Electronic Supplementary Information

Palladium complexes with simple iminopyridines as catalysts for polyketone synthesis

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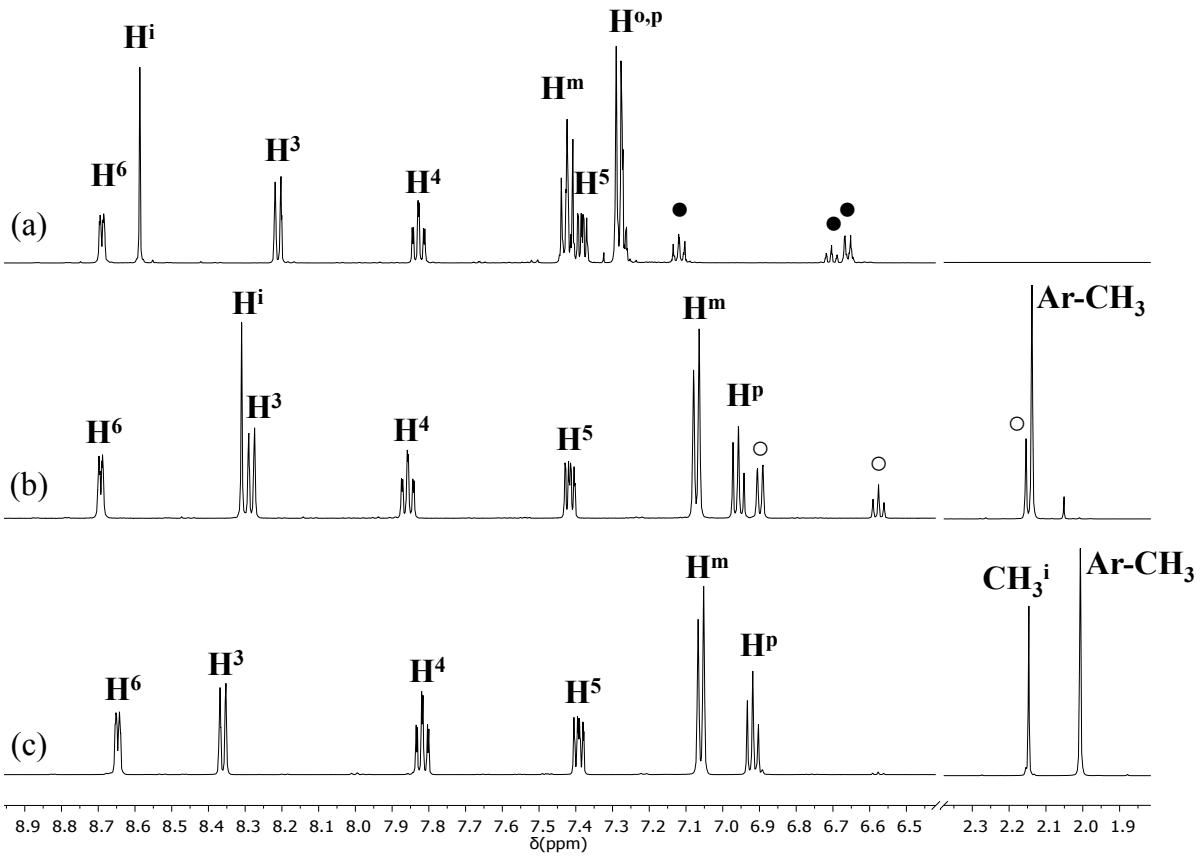

Figure S1. ^{1}H NMR spectra in CD_2Cl_2 at 298 K of (a) **1**; (b) **2**; (c) **4**. Aliphatic and aromatic regions are not on scale.

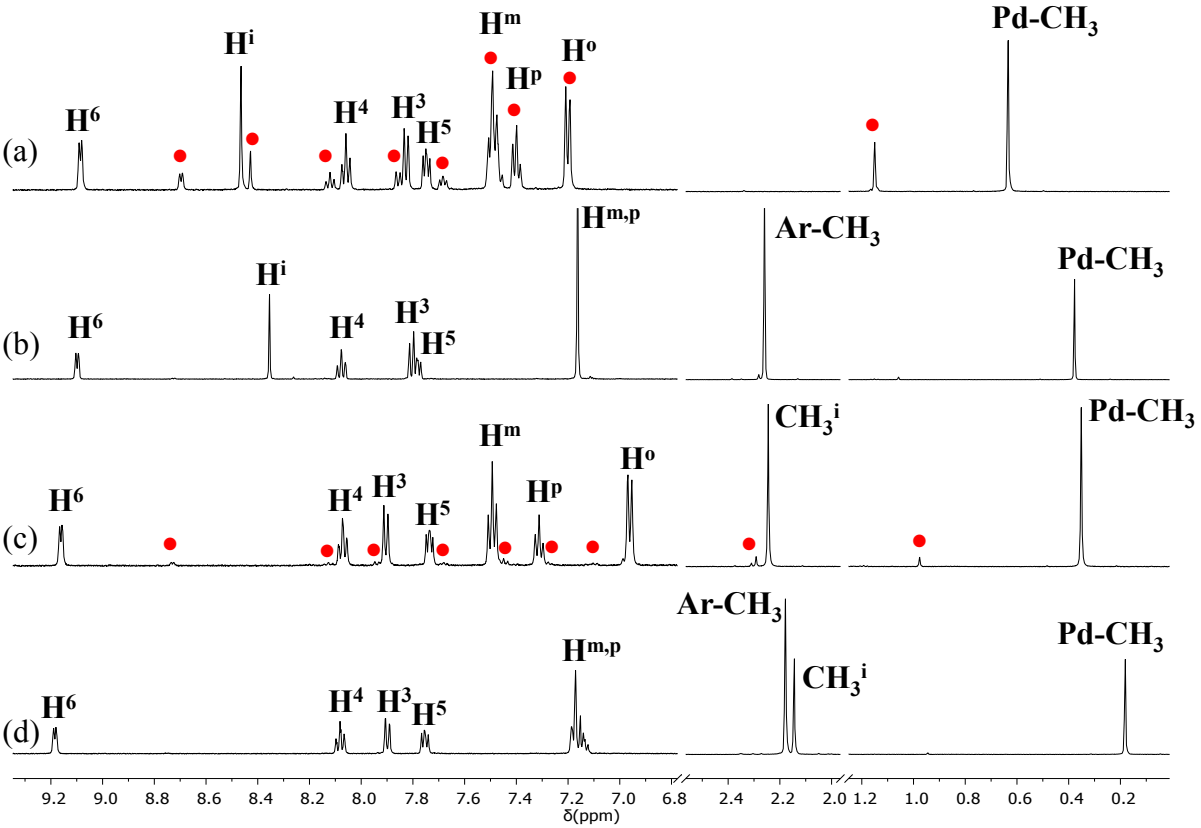

Figure S2. ^{1}H NMR spectra in CD_2Cl_2 at 298 K of (a) **1a**; (b) **2a**; (c) **3a**; (d) **4a**: *cis* (black) and *trans* (red) isomers. Aliphatic and aromatic regions are not on scale.

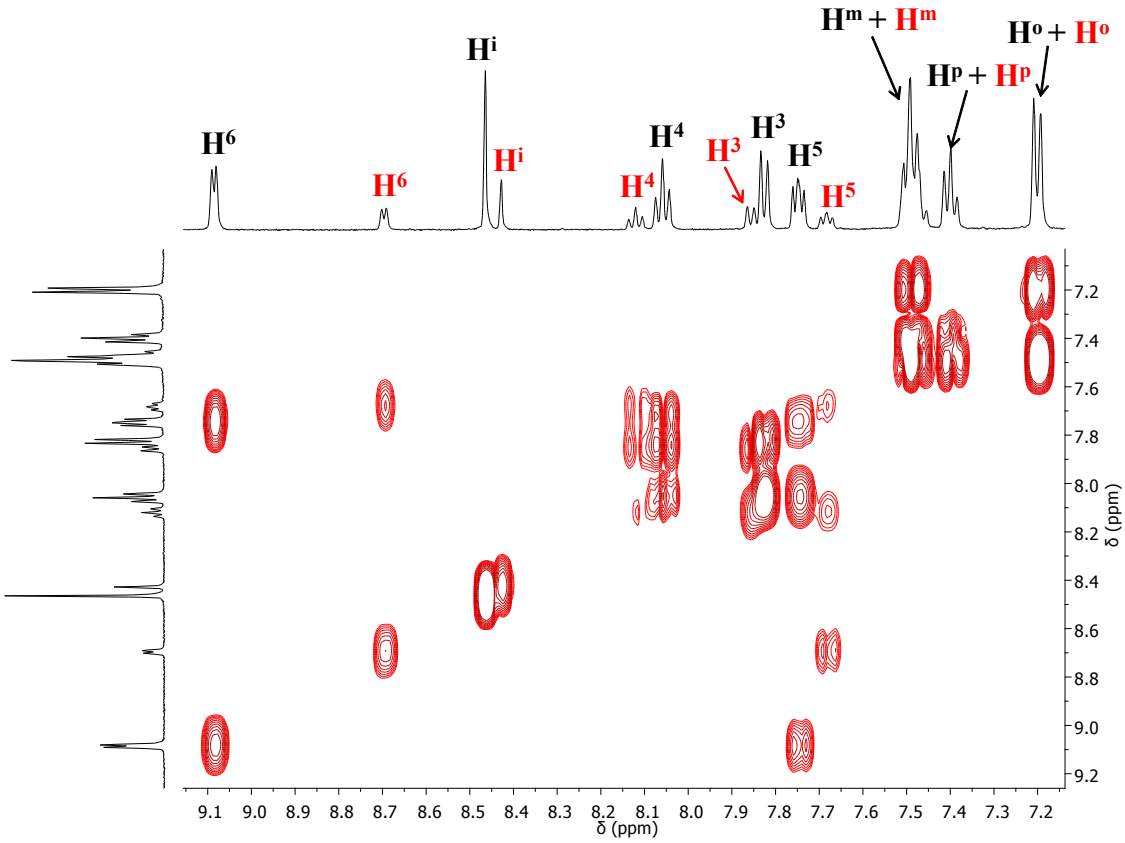

Figure S3. {^{1}H,^{1}H}-COSY spectrum in CD_2Cl_2 at 298 K of **1a**, *cis* (black) and *trans* (red) isomers. Aromatic region.

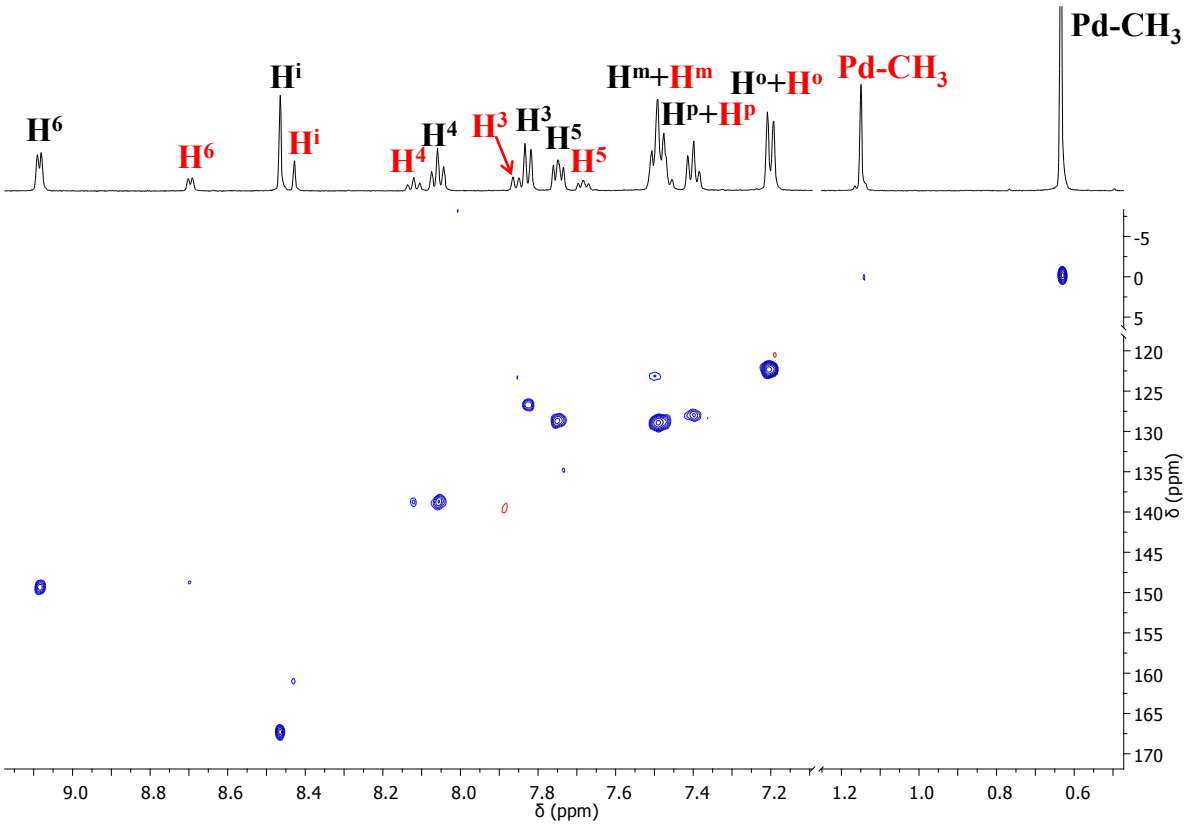

Figure S4. {^{1}H,^{13}C}-HSQC spectrum in CD_2Cl_2 at 298 K of **1a**, *cis* (black) and *trans* (red) isomers.

