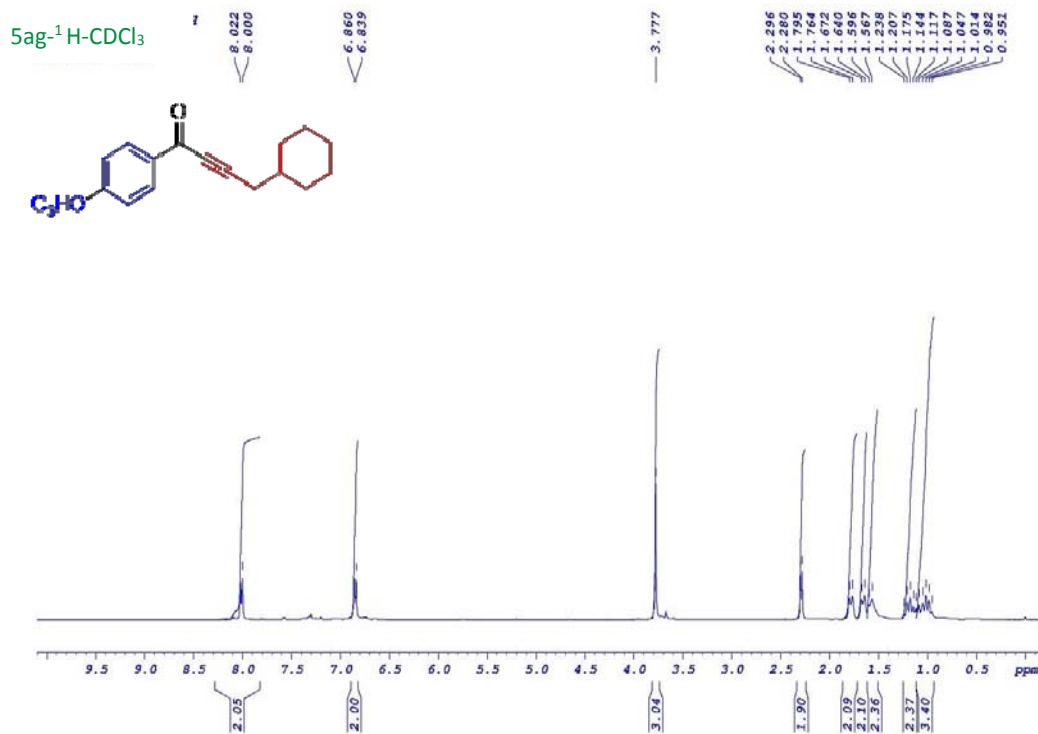


Figure S23. <sup>1</sup>H NMR spectrum for 5ag

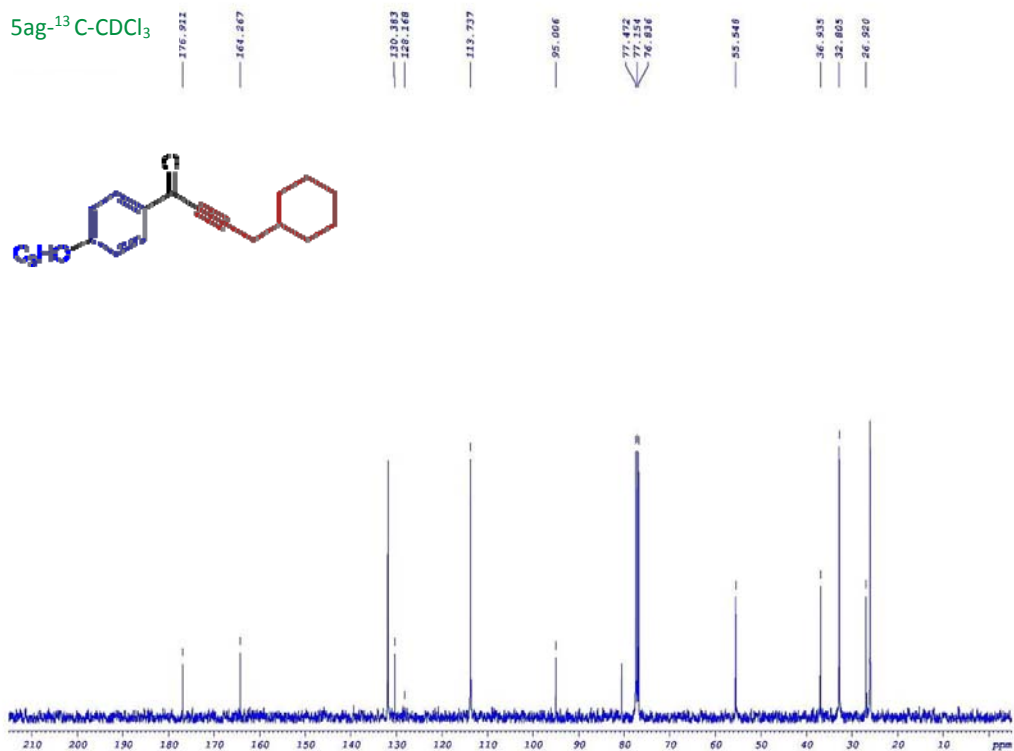


Figure S24. <sup>13</sup>C NMR spectrum for 5ag









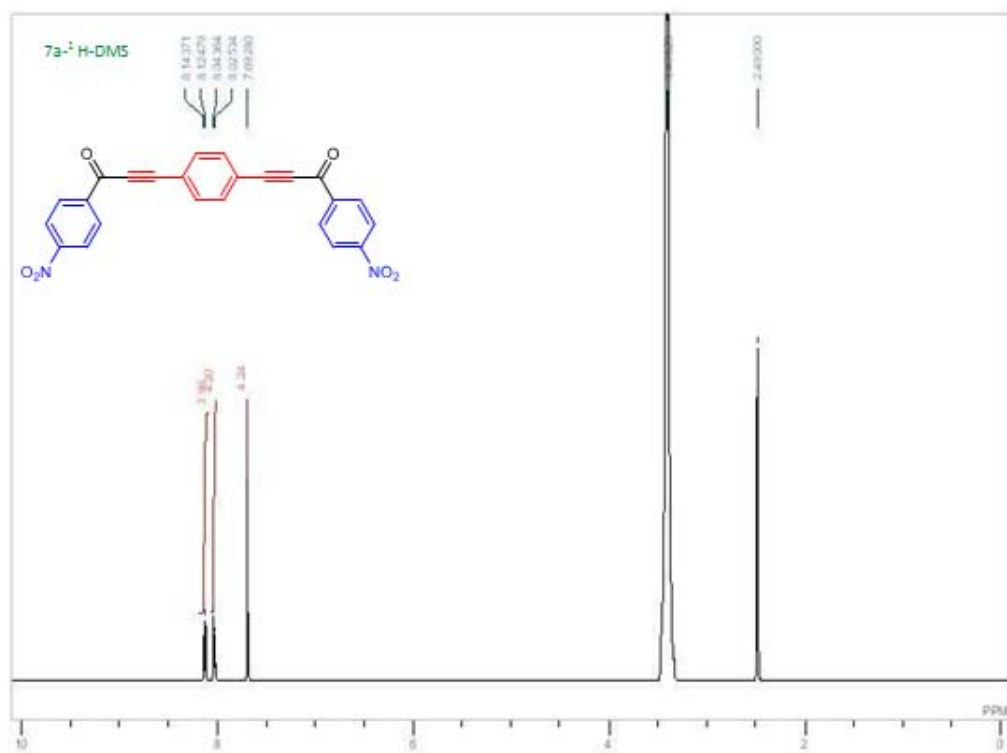


Figure S31. <sup>1</sup>H NMR spectrum for 7a

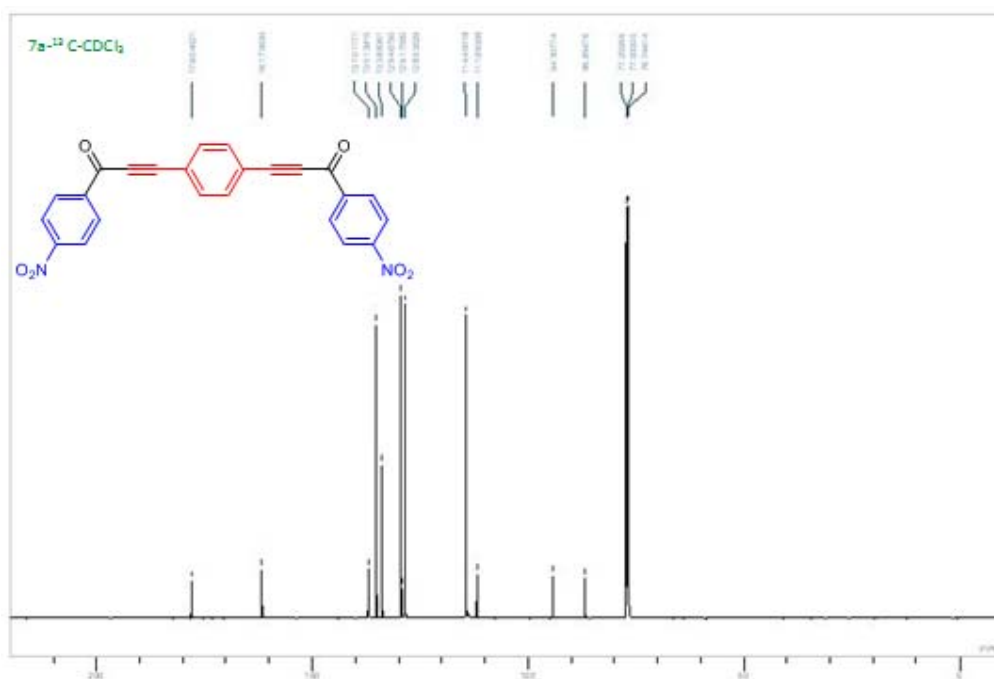


Figure S32. <sup>13</sup>C NMR spectrum for 7a

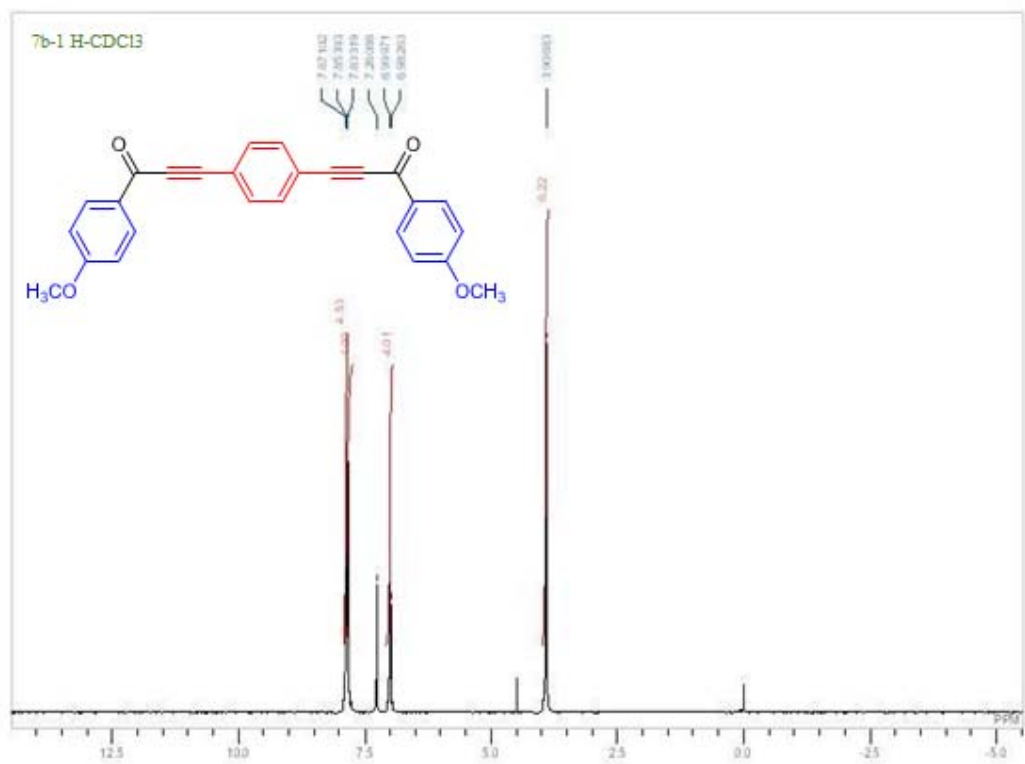


Figure S33. <sup>1</sup>H NMR spectrum for 7b

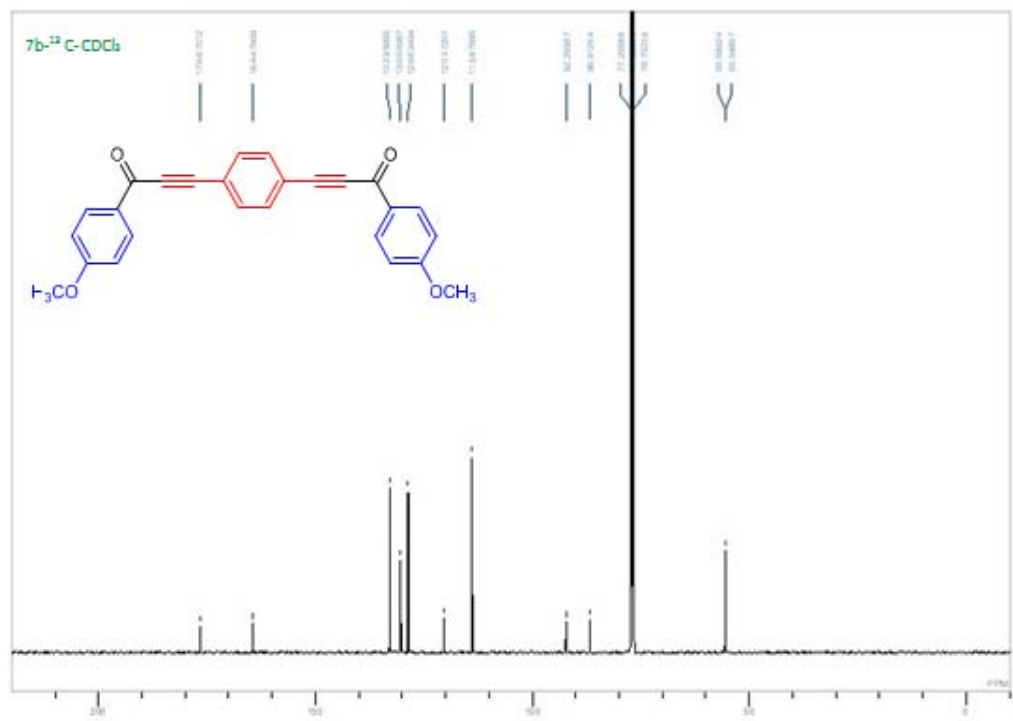


Figure S34. <sup>13</sup>C NMR spectrum for 7b

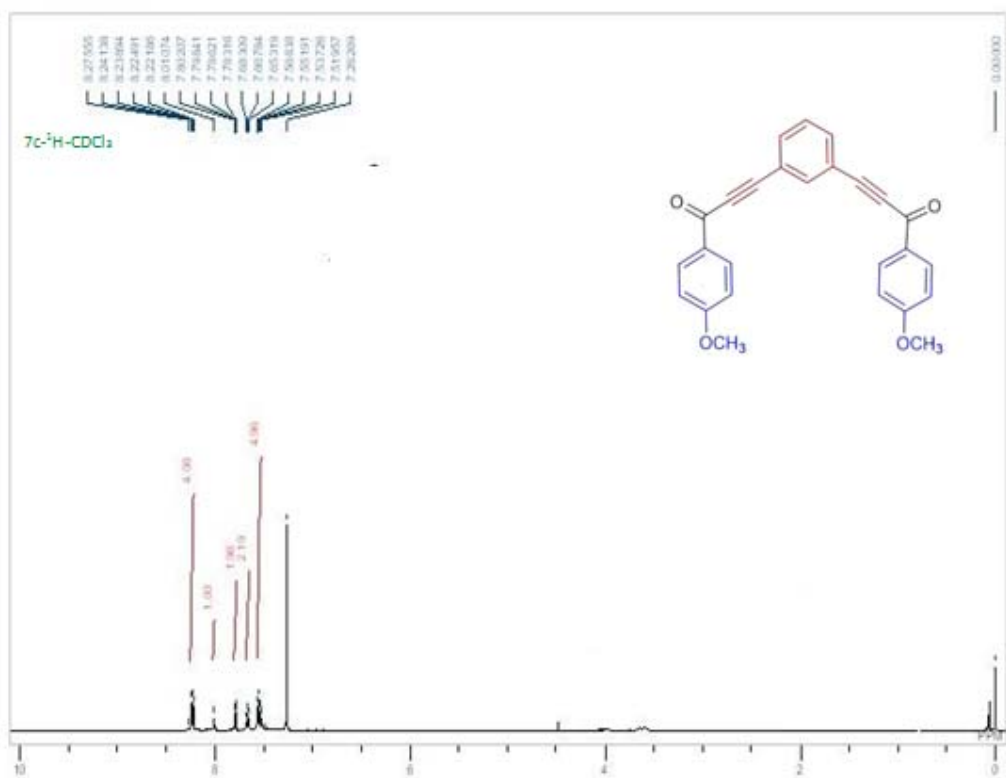


Figure S35. <sup>1</sup>H NMR spectrum for 7c

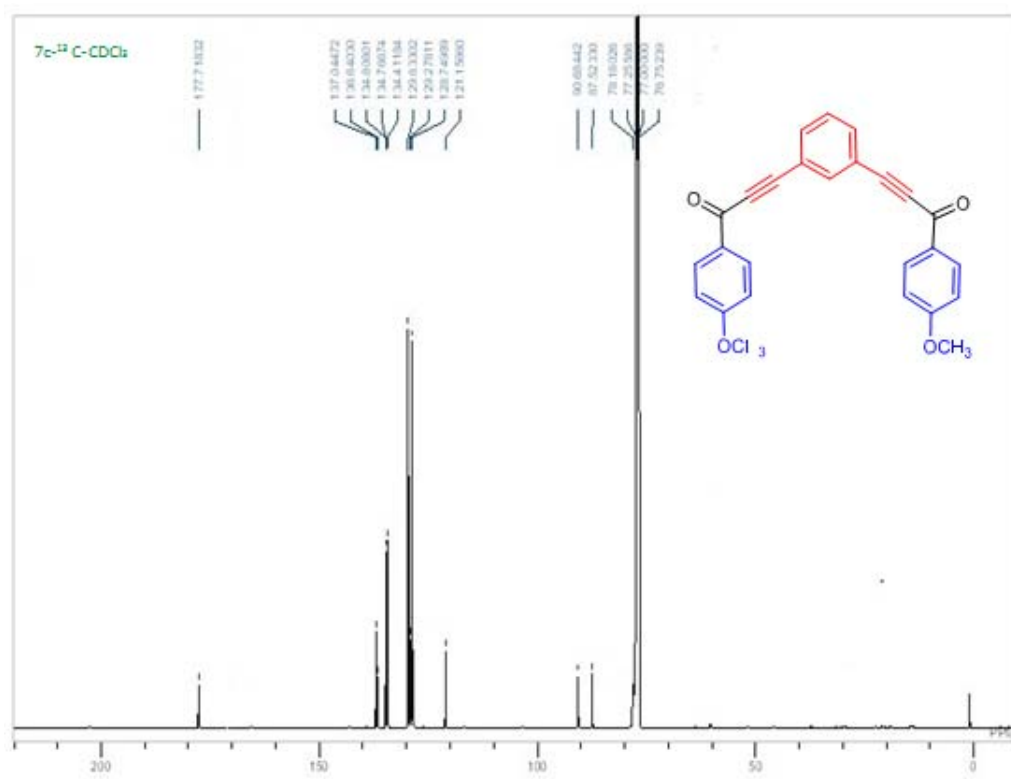


