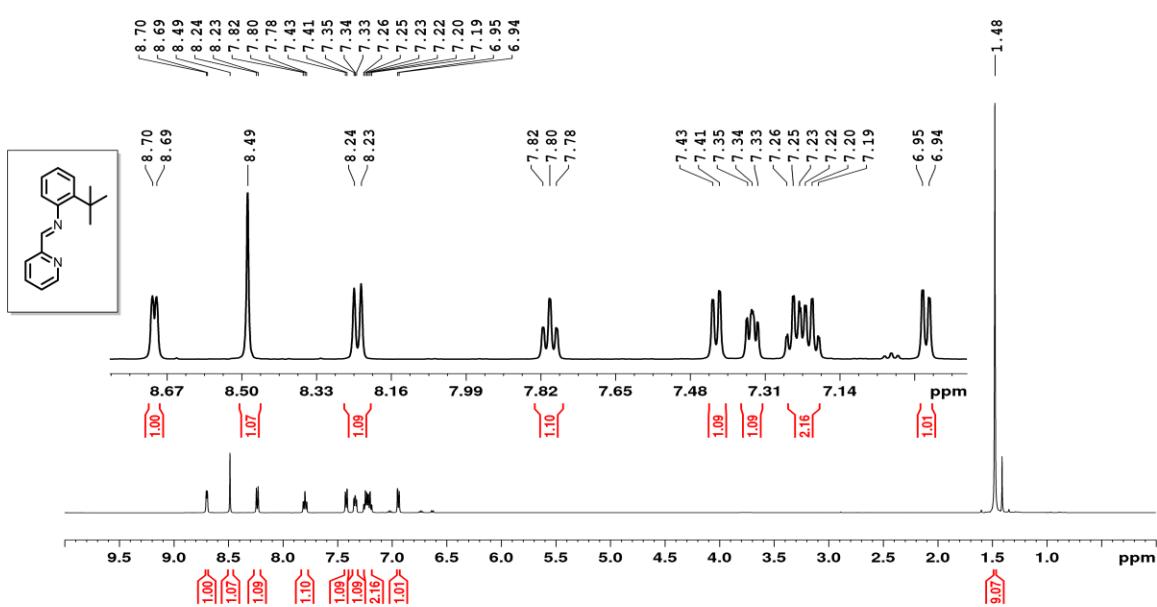


## Supporting Information

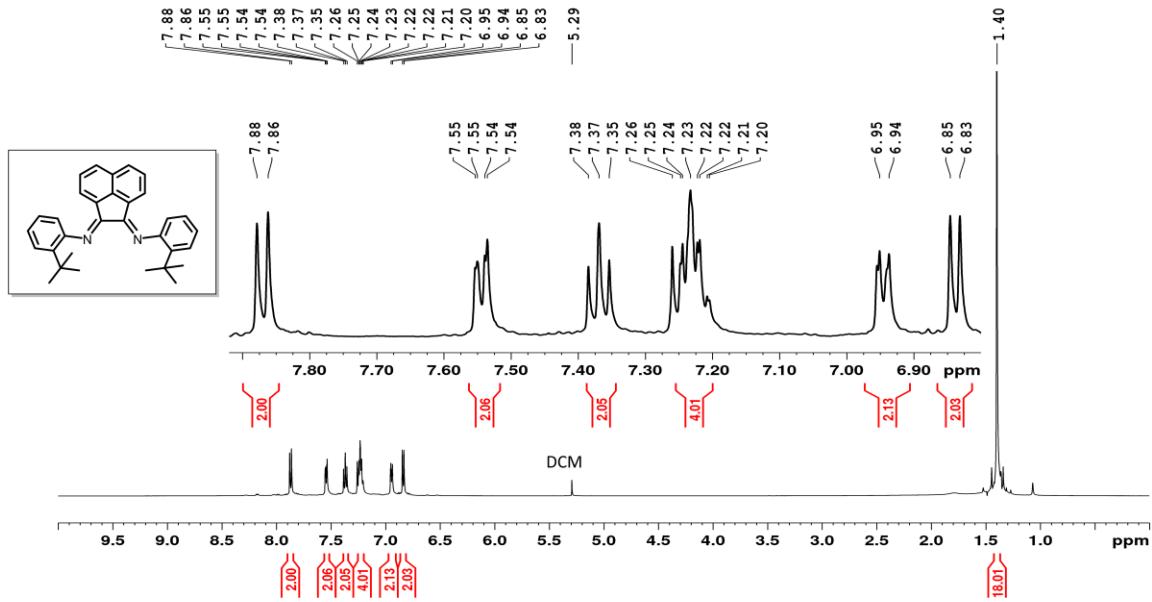
# Ligand Steric Effects of $\alpha$ -Diimine Nickel (II) and Palladium (II) Complexes in the Suzuki–Miyaura Cross-Coupling Reaction

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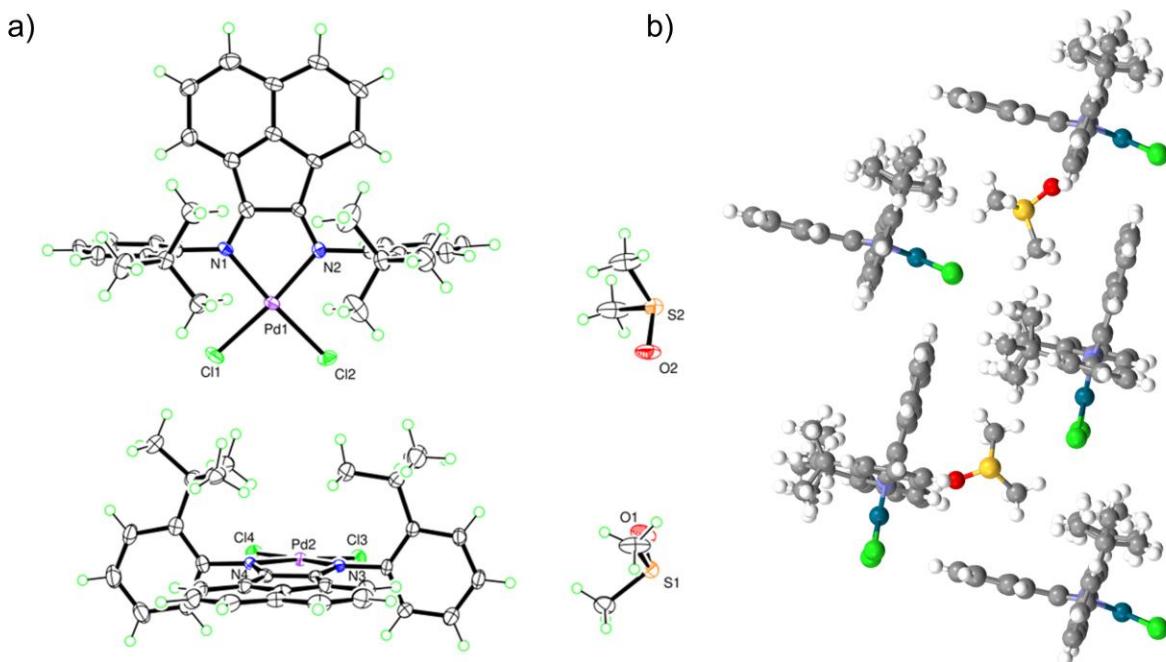
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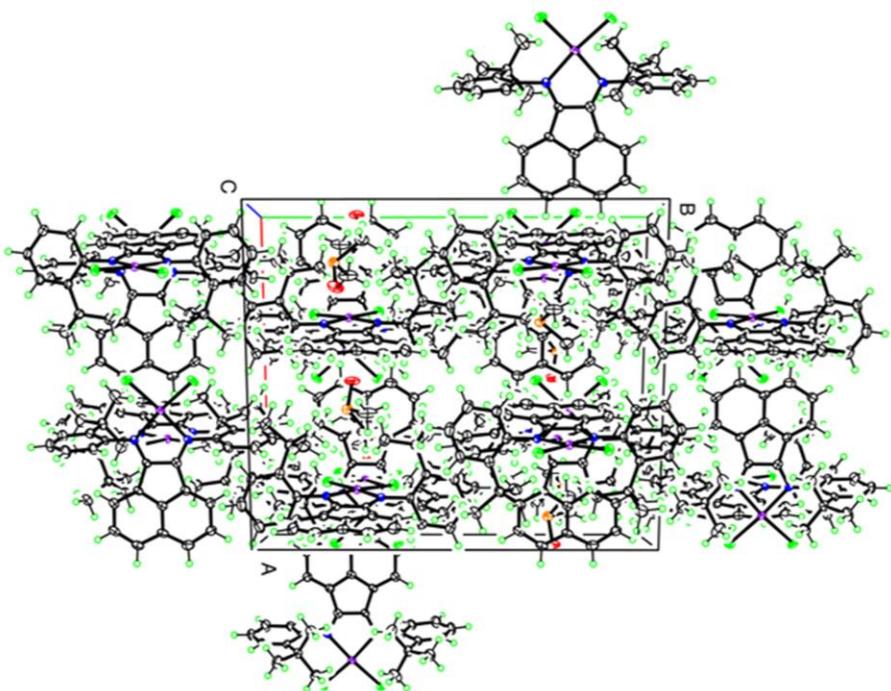
**Figure S1.**  $^1\text{H}$  NMR spectrum of ligand **1a**