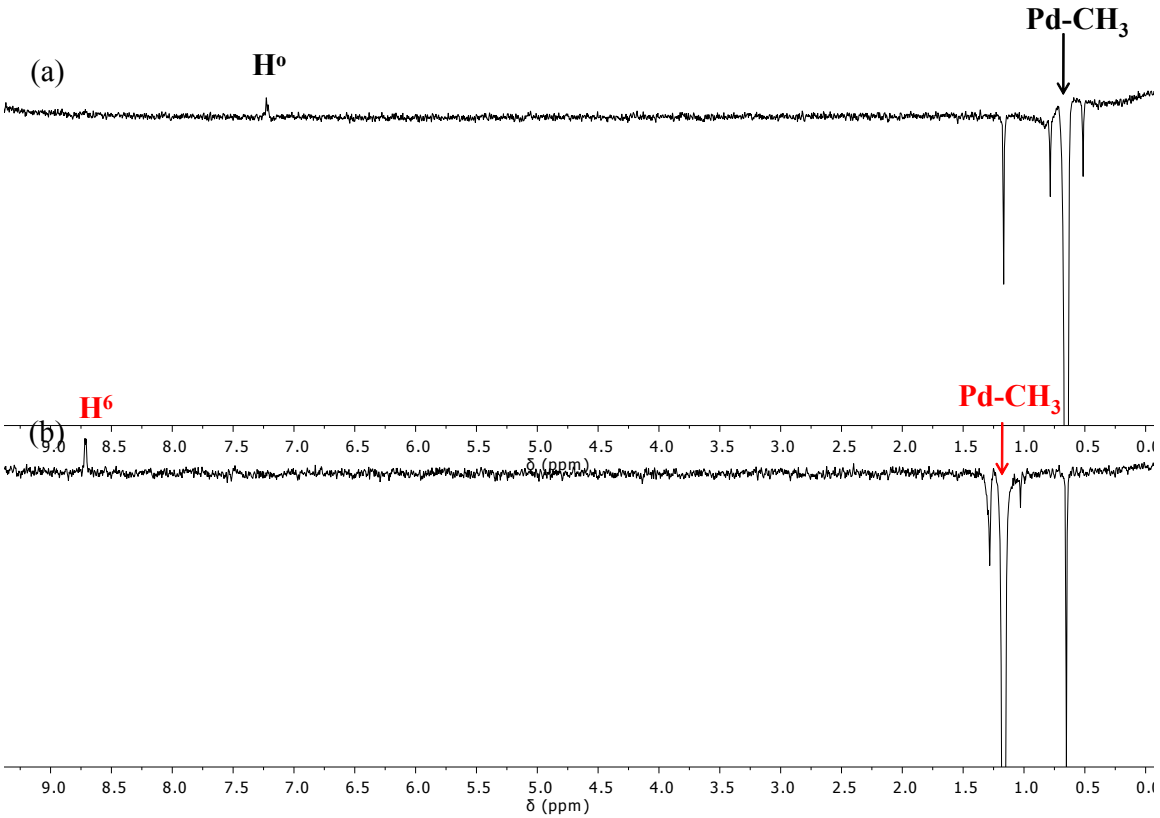

Figure S5. NOE spectra in CD_2Cl_2 at 298 K of **1a** obtained by irradiating the Pd-CH_3 signal of (a) *cis* and (b) *trans* isomer.

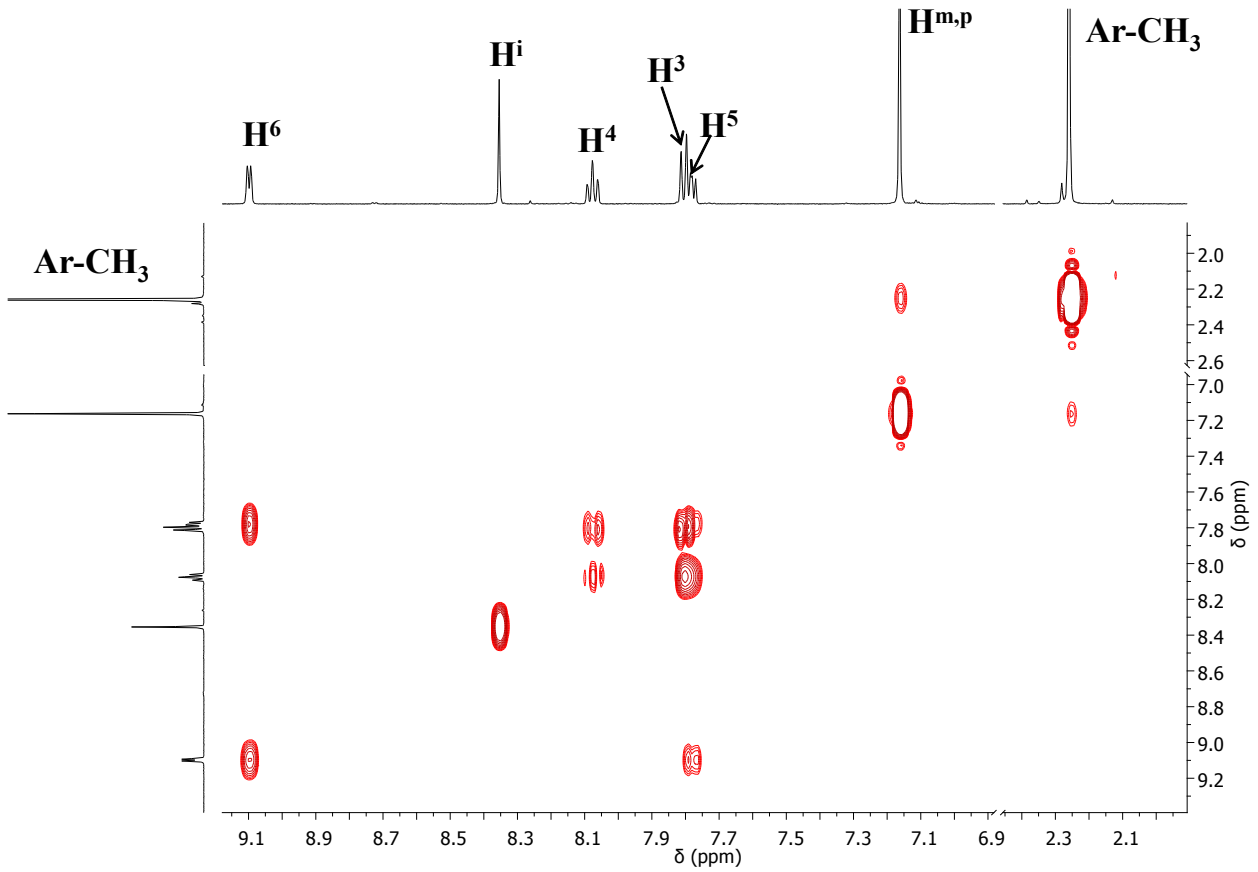

Figure S6. {^{1}H,^{1}H}-COSY spectrum in CD_2Cl_2 at 298 K of **2a**.

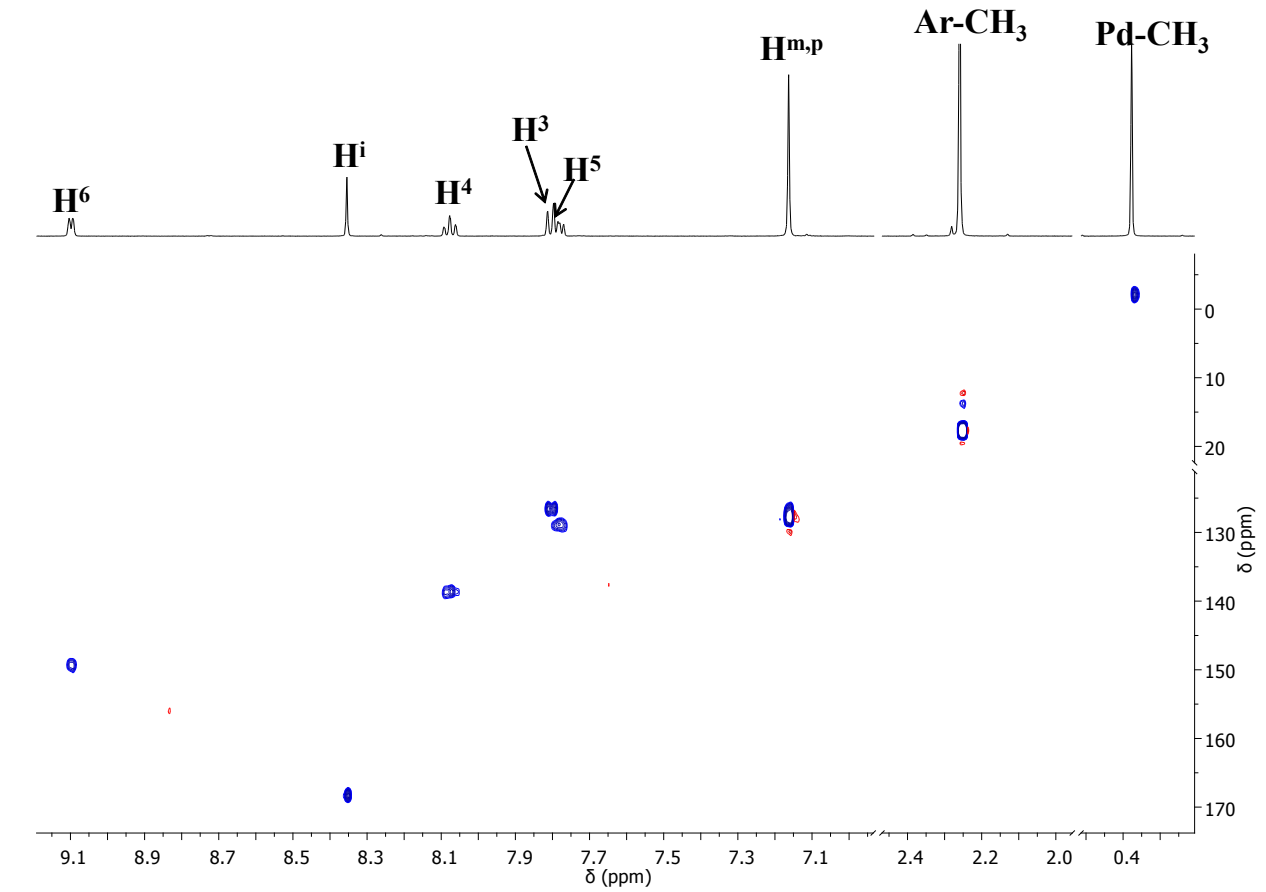

Figure S7. {^{1}H,^{13}C}-HSQC spectrum in CD_2Cl_2 at 298 K of **2a**.

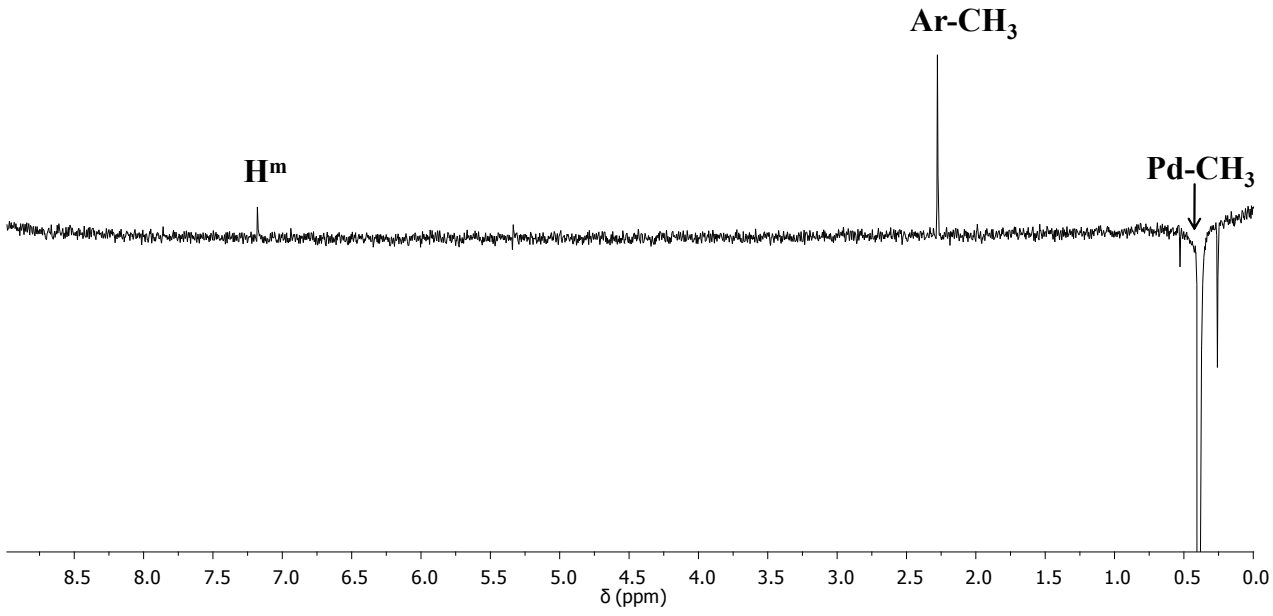

Figure S8. NOE spectra in CD_2Cl_2 at 298 K of **2a** obtained by irradiating the Pd-CH_3 signal.