Figure S36. <sup>13</sup>C NMR spectrum for 7c





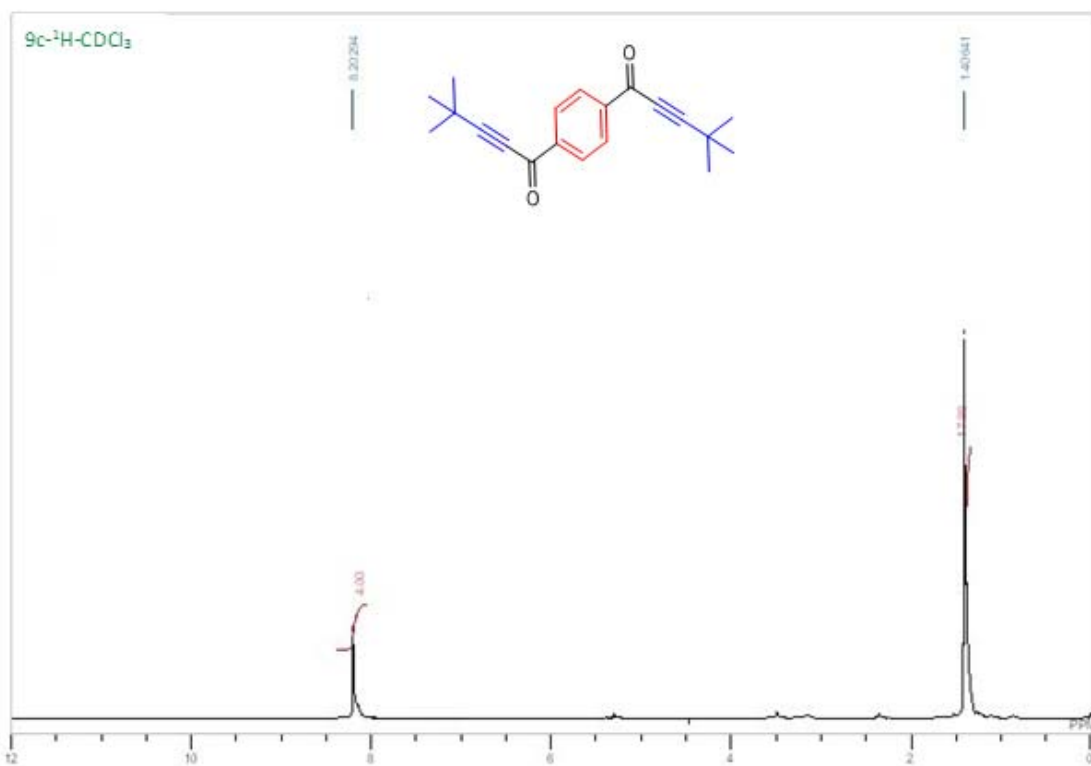


Figure S41. <sup>1</sup>H NMR spectrum for 9c

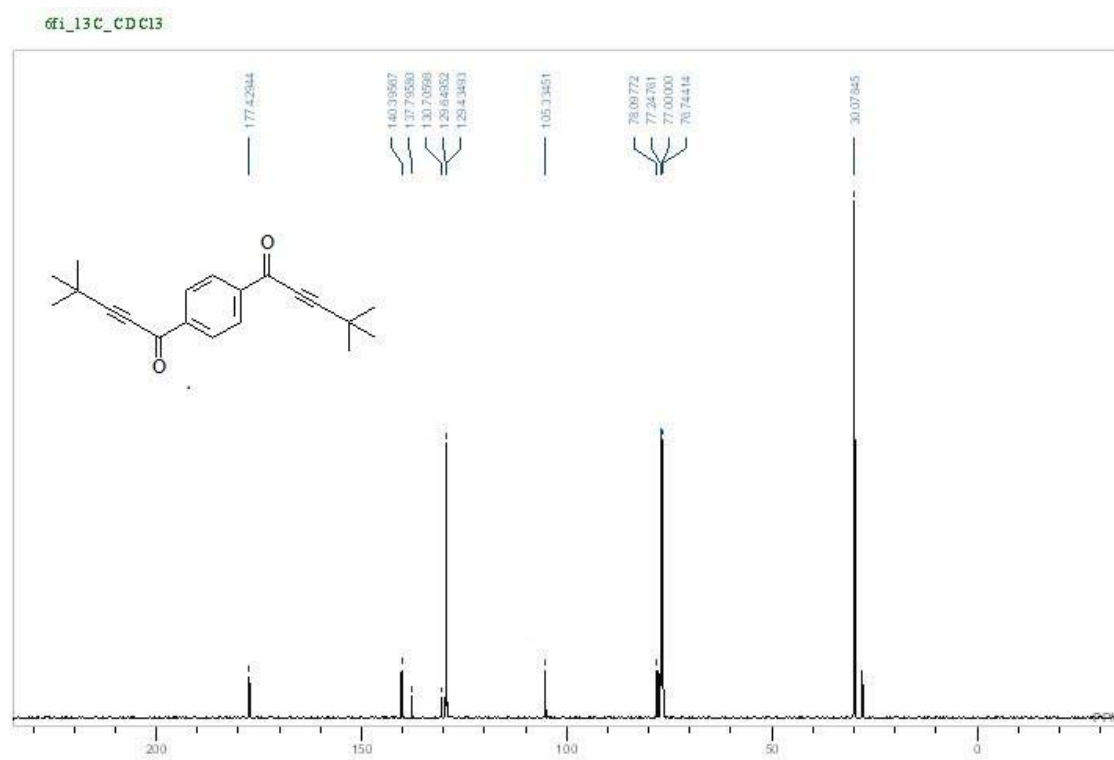
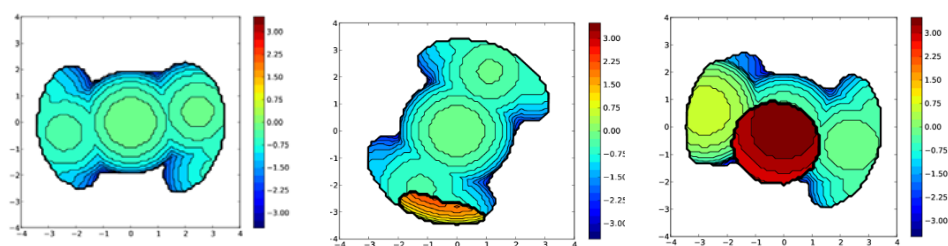


Figure S42. <sup>13</sup>C NMR spectrum for 9c

**Table S1.** Molecular orbital energy diagram for complexes **Pd-C1**, **Pd-C2**, and **Pd-C3** showing the HOMO, LUMO, the HOMO–LUMO gap ( $\Delta E$ ), electronegativity ( $\chi$ ), hardness ( $\eta$ ), and softness ( $S$ ).

| Complex Pd-C | $E_{\text{HOMO}}$ (eV) | $E_{\text{LUMO}}$ (eV) | $\Delta E$ (eV) | $\chi$ (eV)  | $\eta$ (eV)   | $S$ (eV)     |
|--------------|------------------------|------------------------|-----------------|--------------|---------------|--------------|
| <b>1</b>     | <b>-0.218</b>          | <b>-0.0634</b>         | <b>-0.155</b>   | <b>0.141</b> | <b>0.0773</b> | <b>6.468</b> |
| <b>2</b>     | <b>-0.219</b>          | <b>-0.0651</b>         | <b>-0.154</b>   | <b>0.142</b> | <b>0.0770</b> | <b>6.493</b> |
| <b>3</b>     | <b>-0.218</b>          | <b>-0.0653</b>         | <b>-0.153</b>   | <b>0.142</b> | <b>0.0764</b> | <b>6.544</b> |

- **Steric Map of Pd-NHCs-Py complexes: a) Pd-C1, b) Pd-C2 and c) Pd-C3**



a) Pd-C1 N-iPr (28.5%)      b) Pd-C2 N-Benzyl (29.8%)      c) Pd-C3 N-Adamantyl (34.1%)