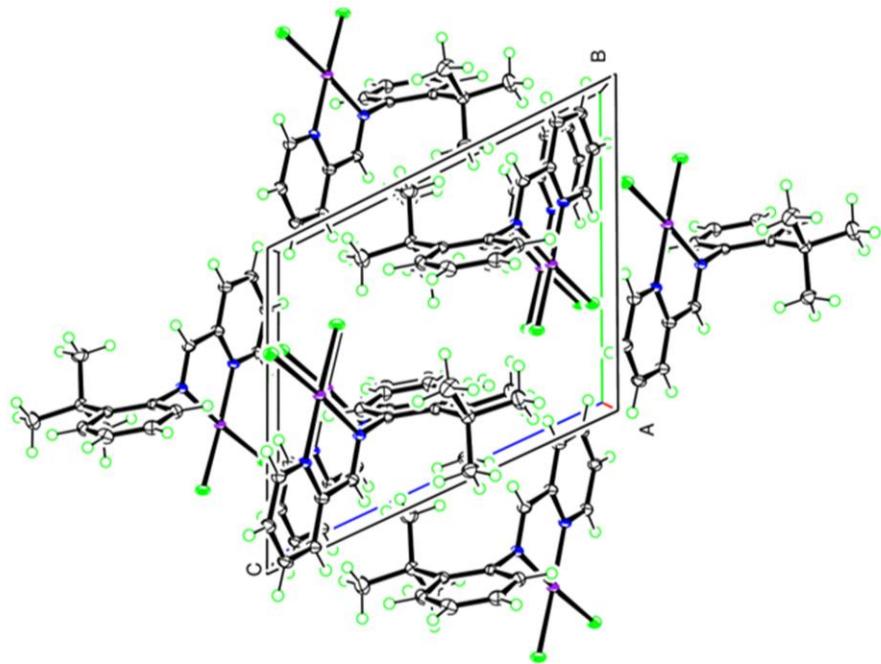
**Figure S2.**  $^1\text{H}$  NMR spectrum of ligand **1b**



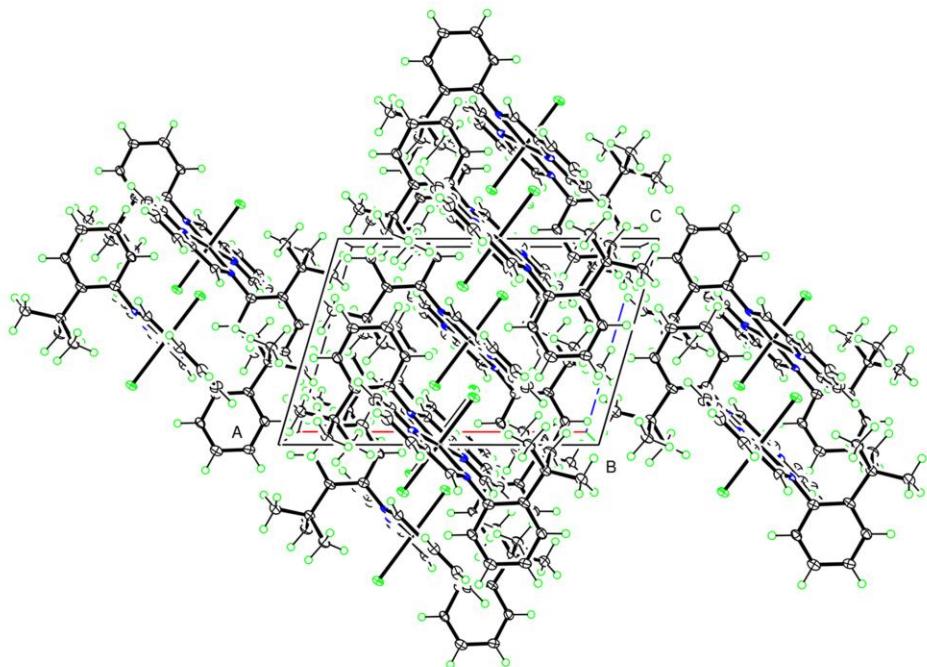
**Figure S3.** (a) Twin ORTEP of complex **Pd B**, (b) Twin packing where DMSO (crystallization solvent) filling structural voids.



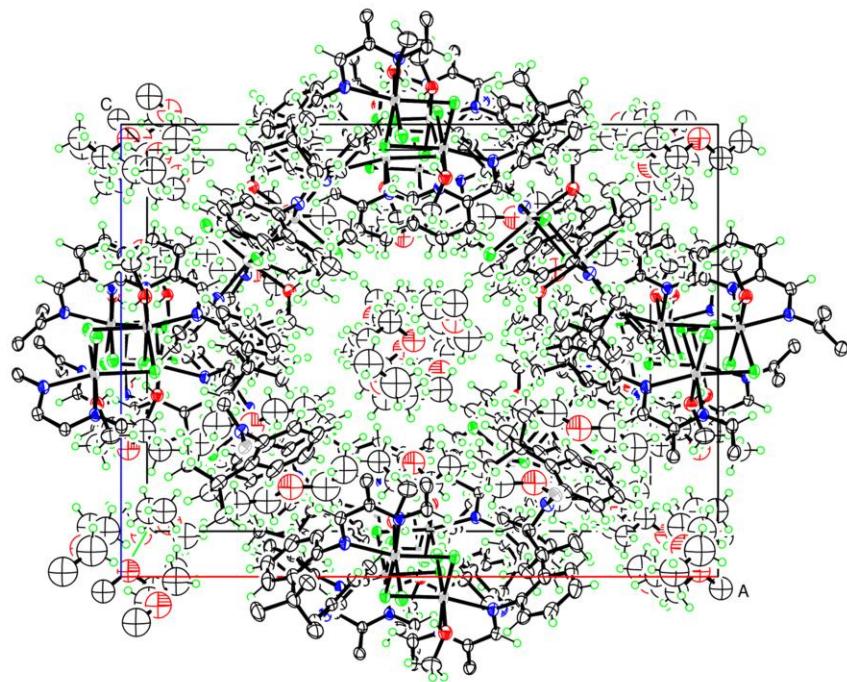
**Figure S4.** Unit cell representation of complex **Pd B**



**Figure S5.** Unit cell representation of complex **Pd A**



**Figure S6.** Unit cell representation of complex **Ni A**



**Figure S7.** Unit cell representation of complex **Ni B**

**Table S1.** Crystal data, data collection and refinement for complex **Ni A** and **Ni B**.

CCDC	2004629	2004628
<b>Complexes</b>	<b>Ni A</b>	<b>Ni B</b>
<b>Crystallized from</b>	Et <sub>2</sub> O/CH <sub>3</sub> OH	Et <sub>2</sub> O/CH <sub>3</sub> OH
<b>Chemical formula</b>	C <sub>32</sub> H <sub>36</sub> Cl <sub>2</sub> N <sub>4</sub> Ni	C <sub>34</sub> H <sub>44</sub> Cl <sub>4</sub> N <sub>4</sub> Ni <sub>2</sub> O <sub>2</sub> ·1.429(C <sub>4</sub> H <sub>10</sub> O)
<b>Formula weight [g mol<sup>-1</sup>]</b>	606.26	905.88
<b>Crystal color, habit</b>	Yellow, Plate	Yellow, Fragment
<b>Crystal size (mm<sup>3</sup>)</b>	0.30 × 0.22 × 0.01	0.36 × 0.24 × 0.12
<b>T (K)</b>	100	100
<b>Crystal system</b>	Monoclinic	Tetragonal
<b>Space group</b>	<i>P</i> 2 <sub>1</sub> /c	<i>I</i> 4 <sub>1</sub> /a
<b>a, b, c (Å)</b>	12.730 (4), 14.003 (4), 8.513 (2)	a = 24.275 (5), c = 18.364 (6)
<b>α, β, γ (°)</b>	β = 106.232 (10)	
<b>V (Å<sup>3</sup>)</b>	1456.9 (7)	10822 (6)
<b>Z</b>	2	8
<b>D<sub>x</sub> (Mg m<sup>-3</sup>)</b>	1.382	1.112
<b>μ (Mo-Kα) (mm<sup>-1</sup>)</b>	0.88	0.93
<b>F (000), θ range (°)</b>	636, 2.2–27.5	3808, 2.5–30.4
<b>No. of measured, independent and observed [I &gt; 2σ(I)] reflections</b>	34420, 34420, 22811	199886, 8273, 6515
<b>R<sub>int</sub></b>	0.123	0.057
<b>Δρ<sub>max</sub>, Δρ<sub>min</sub> (e Å<sup>-3</sup>)</b>	1.65, -1.48	0.79, -0.81
<b>No. of parameters</b>	183	250
<b>Refinement</b>	0.103, 0.261, R[F <sup>2</sup> > 2σ(F <sup>2</sup> )], wR(F <sup>2</sup> ), S	0.053, 0.175, 1.27