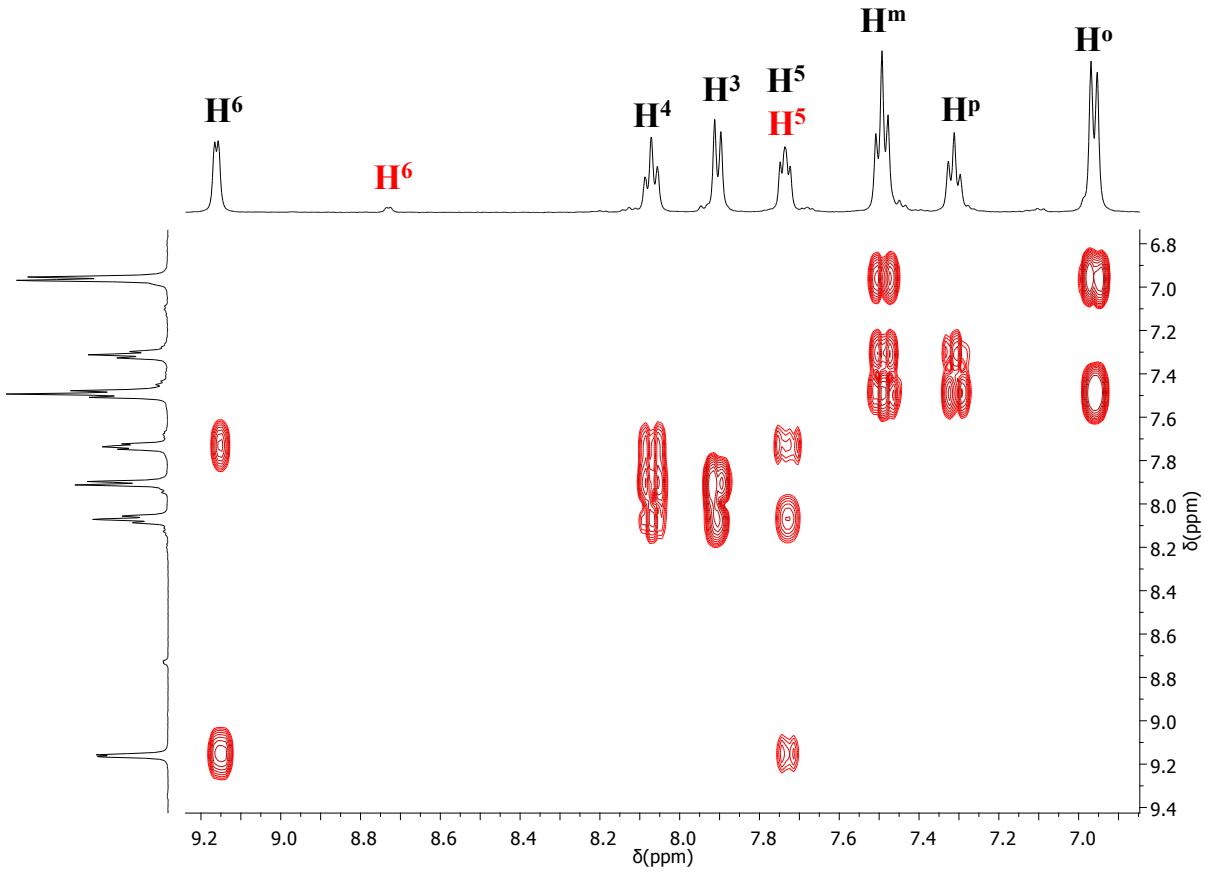

Figure S9. {^{1}H,^{1}H}-COSY spectrum in CD_2Cl_2 at 298 K of **3a**, *cis* (black) and *trans* (red) isomers. Aromatic region.

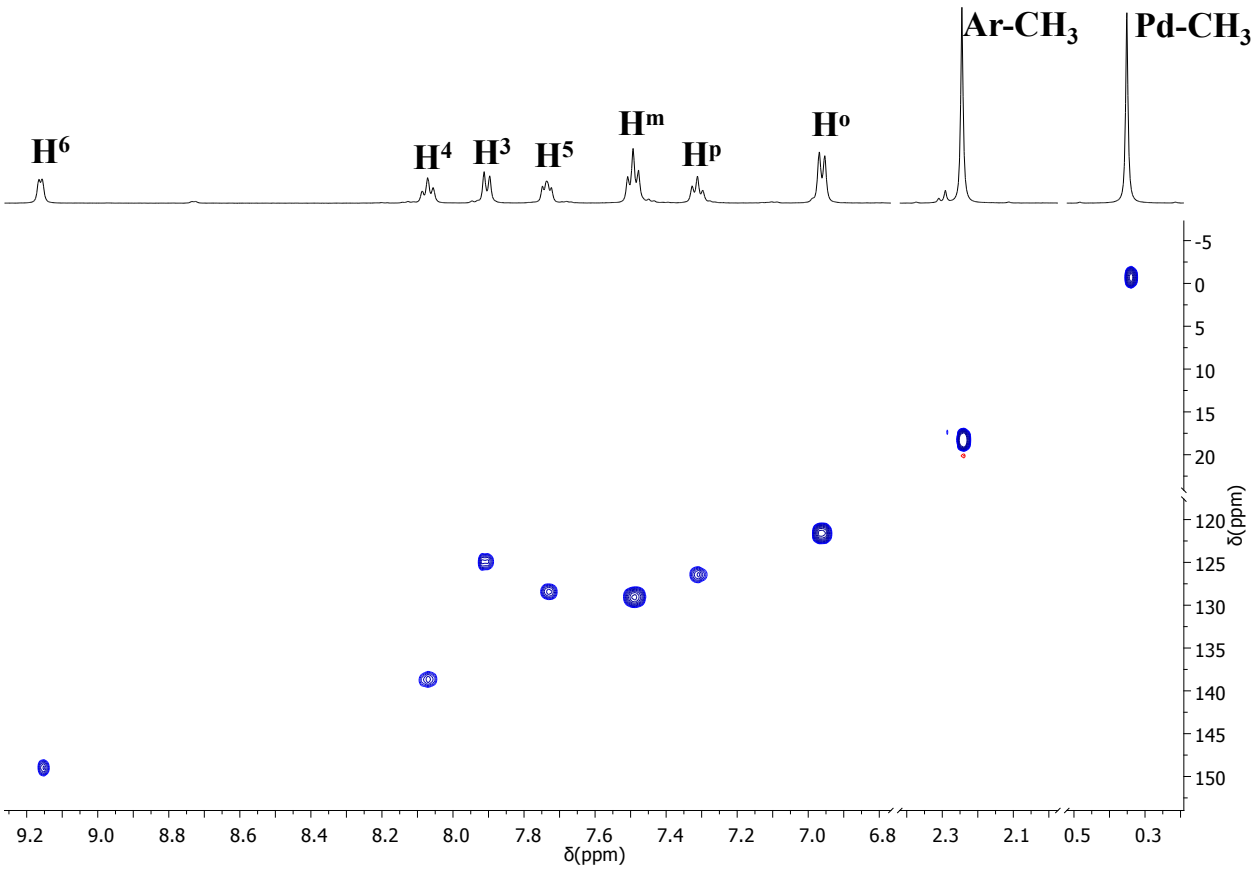

Figure S10. {^{1}H,^{13}C}-HSQC spectrum in CD_2Cl_2 at 298 K of **3a**.

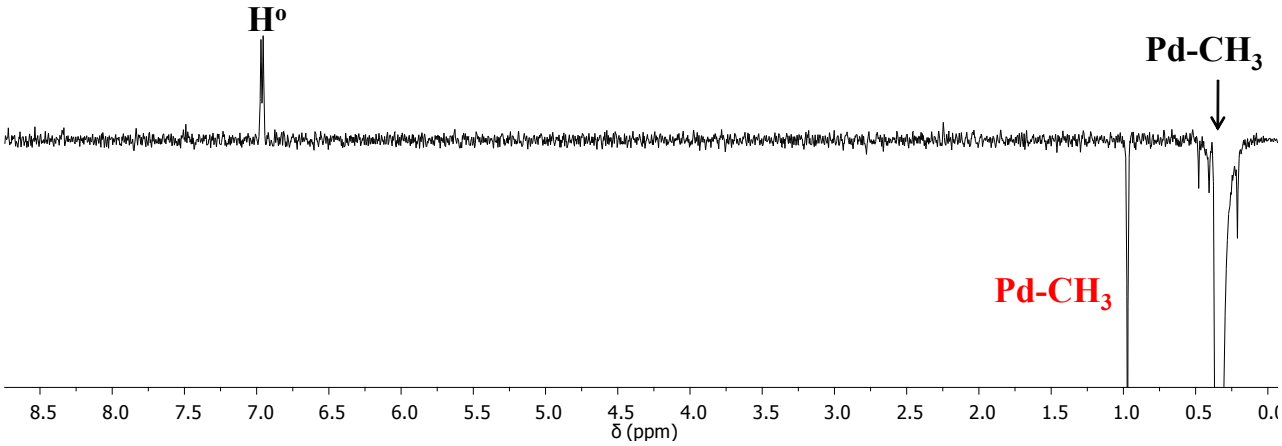

Figure S11. NOE spectrum in CD_2Cl_2 at 298 K of **3a** obtained by irradiating the Pd-CH_3 signal of the *cis* isomer (black).

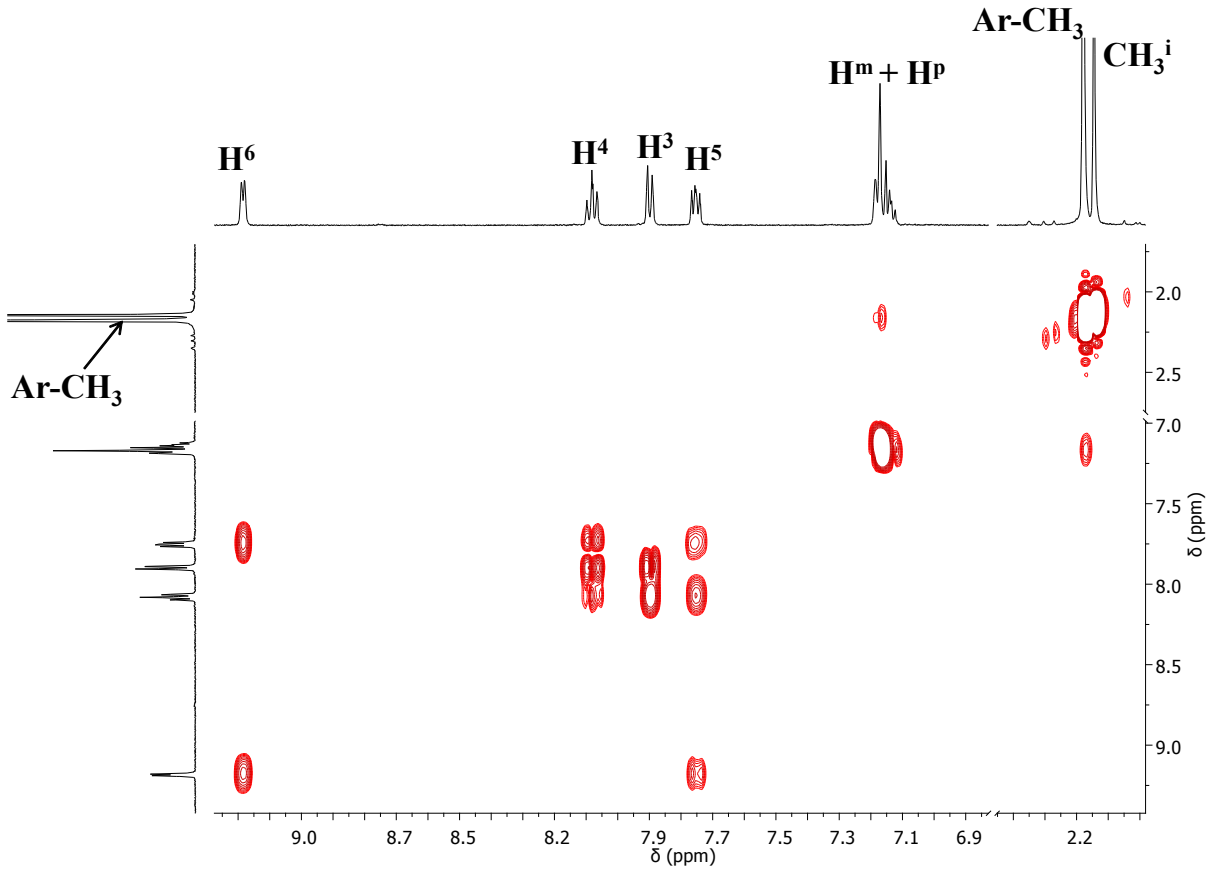

Figure S12. {^{1}H,^{1}H}-COSY spectrum in CD_2Cl_2 at 298 K of **4a**.

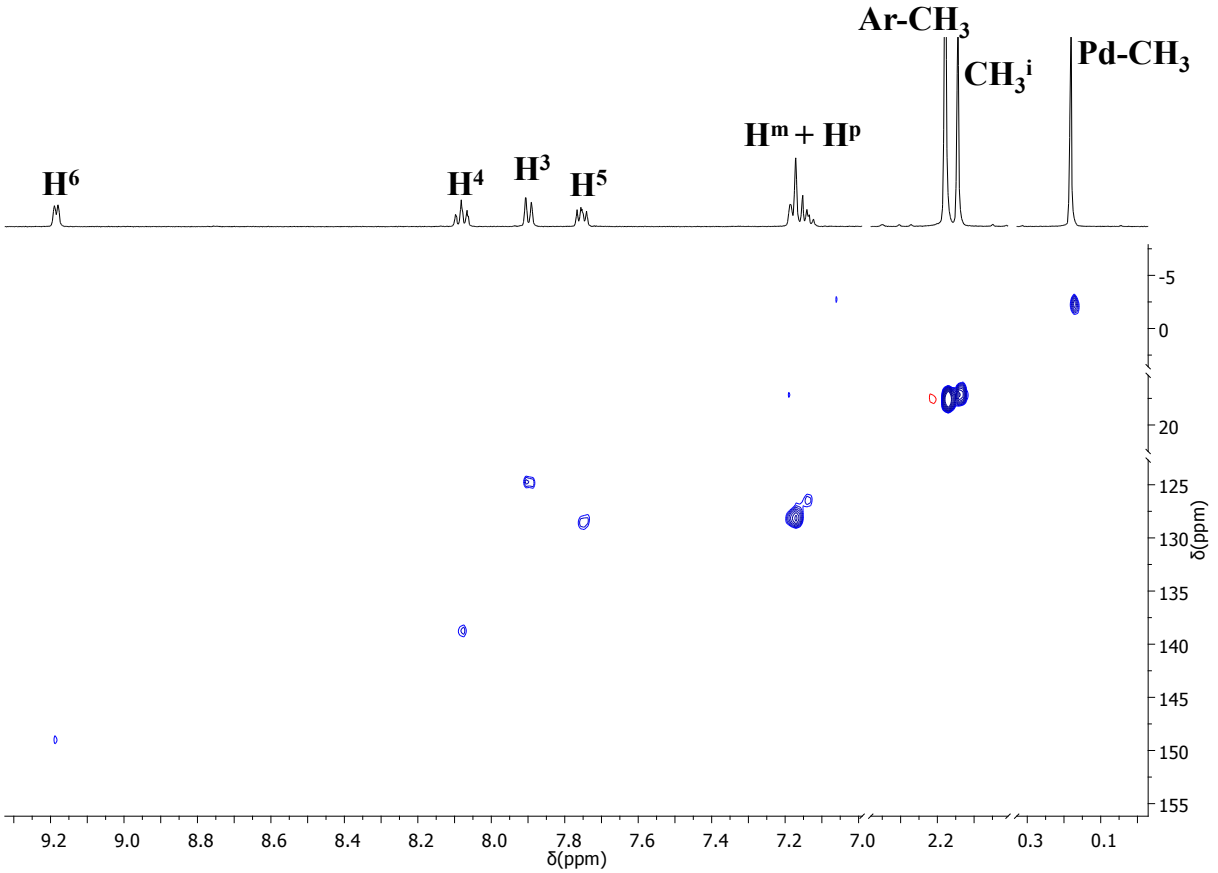

Figure S13. {^{1}H,^{13}C}-HSQC spectrum in CD_2Cl_2 at 298 K of **4a**. Aromatic region, aliphatic region in the box.