Figure S43. Steric Map of Pd-NHCs-Py complexes: a) Pd-C1, b) Pd-C2 and c) Pd-C



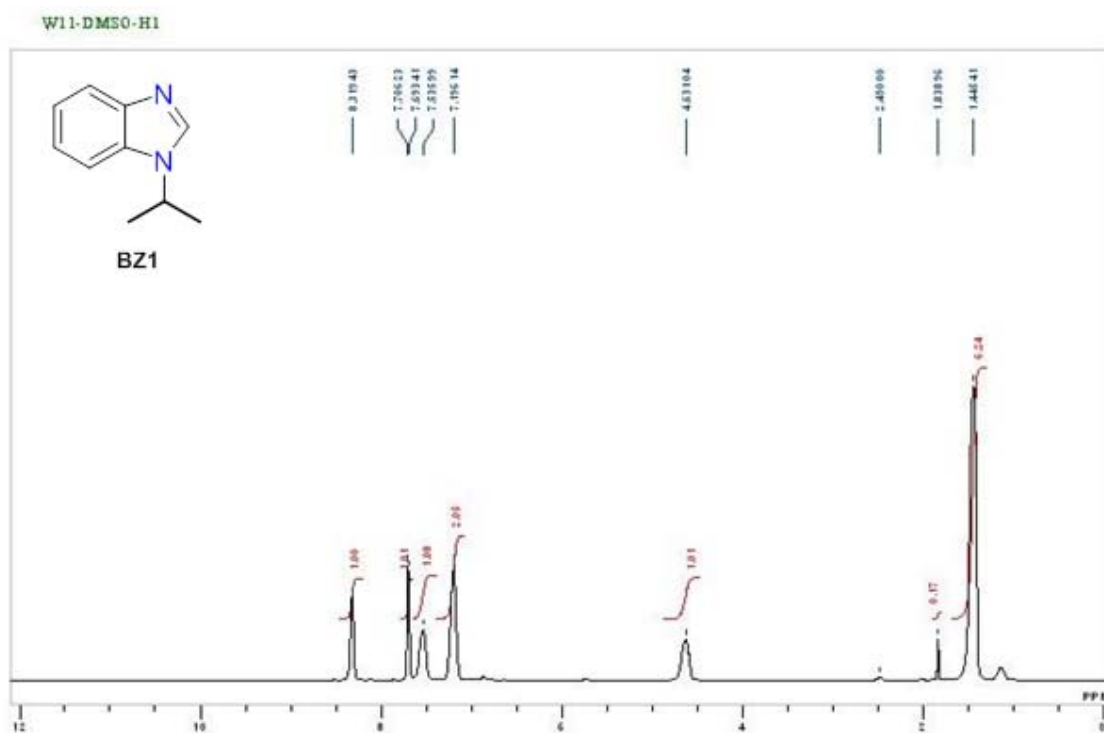


Figure S44. <sup>1</sup>H NMR spectrum for BZ1

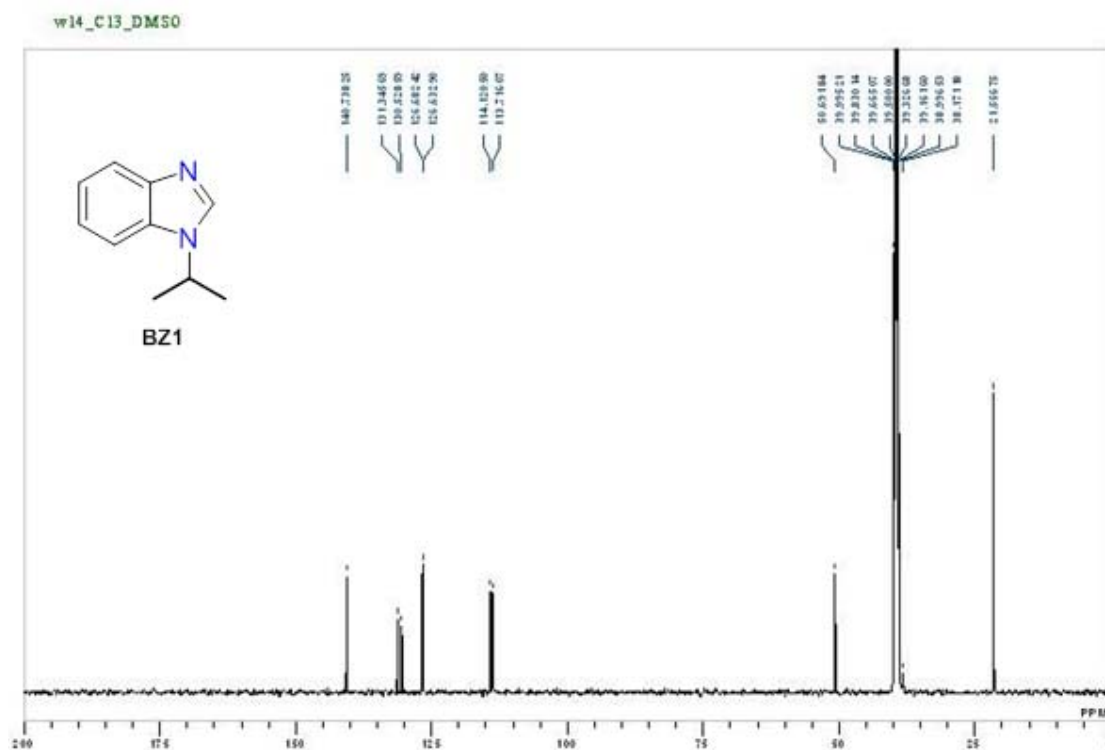


