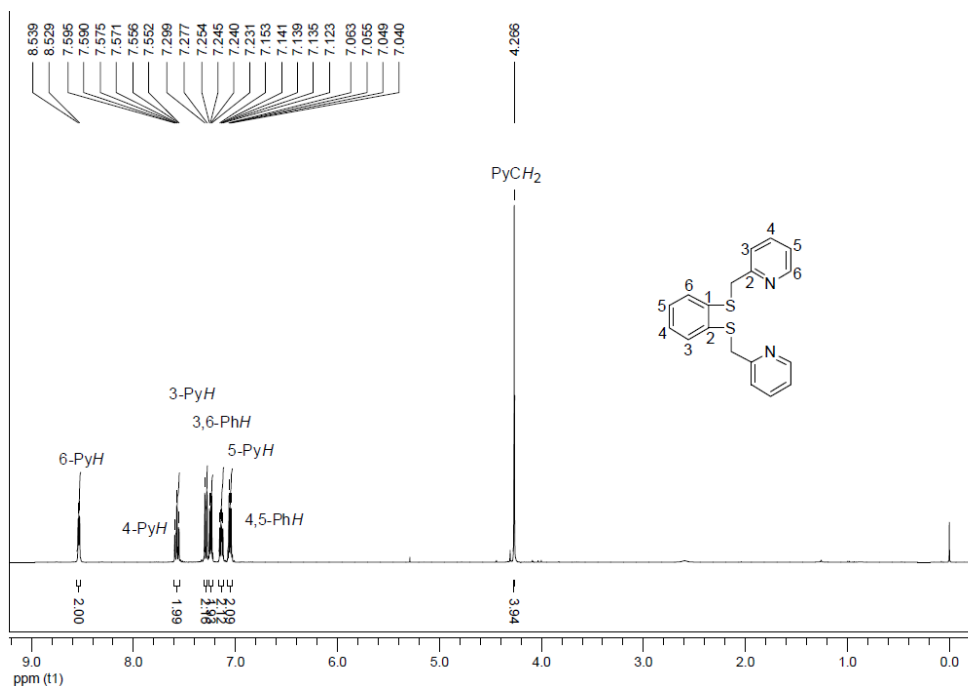
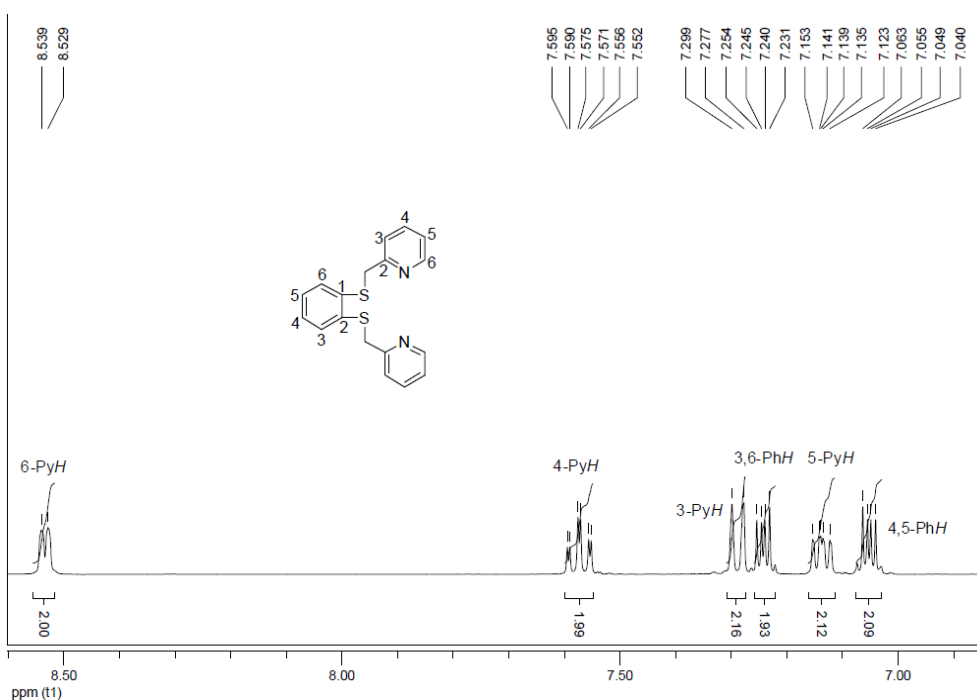


## Supplementary Information

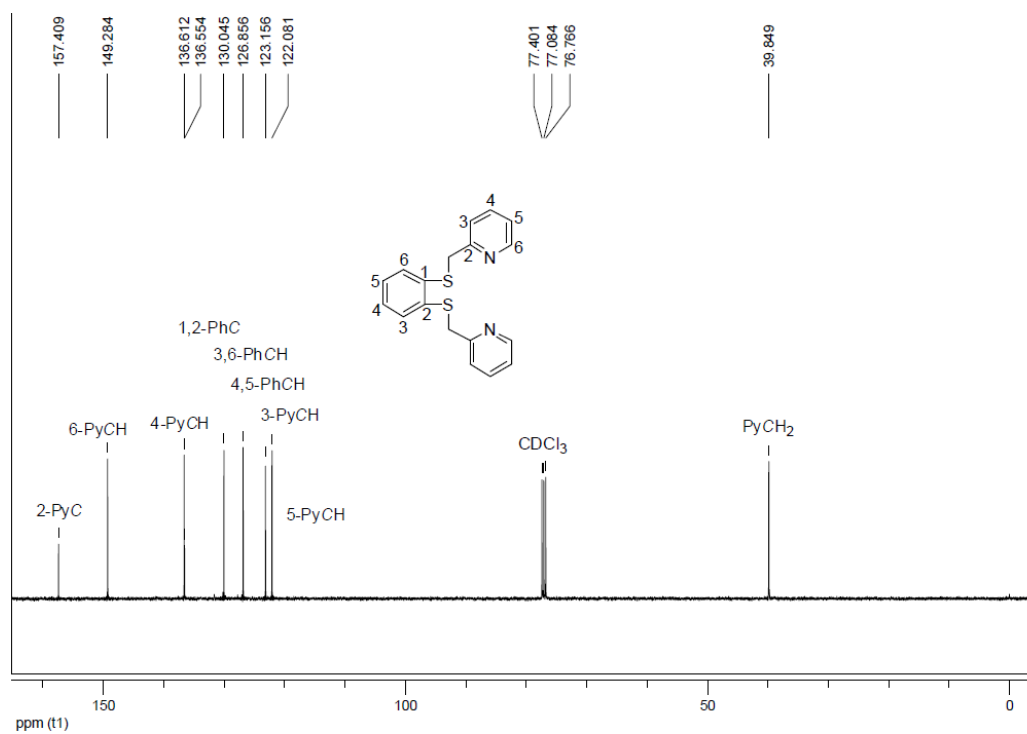
For 1D  $^1\text{H}$  and  $^{13}\text{C}$ -NMR spectra of ligand **L**, see Figs S1–S10:



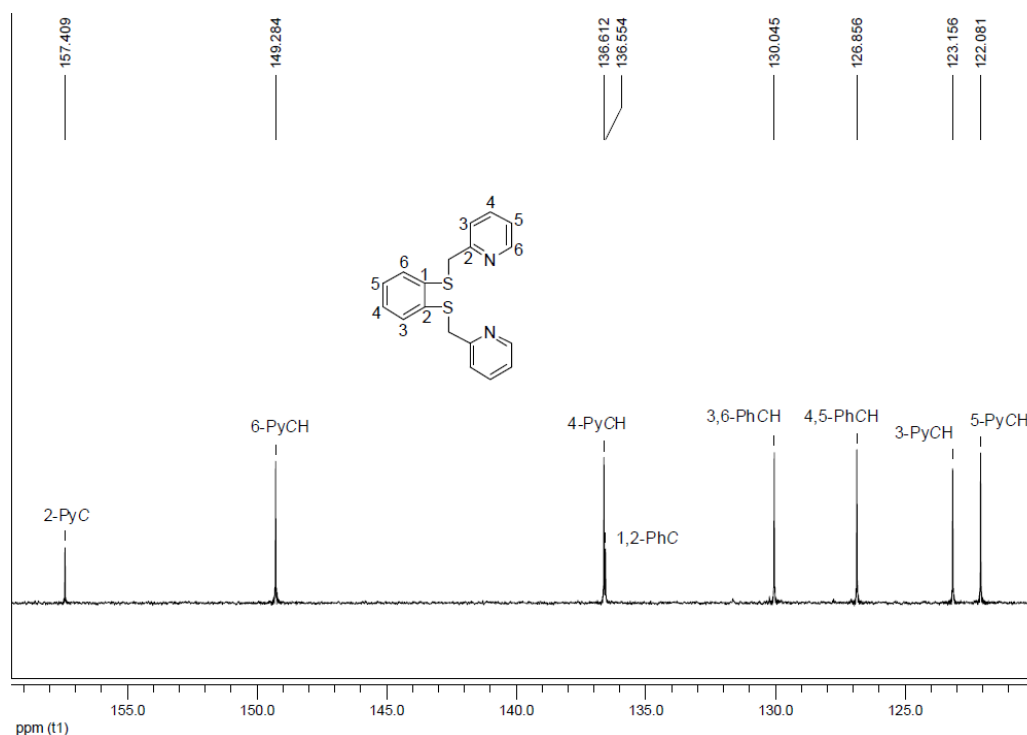
**Figure S1**  $^1\text{H}$ -NMR(CDCl<sub>3</sub>) spectrum of ligand **L**



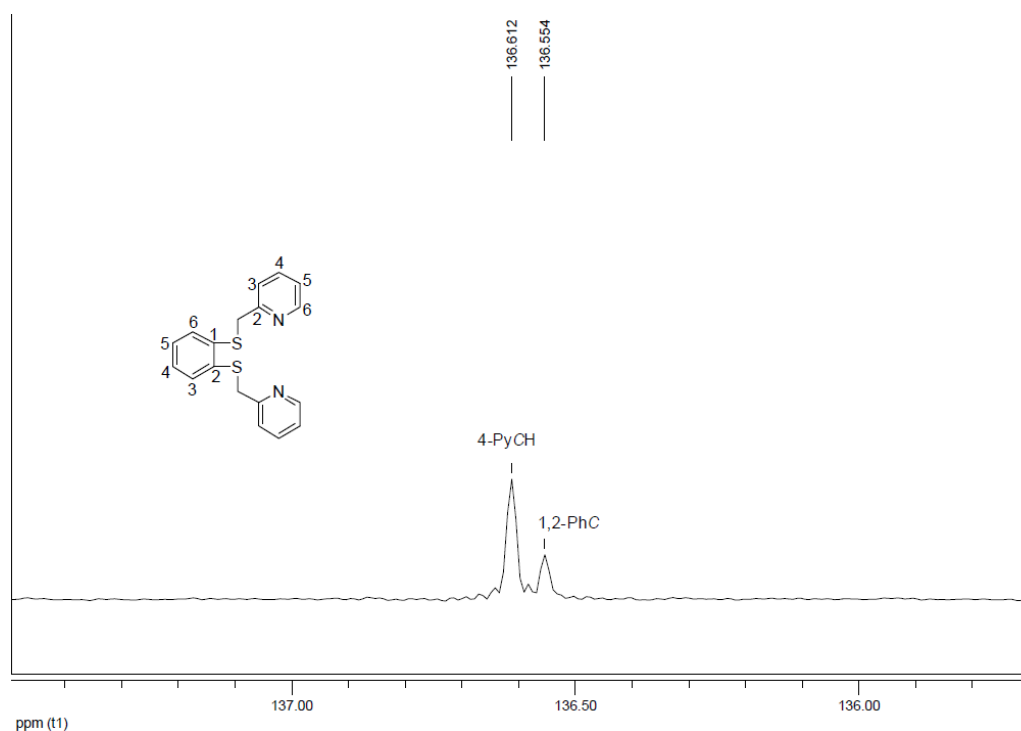
**Figure S2** The expansion of  $^1\text{H}$ -NMR(CDCl<sub>3</sub>) spectrum of ligand **L**



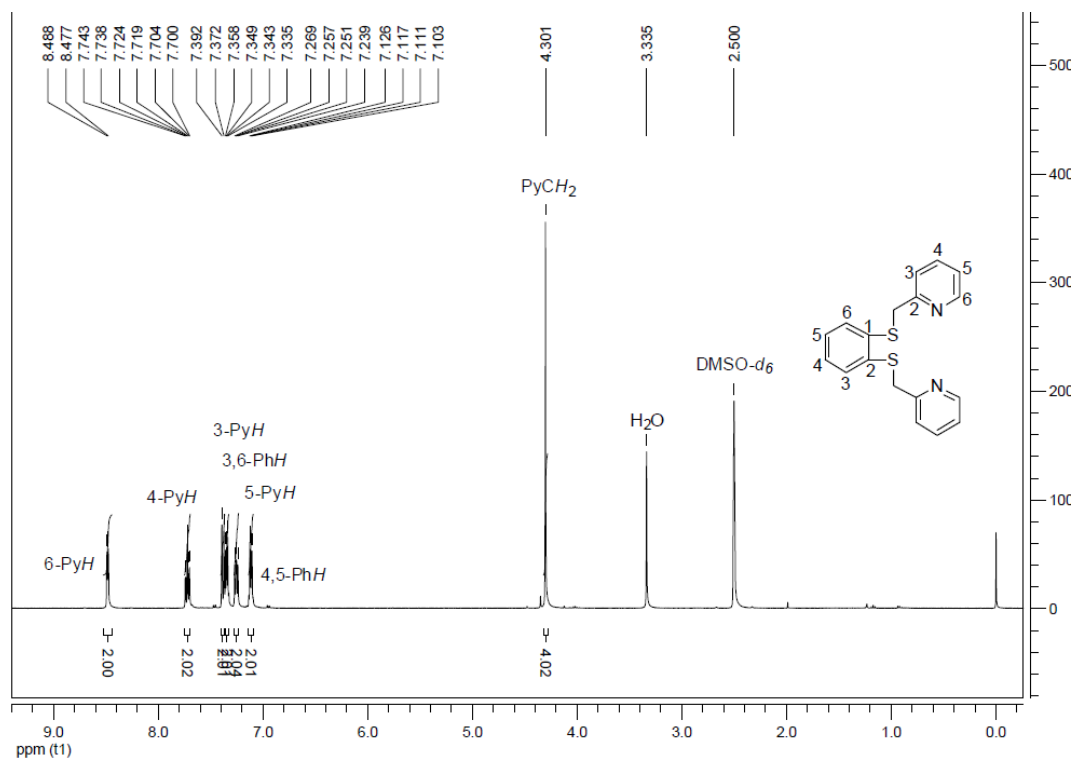
**Figure S3**  $^{13}\text{C}$ -NMR( $\text{CDCl}_3$ ) spectrum of ligand **L**



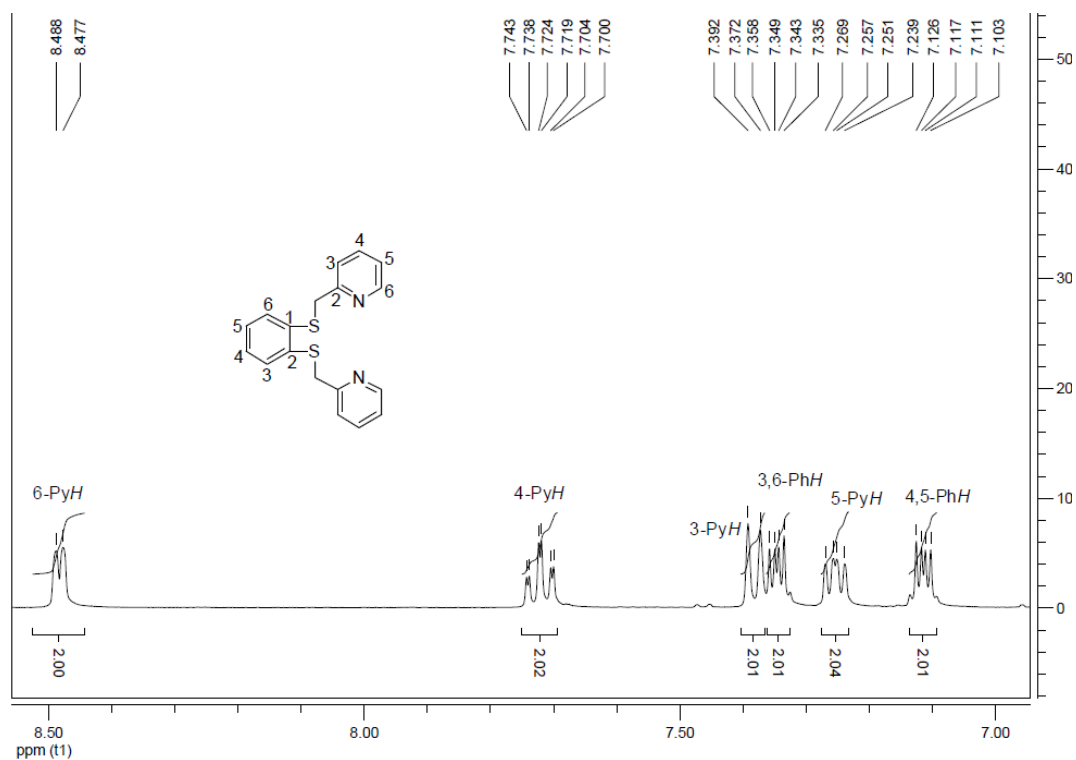
**Figure S4** The expansion of  $^{13}\text{C}$ -NMR( $\text{CDCl}_3$ ) spectrum of ligand **L**