**Table S2.** Crystal data, data collection and refinement for complex **Pd A** and **Pd B**.

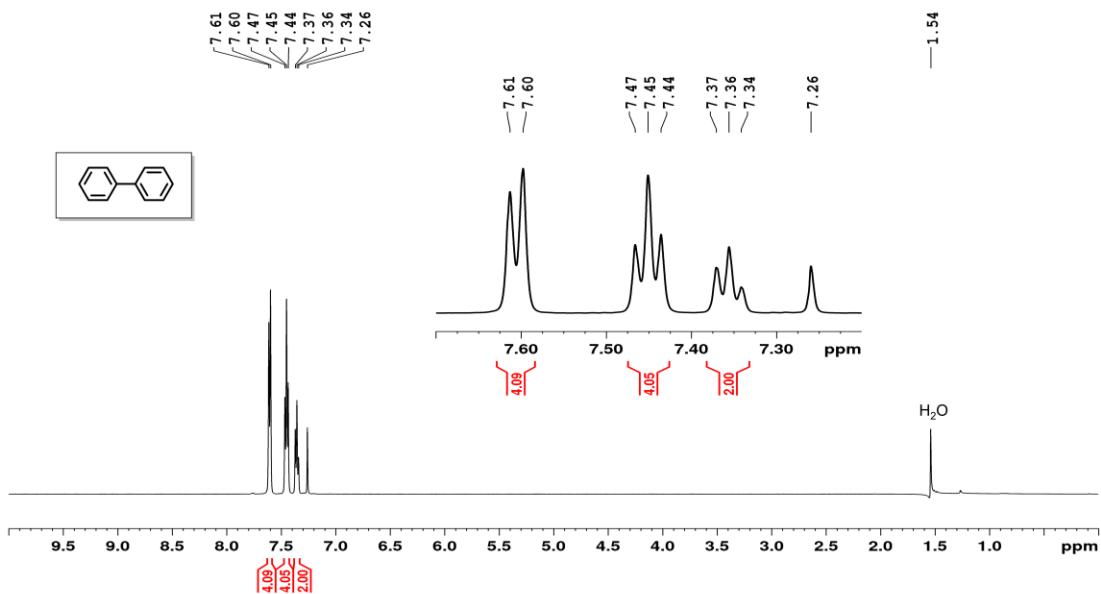
CCDC	2004630	2004631
Complexes	Pd A	Pd B
Crystallized from	DMSO	DMSO
Chemical formula	C <sub>16</sub> H <sub>18</sub> Cl <sub>2</sub> N <sub>2</sub> Pd	C <sub>32</sub> H <sub>32</sub> Cl <sub>2</sub> N <sub>2</sub> Pd·C <sub>2</sub> H <sub>6</sub> OS
Formula weight [g mol <sup>-1</sup> ]	415.62	700.02
Crystal color, habit	Yellow, Tablet	Orange, Fragment
Crystal size (mm <sup>3</sup> )	0.34 × 0.16 × 0.04	0.20 × 0.15 × 0.07
T (K)	100	100
Crystal system	Triclinic	Monoclinic
Space group	$P\bar{1}$	$P2_1/n$
<b>a, b, c (Å)</b>	8.623 (3), 9.493 (3), 11.552 (4)	19.383 (4), 20.236 (4), 19.392 (4)
<b>α, β, γ (°)</b>	112.209 (10), 107.067 (9), 96.813 (10)	β = 119.84 (1)
<b>V (Å<sup>3</sup>)</b>	808.2 (4)	6598 (3)
<b>Z</b>	2	8
<b>D<sub>x</sub> (Mg m<sup>-3</sup>)</b>	1.708	1.409
<b>μ (Mo-Kα) (mm<sup>-1</sup>)</b>	1.47	0.82
<b>F (000), θ range (°)</b>	416, 2.4–30.5	2880, 2.3–26.9
No. of measured, independent and observed [ <i>I</i> > 2σ( <i>I</i> )] reflections	25531, 4950, 4558	110929, 15135, 13225
<b>R<sub>int</sub></b>	0.034	0.069
<b>Δρ<sub>max</sub>, Δρ<sub>min</sub> (e Å<sup>-3</sup>)</b>	0.81, -0.99	1.53, -1.02
No. of parameters	194	756
Refinement R[F <sup>2</sup> > 2σ(F <sup>2</sup> )], wR(F <sup>2</sup> ), S	0.022, 0.054, 1.12	0.040, 0.095, 1.07

**Table S3.** Selected bond lengths and angles for complexes **Ni A** and **Ni B**

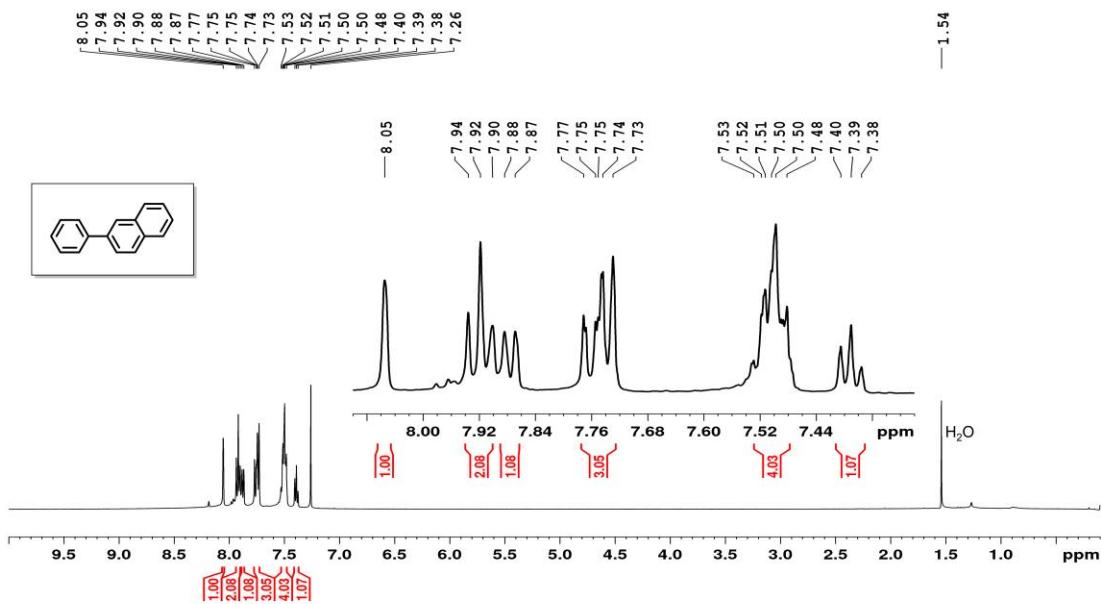
Complex	Selected bond distances ( $\text{\AA}$ )	Selected bond angles [°]
<b>Ni A</b>	Ni1—N1 <sup>i</sup> 2.099 (6), Ni1—N1 2.099 (6), Ni1—N2 2.188 (6), Ni1—N2 <sup>i</sup> 2.188 (6), Ni1—Cl1 <sup>i</sup> 2.373 (2), Ni1—Cl1 2.373 (2)	N1 <sup>i</sup> —Ni1—N1 180.0, N1 <sup>i</sup> —Ni1—N2 101.6 (2), N1—Ni1—N2 78.4 (2), N1 <sup>i</sup> —Ni1—N2 <sup>i</sup> 78.4 (2), N1—Ni1—N2 <sup>i</sup> 101.6 (2), N2—Ni1—N2 <sup>i</sup> 180.0 (3), N1 <sup>i</sup> —Ni1—Cl1 <sup>i</sup> 87.47 (18), N1—Ni1—Cl1 <sup>i</sup> 92.53 (18), N2—Ni1—Cl1 <sup>i</sup> 87.14 (17), N2 <sup>i</sup> —Ni1—Cl1 <sup>i</sup> 92.86 (17), N1 <sup>i</sup> —Ni1—Cl1 92.53 (18), N1—Ni1—Cl1 87.47 (18), N2—Ni1—Cl1 92.86 (17), N2 <sup>i</sup> —Ni1—Cl1 87.14 (17), Cl1 <sup>i</sup> —Ni1—Cl1 180.0
<b>Ni B</b>	Ni1—N1 2.060 (2), Ni1—N2 2.111 (2), Ni1—Cl1 2.3765 (8), Ni1—Cl2 2.3850 (9), Ni1—Cl1 <sup>i</sup> 2.4344 (8), Cl1—Ni1 <sup>i</sup> 2.4343 (8)	N1—Ni1—N2 79.16 (8), N1—Ni1—Cl1 174.14 (6), N2—Ni1—Cl1 95.05 (6), N1—Ni1—Cl2 90.46 (7), N2—Ni1—Cl2 100.09 (7), Cl1—Ni1—Cl2 91.40 (3), N1—Ni1—Cl1 <sup>i</sup> 94.46 (6), N2—Ni1—Cl1 <sup>i</sup> 167.34 (7), Cl1—Ni1—Cl1 <sup>i</sup> 91.06 (2), Cl2—Ni1—Cl1 <sup>i</sup> 90.81 (2), Ni1—Cl1—Ni1 <sup>i</sup> 88.94 (2)