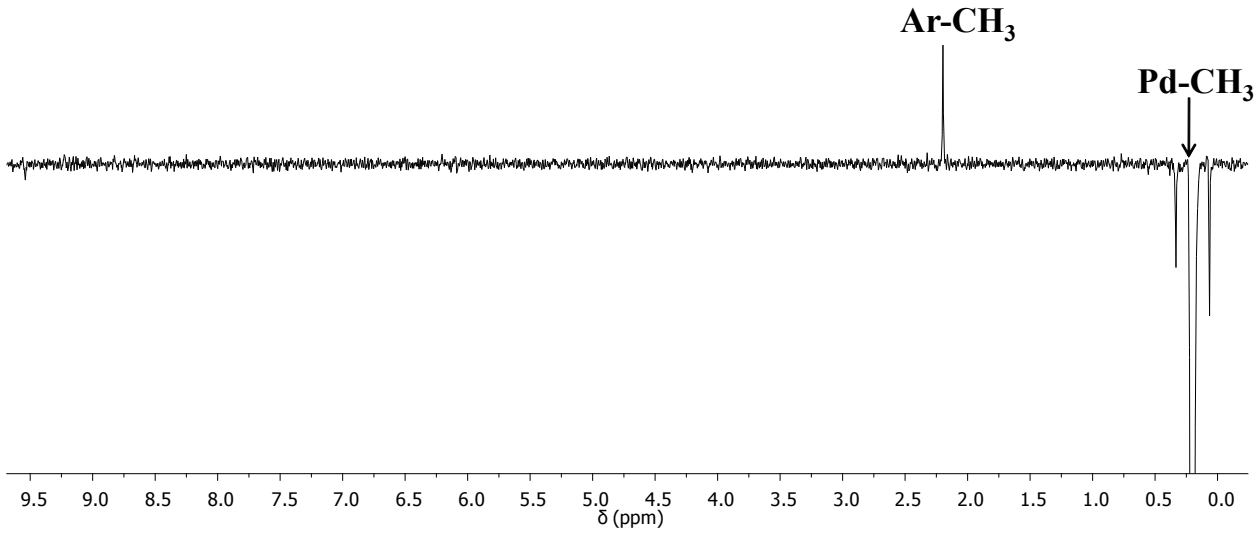

Figure S14. NOE spectrum in CD_2Cl_2 at 298 K of **4a** obtained by irradiating the Pd-CH_3 signal.

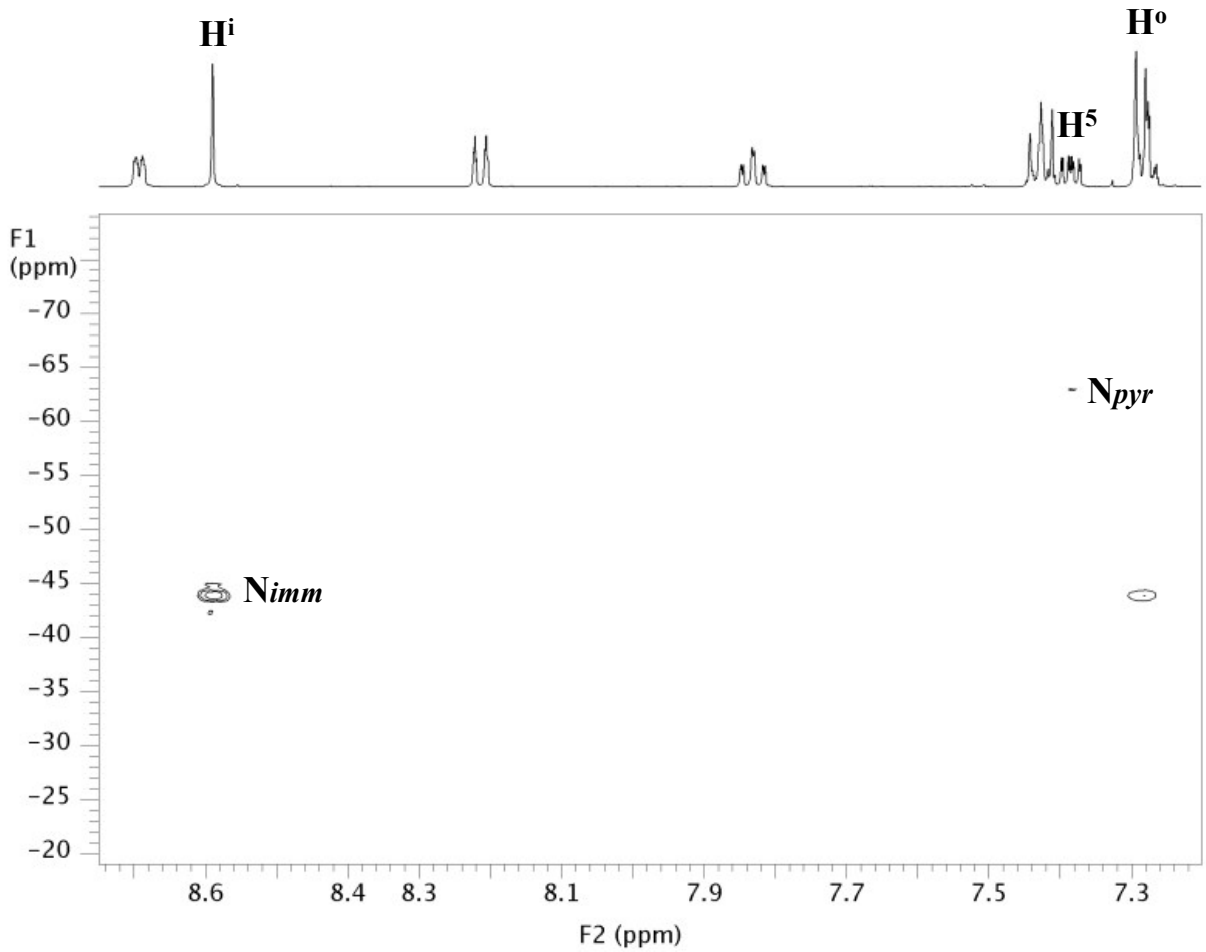

Figure S15. {^{1}H,^{15}N}-HMBC spectrum in CD_2Cl_2 at 298 K of ligand **1**. J = 3 Hz.

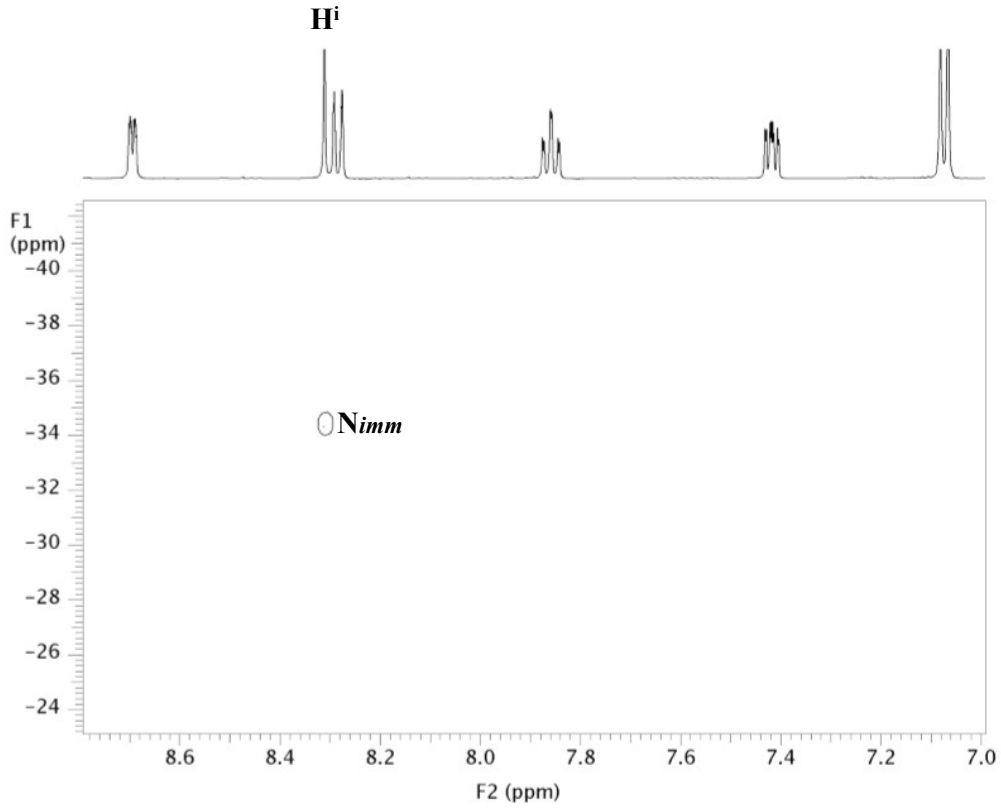

Figure S16. {^{1}H,^{15}N}-HMBC spectrum in CD_2Cl_2 at 298 K of ligand **2**. J = 3 Hz.

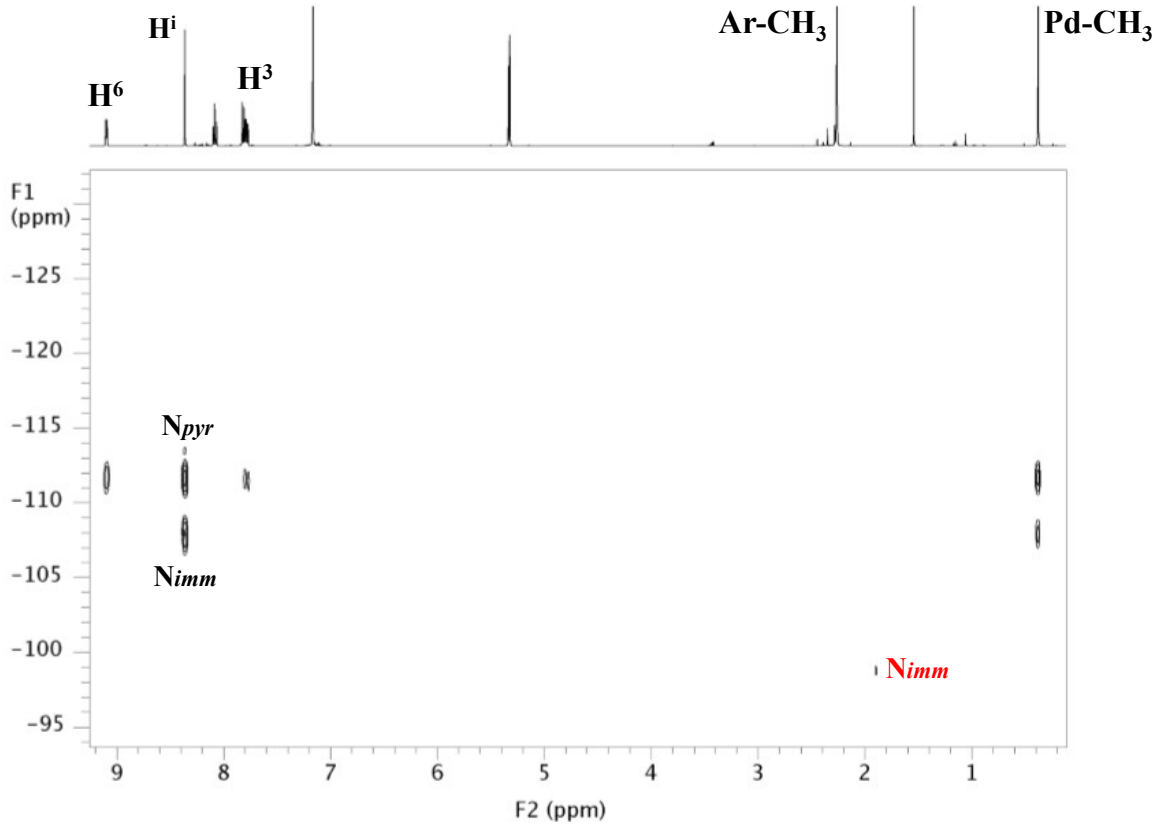

Figure S17. {^{1}H,^{15}N}-HMBC spectrum in CD_2Cl_2 at 298 K of **2a**. J = 5 Hz. *cis* (black) and *trans* (red) isomers.

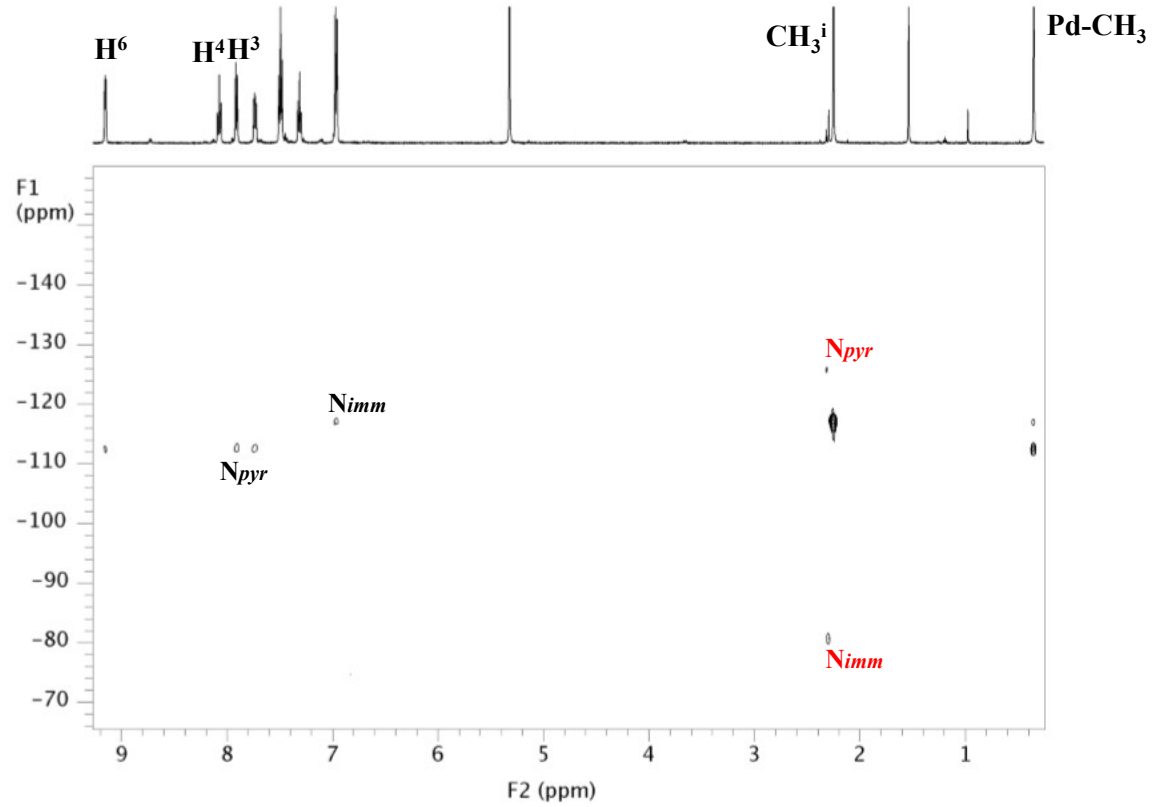

Figure S18. {^{1}H,^{15}N}-HMBC spectrum in CD_2Cl_2 at 298 K of **3a**. J = 4 Hz. *cis* (black) and *trans* (red) isomers.