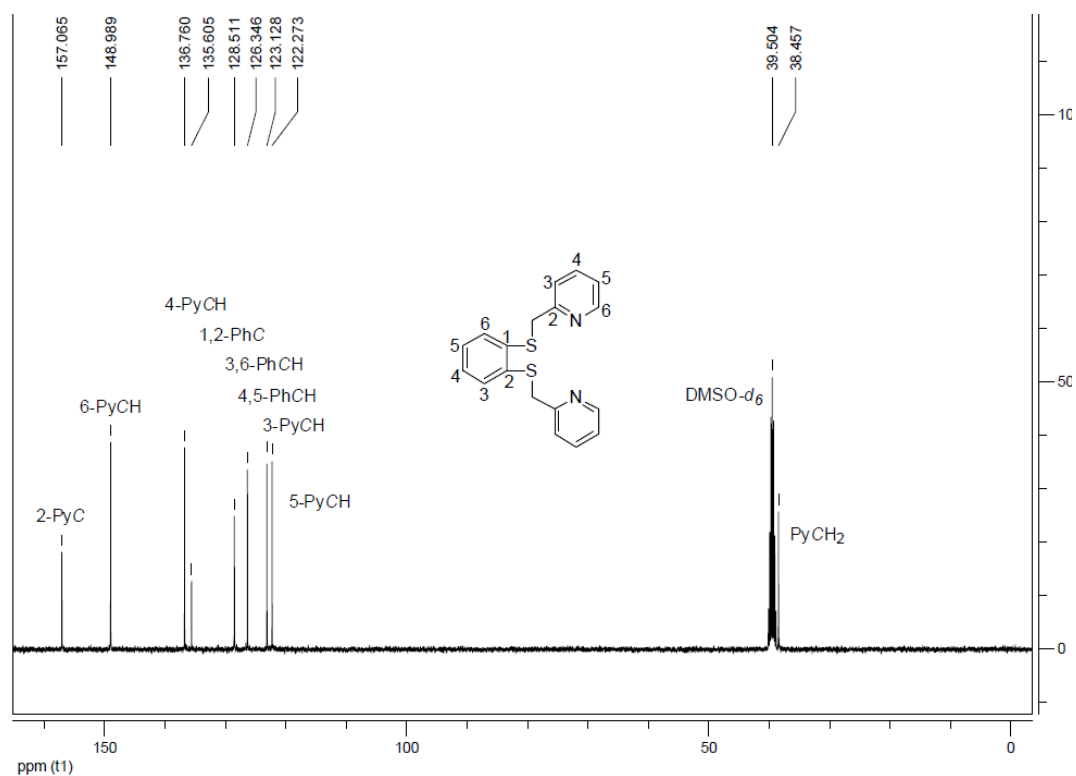
**Figure S5** The expansion of  $^{13}\text{C}$ -NMR( $\text{CDCl}_3$ ) spectrum of ligand **L**



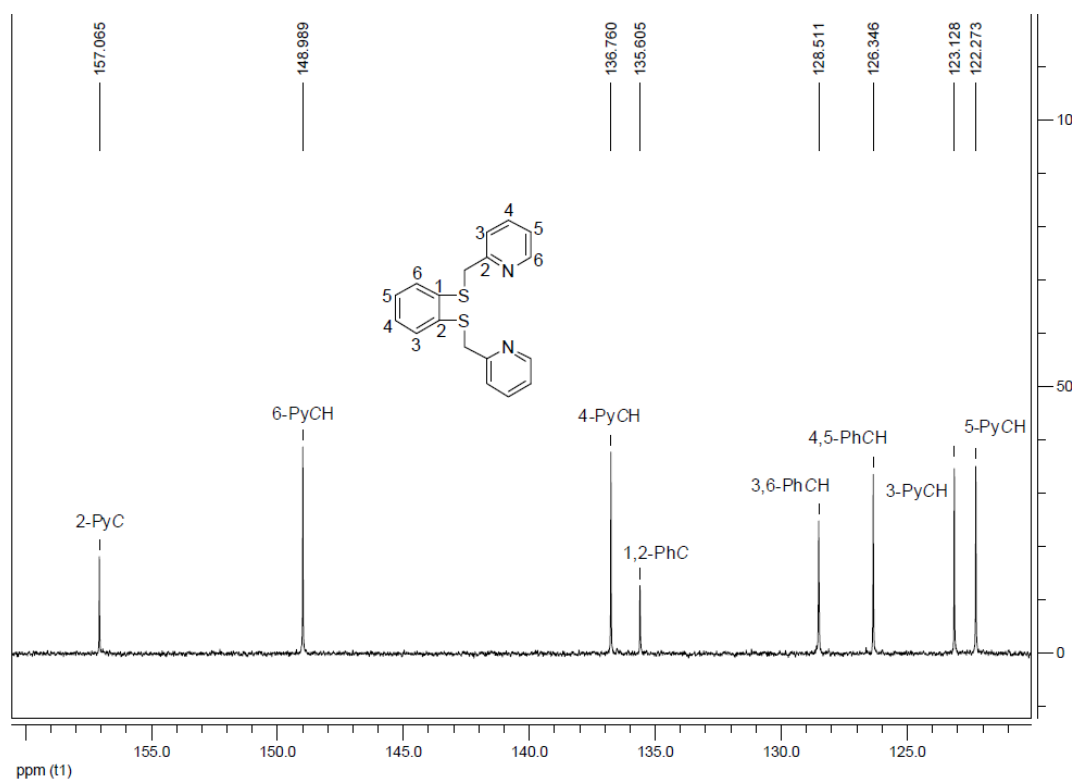
**Figure S6**  $^1\text{H}$ -NMR( $\text{DMSO-}d_6$ ) spectrum of ligand **L**



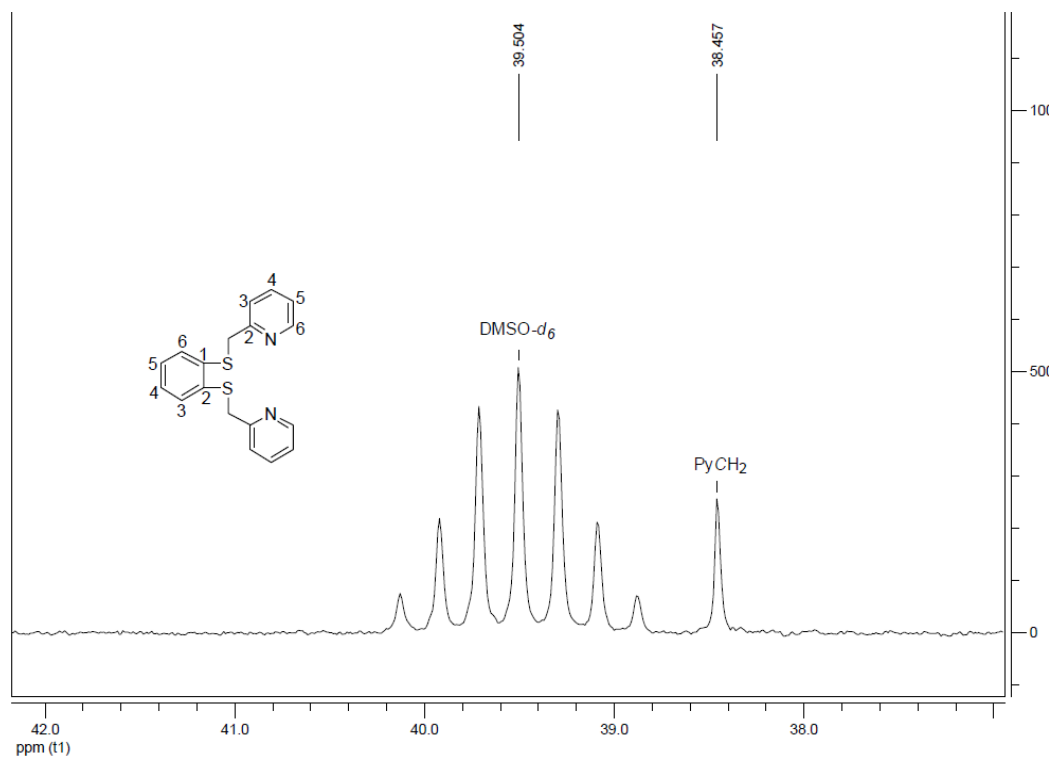
**Figure S7** The expansion of <sup>1</sup>H-NMR(DMSO-*d*<sub>6</sub>) spectrum of ligand L



**Figure S8** <sup>13</sup>C-NMR(DMSO-*d*<sub>6</sub>) spectrum of ligand L

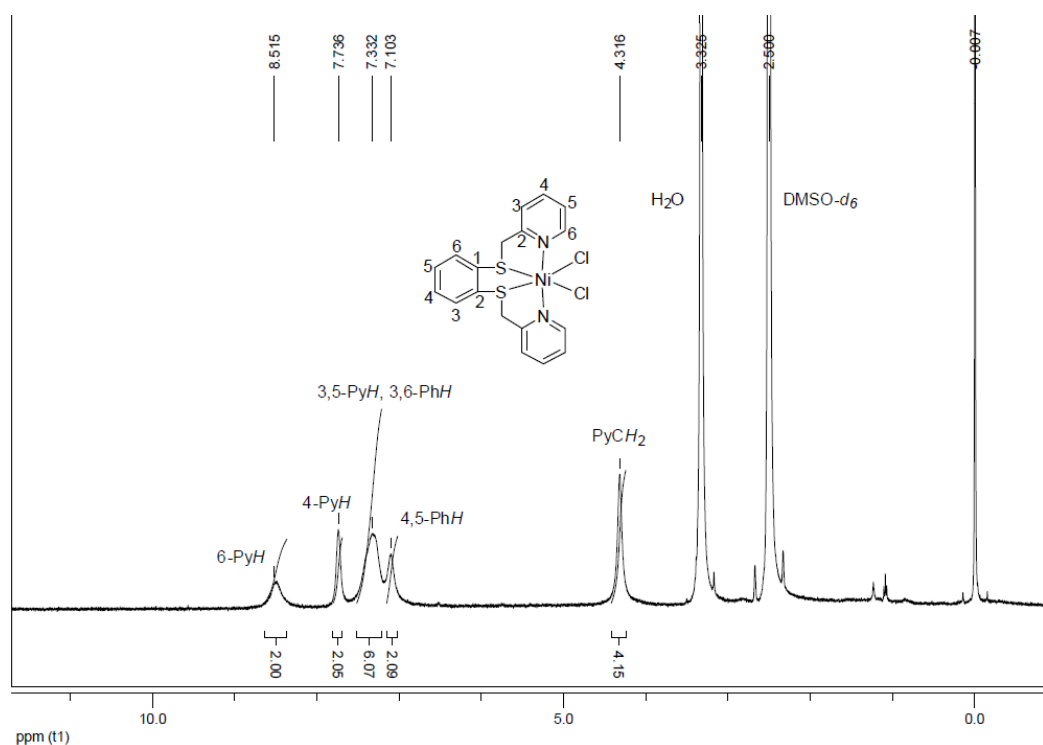


**Figure S9** The expansion of  $^{13}\text{C}$ -NMR(DMSO- $d_6$ ) spectrum of ligand **L**

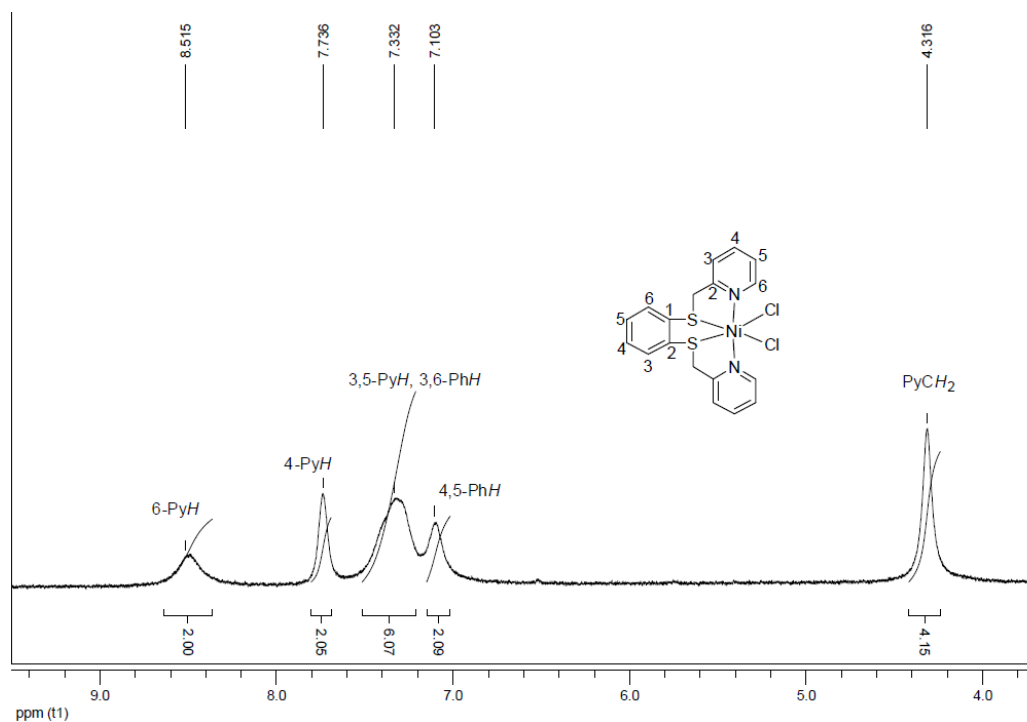


**Figure S10** The expansion of  $^{13}\text{C}$ -NMR(DMSO- $d_6$ ) spectrum of ligand **L**

For 1D  $^1\text{H}$ -NMR spectra of compound **1**, see Figs S11–S12:

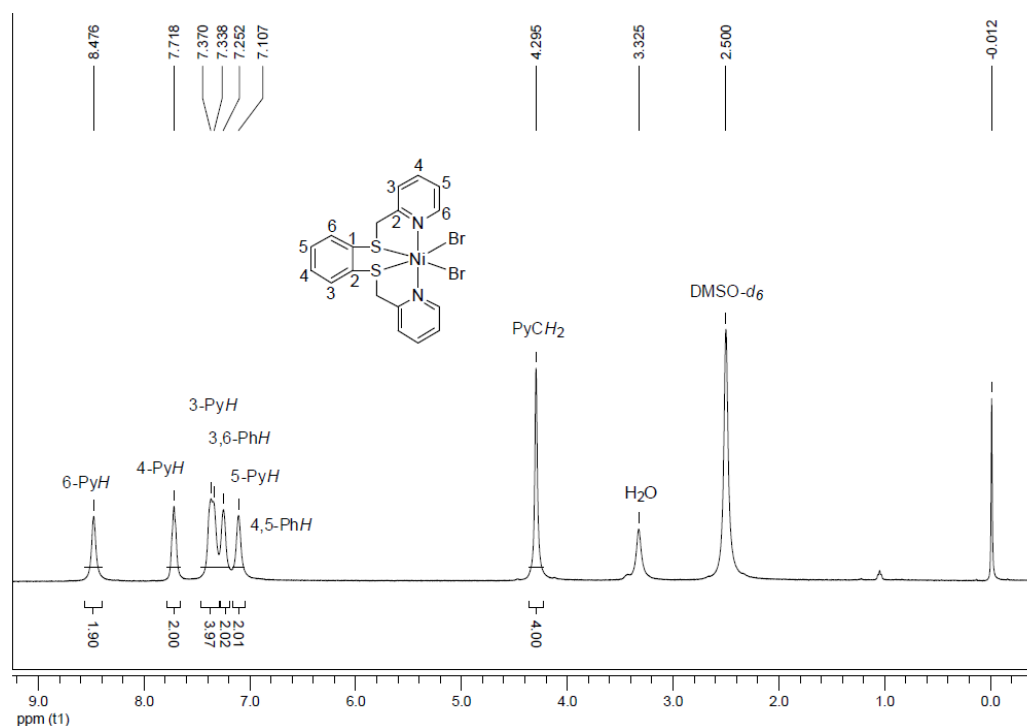


**Figure S11**  $^1\text{H}$ -NMR(DMSO- $d_6$ ) spectrum of compound **1**

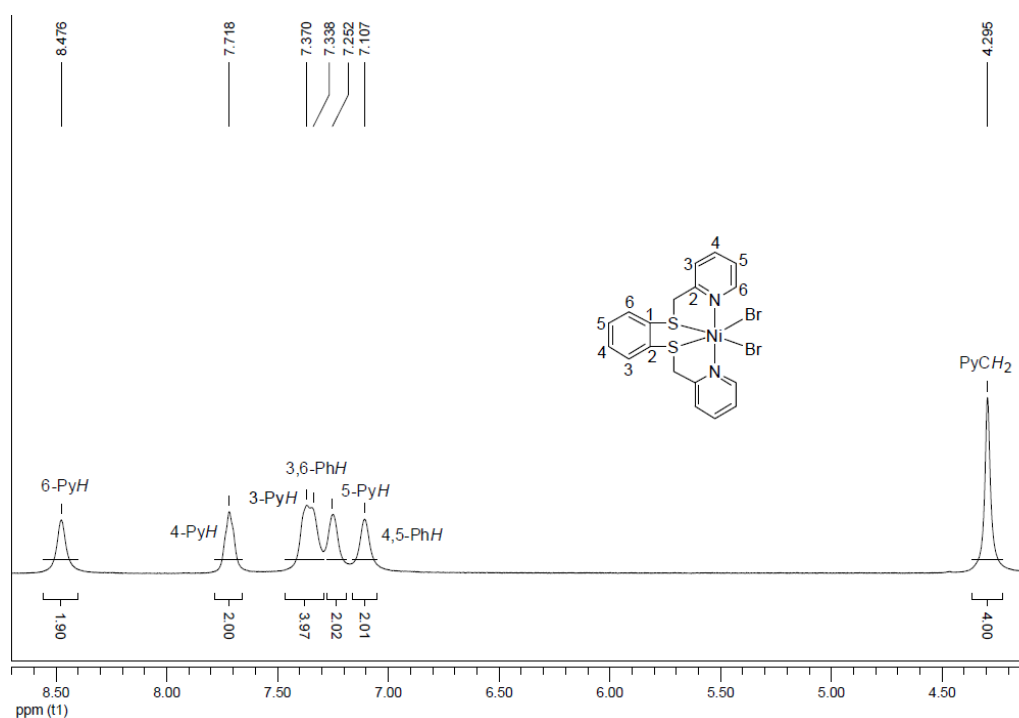


**Figure S12** The expansion of  $^1\text{H}$ -NMR(DMSO- $d_6$ ) spectrum of compound **1**

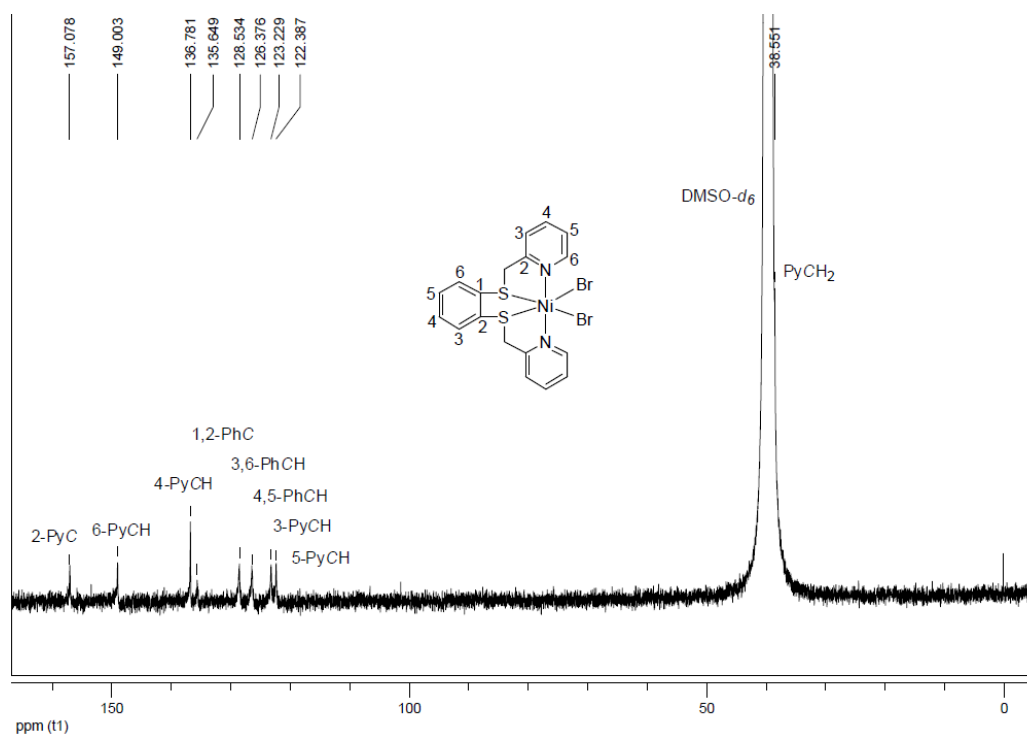
For 1D  $^1\text{H}$  and  $^{13}\text{C}$ -NMR spectra of compound **2**, see Figs S13–S17:



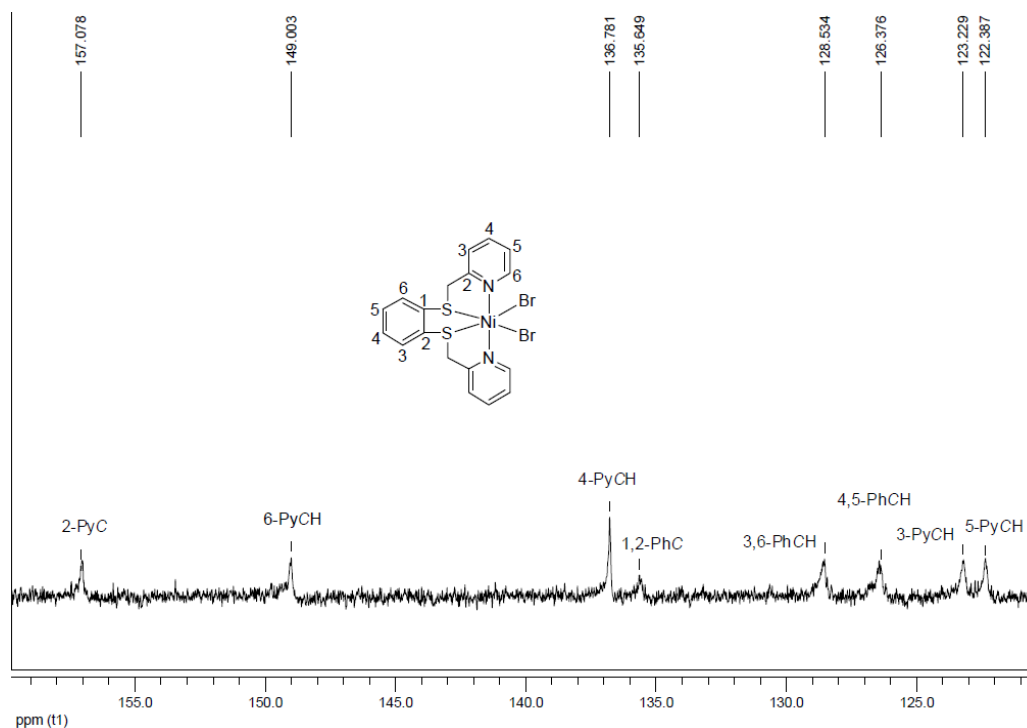
**Figure S13**  $^1\text{H}$ -NMR(DMSO- $d_6$ ) spectrum of compound **2**



**Figure S14** The expansion of  $^1\text{H}$ -NMR(DMSO- $d_6$ ) spectrum of compound **2**

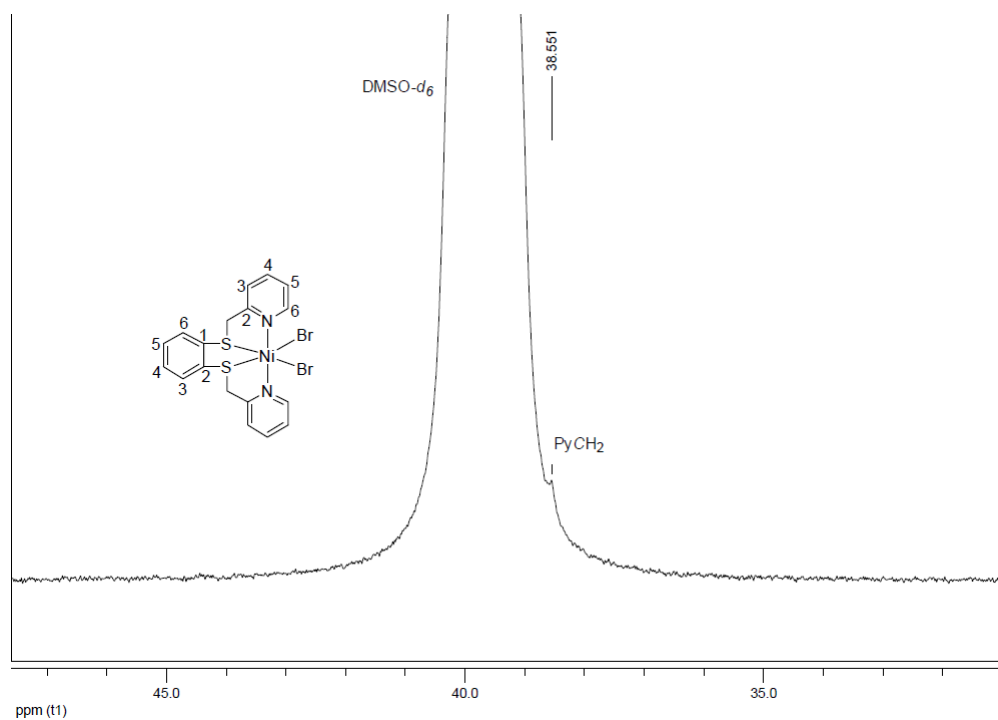


**Figure S15**  $^{13}\text{C}$ -NMR(DMSO- $d_6$ ) spectrum of compound **2**



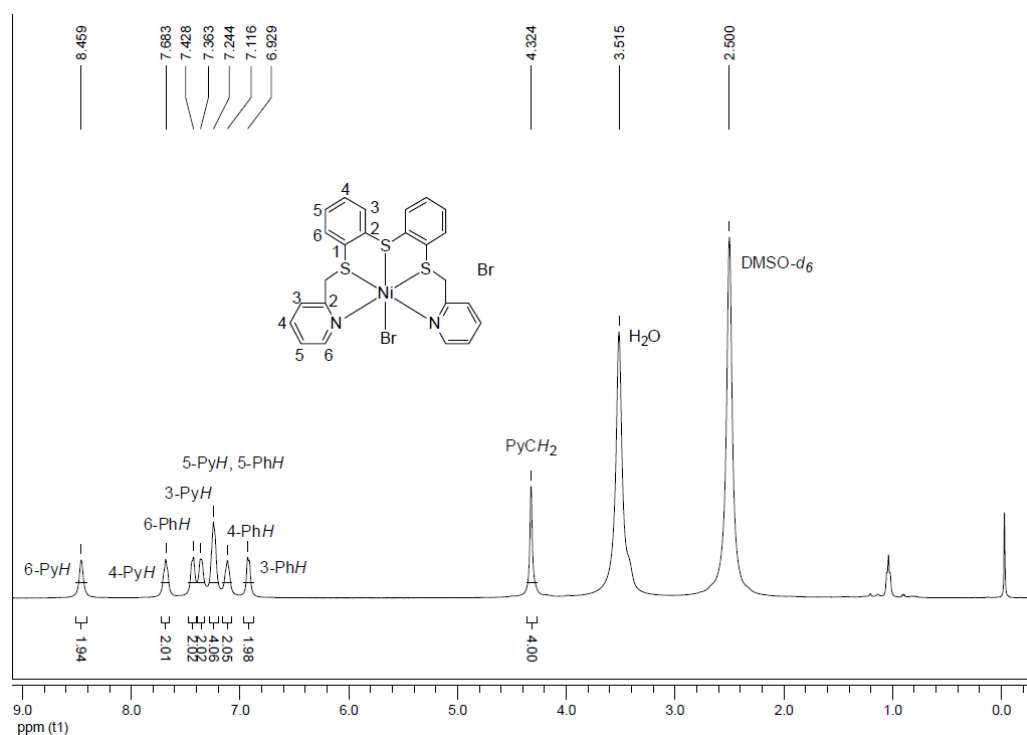
**Figure S16** The expansion of  $^{13}\text{C}$ -NMR(DMSO- $d_6$ ) spectrum of compound **2**



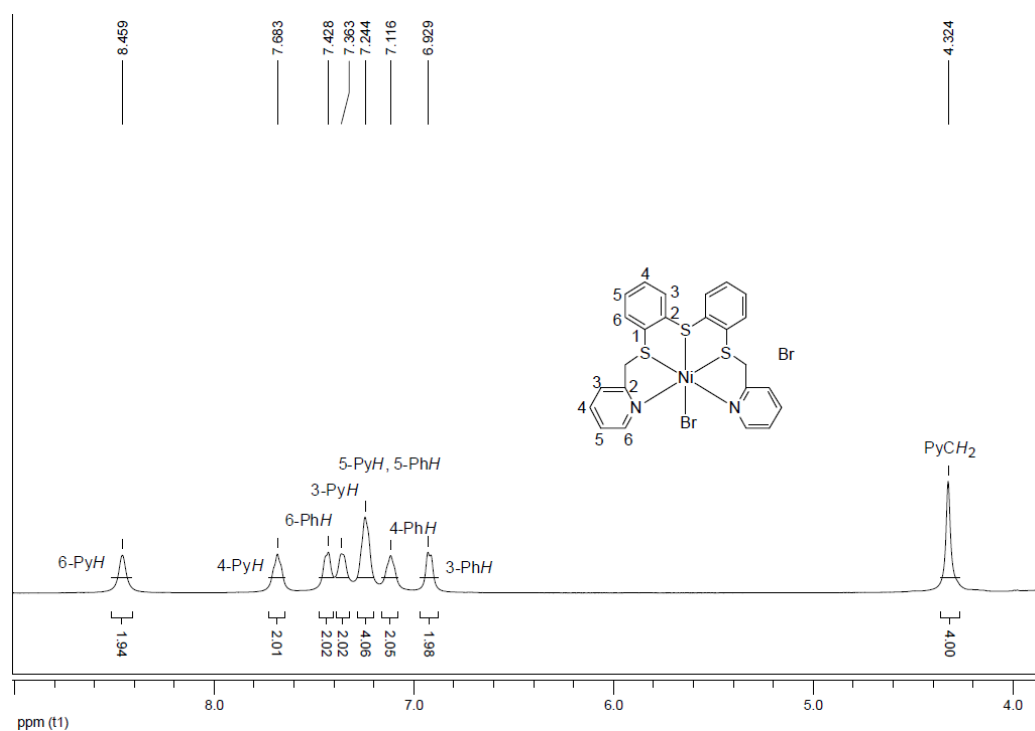


**Figure S17** The expansion of <sup>13</sup>C-NMR(DMSO-*d*<sub>6</sub>) spectrum of compound **2**

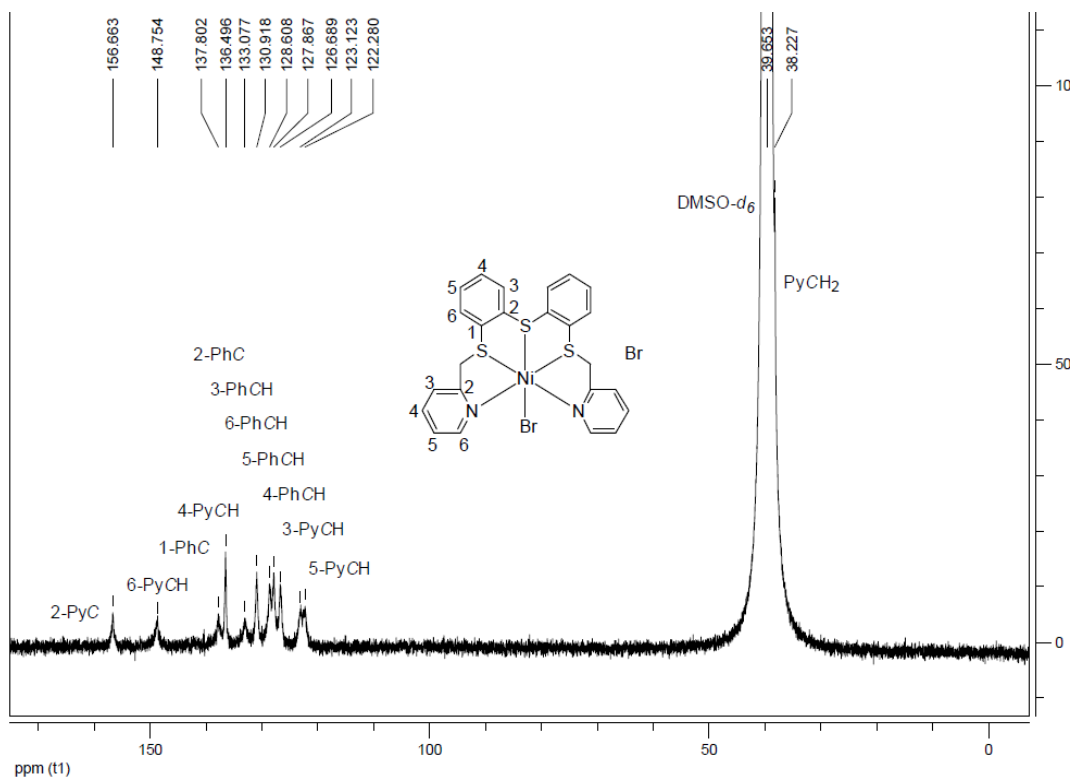
For 1D <sup>1</sup>H and <sup>13</sup>C-NMR spectra of compound **2**<sup>\*</sup>, see Figs S18-S22:



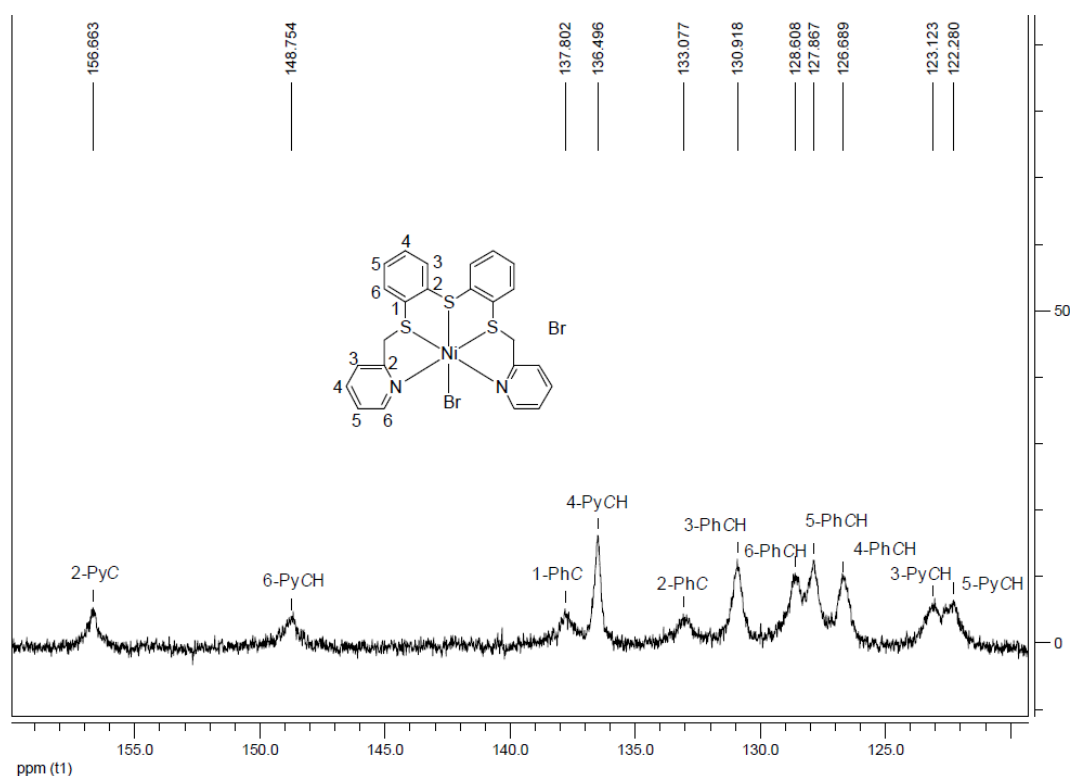
**Figure S18** <sup>1</sup>H-NMR(DMSO-*d*<sub>6</sub>) spectrum of compound **2**<sup>\*</sup>



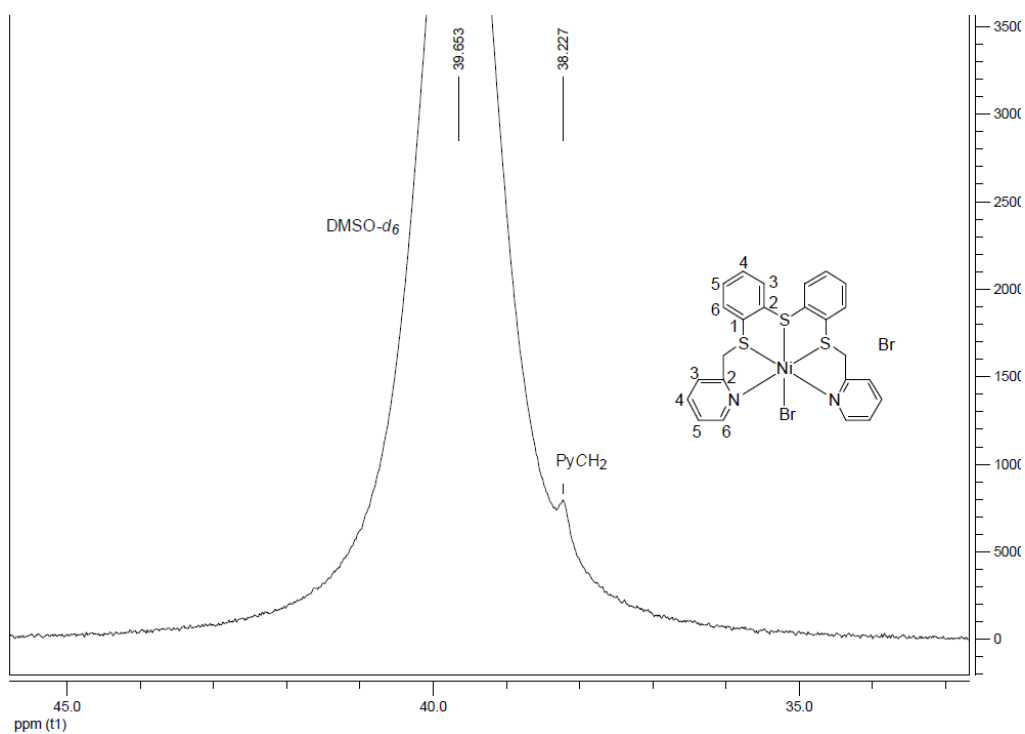
**Figure S19** The expansion of <sup>1</sup>H-NMR(DMSO-*d*<sub>6</sub>) spectrum of compound 2\*