Figure S45. <sup>13</sup>C NMR spectrum for BZ1

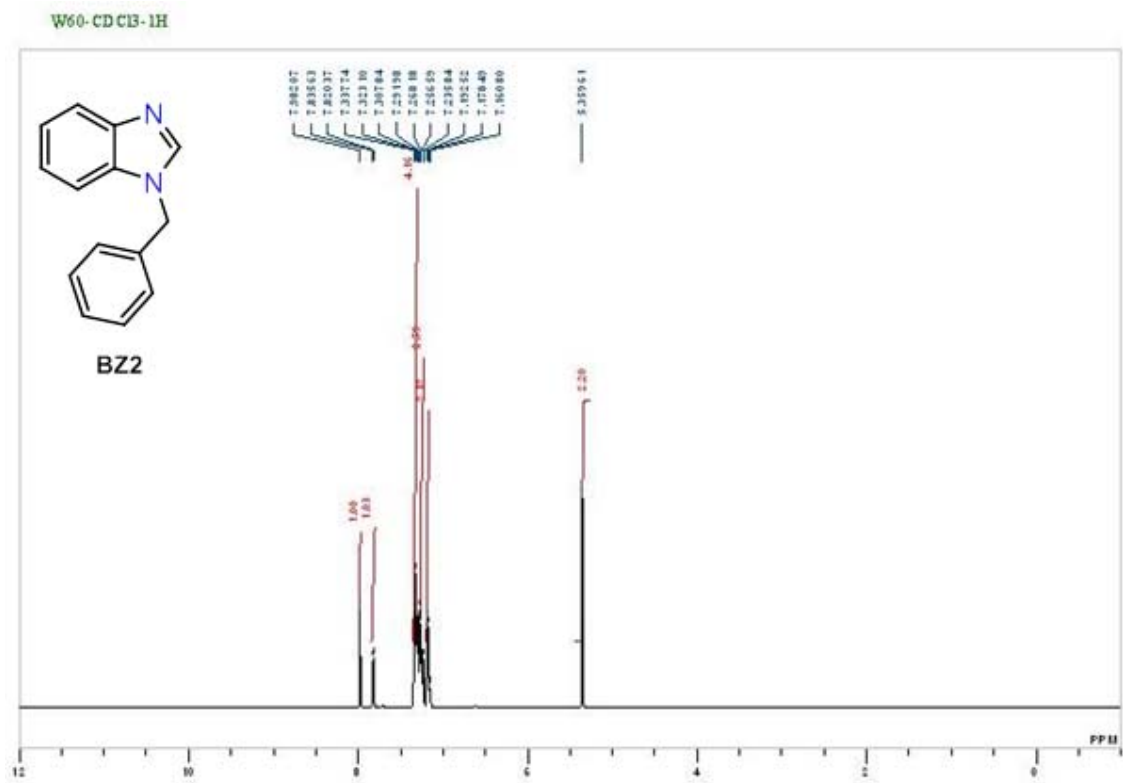


Figure S46. <sup>1</sup>H NMR spectrum for BZ2

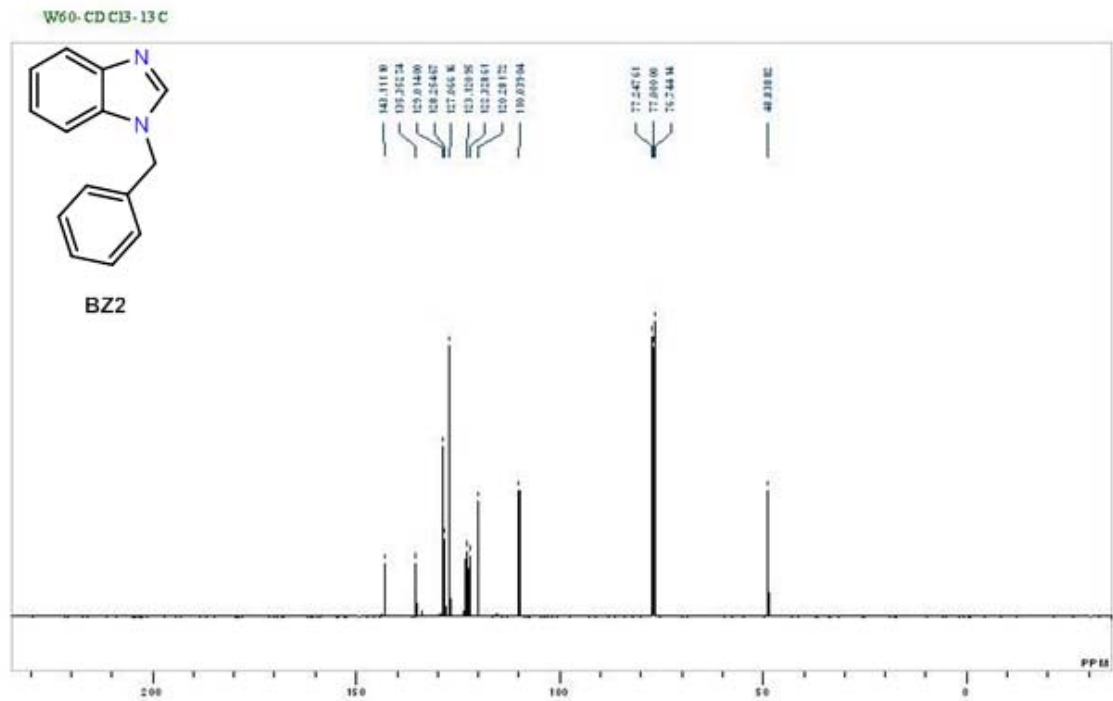
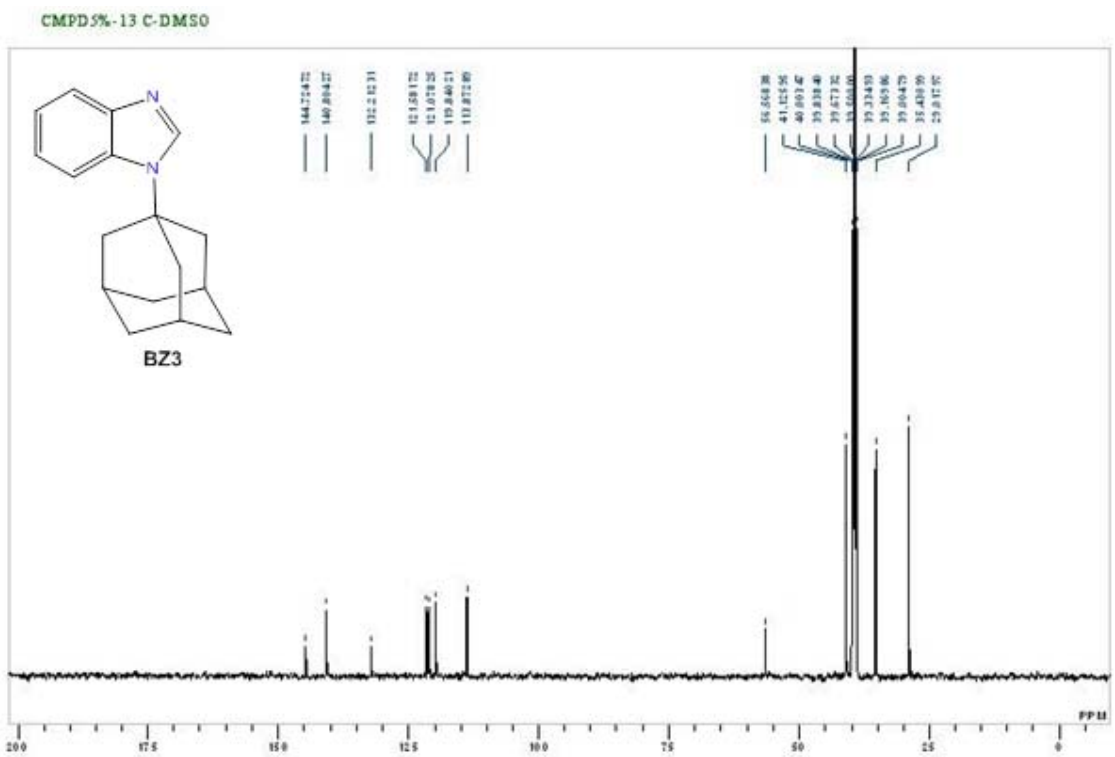
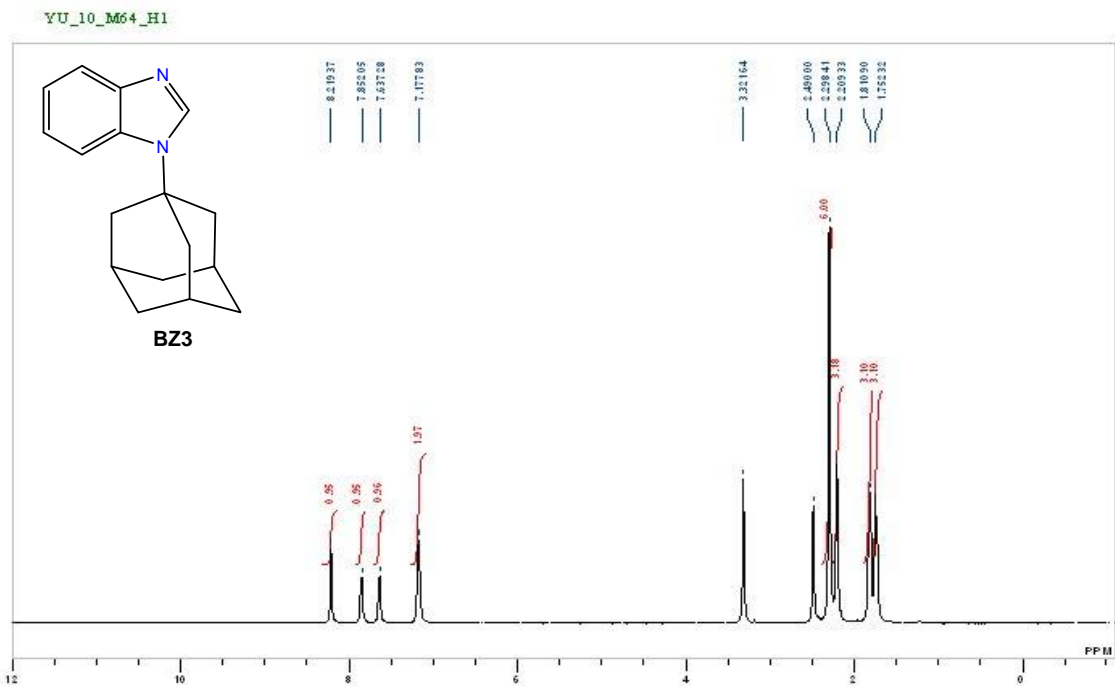