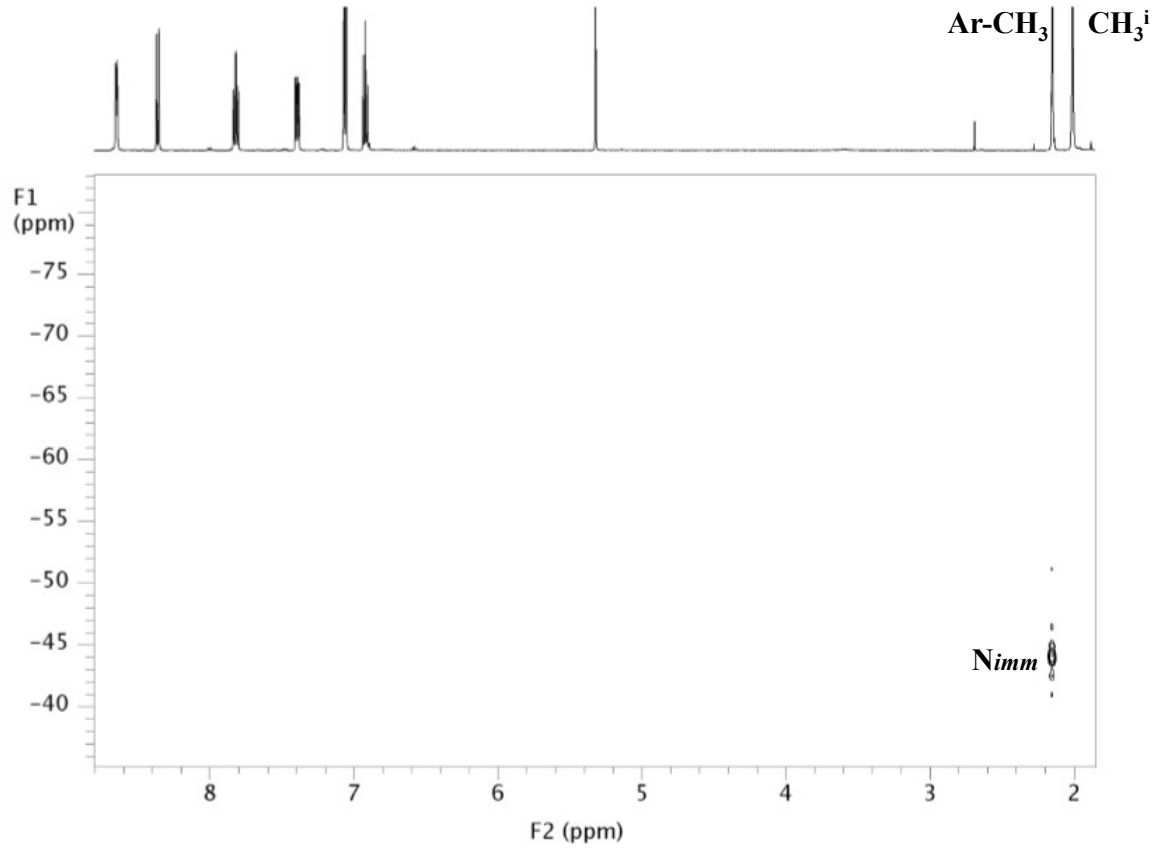

Figure S19. {^{1}H,^{15}N}-HMBC spectrum in CD_2Cl_2 at 298 K of **4**. J = 2 Hz.

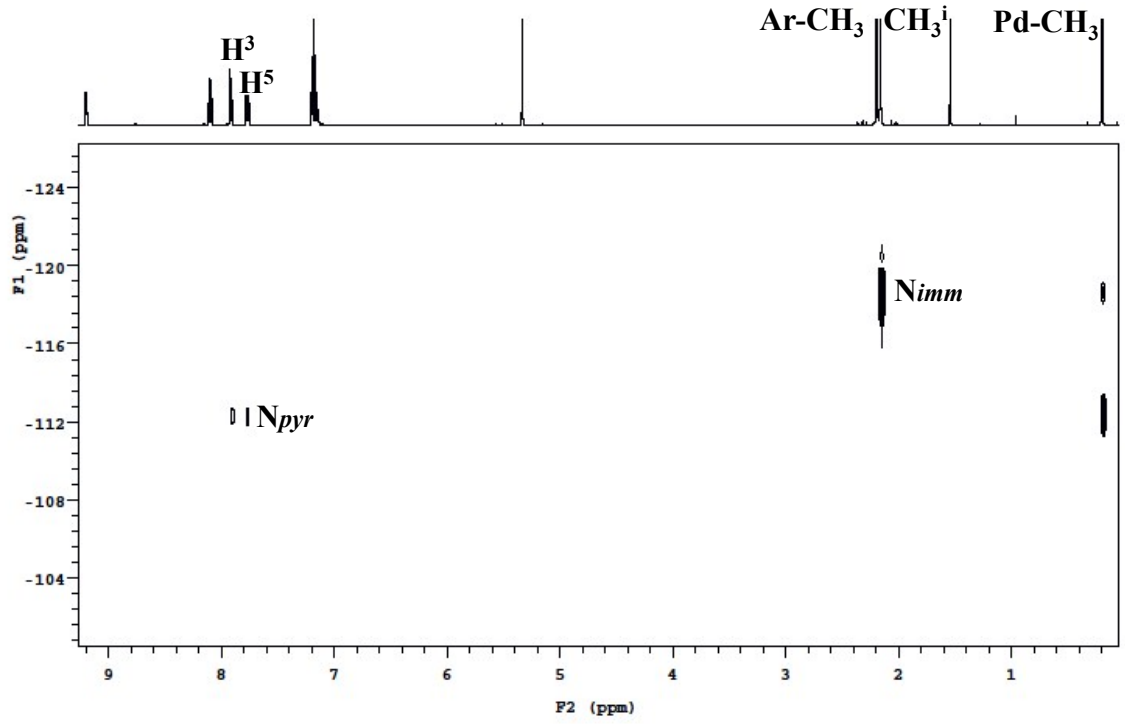

Figure S20. {^{1}H,^{15}N}-HMBC spectrum in CD_2Cl_2 at 298 K of **4a**. ^{2}J = 4 Hz.

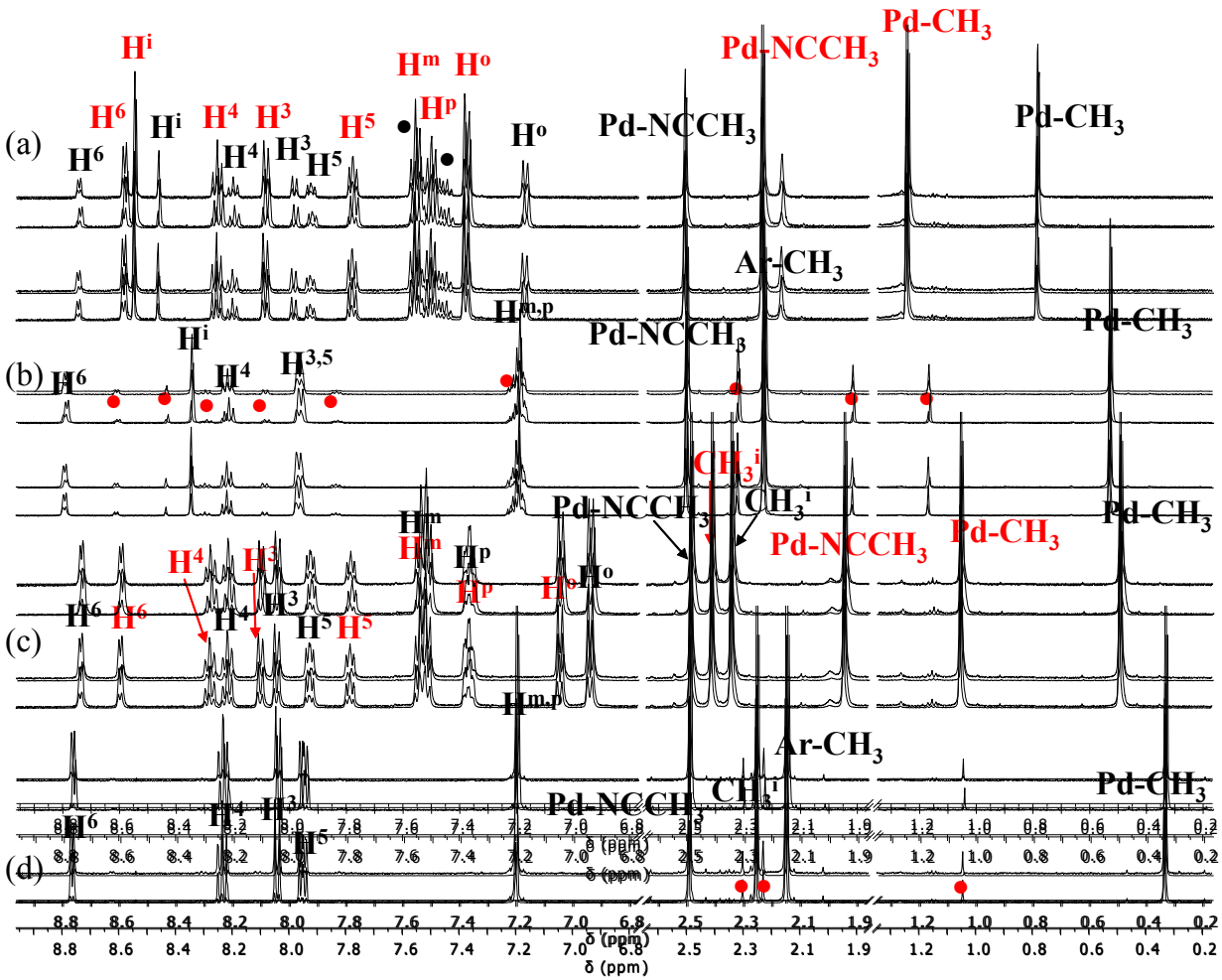

Figure S21. ^{1}H NMR spectra in CD_2Cl_2 at 298 K of (a) **1b**; (b) **2b**; (c) **3b**; (d) **4b**: *cis* (black) and *trans* (red) isomers. Aliphatic and aromatic regions are not on scale.

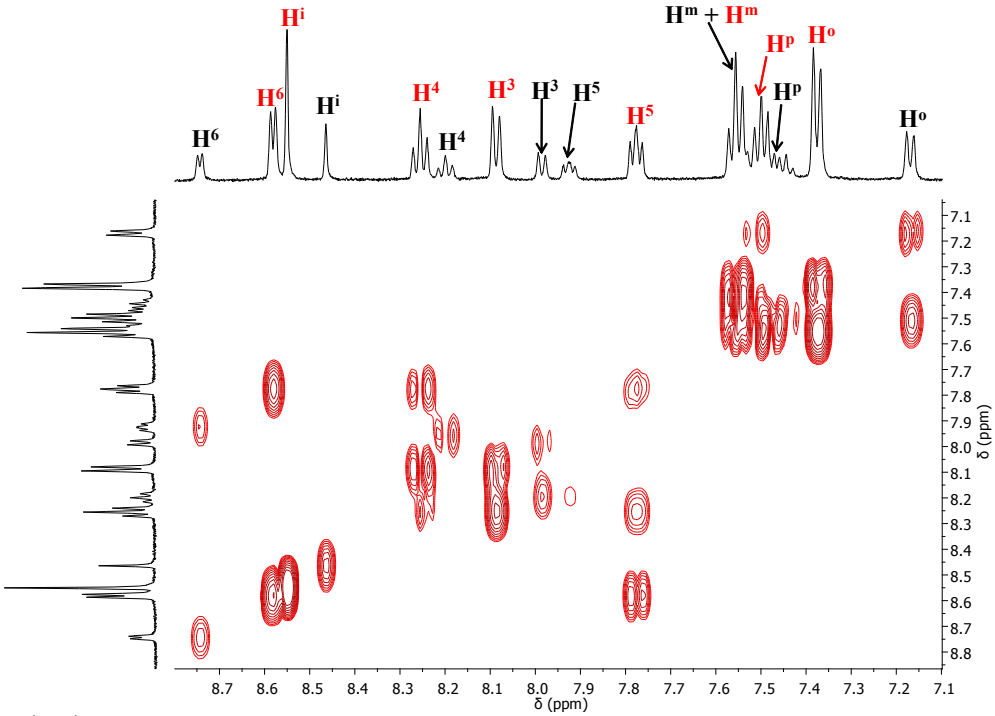

Figure S22. {^{1}H,^{1}H}-COSY spectrum in CD_2Cl_2 at 298 K of **1b**, *cis* (black) and *trans* (red) isomers. Aromatic region.