**Figure S20** <sup>13</sup>C-NMR(DMSO-*d*<sub>6</sub>) spectrum of compound 2\*

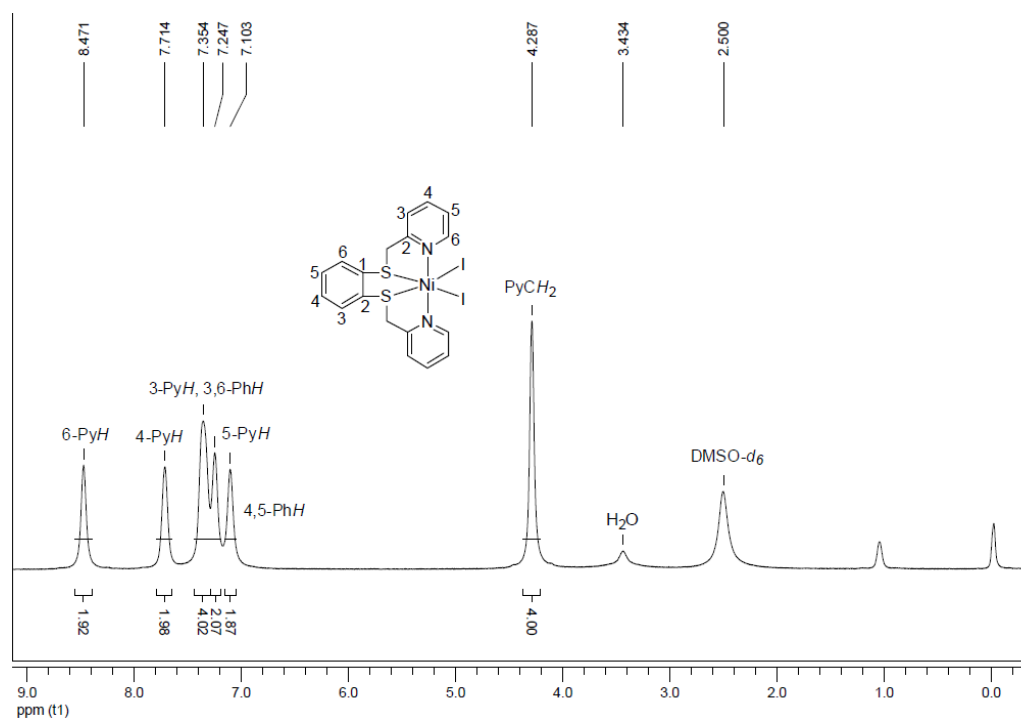


**Figure S21** The expansion of  $^{13}\text{C}$ -NMR(DMSO- $d_6$ ) spectrum of compound **2\***

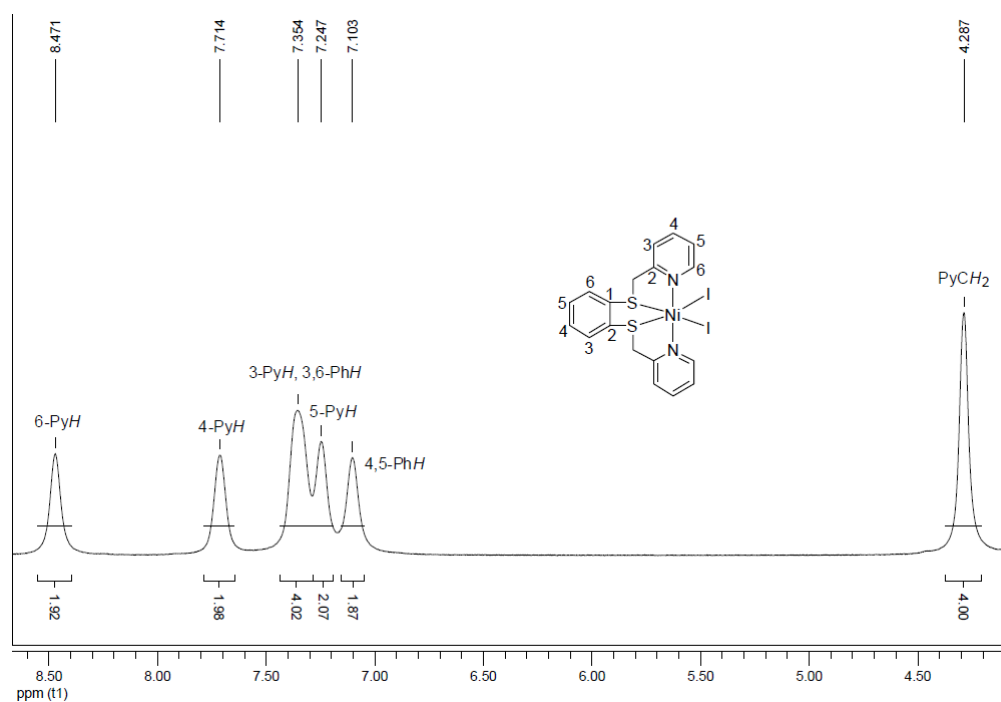


**Figure S22** The expansion of  $^{13}\text{C}$ -NMR(DMSO- $d_6$ ) spectrum of compound **2\***

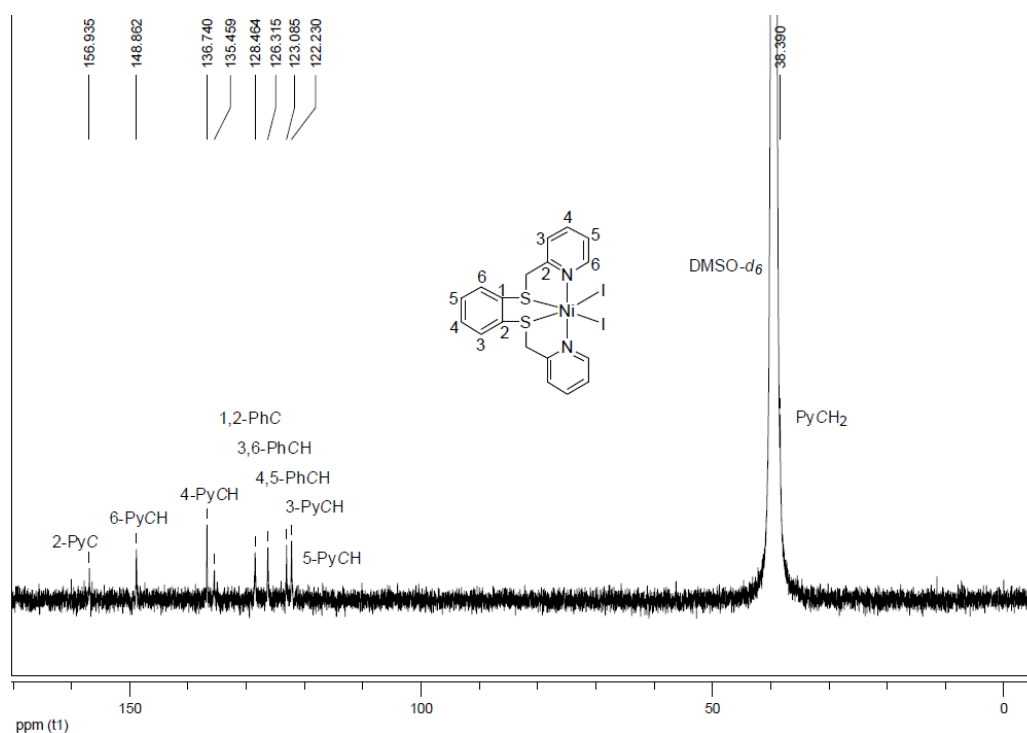
For 1D  $^1\text{H}$  and  $^{13}\text{C}$ -NMR spectra of compound **3**, see Figs S23–S27:



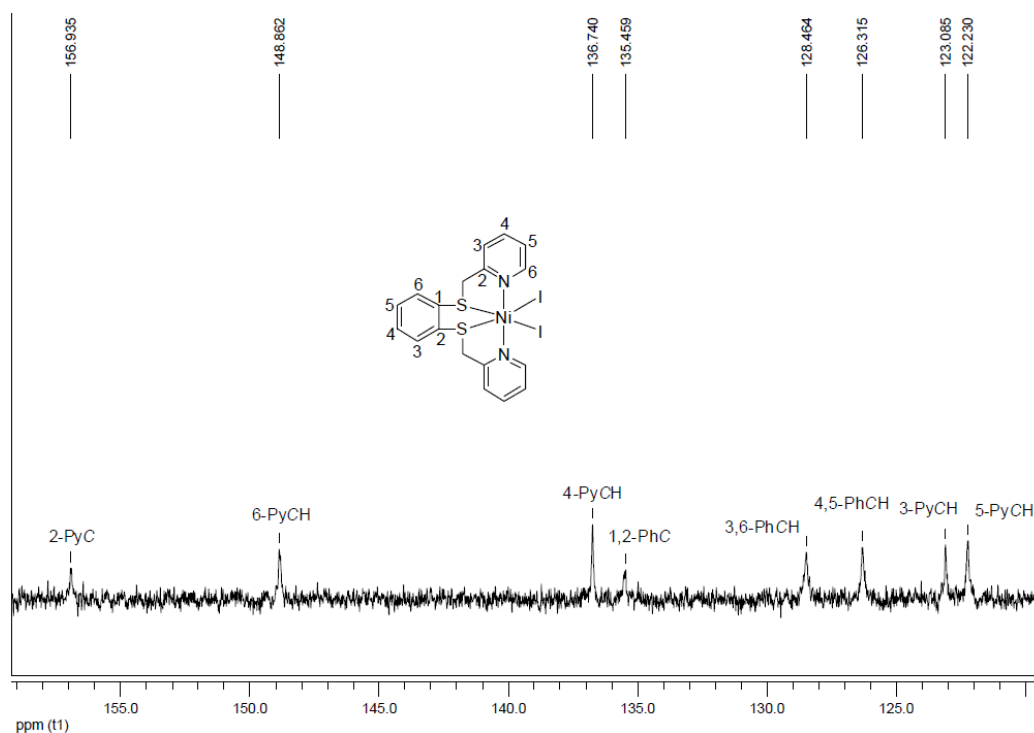
**Figure S23**  $^1\text{H}$ -NMR(DMSO-*d*<sub>6</sub>) spectrum of compound **3**



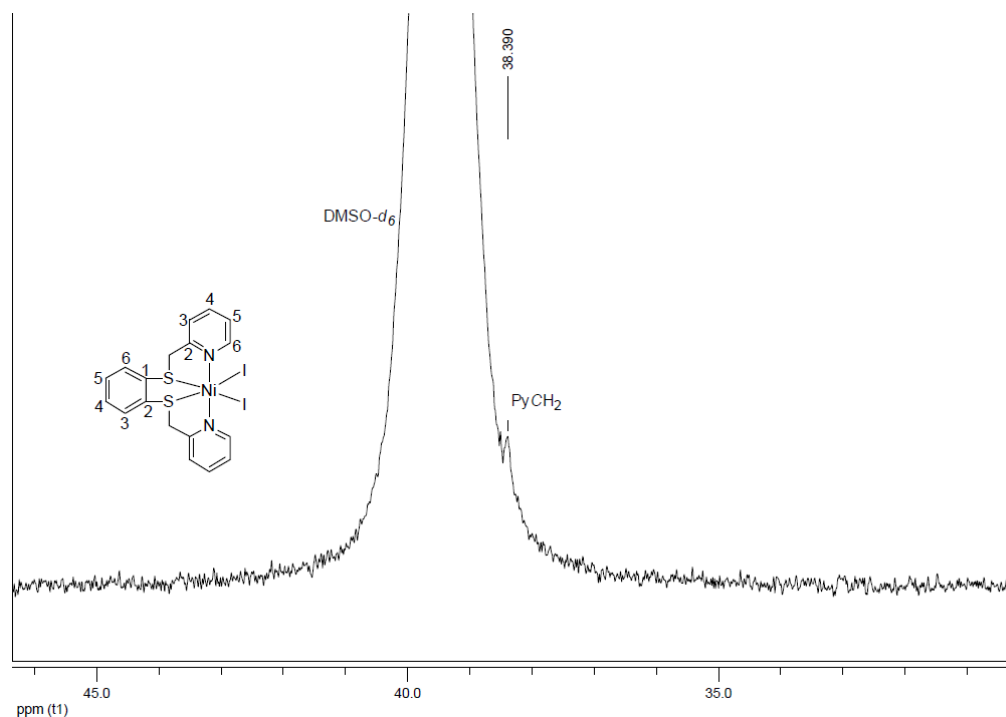
**Figure S24** The expansion of  $^1\text{H}$ -NMR(DMSO-*d*<sub>6</sub>) spectrum of compound **3**



**Figure S25**  $^{13}\text{C}$ -NMR(DMSO- $d_6$ ) spectrum of compound **3**

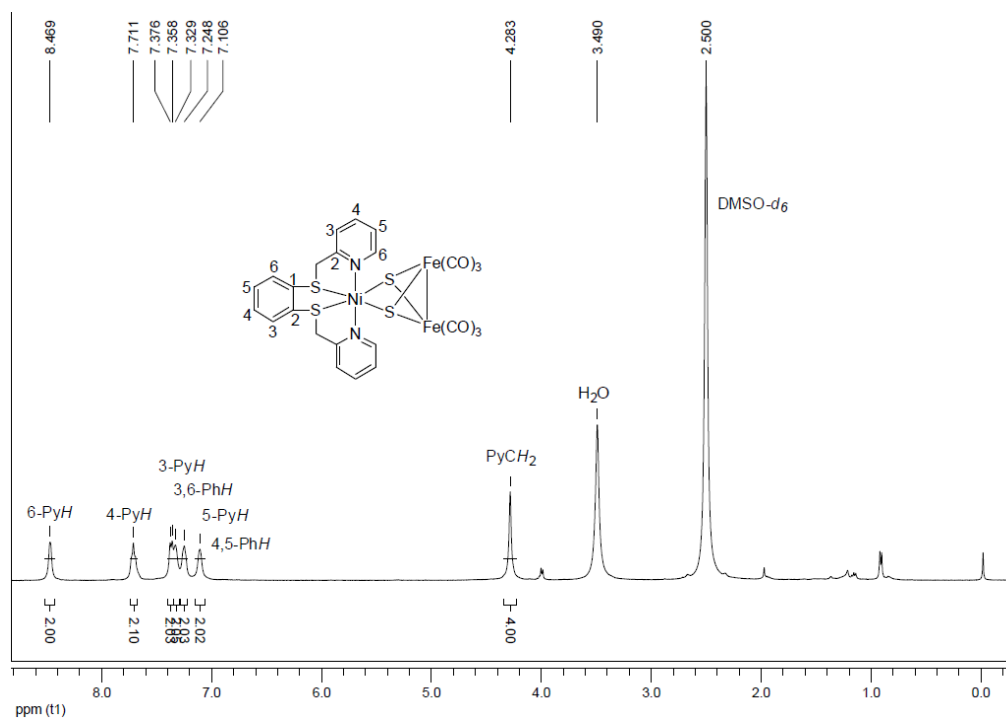


**Figure S26** The expansion of  $^{13}\text{C}$ -NMR(DMSO- $d_6$ ) spectrum of compound **3**

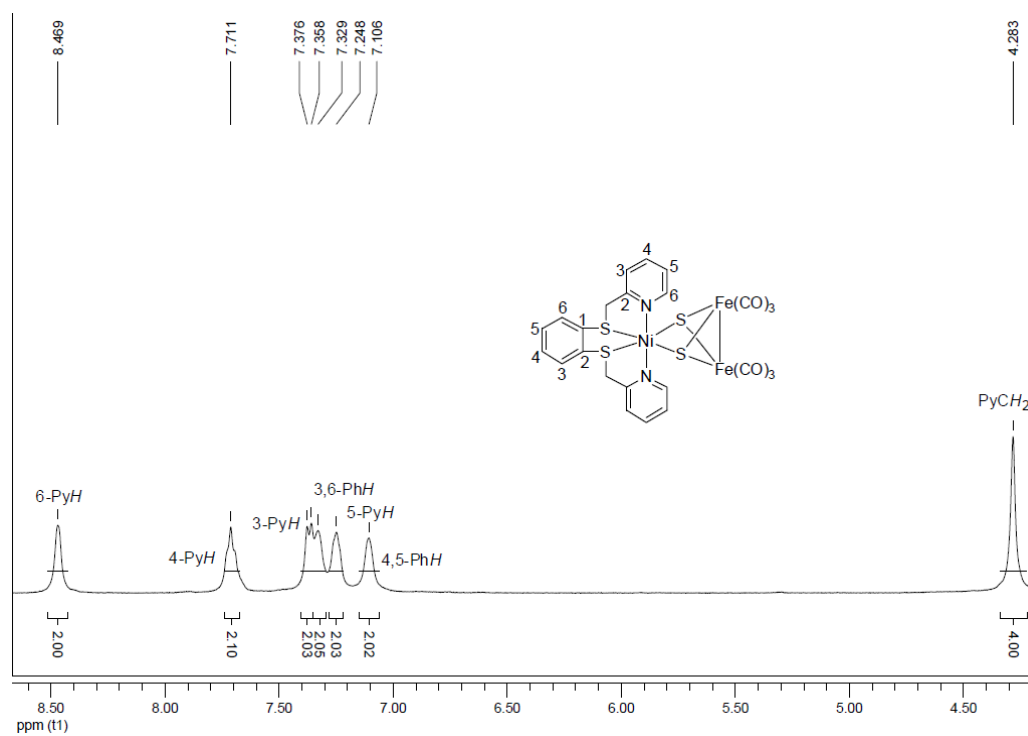


**Figure S27** The expansion of  $^{13}\text{C}$ -NMR( $\text{DMSO-}d_6$ ) spectrum of compound **3**

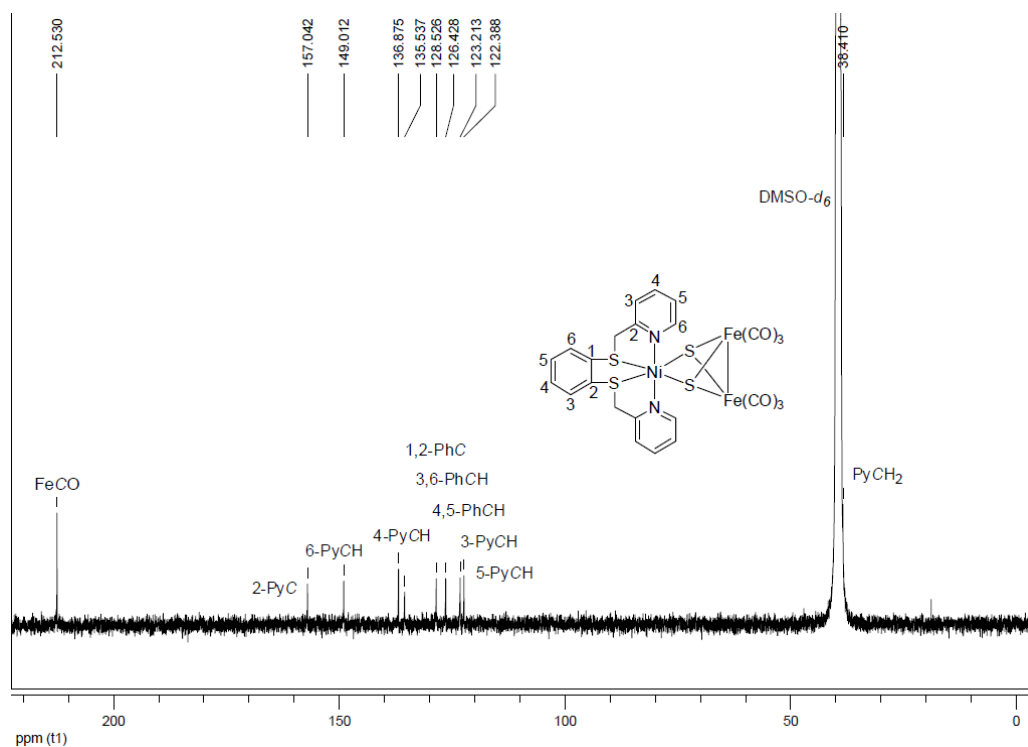
For 1D  $^1\text{H}$  and  $^{13}\text{C}$ -NMR spectras of compound **4**, see Figs S28-S32:



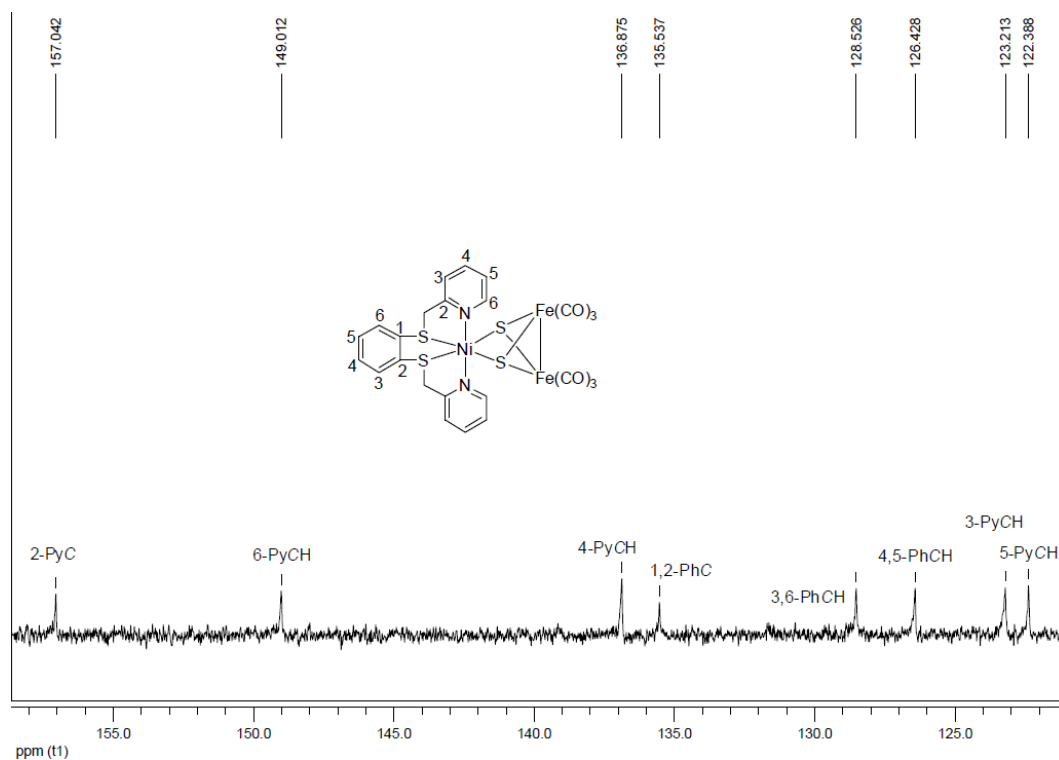
**Figure S28**  $^1\text{H}$ -NMR( $\text{DMSO-}d_6$ ) spectrum of compound **4**



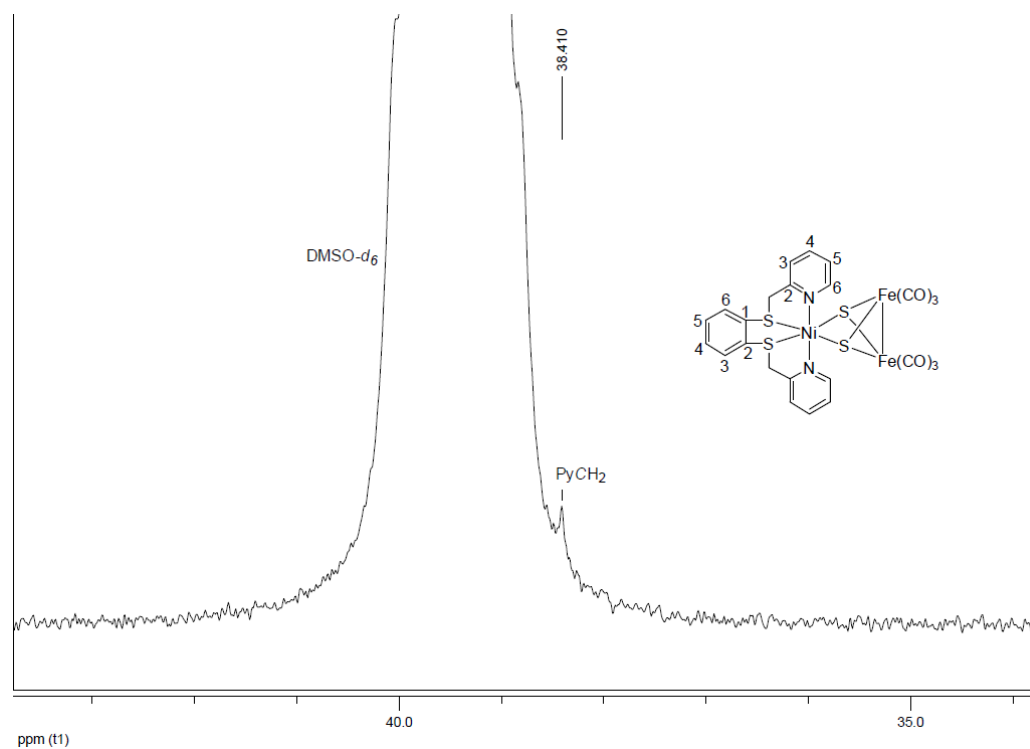
**Figure S29** The expansion of <sup>1</sup>H-NMR(DMSO-*d*<sub>6</sub>) spectrum of compound **4**



**Figure S30** <sup>13</sup>C-NMR(DMSO-*d*<sub>6</sub>) spectrum of compound **4**



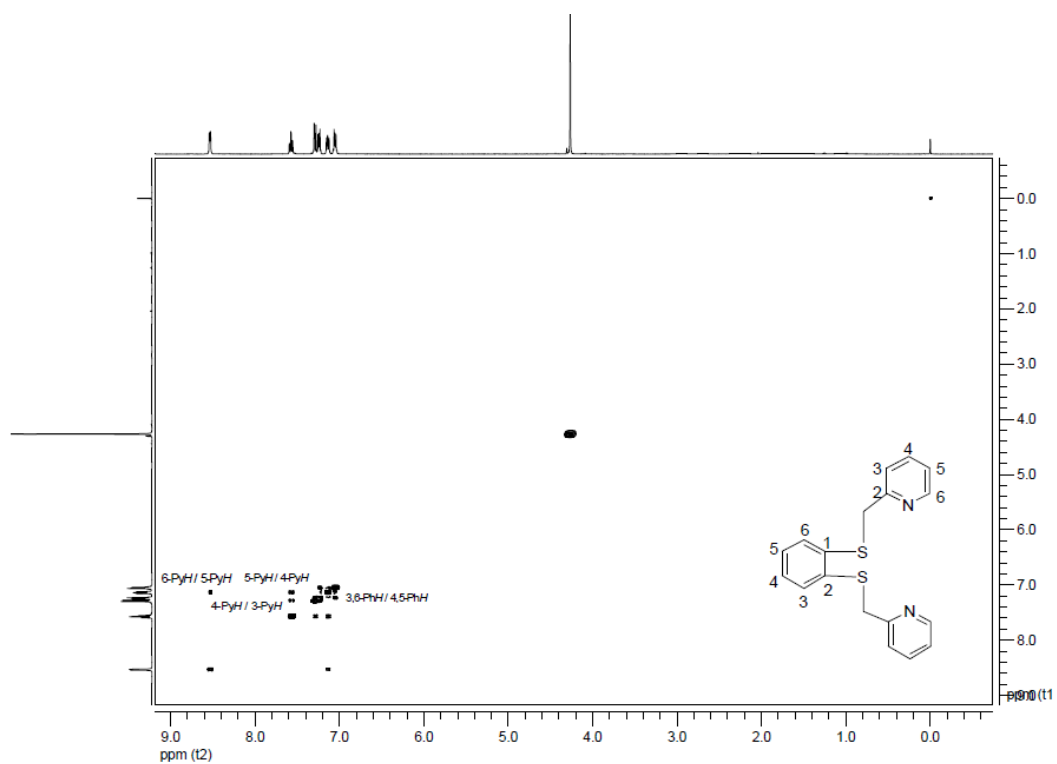
**Figure S31** The expansion of  $^{13}\text{C}$ -NMR( $\text{DMSO-}d_6$ ) spectrum of compound **4**



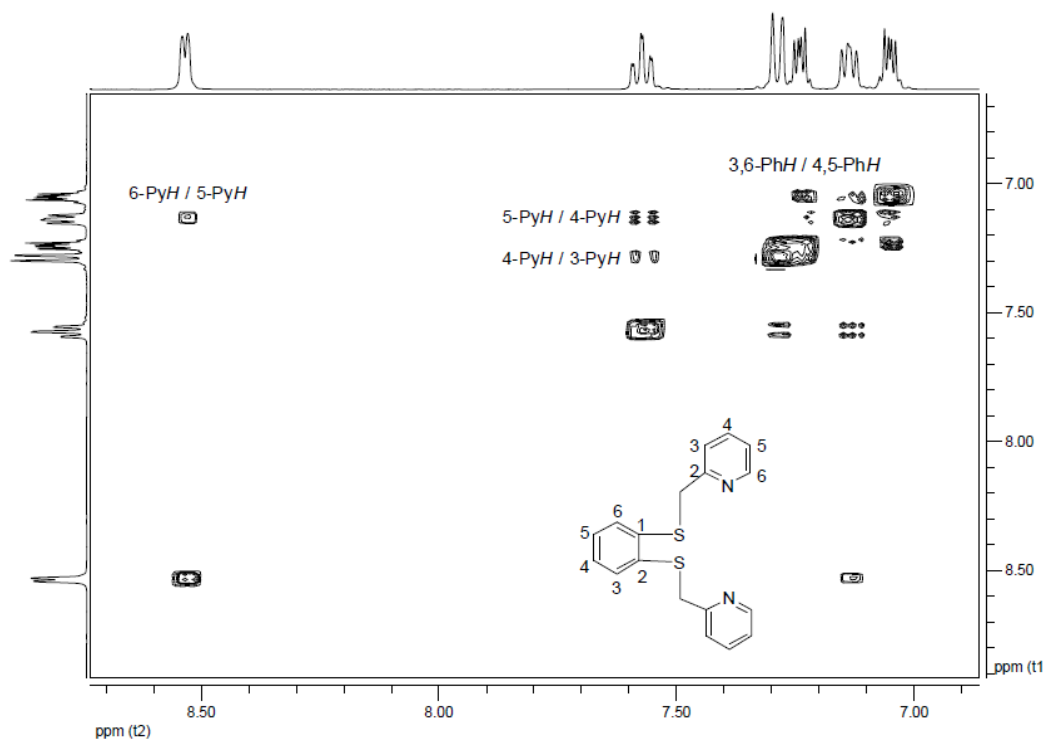
**Figure S32** The expansion of  $^{13}\text{C}$ -NMR( $\text{DMSO-}d_6$ ) spectrum of compound **4**



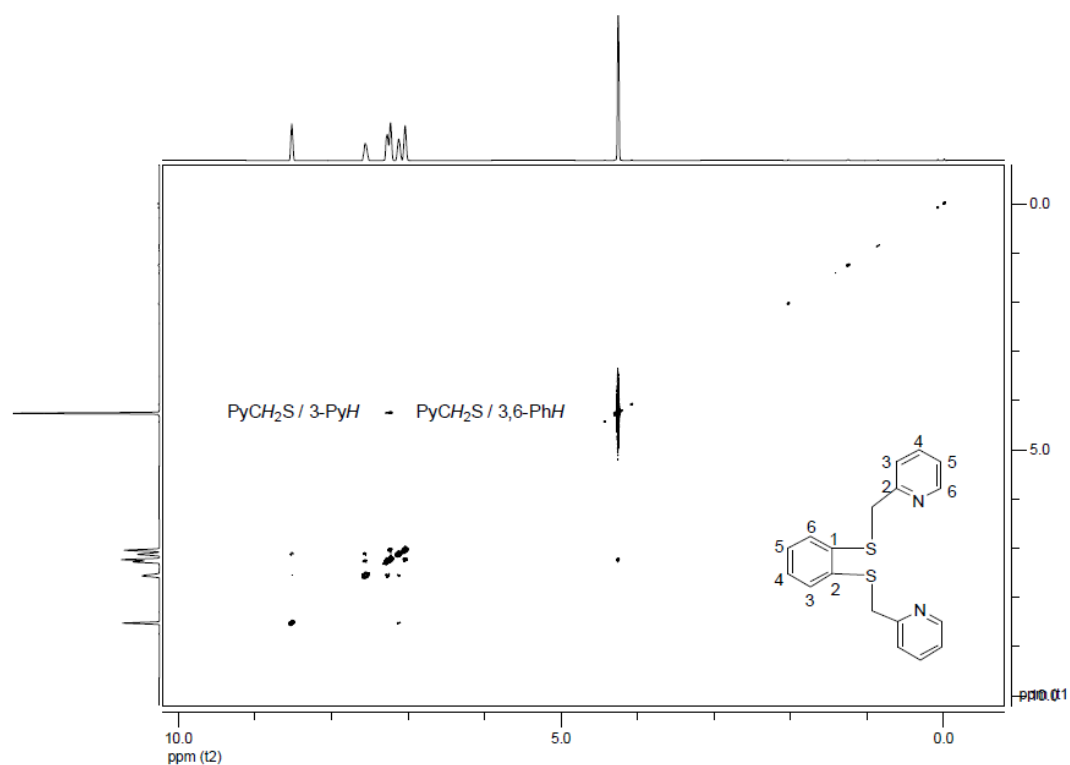
For 2D-NMR spectra of ligand **L**, see Figs S33-S40:



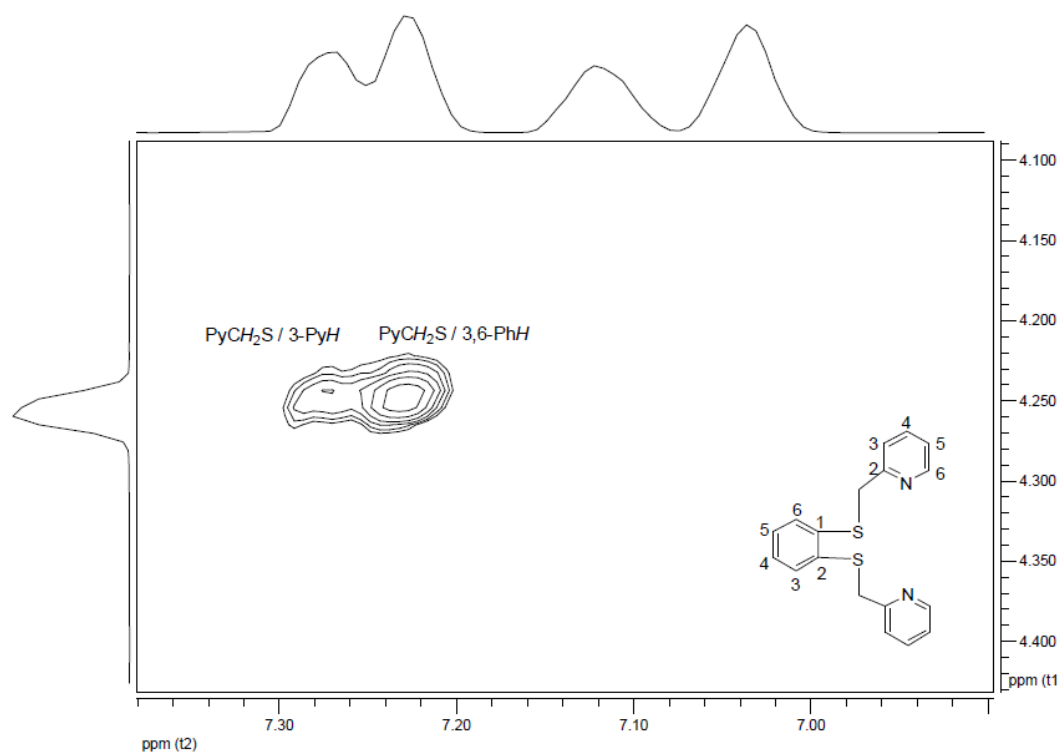
**Figure S33**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of ligand **L**