**Table S4.** Selected bond lengths and angles for complexes **Pd A** and **Pd B**.

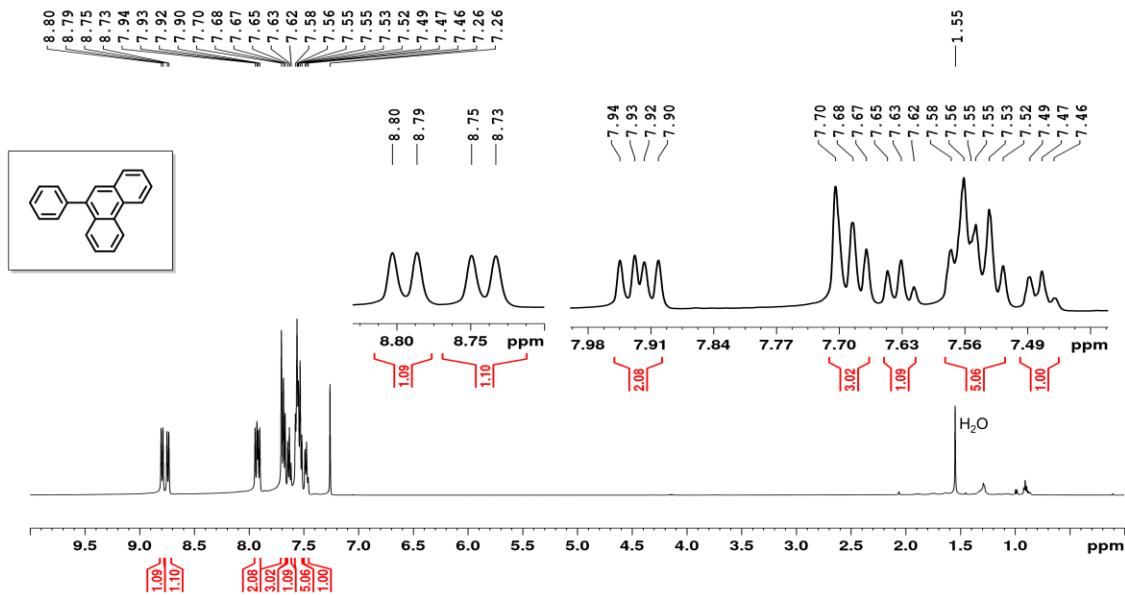
Complex	Selected bond distances ( $\text{\AA}$ ): Pd1—N1, Pd1—N2, Pd1—Cl2, Pd1—Cl1	Selected bond angles [°]: N1—Pd1—N2, N1—Pd1—Cl2, N2—Pd1—Cl2, N1—Pd1—Cl1, N2—Pd1—Cl1, Cl2—Pd1—Cl1
<b>Pd A</b>	2.0383 (15), 2.0392 (15), 2.2694 (7), 2.2929 (8)	80.72 (6), 173.55 (4), 93.50 (5), 95.22 (5), 175.92 (4), 90.54 (3)
<b>Pd B</b>	2.062 (3), 2.054 (3), 2.2830 (11), 2.2769 (11)	81.32 (13), 175.42 (9), 94.42 (10), 92.92 (9), 173.44 (10), 91.24 (4)



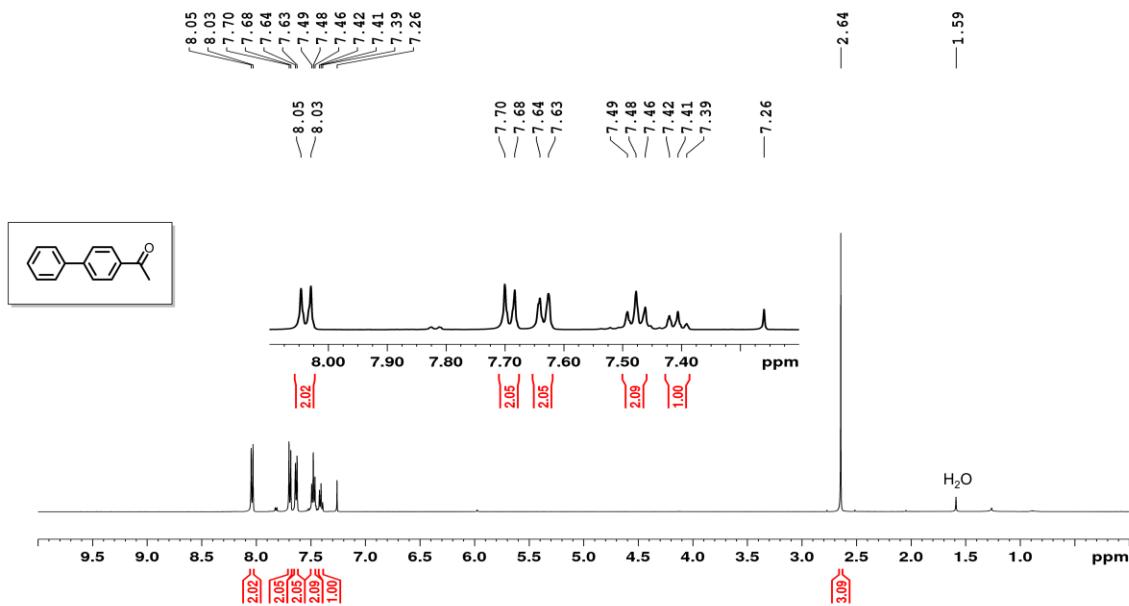
**Figure S8.** <sup>1</sup>H NMR spectrum of 1A1



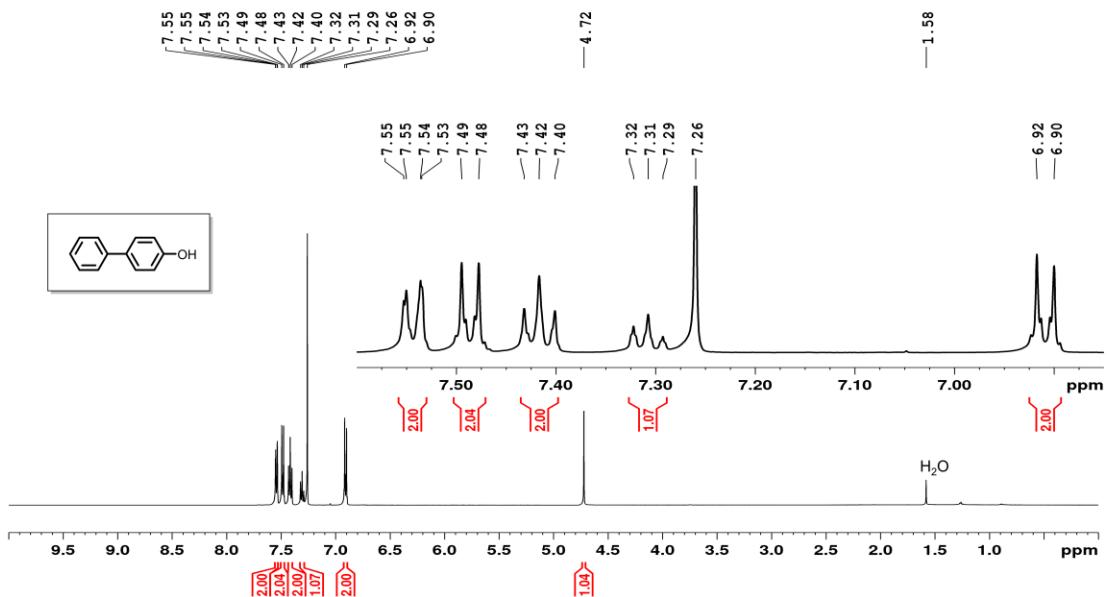
**Figure S9.** <sup>1</sup>H NMR spectrum of 1A2 & 2A1



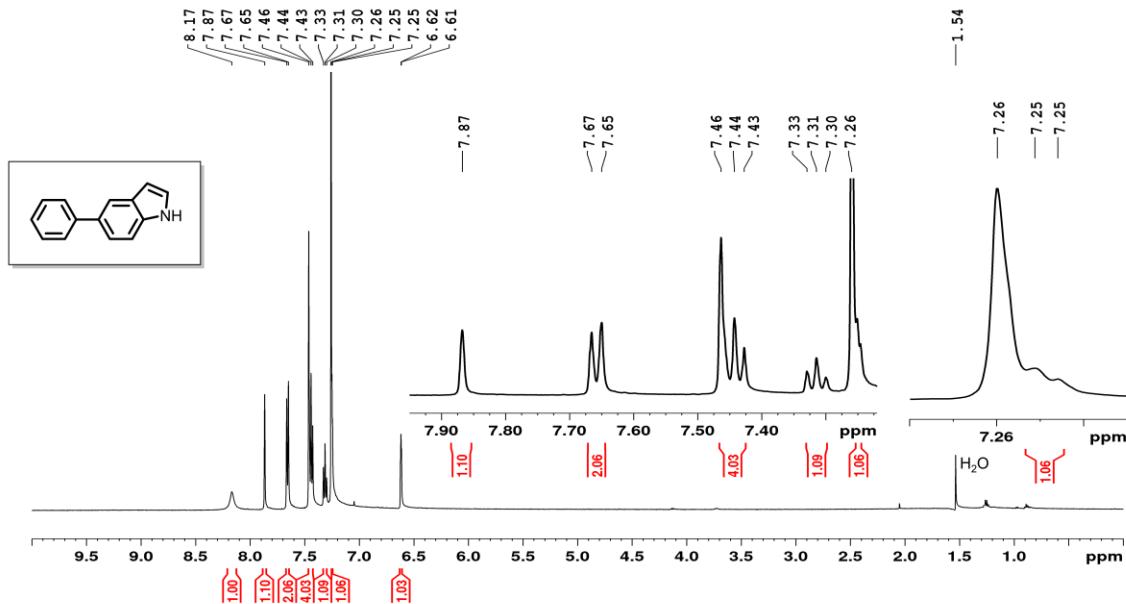
**Figure S10.** <sup>1</sup>H NMR spectrum of 1A3 & 3A1