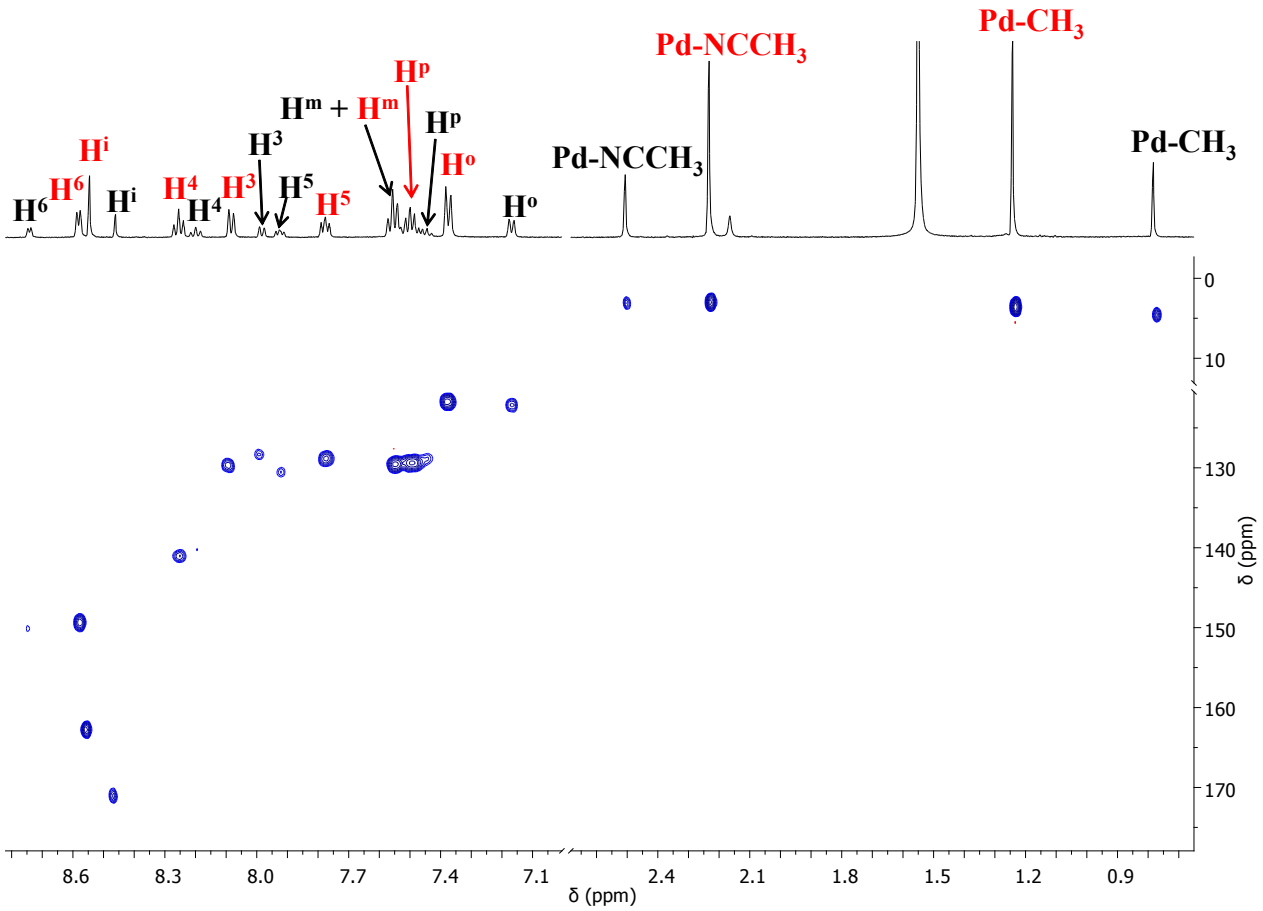

Figure S23. {^{1}H,^{13}C}-HSQC spectrum in CD_2Cl_2 at 298 K of **1b**, *cis* (black) and *trans* (red) isomers.

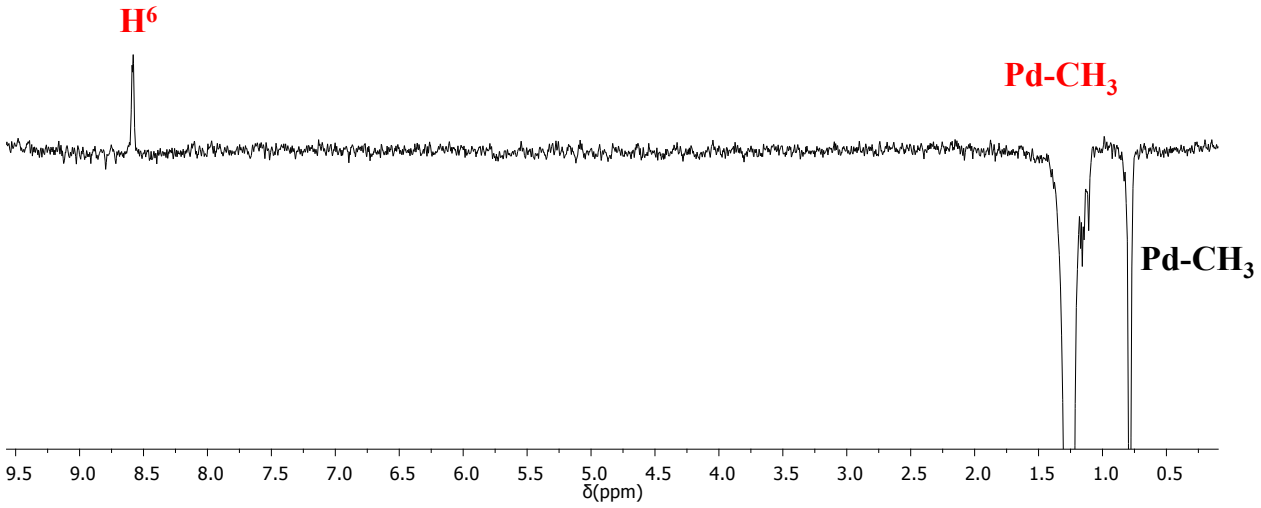

Figure S24. NOE spectrum in CD_2Cl_2 at 298 K of **1b** obtained by irradiating the Pd-CH_3 signal of the *trans* isomer.

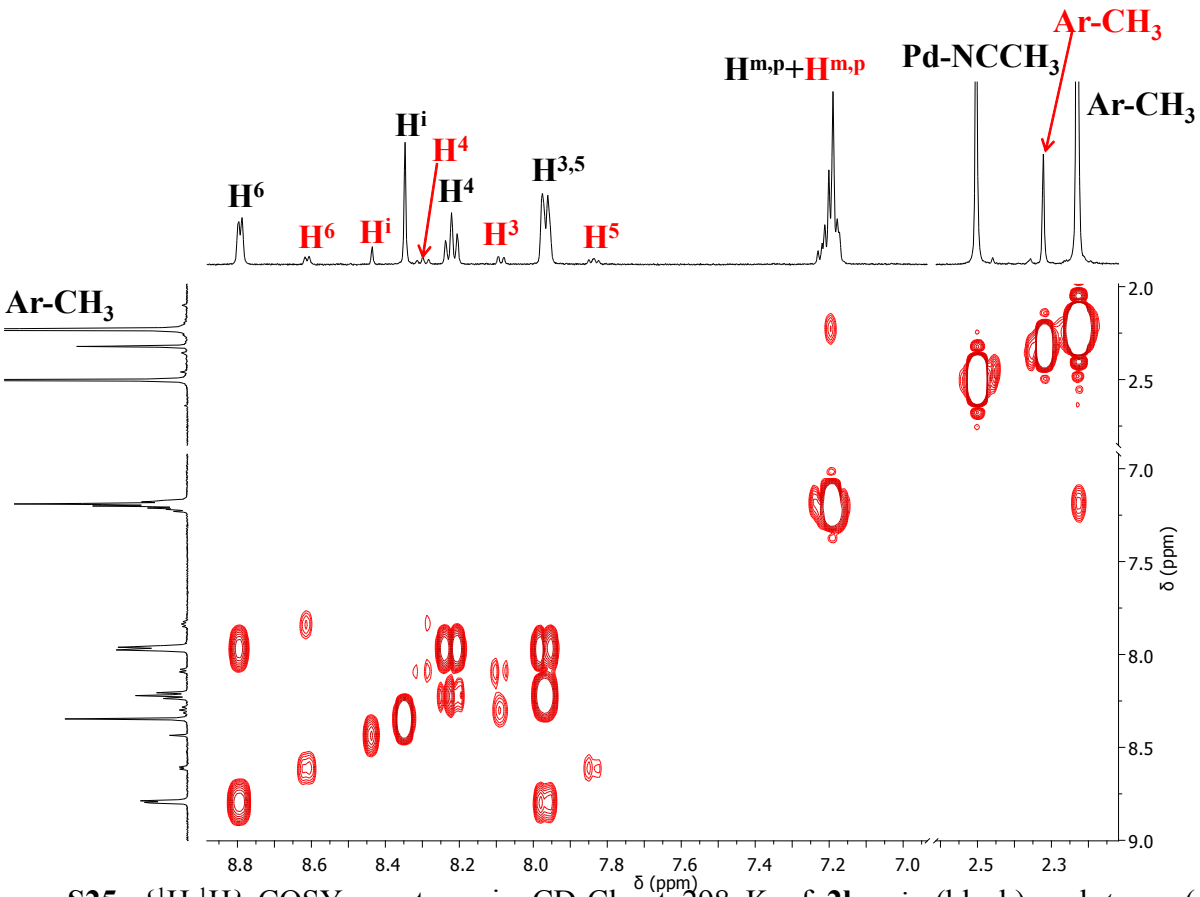

Figure S25. {^{1}H,^{1}H}-COSY spectrum in CD_2Cl_2 at 298 K of **2b**, *cis* (black) and *trans* (red) isomers.

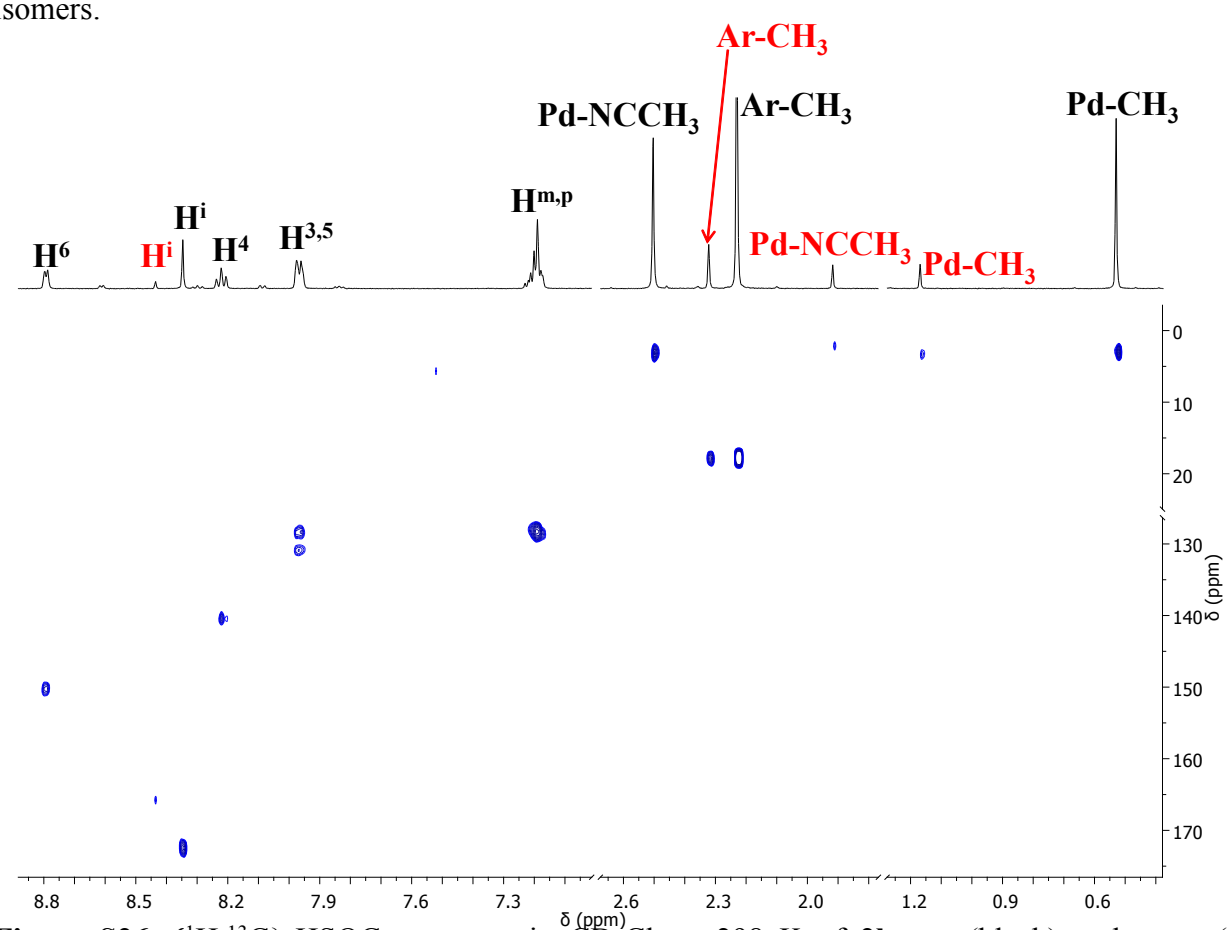

Figure S26. {^{1}H,^{13}C}-HSQC spectrum in CD_2Cl_2 at 298 K of **2b**, *cis* (black) and *trans* (red) isomers.