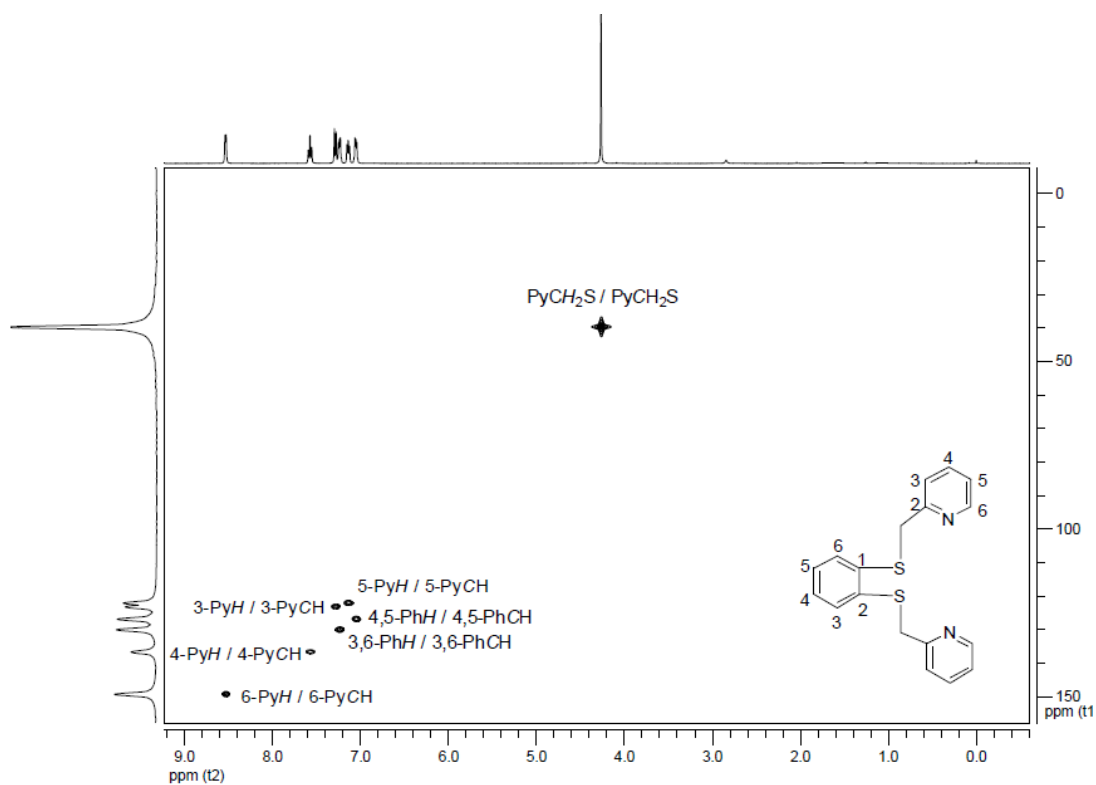
**Figure S34** The expansion of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of ligand **L**



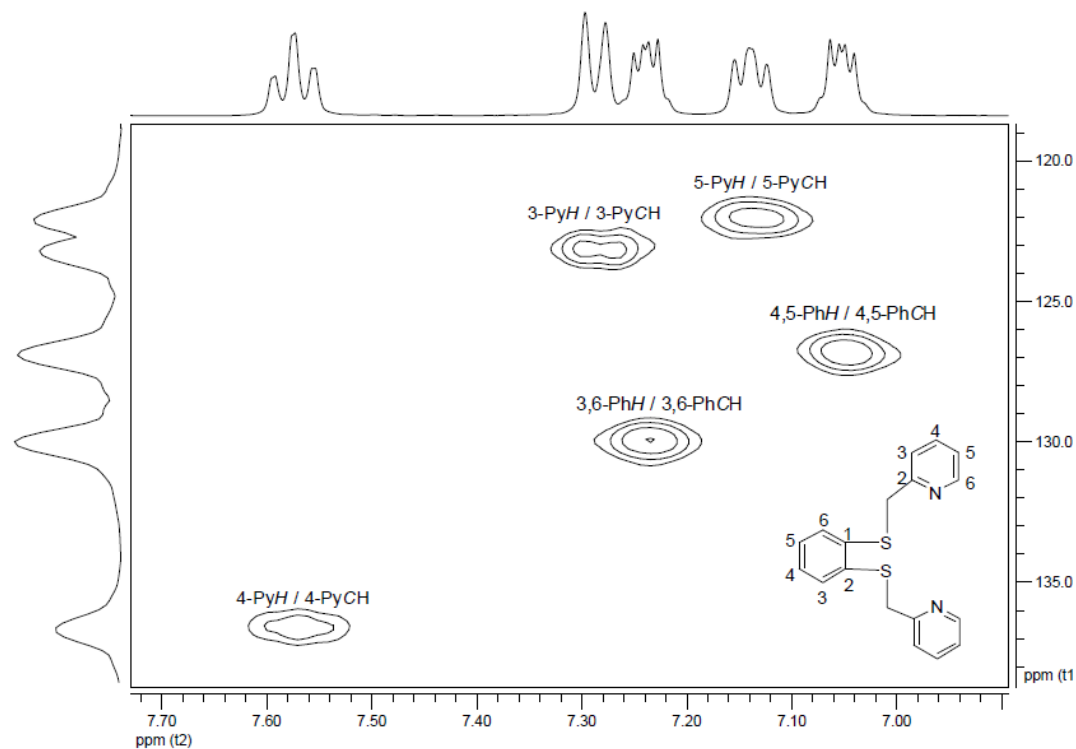
**Figure S35**  $^1\text{H}$ - $^1\text{H}$  NOESY spectrum of ligand **L**



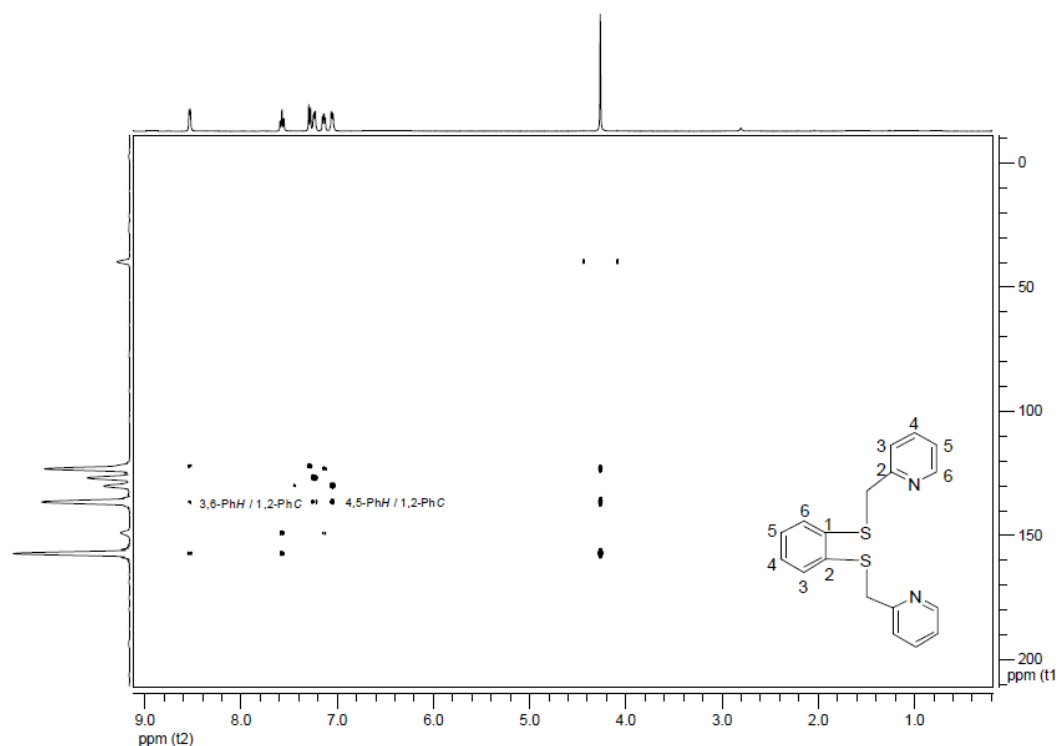
**Figure S36** The expansion of  $^1\text{H}$ - $^1\text{H}$  NOESY spectrum of ligand **L**



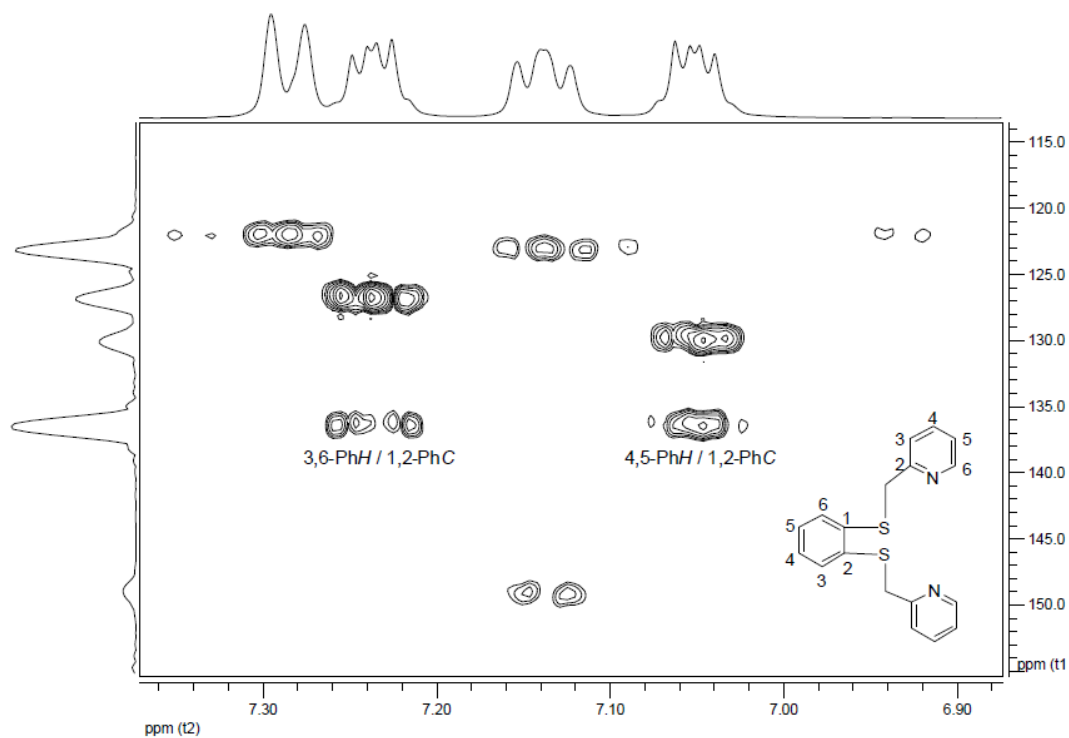
**Figure S37** HMQC spectrum of ligand **L**



**Figure S38** The expansion of HMQC spectrum of ligand **L**

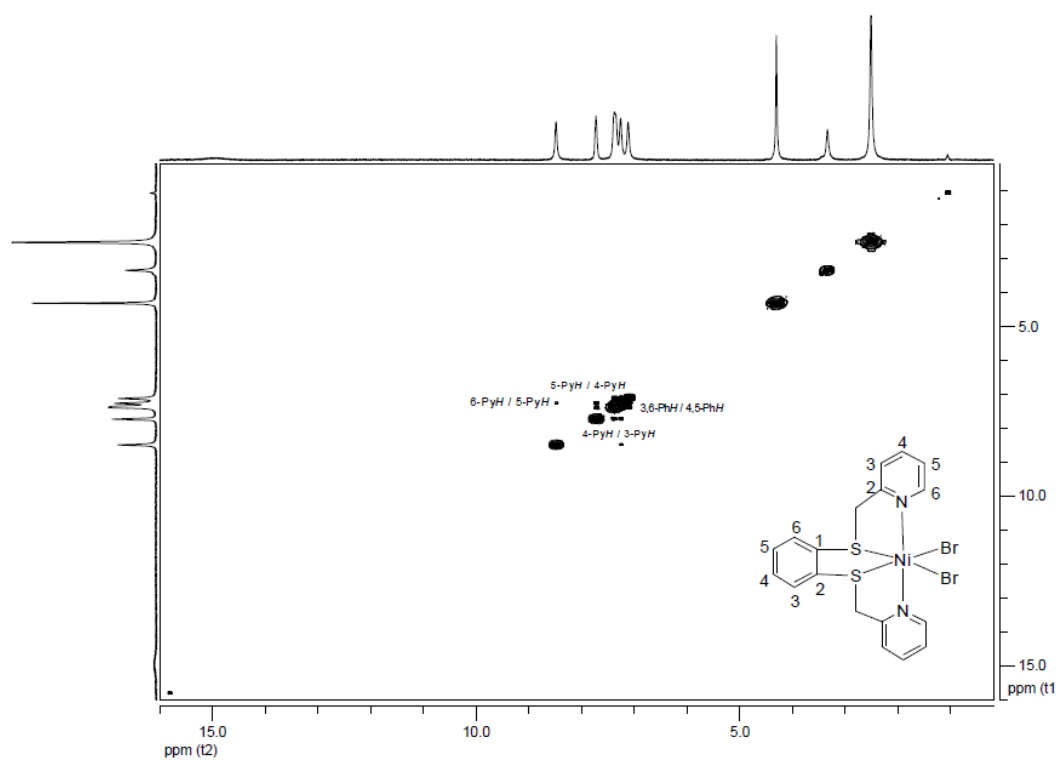


**Figure S39** HMBC spectrum of ligand **L**

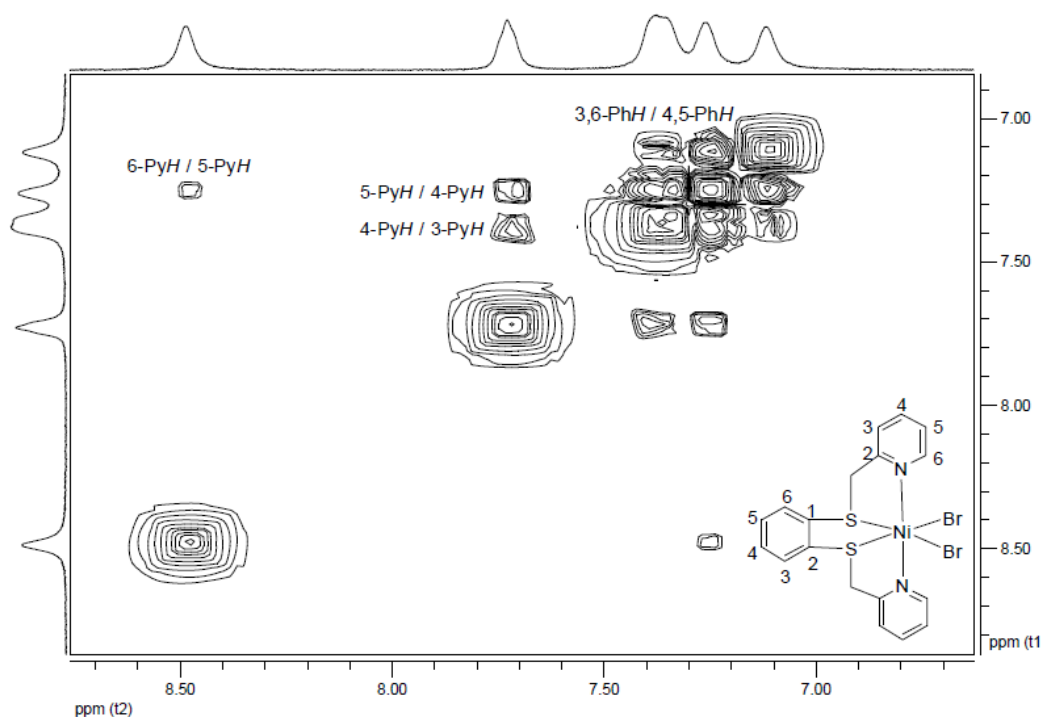


**Figure S40** The expansion of HMBC spectrum of ligand **L**

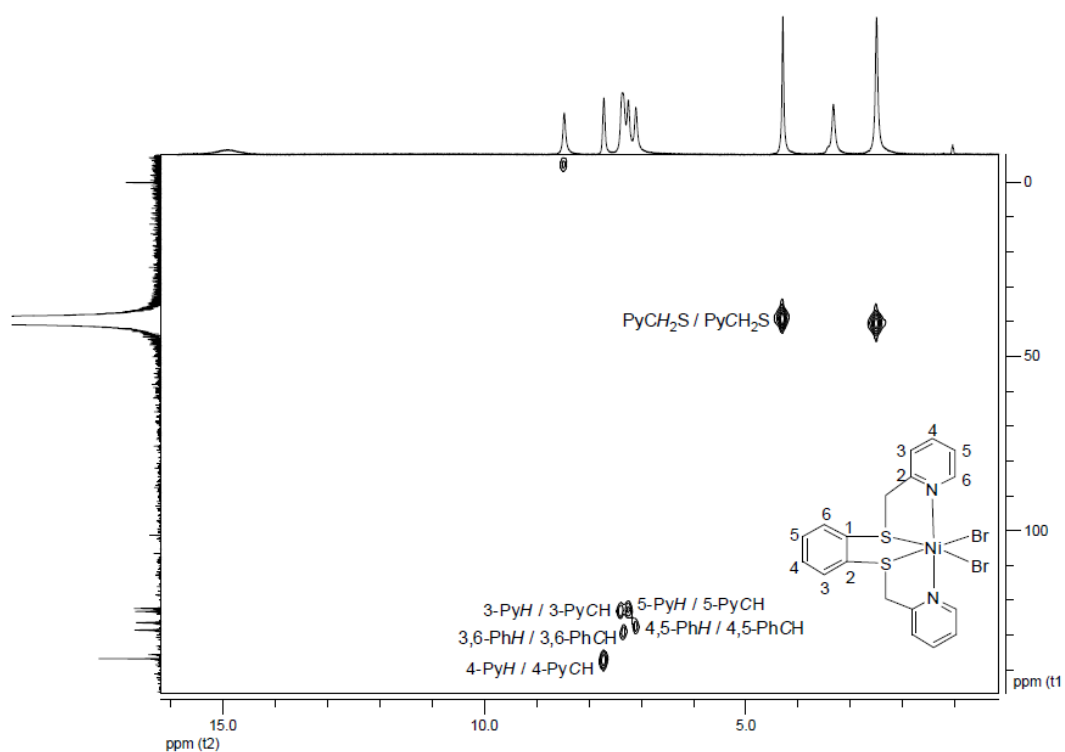
For 2D-NMR spectra of compound **2**, see Figs S41–S44:



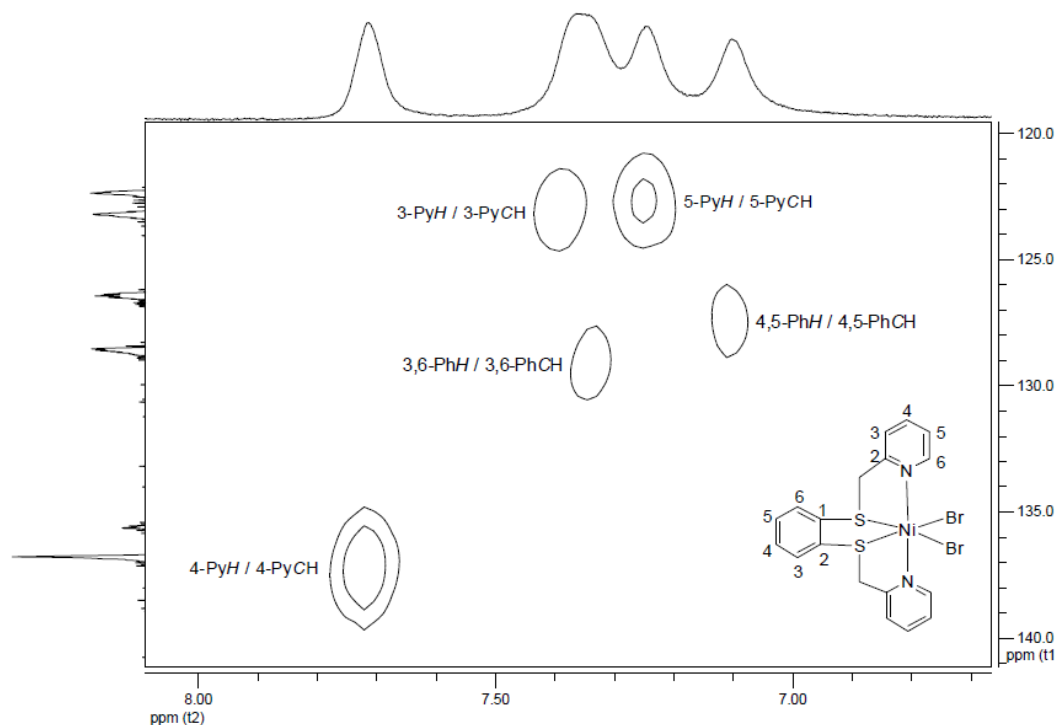
**Figure S41**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2**