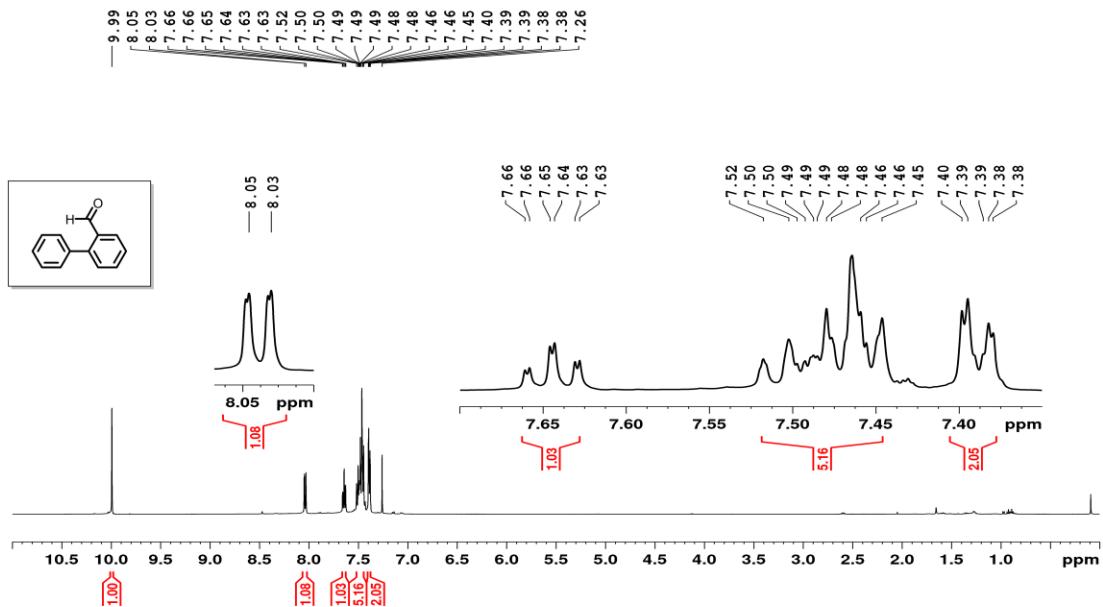
**Figure S11.** <sup>1</sup>H NMR spectrum of 1A4



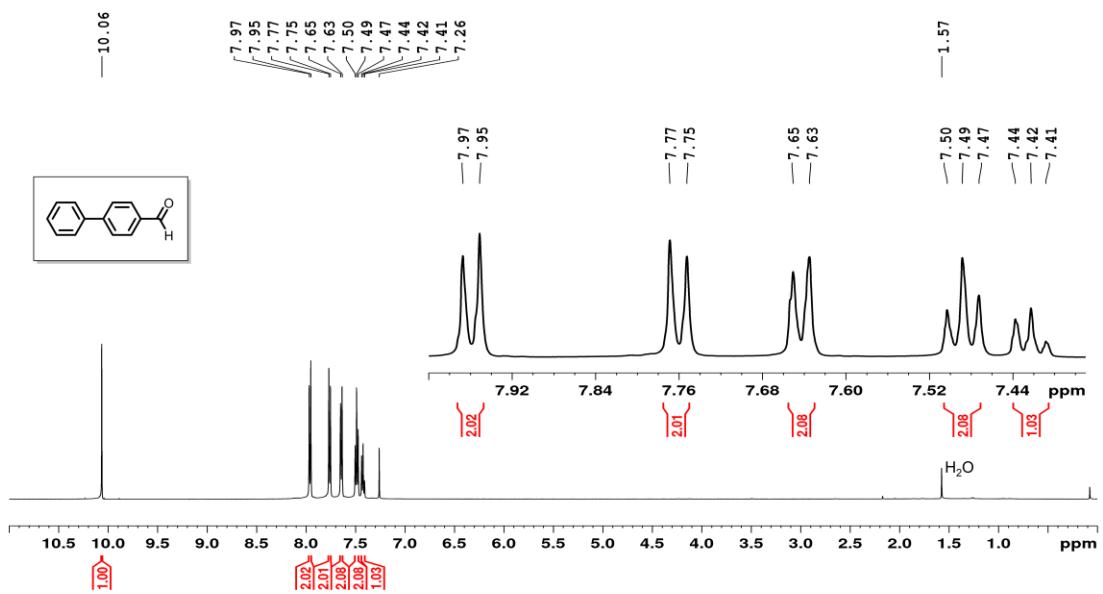
**Figure S12.** <sup>1</sup>H NMR spectrum of 1A5



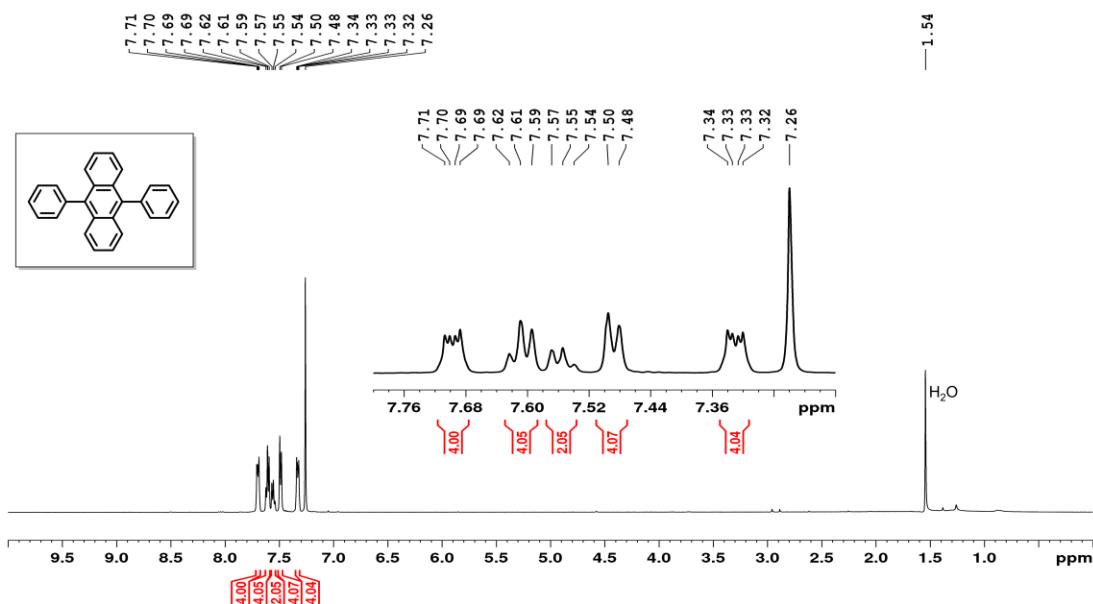
**Figure S13.** <sup>1</sup>H NMR spectrum of 1A6



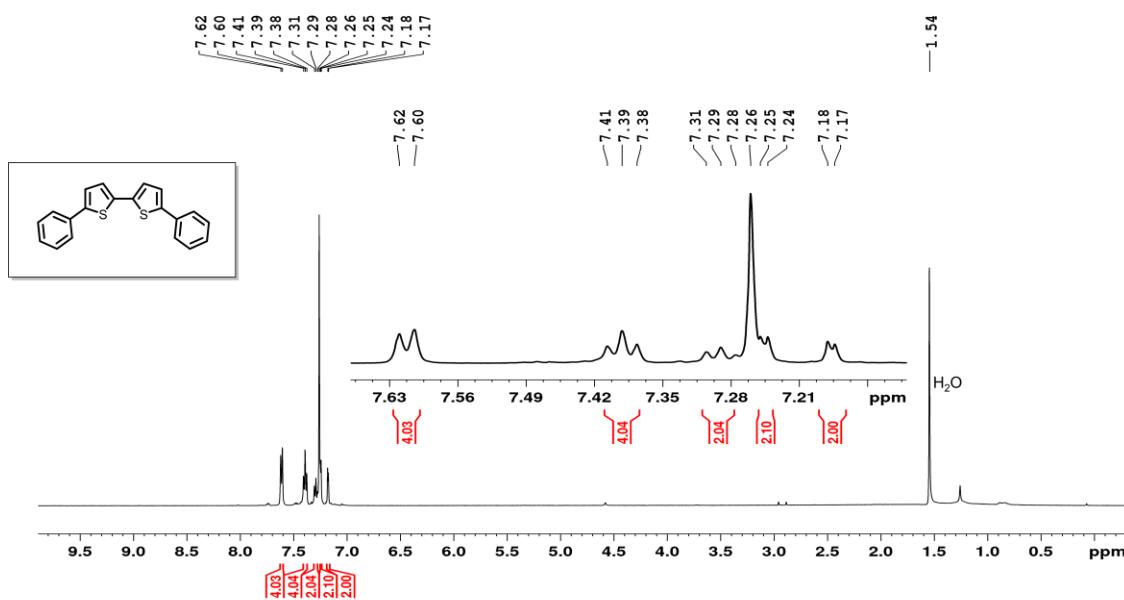
**Figure S14.**  $^1\text{H}$  NMR spectrum of **1A7**



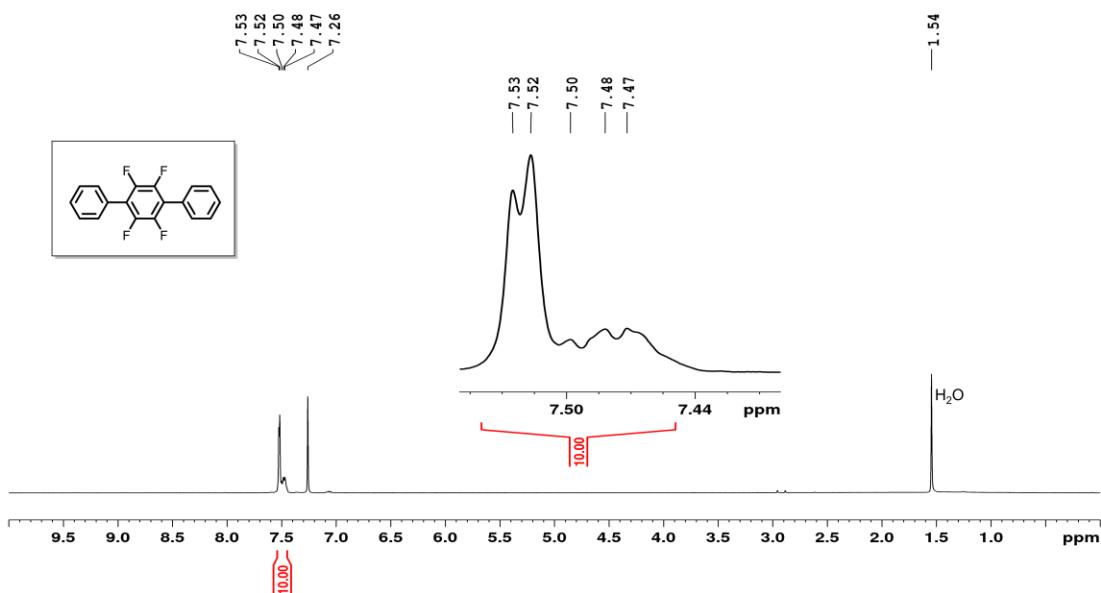
**Figure S15.**  $^1\text{H}$  NMR spectrum of **1A8**