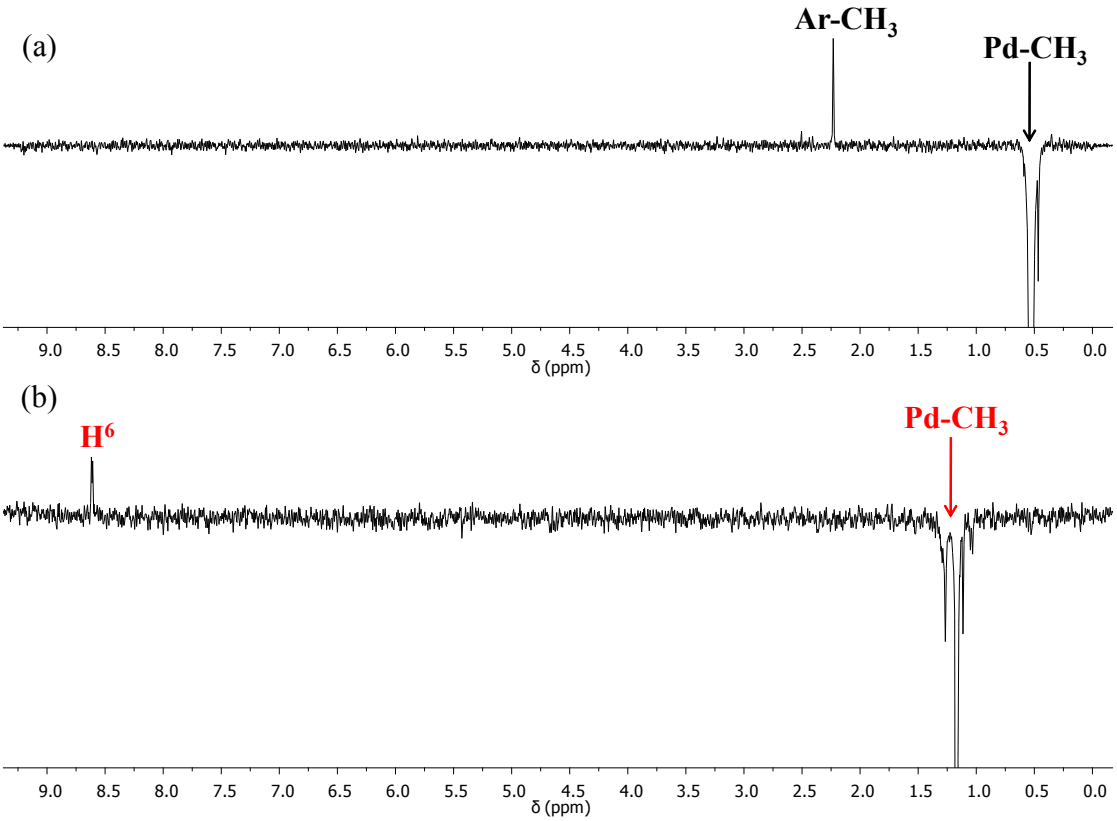

Figure S27. NOE spectra in CD_2Cl_2 at 298 K of **2b** obtained by irradiating the Pd-CH_3 signal of (a) *cis* and (b) *trans* isomer.

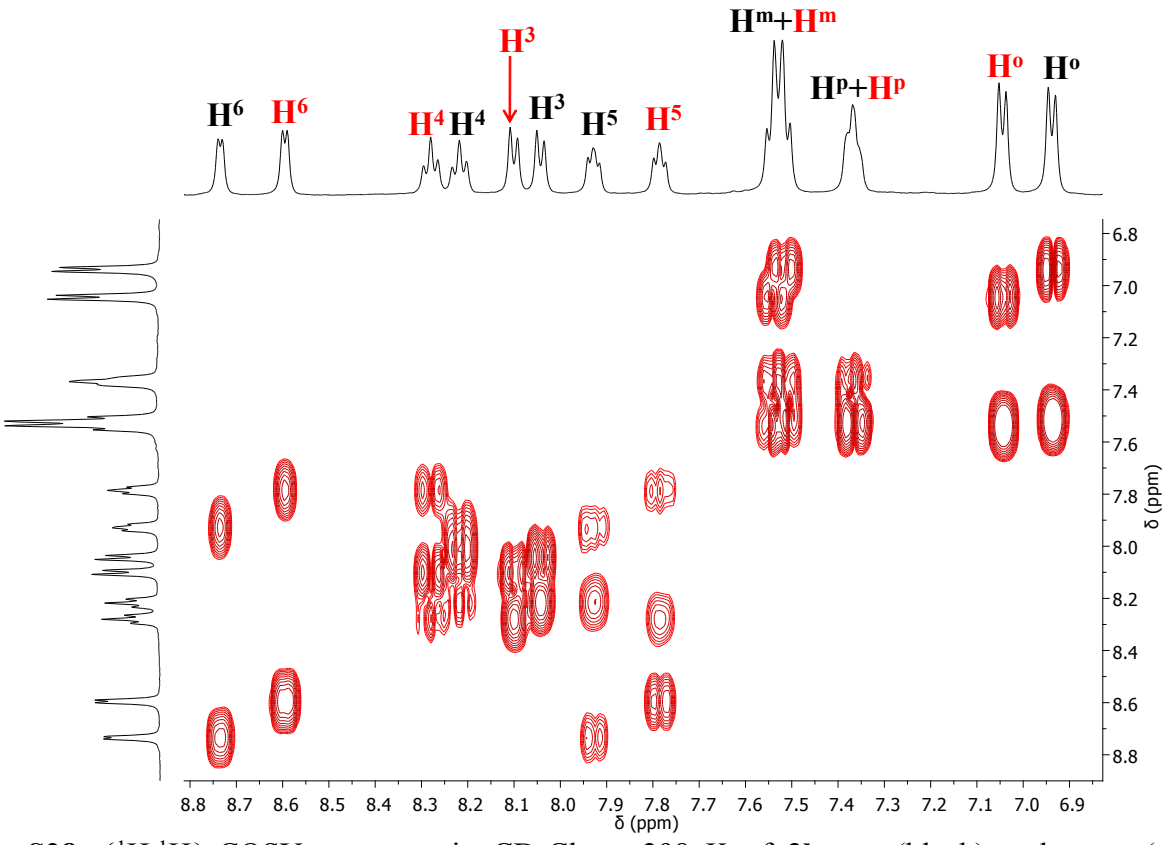

Figure S28. {^{1}H,^{1}H}-COSY spectrum in CD_2Cl_2 at 298 K of **3b**, *cis* (black) and *trans* (red) isomers. Aromatic region.

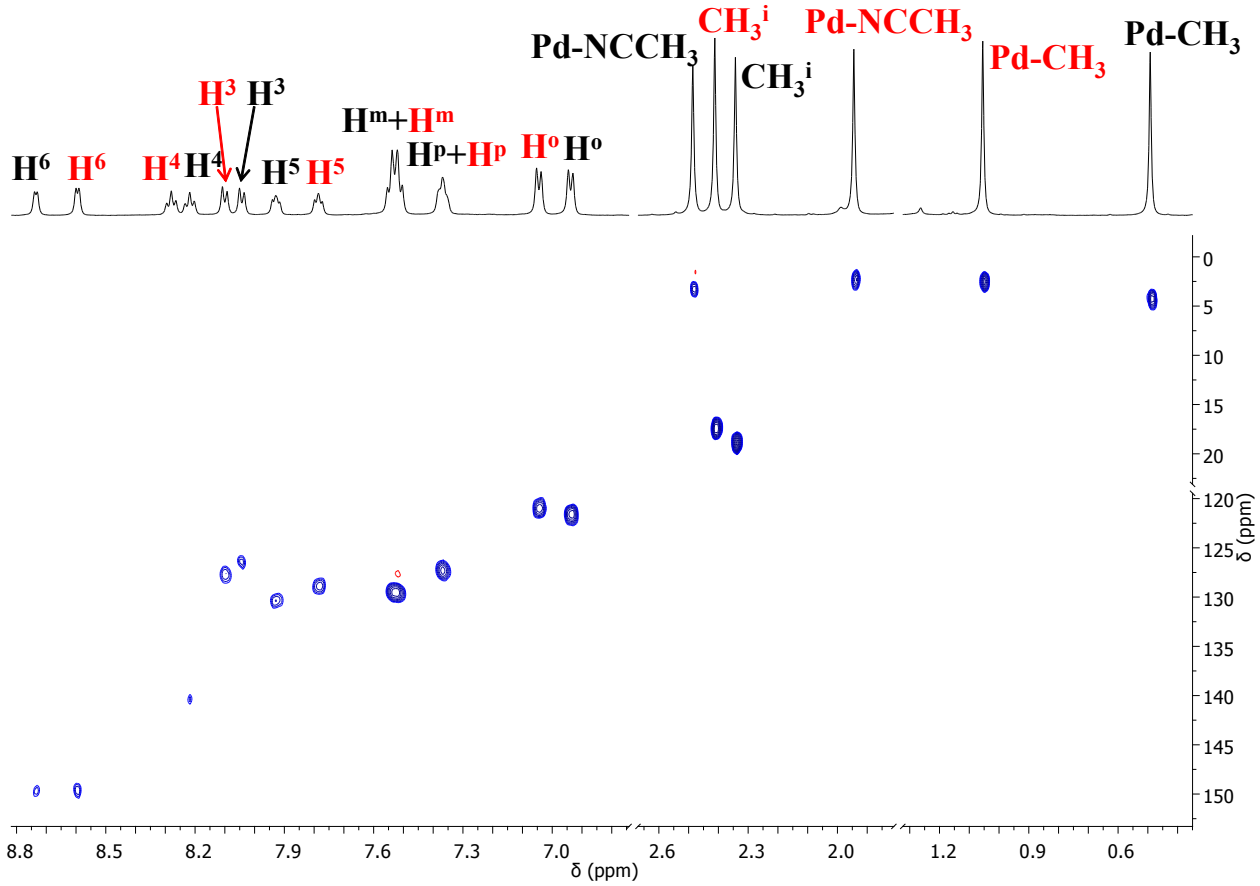

Figure S29. {^{1}H,^{13}C}-HSQC spectrum in CD_2Cl_2 at 298 K of **3b**, *cis* (black) and *trans* (red) isomers.

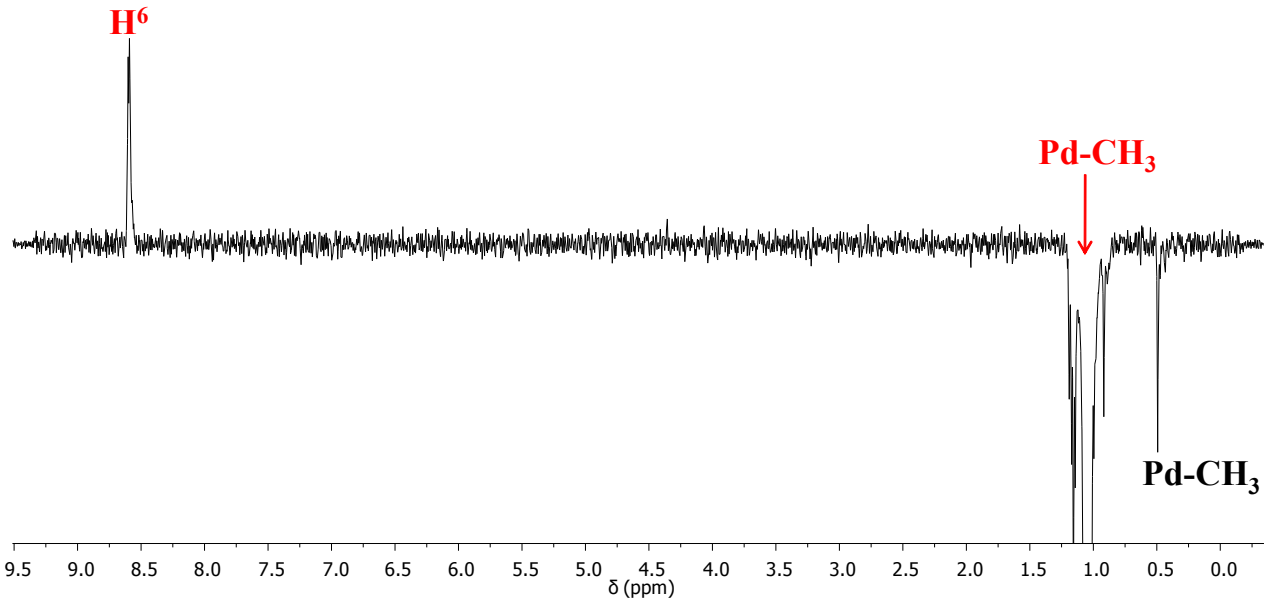

Figure S30. NOE spectrum in CD_2Cl_2 at 298 K of **3b** obtained by irradiating the Pd-CH_3 signal of the *trans* isomer.

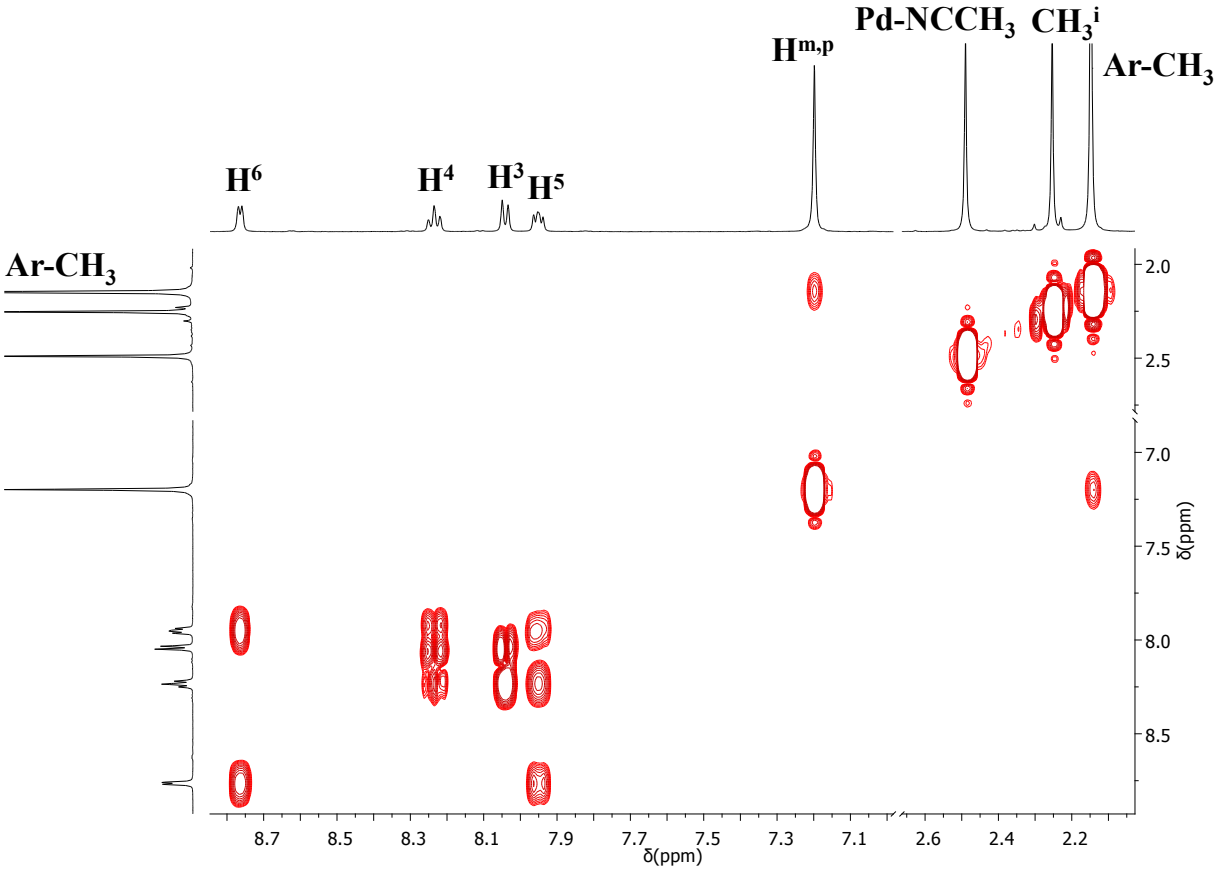

Figure S31. {^{1}H,^{1}H}-COSY spectrum in CD_2Cl_2 at 298 K of **4b**.