**Figure S42** The expansion of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2**

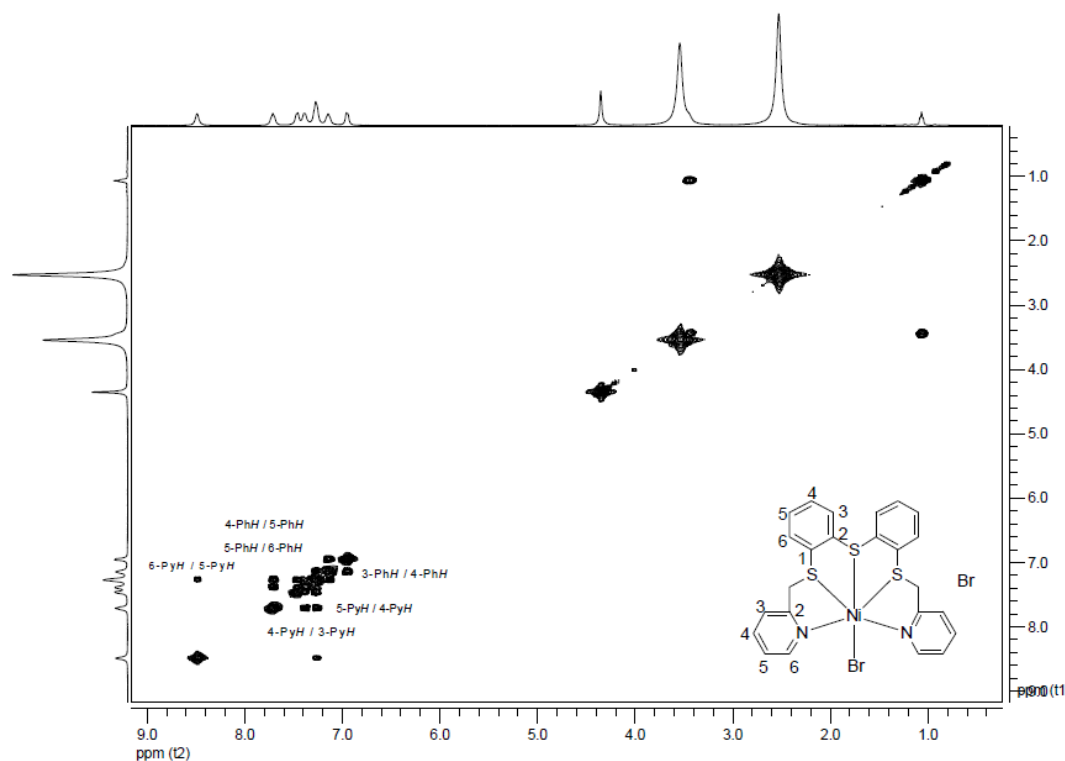


**Figure S43** HMQC spectrum of compound **2**

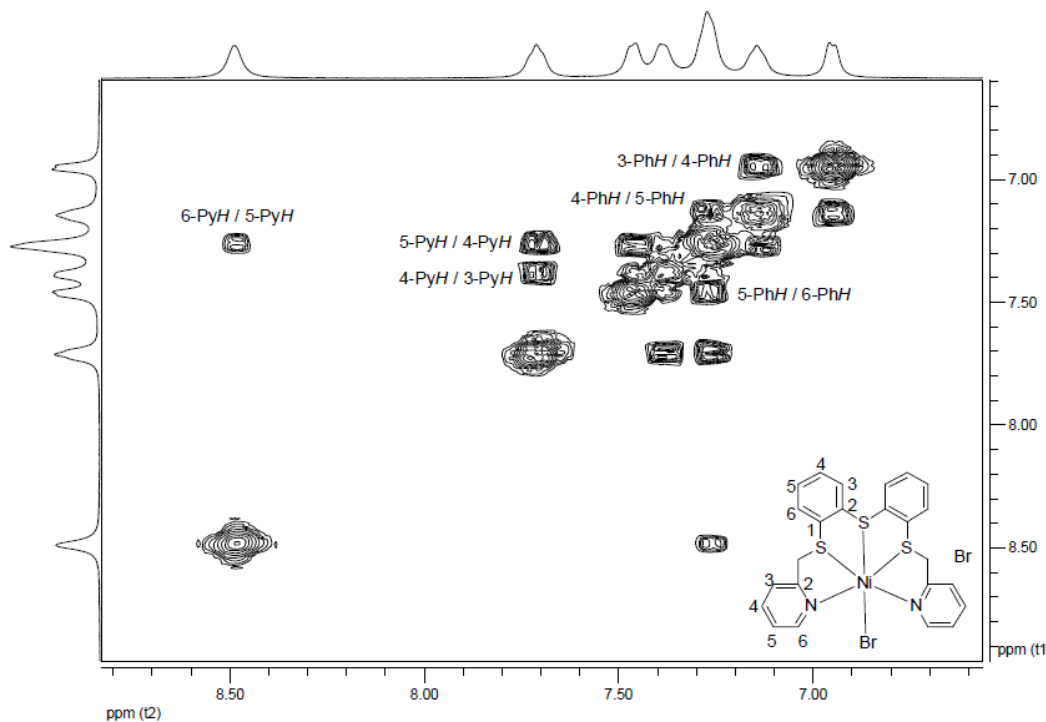


**Figure S44** The expansion of HMQC spectrum of compound **2**

For 2D-NMR spectra of compound **2**<sup>\*</sup>, see Figs S45–S46:

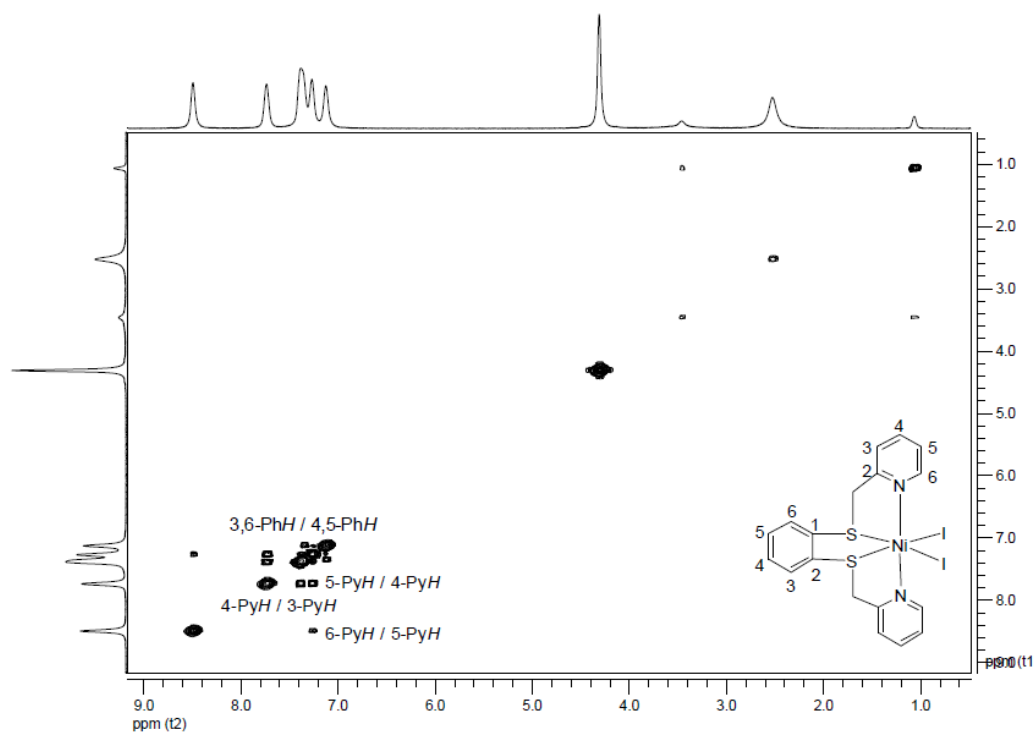


**Figure S45**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2**<sup>\*</sup>

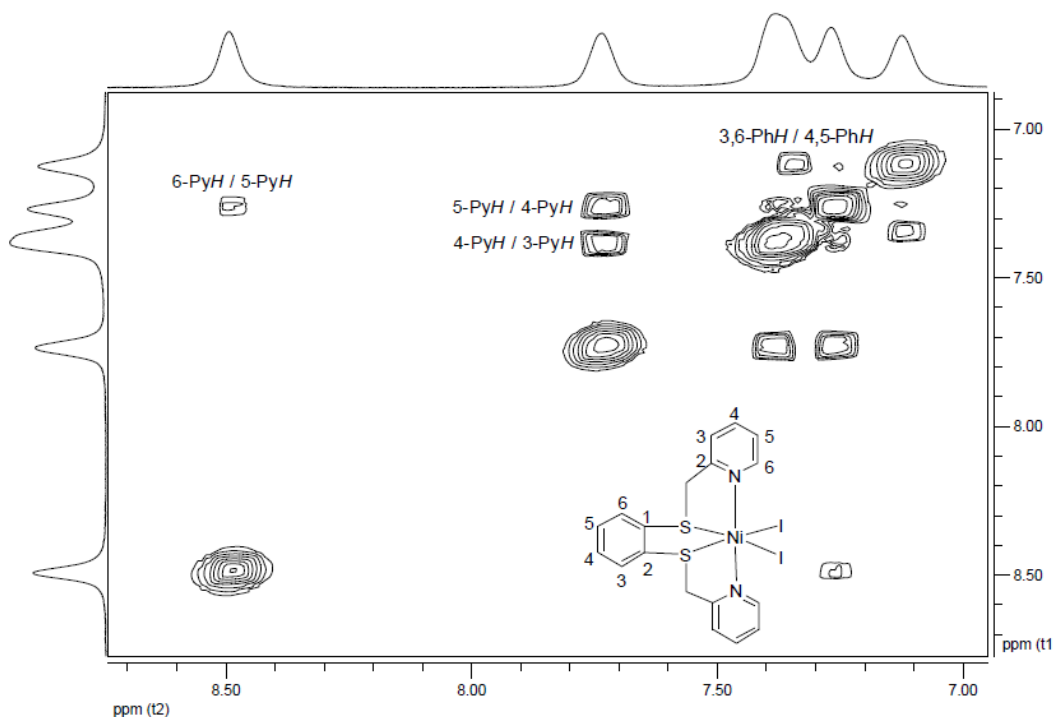


**Figure S46** The expansion of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **2**<sup>\*</sup>

For 2D-NMR spectra of compound **3**, see Figs S47–S50:

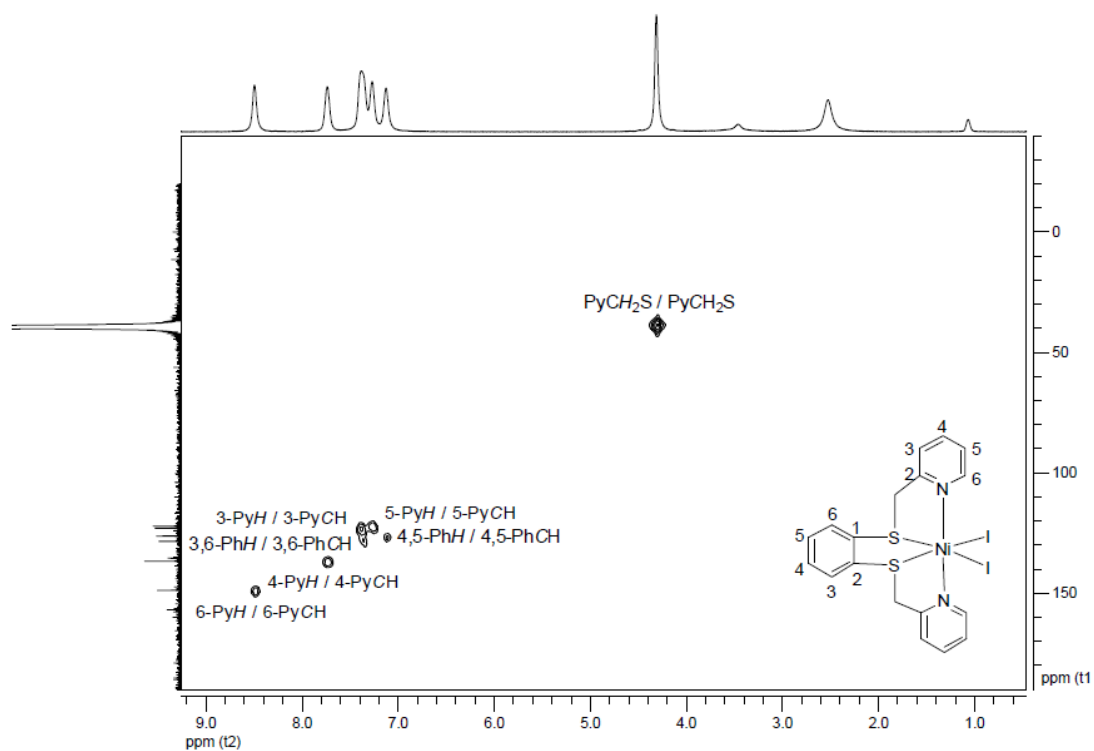


**Figure S47**  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **3**

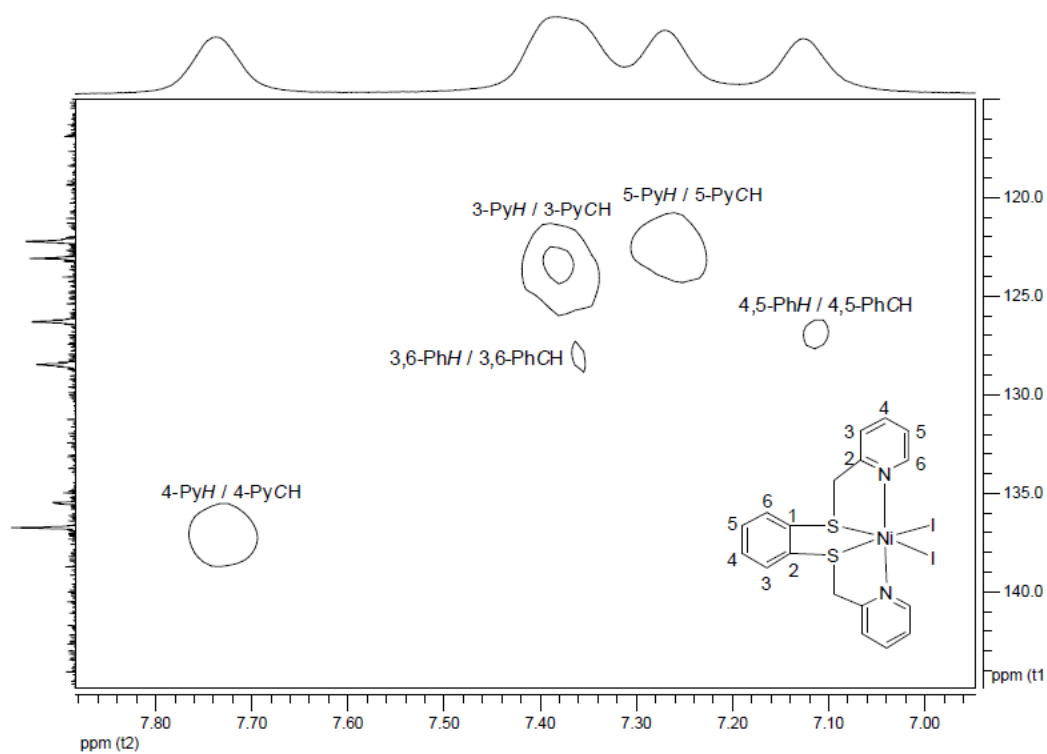


**Figure S48** The expansion of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **3**





**Figure S49** HMQC spectrum of compound **3**



**Figure S50** The expansion of HMQC spectrum of compound **3**

For 2D-NMR spectra of compound **4**, see Figs S51–S56:

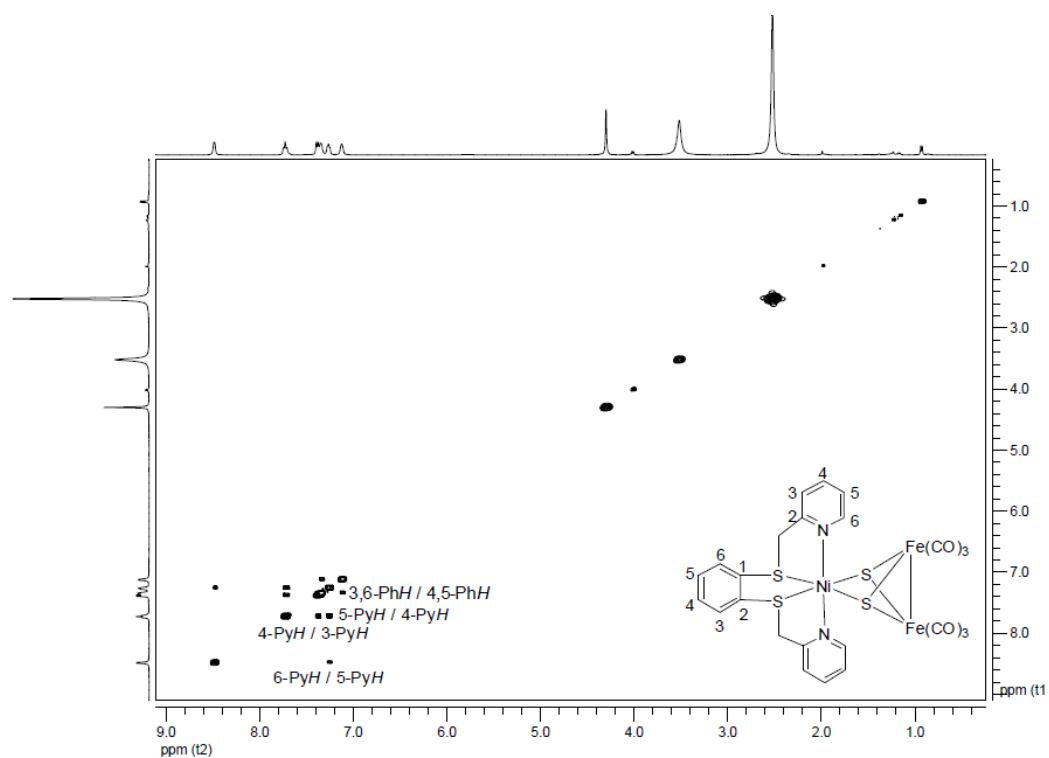


Figure S51  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **4**

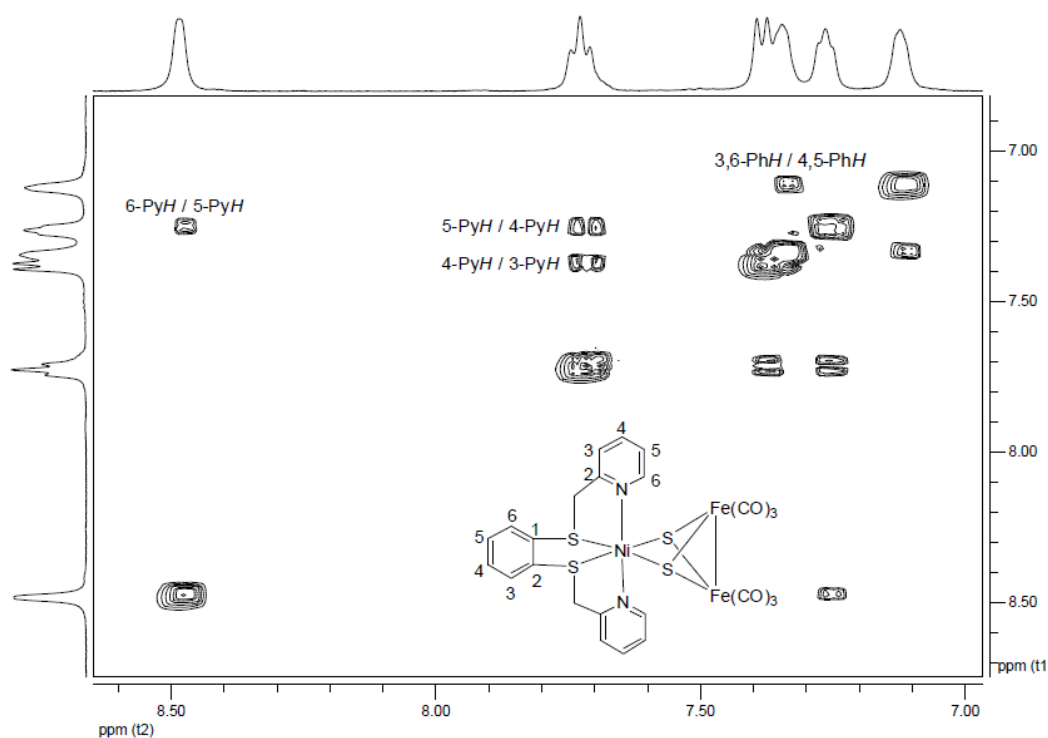
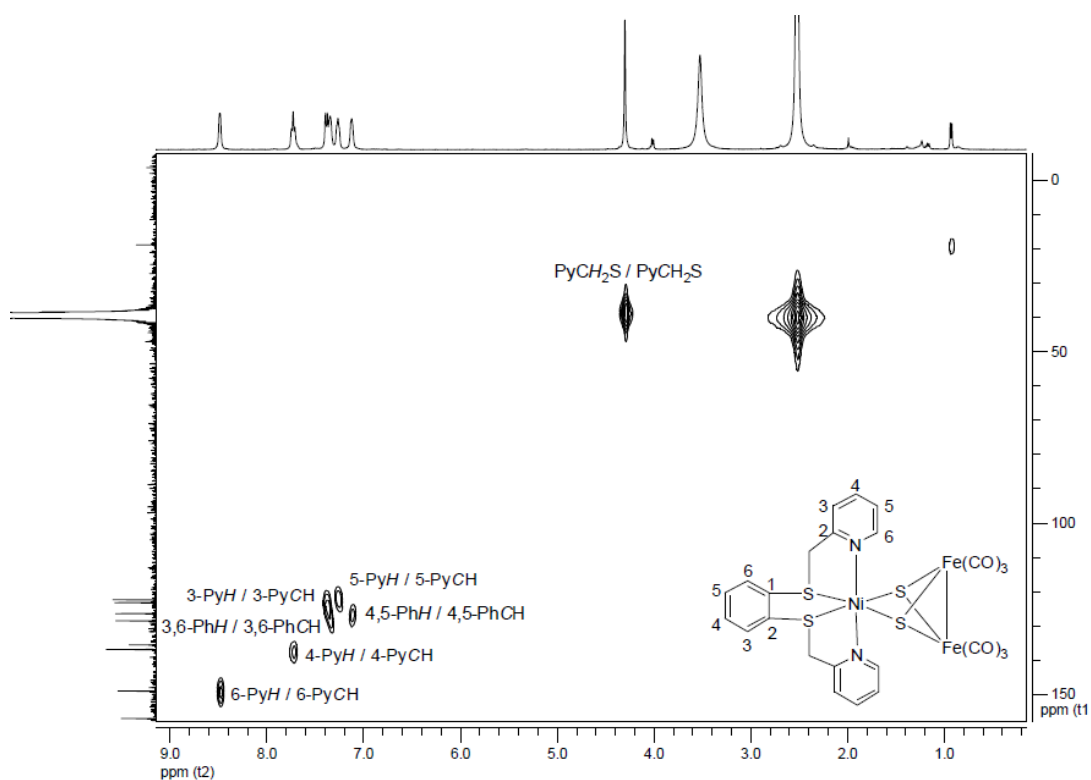
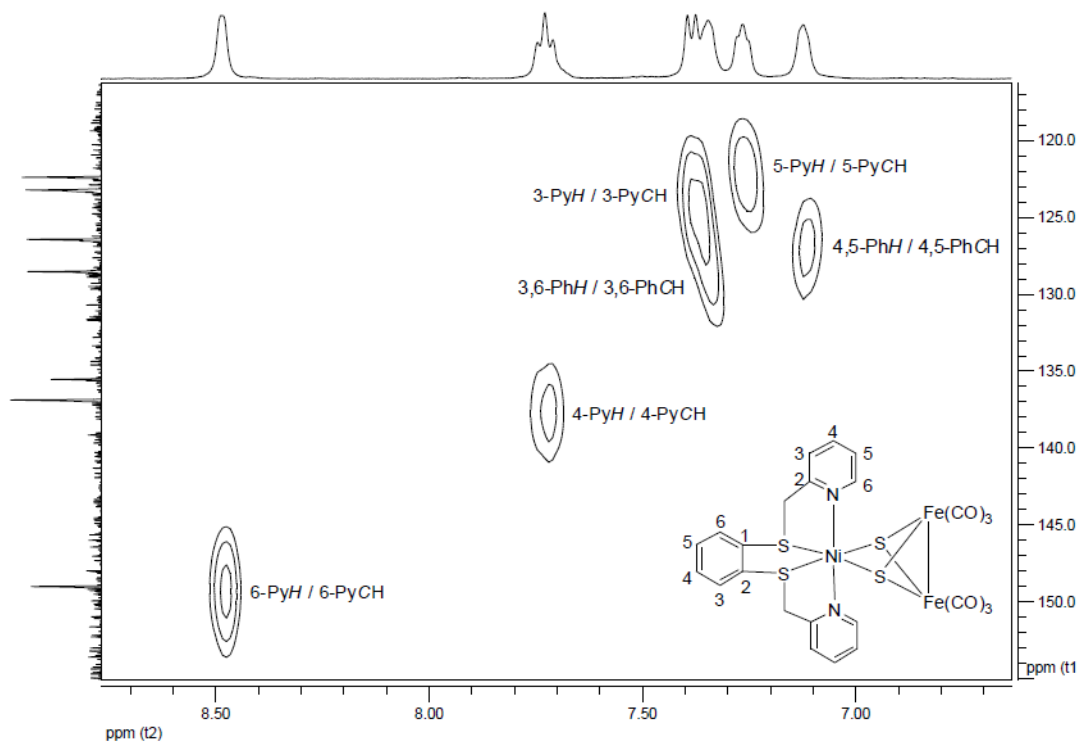


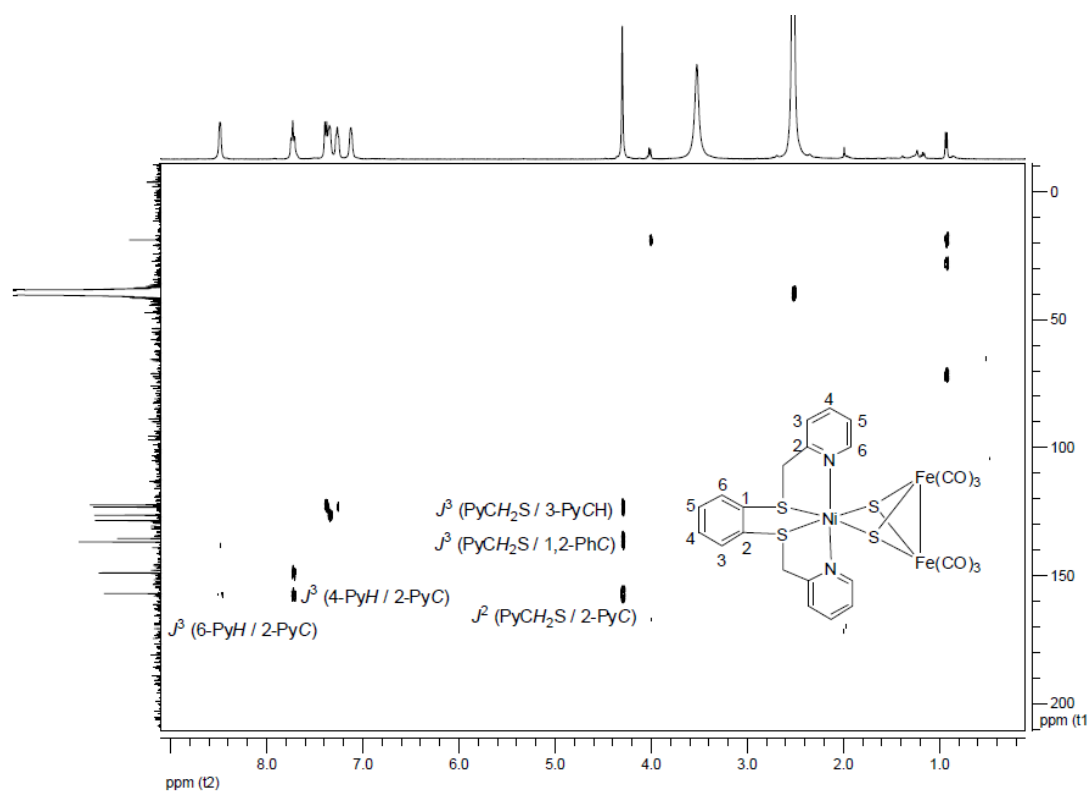
Figure S52 The expansion of  $^1\text{H}$ - $^1\text{H}$  COSY spectrum of compound **4**



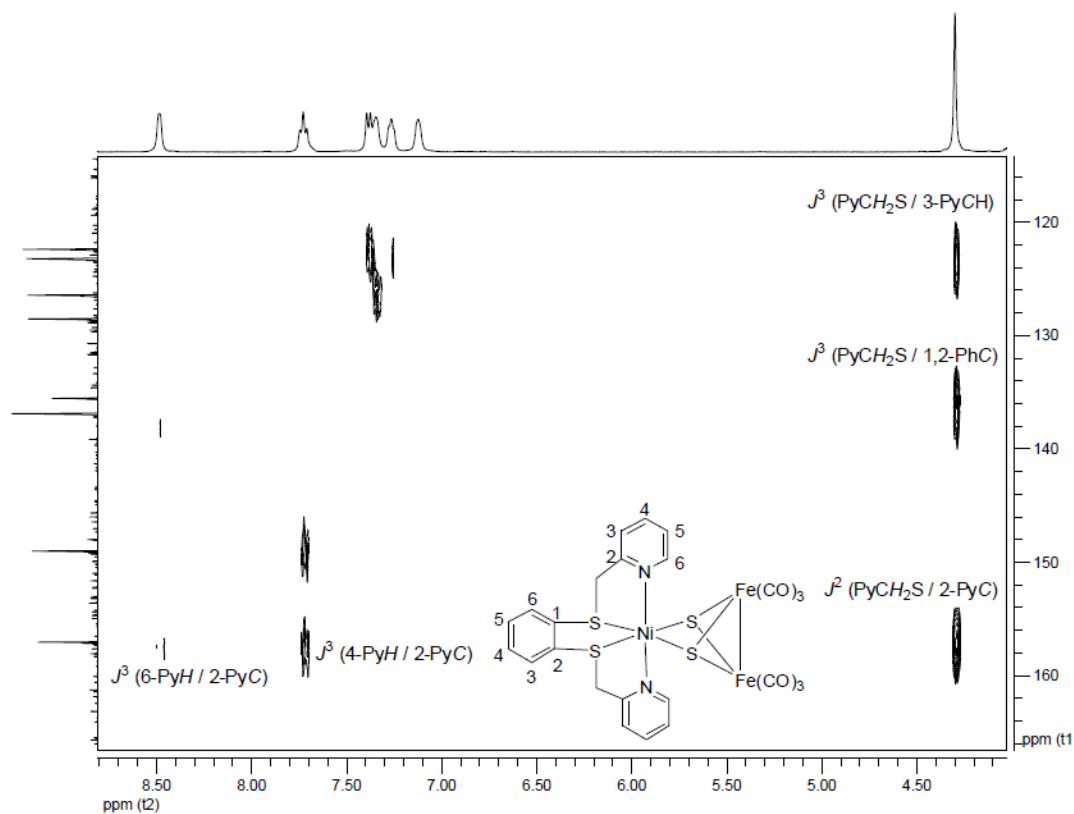
**Figure S53** HMQC spectrum of compound **4**



**Figure S54** The expansion of HMQC spectrum of compound **4**

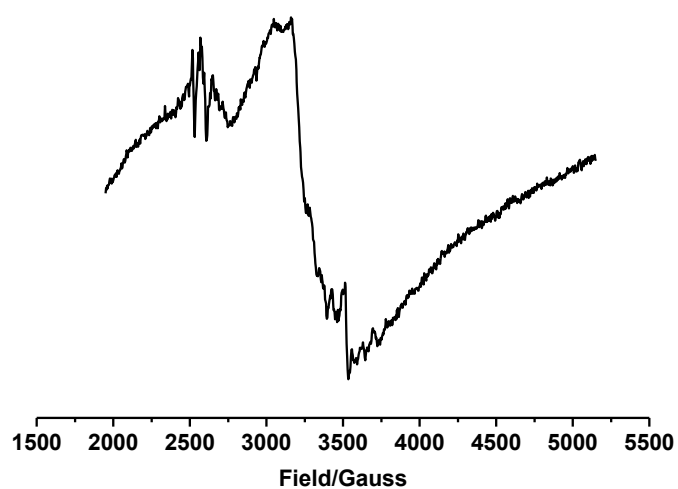


**Figure S55** HMBC spectrum of compound **4**

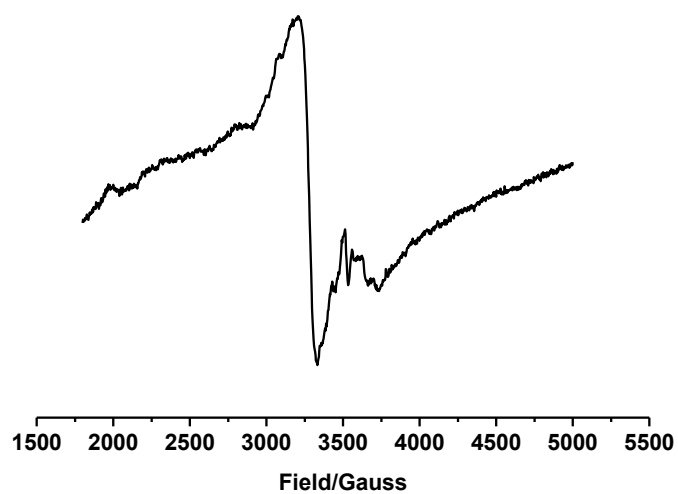


**Figure S56** The expansion of HMBC spectrum of compound **4**

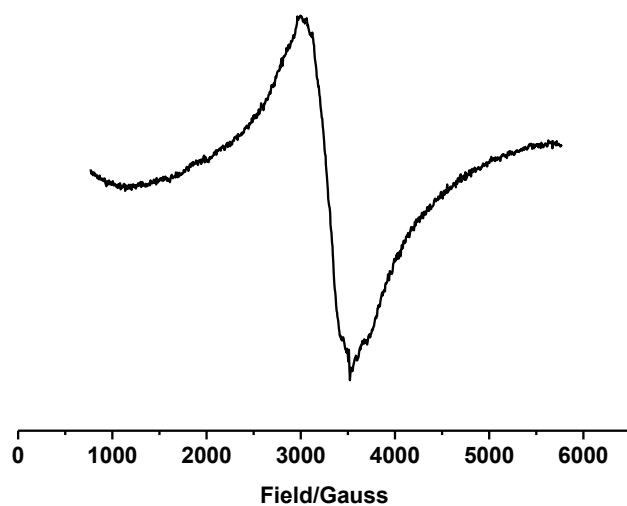
**For EPR Spectra of complexes 1, 2\*, 3 and 4, see Figs S57–S60:**



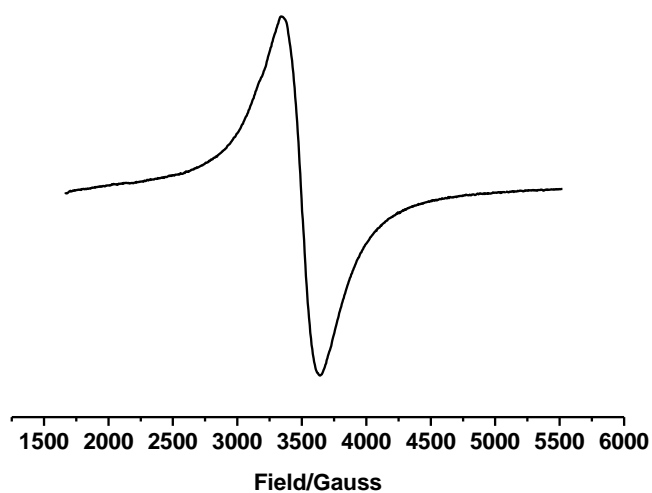
**Figure S57** X-band EPR spectrum of complex **1** with  $g = 2.161$  at room temperature.



**Figure S58** X-band EPR spectrum of complex **2\*** with  $g = 2.141$  at room temperature.



**Figure S59** X-band EPR spectrum of complex **3** with  $g = 2.134$  at room temperature.



**Figure S60** X-band EPR spectrum of complex **4** with  $g = 2.003$  at room temperature.