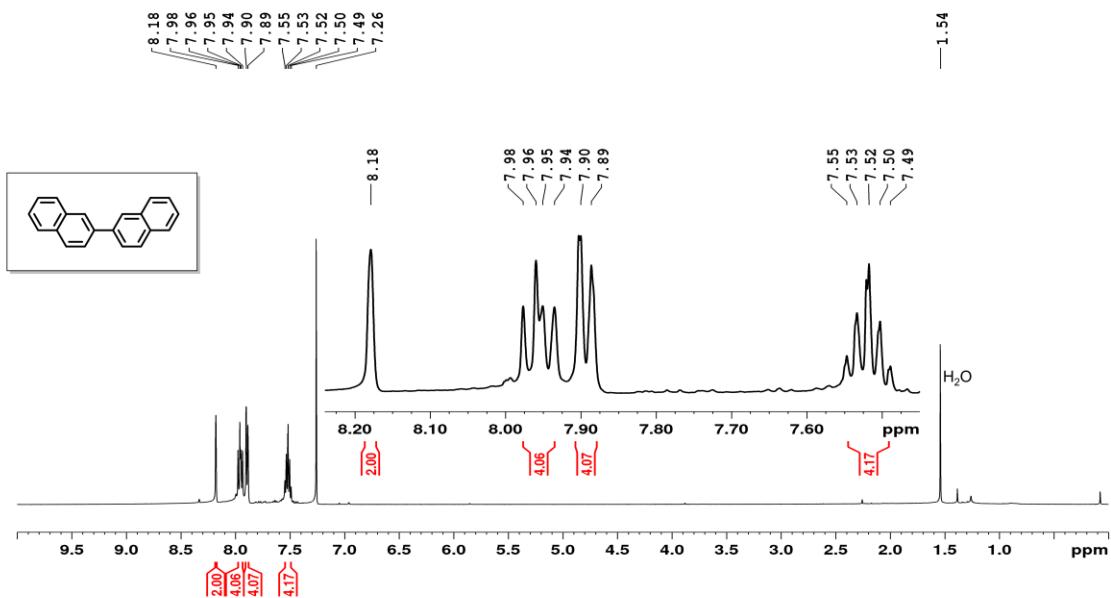
**Figure S16.**  $^1\text{H}$  NMR spectrum of **1A9**



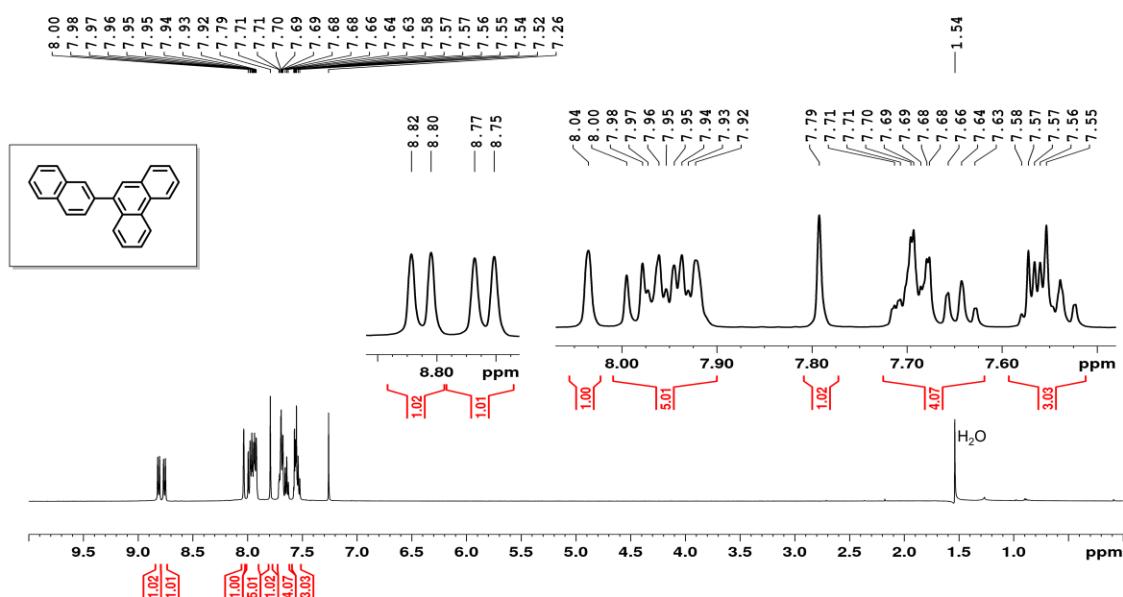
**Figure S17.**  $^1\text{H}$  NMR spectrum of **1A10**



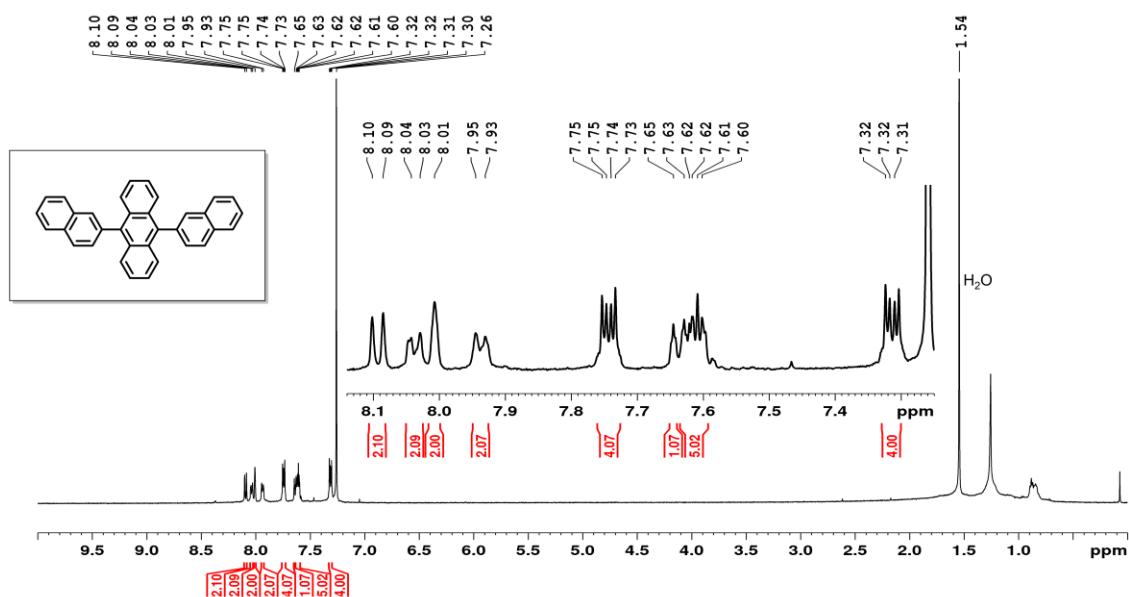
**Figure S18.** <sup>1</sup>H NMR spectrum of 1A11



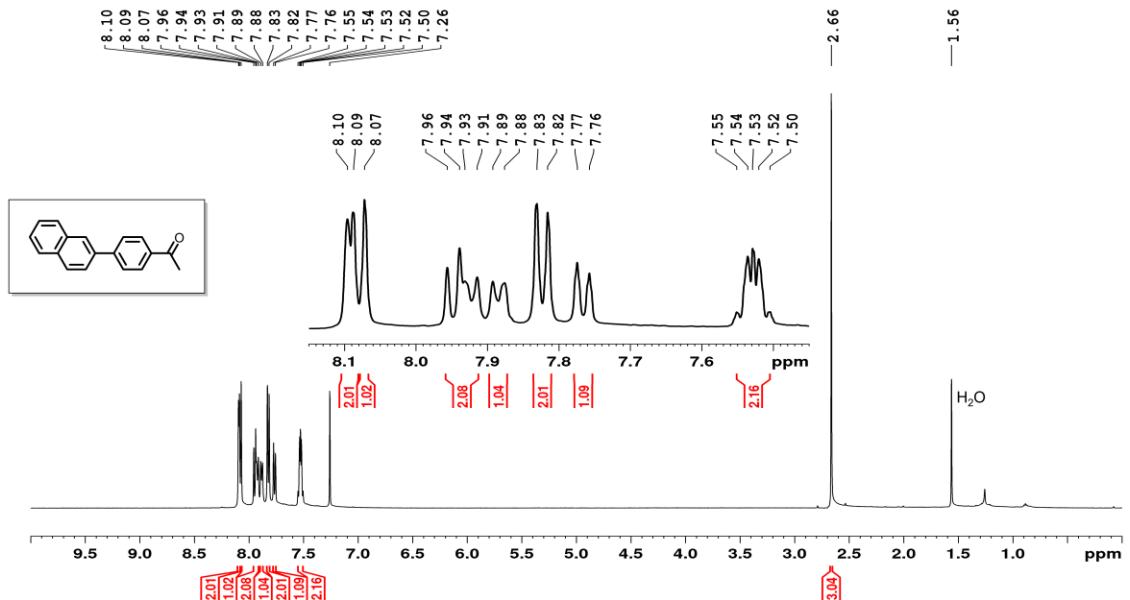
**Figure S19.** <sup>1</sup>H NMR spectrum of 2A2