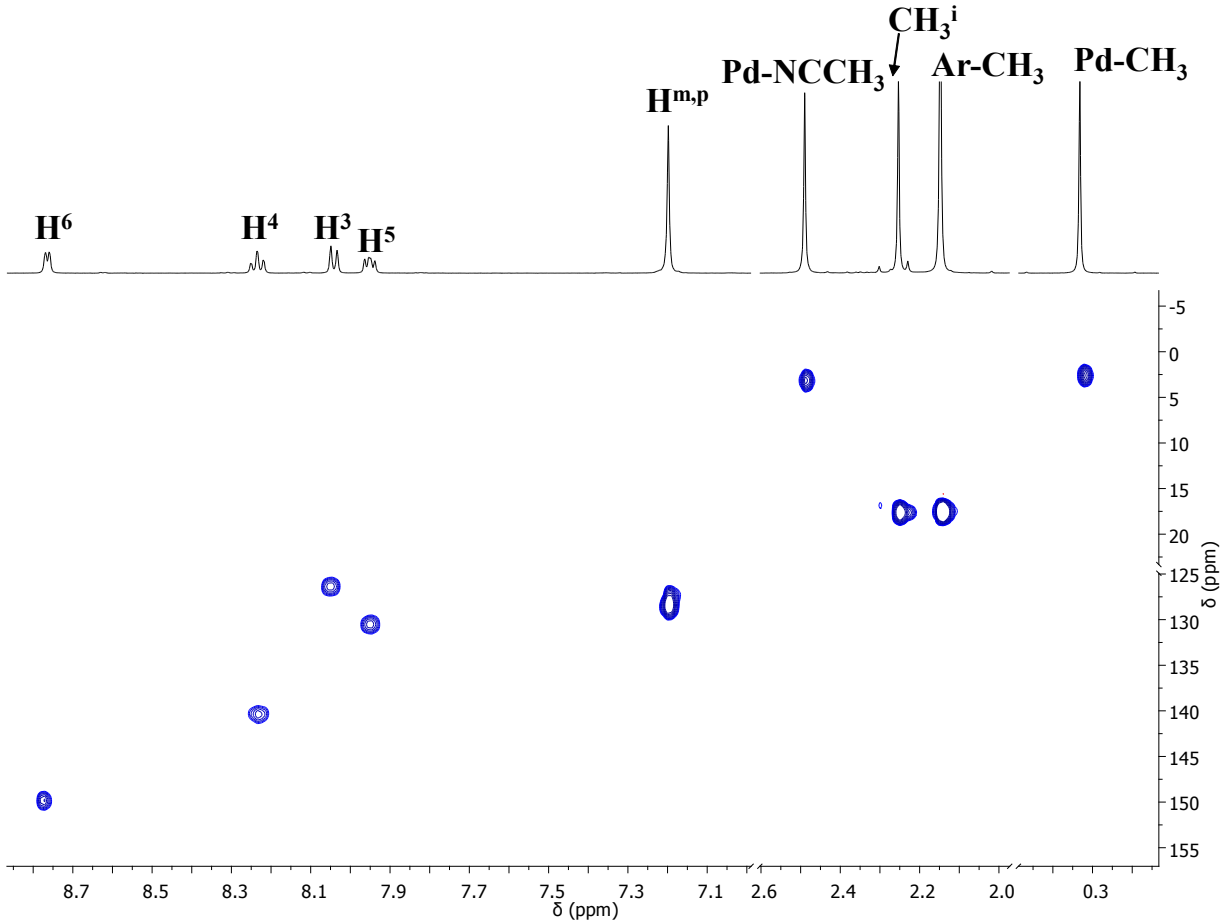

Figure S32. {^{1}H,^{13}C}-HSQC spectrum in CD_2Cl_2 at 298 K of **4b**.

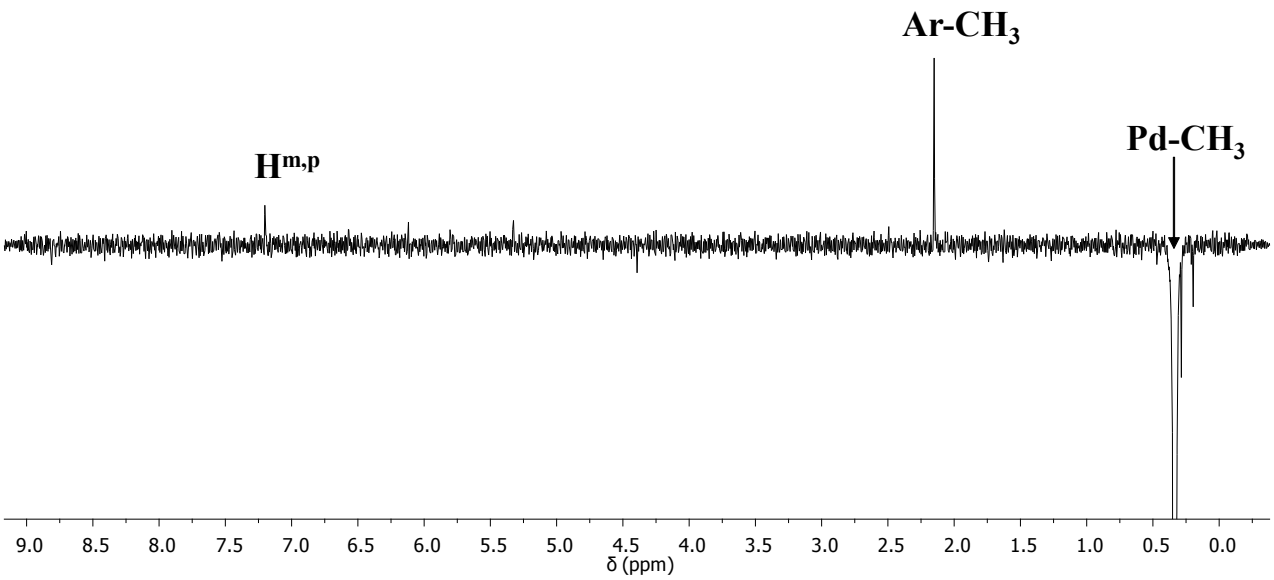

Figure S33. NOE spectrum in CD_2Cl_2 at 298 K of **4b** obtained by irradiating the Pd-CH_3.

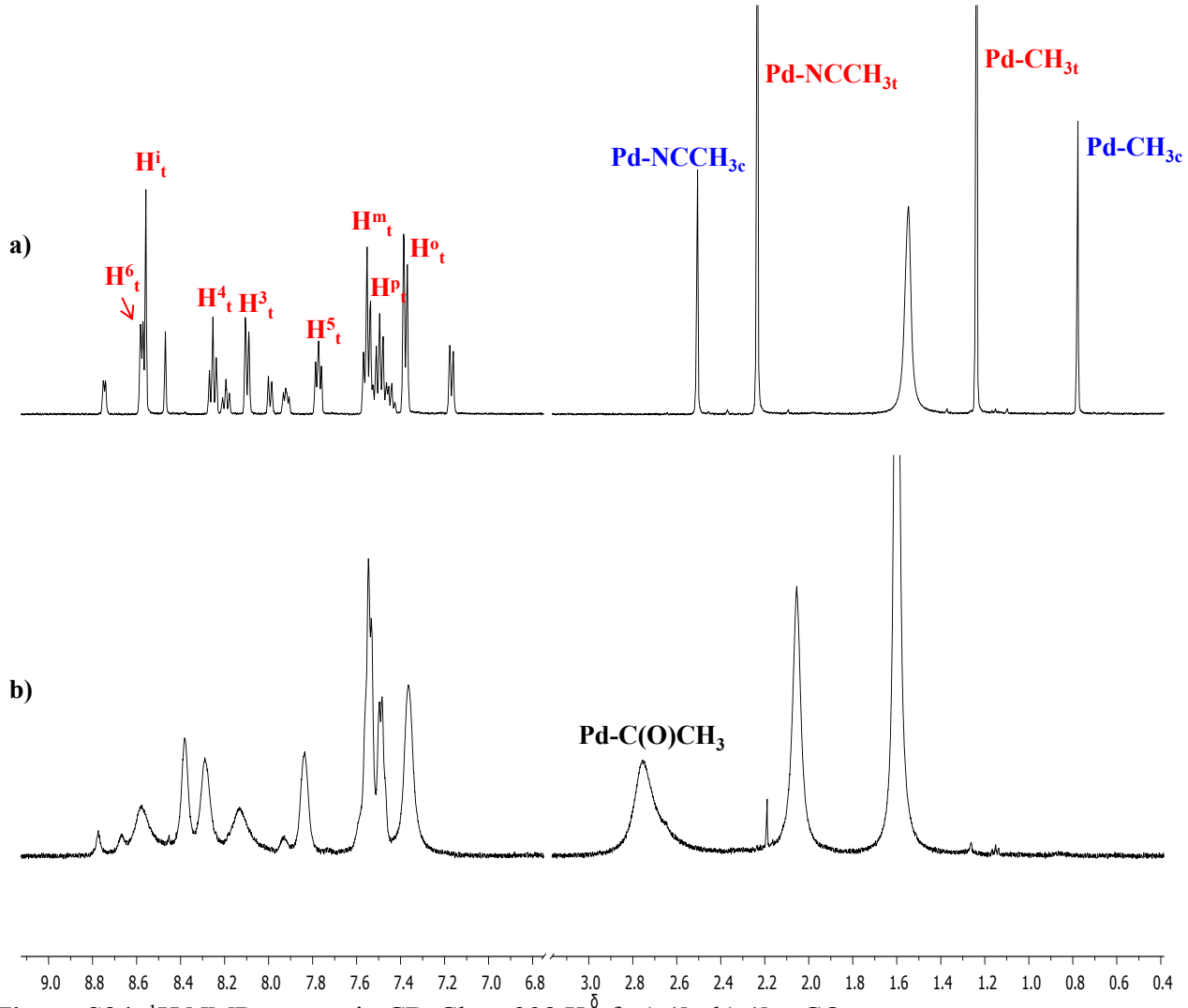

Figure S34. ^{1}H NMR spectra in CD_2Cl_2 at 298 K of: a) **1b**; b) **1b** +CO.

Table S1. X ray diffraction data for complexes **1a-4a**.

	1a	**2a**	**3a**	**4a**
Formula	$PdClC_{13}H_{13}N_2 \cdot CH_2Cl_2$	$PdClC_{15}H_{17}N_2 \cdot \frac{1}{2}CH_2Cl_2$	$PdClC_{14}H_{15}N_2$	$PdClC_{16}H_{19}N_2$
Formula weight (Da)	424.03	409.65	353.13	381.18
Temperature (K)	100(2)	100(2)	100(2)	100(2)
Wavelength ($\AA$)	0.700	0.700	0.700	0.700
Crystal system	Monoclinic	Monoclinic	Monoclinic	Monoclinic
Space Group	P 21/n	P 2/c	P 21/n	P 21/n
a ($\AA$)	11.948(2)	11.000(9)	9.743(2)	7.488(2)
b ($\AA$)	7.674(2)	7.808(3)	18.454(1)	12.883(1)
c ($\AA$)	17.388(3)	19.367(5)	15.501(2)	16.337(1)
α (deg)	90	90	90	90
β (deg)	96.537(4)	104.43(2)	100.64(1)	100.720(5)
γ (deg)	90	90	90	90
V ($\AA^3$)	1583.9(6)	1610(2)	2739.1(6)	1548.5(4)
Z	4	4	8	4
ρ (g/cm^{-3})	1.778	1.689	1.713	1.635
F (000)	840	820	1408	768
μ (mm^{-1})	1.578	1.397	1.451	1.290
θ min,max(deg)	1.938,29.951	1.883,29.986	1.707,29.981	1.996,29.983
Resolution ($\AA$)	0.70	0.70	0.70	0.70
Total refl. collctd	28341	68618	99089	55460
Independent refl.	4766	4798	8290	4667
Obs. Refl. ($F_o > 4\sigma F_o$)	4762	4764	8289	4642
I/σ_I (all data)	55.92	58.13	105.57	72.13
I/σ_I (max resltn)	43.78	43.05	76.60	54.93
R_{merge} (all data)	2.6%	4.2%	2.0%	2.7%
R_{merge} (max resltn)	2.3%	4.5%	1.7%	2.3%
Completeness (all data)	0.988	0.985	0.990	0.982
Completeness (max resltn)	0.991	0.975	0.994	0.989
Multiplicity (all data)	5.8	14.2	11.8	11.6
Multiplicity (max resltn)	4.6	11.2	8.9	8.9
Data/restraint/parameters	4766/0/182	4798/0/187	8290/0/326	4667/0/182
$R_{(I>2\sigma(I))}$,$wR2_{(I>2\sigma(I))}$	0.0288,0.0823	0.0216,0.0578	0.0257,0.0703	0.0258,0.0745
R (all data), wR_2 (all data)	0.0288,0.0824	0.0217,0.0579	0.0257,0.0703	0.0259,0.0746
GooF	1.051	1.215	1.190	1.092