Figure S47. <sup>13</sup>C NMR spectrum for BZ2



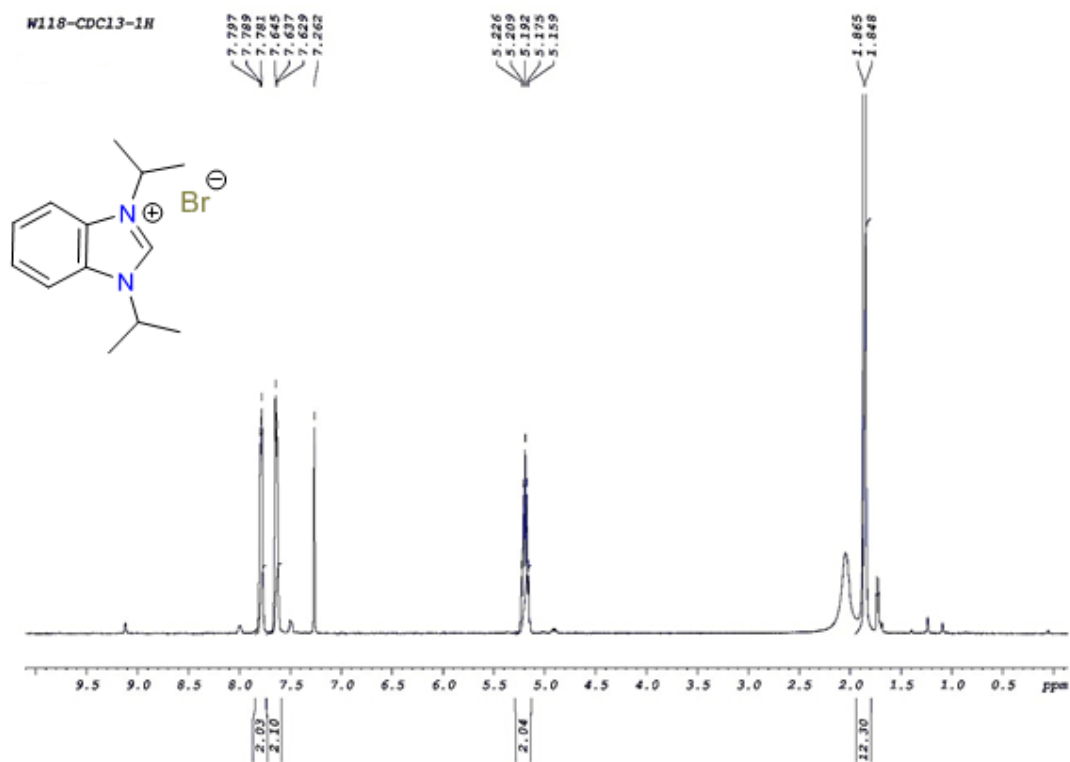


Figure S50. <sup>1</sup>H NMR spectrum for NHC1

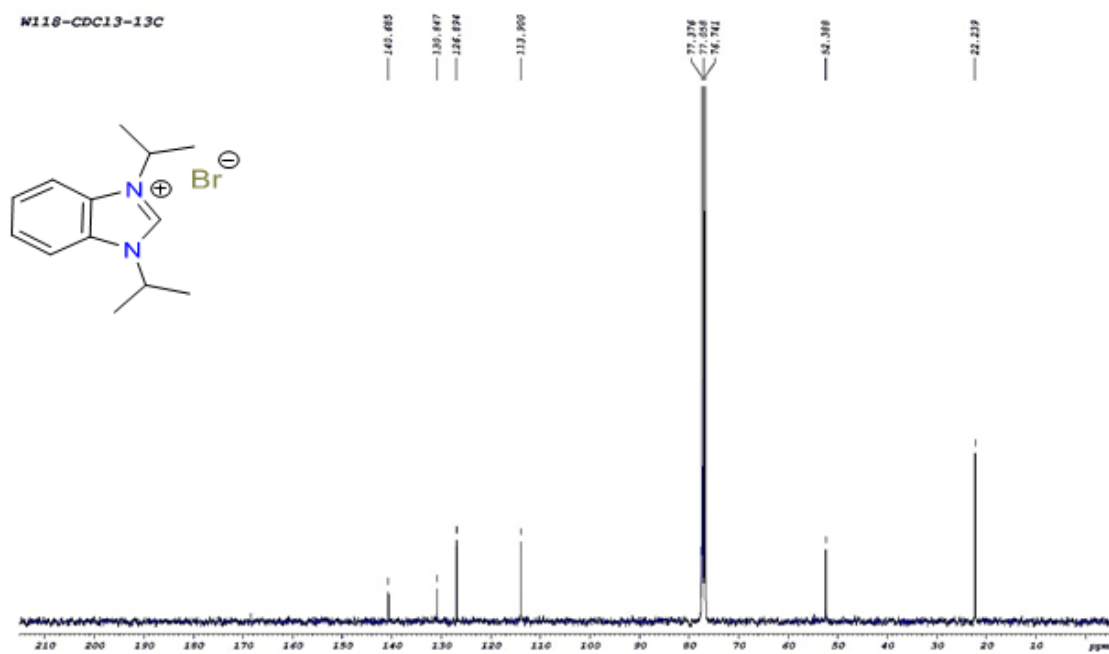


Figure S51. <sup>13</sup>C NMR spectrum for NHC1

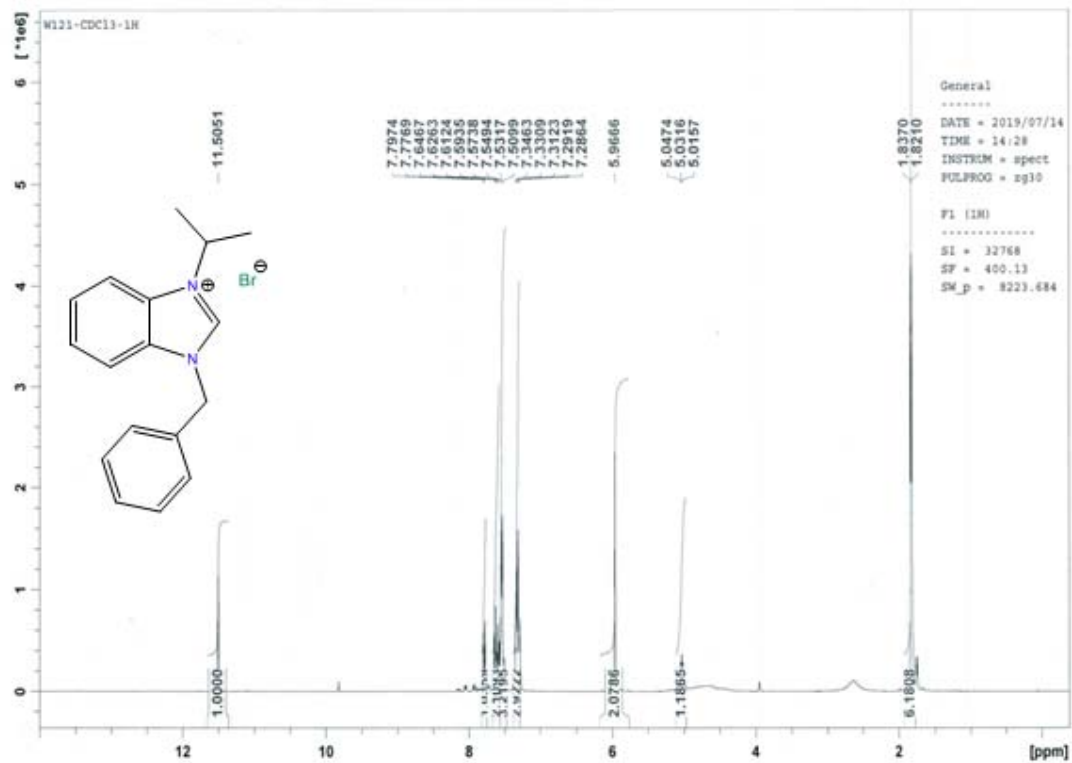


Figure S52. <sup>1</sup>H NMR spectrum for NHC2

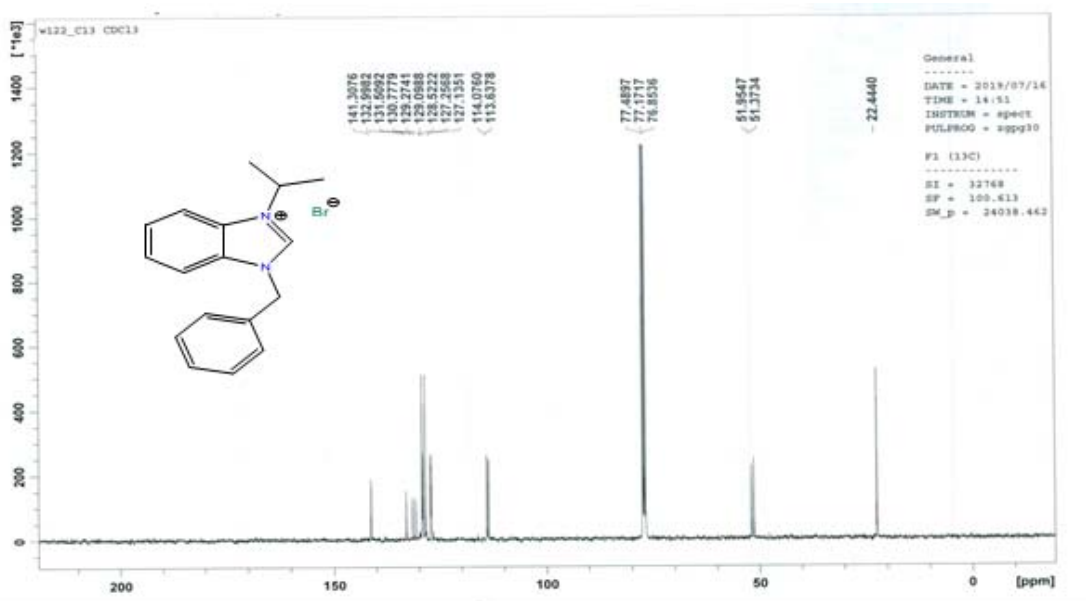