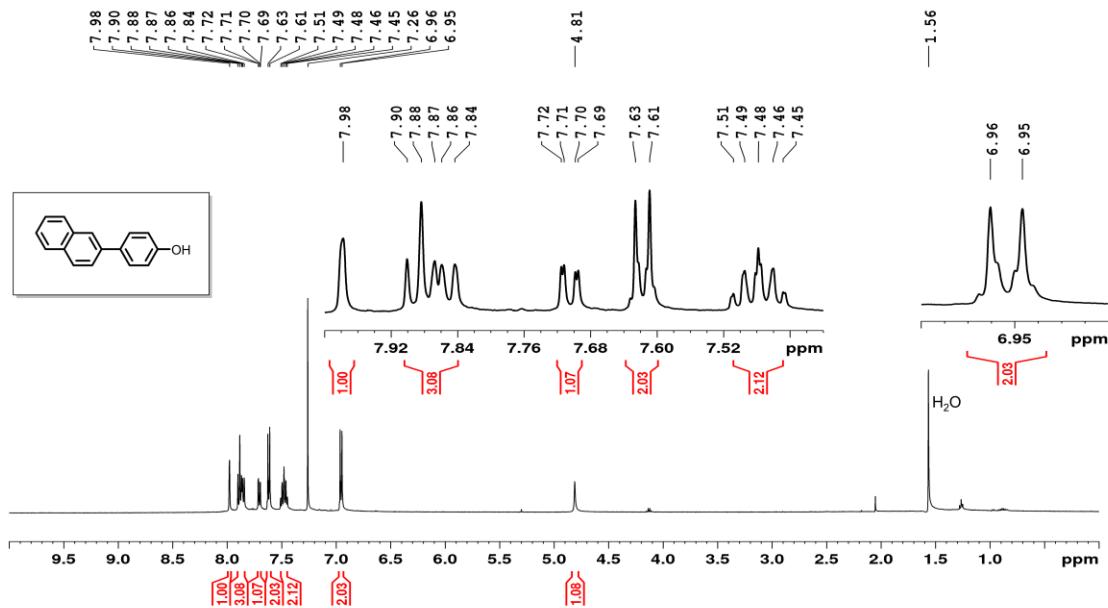
**Figure S20.** <sup>1</sup>H NMR spectrum of 2A3 & 3A2



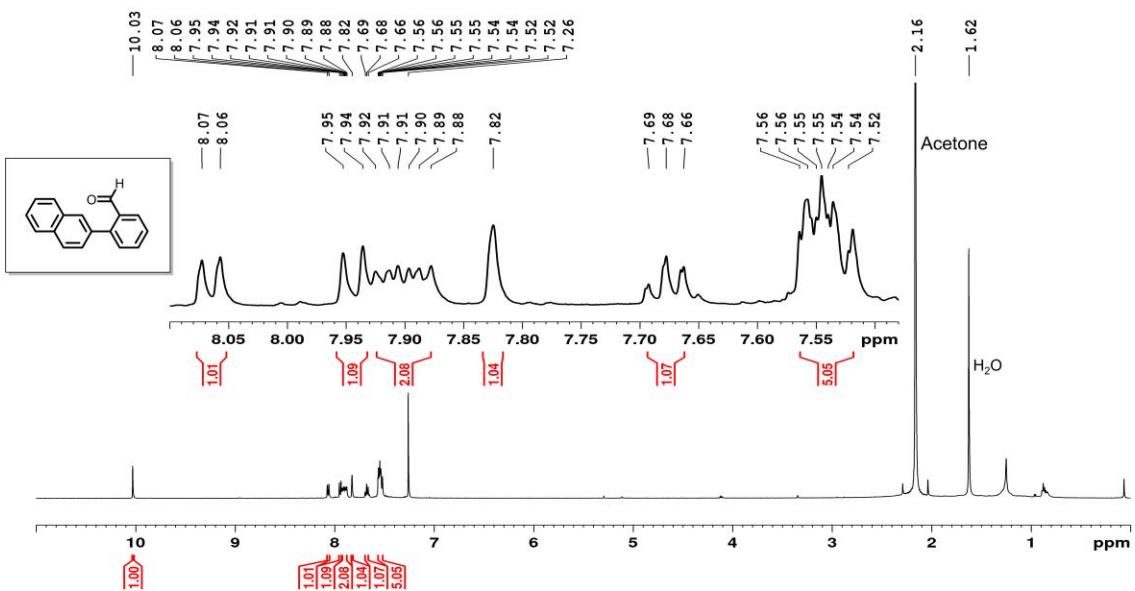
**Figure S21.** <sup>1</sup>H NMR spectrum of 2A4



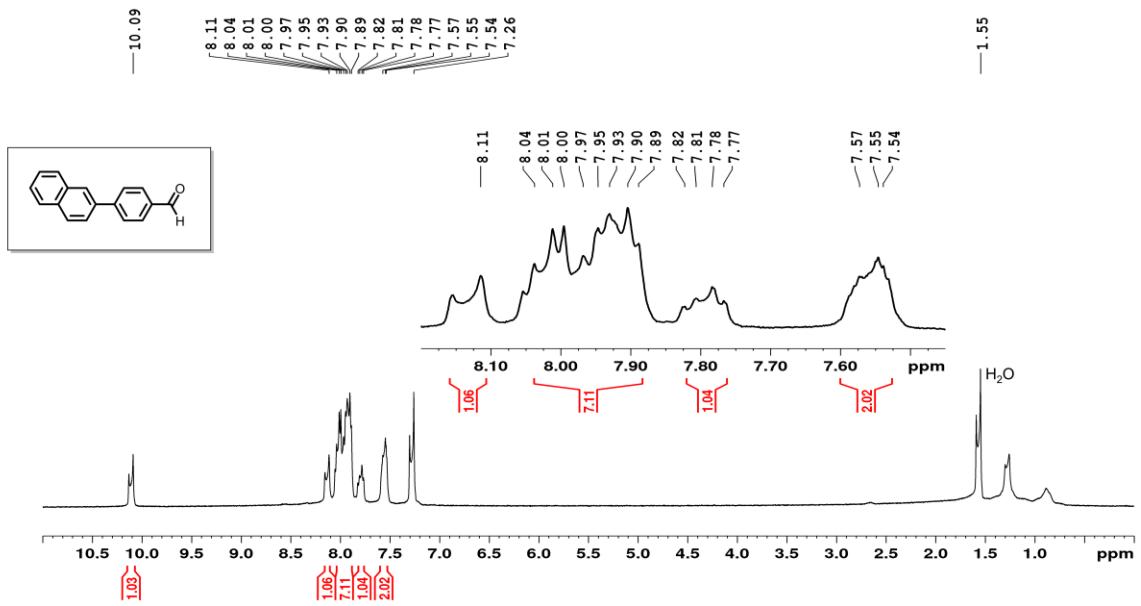
**Figure S22.** <sup>1</sup>H NMR spectrum of 2A5



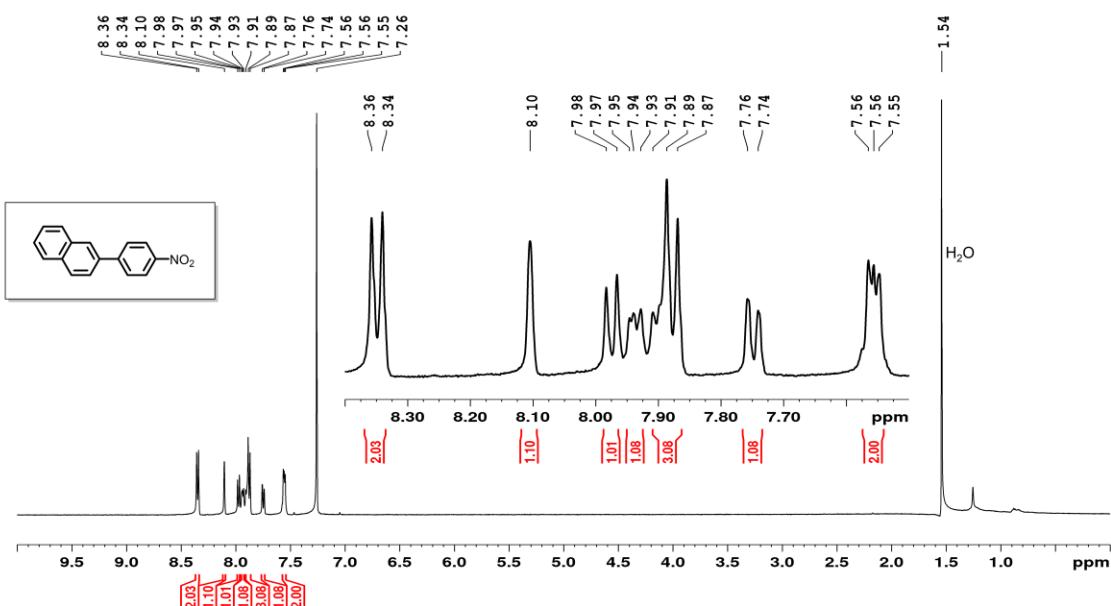
**Figure S23.** <sup>1</sup>H NMR spectrum of 2A6