Figure S53. <sup>13</sup>C NMR spectrum for NHC2

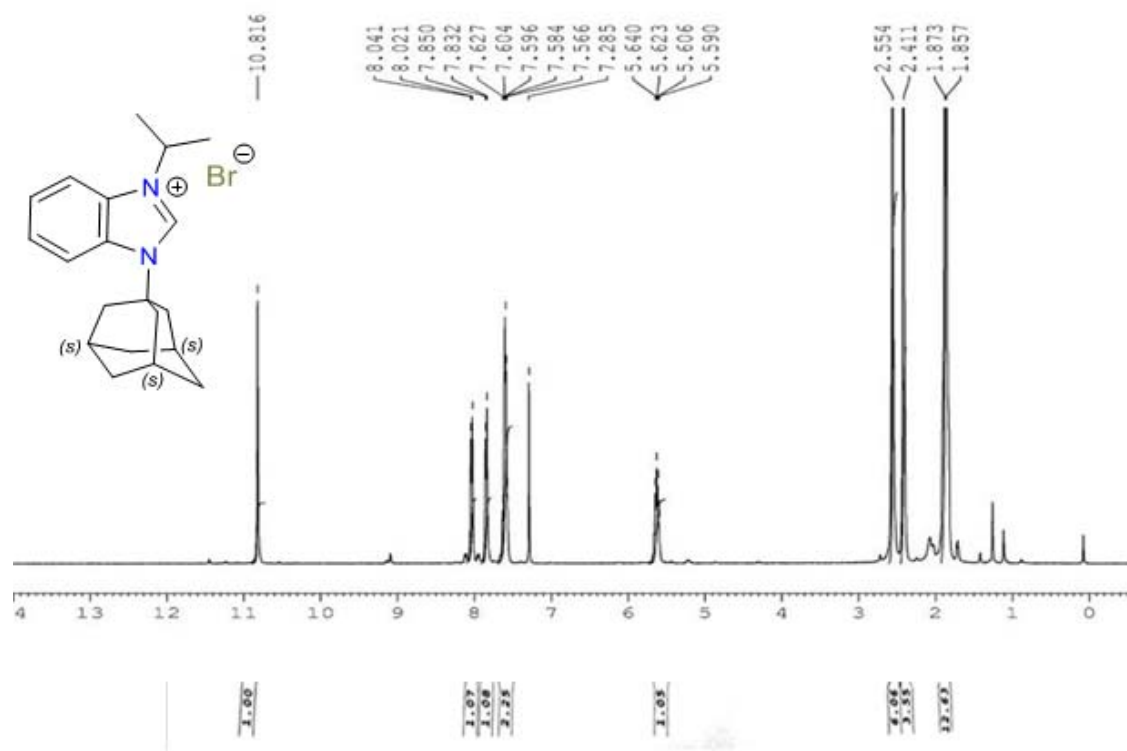


Figure S54. <sup>1</sup>H NMR spectrum for NHC3

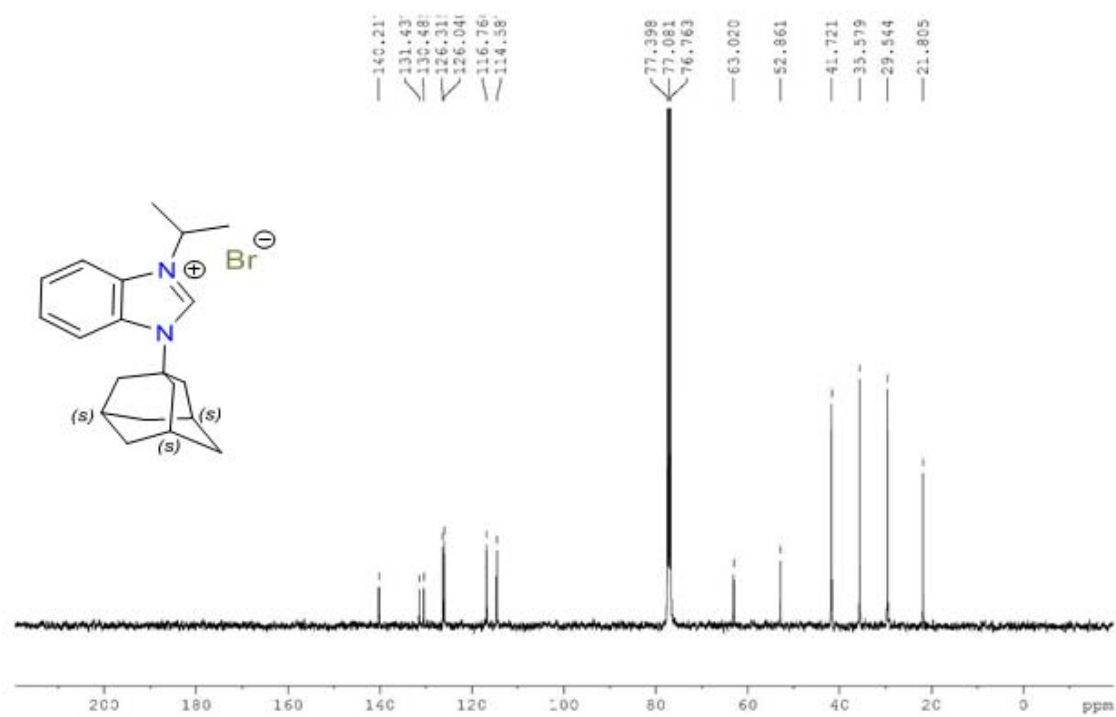


Figure S55. <sup>13</sup>C NMR spectrum for NHC3

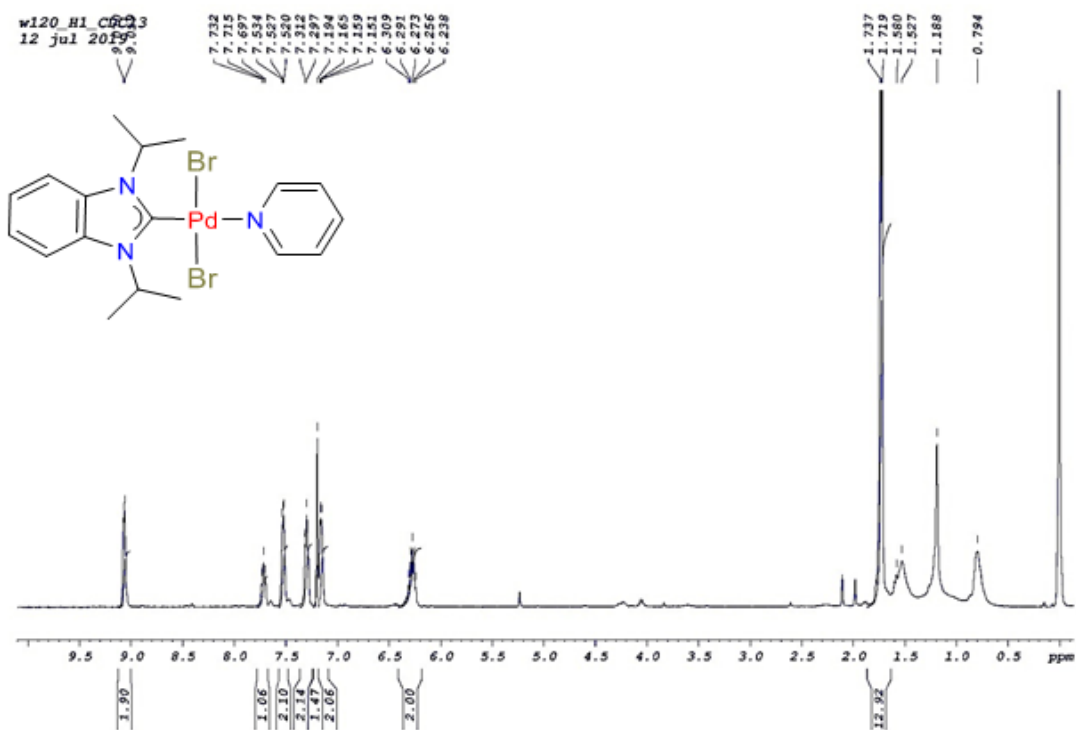


Figure S56.  $^1\text{H}$  NMR spectrum for Pd-C1

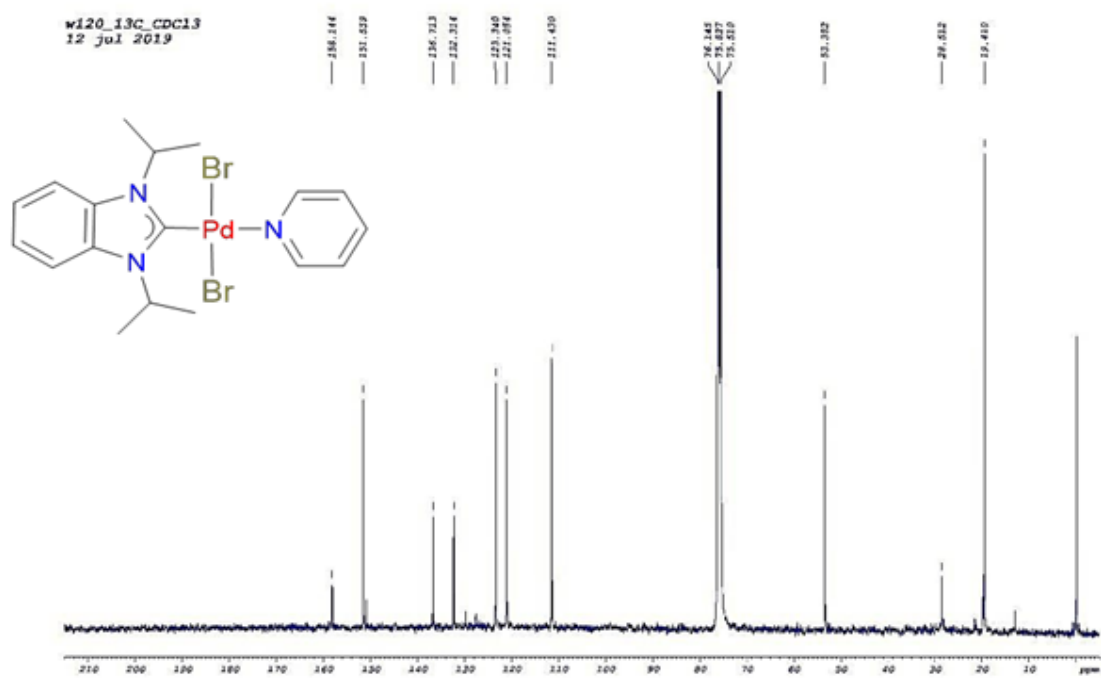


Figure S57.  $^{13}\text{C}$  NMR spectrum for Pd-C1

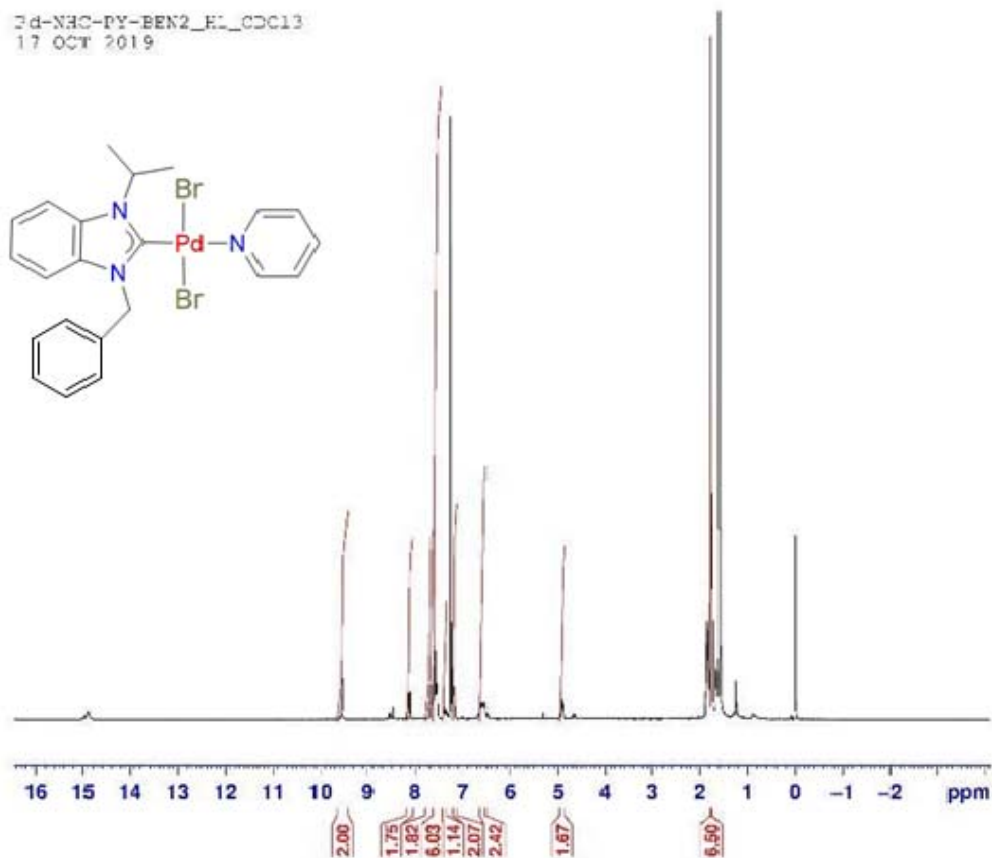


Figure S58. <sup>1</sup>H NMR spectrum for Pd-C2

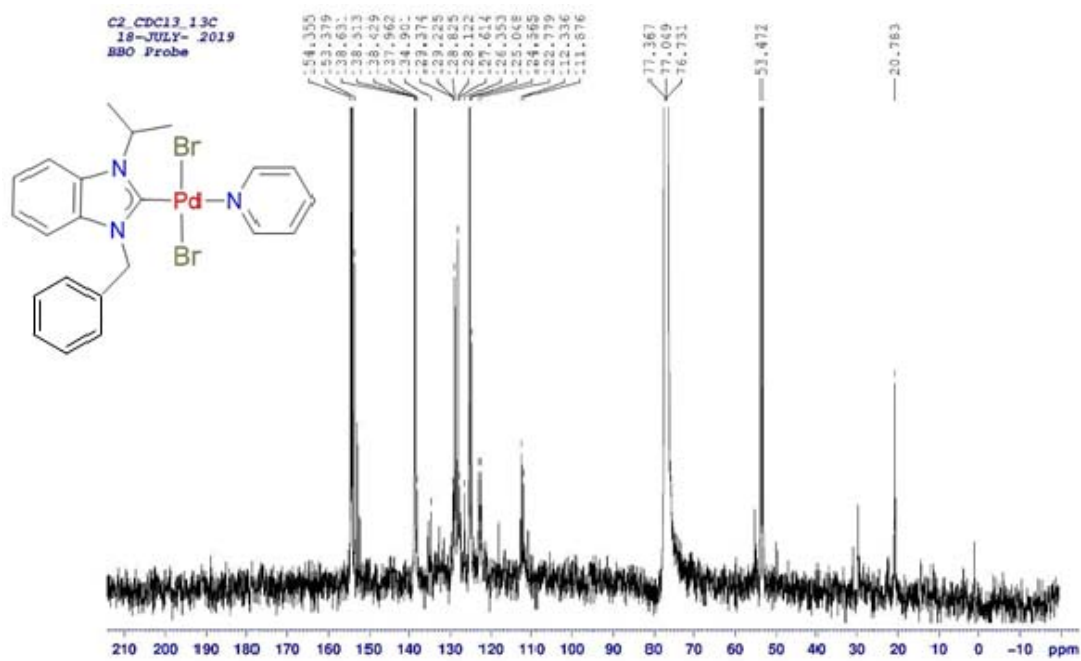


Figure S59. <sup>13</sup>C NMR spectrum for Pd-C2



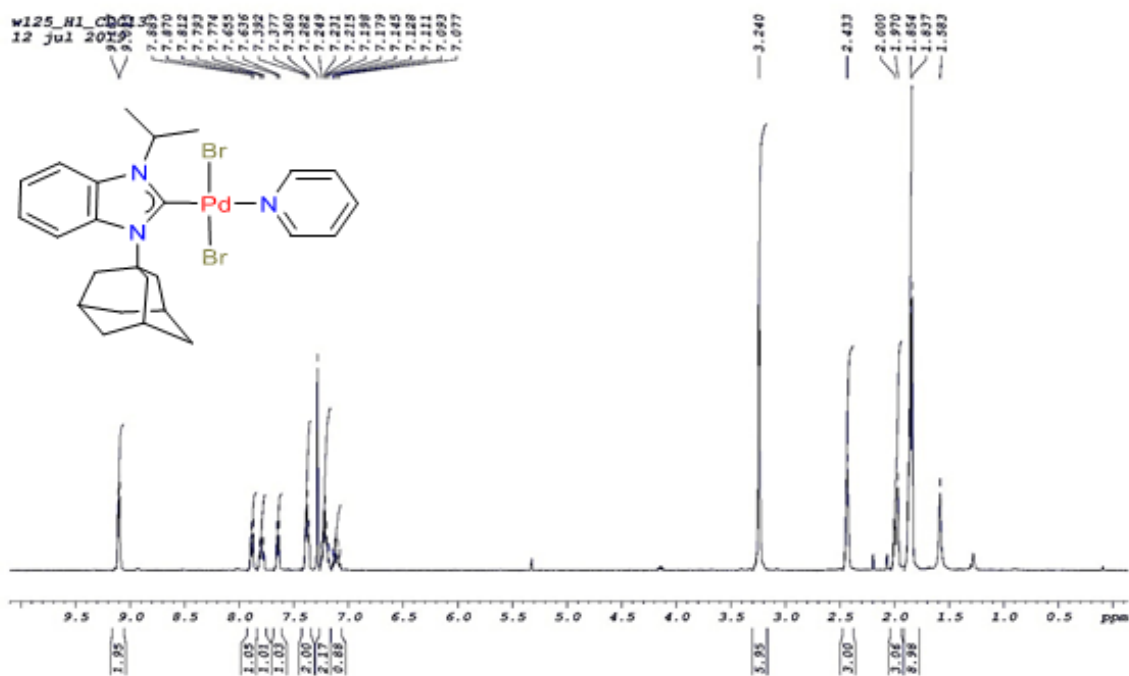


Figure 60.  $^1\text{H}$  NMR spectrum of Pd-C3

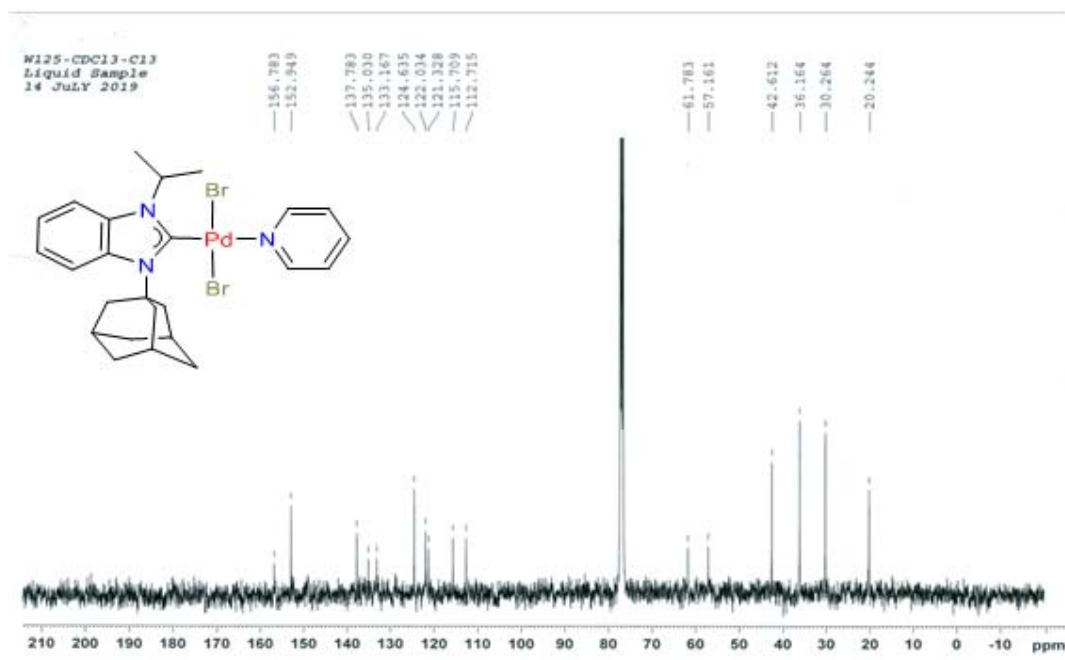


Figure 61.  $^{13}\text{C}$  NMR spectrum of Pd-C3