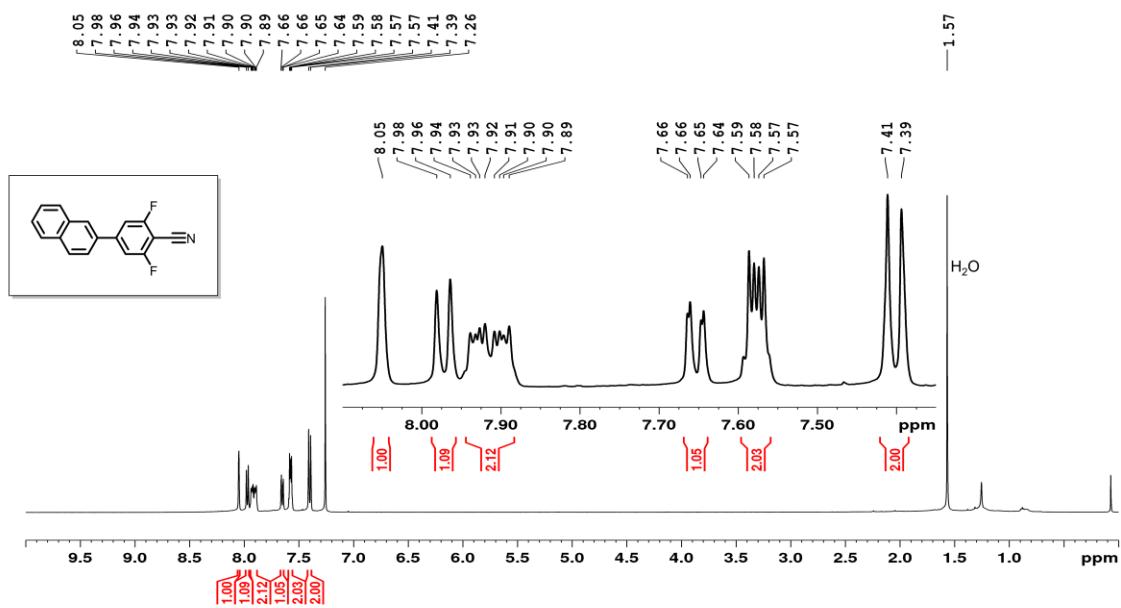
**Figure S24.** <sup>1</sup>H NMR spectrum of 2A7



**Figure S25.** <sup>1</sup>H NMR spectrum of 2A8

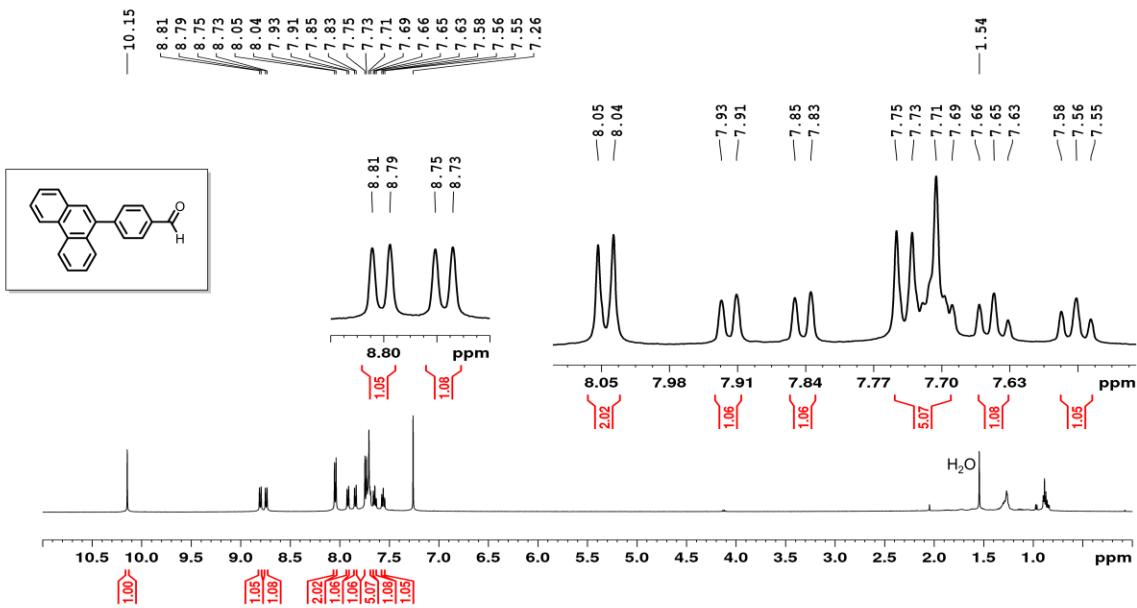


**Figure S26.** <sup>1</sup>H NMR spectrum of 2A9

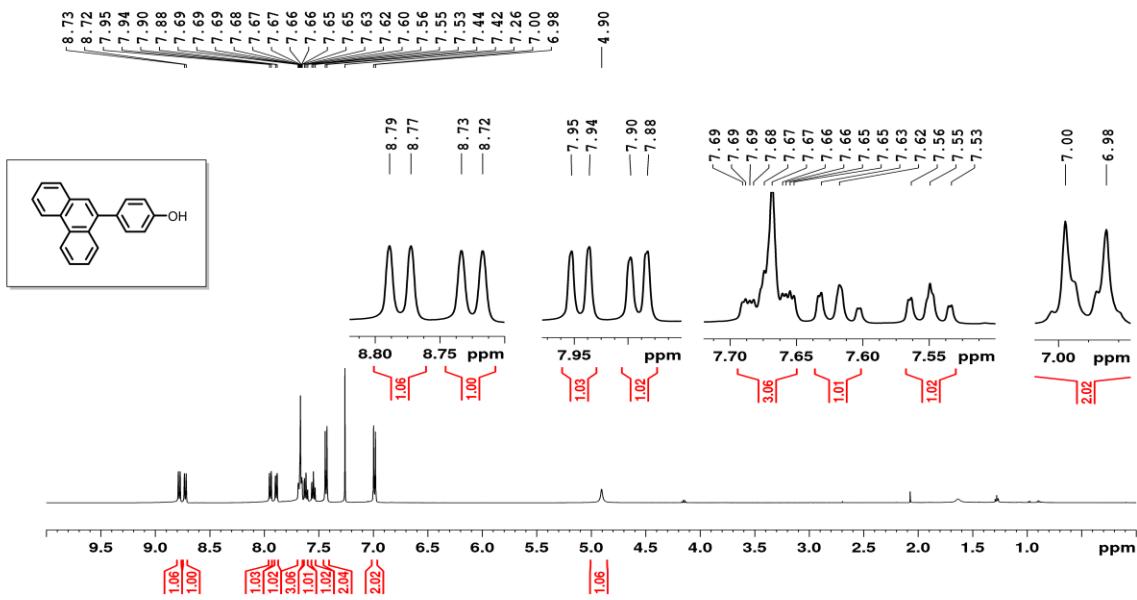


**Figure S27.** <sup>1</sup>H NMR spectrum of 2A10

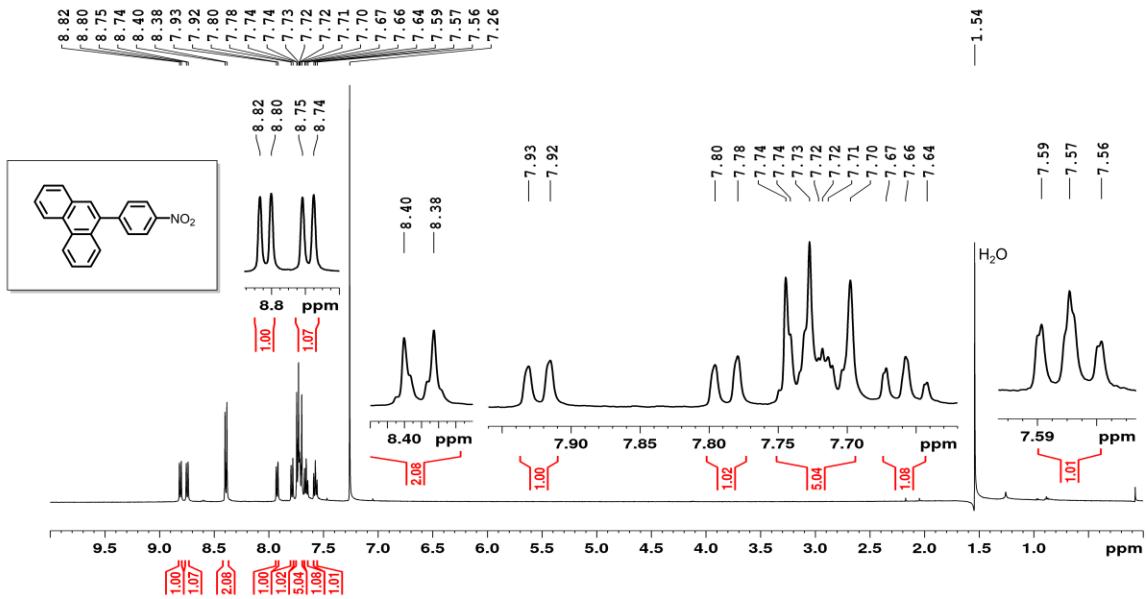




**Figure S30.**  $^1\text{H}$  NMR spectrum of **3A5**



**Figure S31.**  $^1\text{H}$  NMR spectrum of **3A6**



**Figure S32.** <sup>1</sup>H NMR spectrum of 3A7