Electronic supplementary information

Nitron-Derivative-Based Palladium Carbene Complexes: Structural Characterizations, Theoretical Calculations, and Catalytic Applications in the Mizoroki-Heck Coupling Reaction

Ming-Yi Lee, Chih-Hsiang Liao, Hsiu-Yu Hung, Jhen-Yi Lee,* and Hon Man Lee*

Department of Chemistry, National Changhua University of Education, Changhua 500, Taiwan

Email: leehm@cc.ncue.edu.tw

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1. Crystallographic data

Table S1. Crystallographic data

	1a	**1b**	**1c**	**2**	**4**
empirical formula	$C_{44}H_{36}N_8O_4Pd$	$C_{26}H_{46}N_8O_3Pd \cdot 5.5H_2O$	$C_{38}H_{54}N_8O_3Pd$	$C_{26}H_{44}N_8O_3Pd$	$C_{25}H_{21}I_2N_5Pd \cdot CH_2Cl_2$
formula weight	847.21	667.57	777.29	623.09	836.59
crystal system	triclinic	Orthorhombic	monoclinic	triclinic	Orthorhombic
space group	$P\bar{1}$	*Pbca*	$P2_1/c$	$P\bar{1}$	$Pca2_1$
a, Å	10.1350(4)	20.866(5)	15.7355(2)	10.7070(3)	18.6757(7)
b, Å	12.5937(5)	11.513(3)	26.5299(3)	11.5157(3)	10.0915(4)
c, Å	16.0612(6)	29.853(6)	18.7343(2)	12.8117(3)	15.2442(6)
α, deg	109.954(2)	90	90	79.913(2)	90
β, deg	97.699(2)	90	103.4930(10)	77.412(2)	90
γ, deg	95.951(2)	90	90	75.138(2)	90
V, Å^3	1884.85(13)	7172(3)	7604.98(16)	1478.17(7)	2873.01(19)
T, K	150(2)	150(2)	100(2)	100(2)	150(2)
Z	2	8	8	2	4
F(000)	868	2792	3264	652	1600
no. of unique data	8216	7827	13586	5255	7483
no. of params refined	517	381	914	355	326
R_1[a] [$I > 2\sigma I$]	0.0449	0.0688	0.0882	0.0271	0.0277
wR_2[b] (all data)	0.1165	0.2035	0.2227	0.0720	0.0582

[a] $R_1 = \Sigma(||F_o| - |F_c||)/\Sigma|F_o|$. [b] $wR_2 = [\Sigma(|F_o|^2 - |F_c|^2)^2/\Sigma(F_o^2)]^{1/2}$

2. Time-yield curves

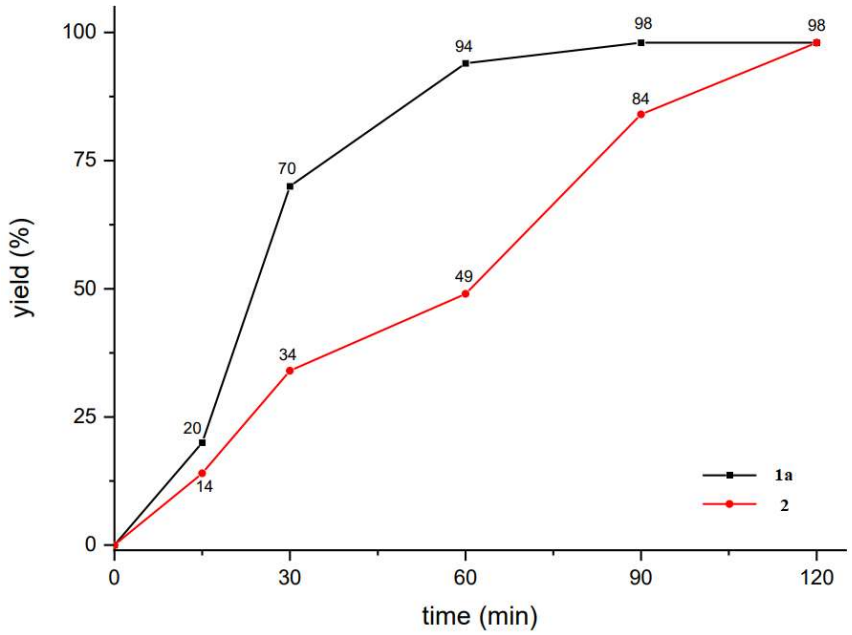
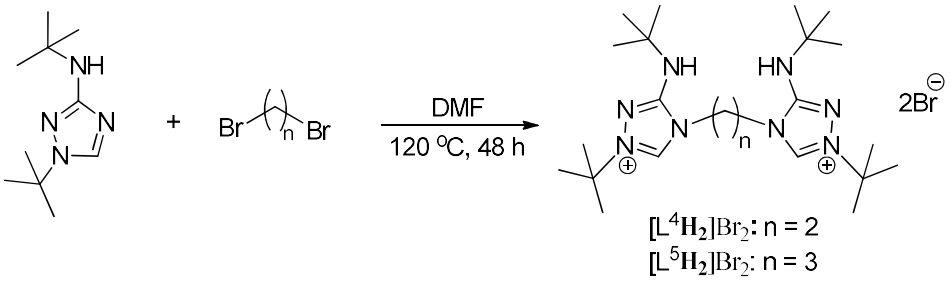


Figure S1. Time-yield curves of the Mizoroki-Heck coupling reaction between 4-chloroacetophenone and styrene at 120 °C catalyzed complexes **1a** and **2**.

3. Synthesis of new ligand precursors.



Scheme S1. Synthesis of ligand precursors

Scheme 1 outlines the synthetic route for preparing the unknown bis(carbene) ligand precursors $[L^4\mathbf{H}_2]Br_2$ and $[L^5\mathbf{H}_2]Br_2$ (L^4 and L^5 = bis(carbene) ligands with ethylene and propylene bridges,

respectively). The synthesis involved nucleophilic substitution reactions of 3-*tert*-butylamino-1-*tert*-butyl-1,2,4-triazole with respective dialkyl bromides in DMF as the solvent. The successful formation of these compounds was confirmed by the presence of characteristic downfield signals in the proton nuclear magnetic resonance (NMR) spectra. Specifically, the NC*H*N signals appeared at 10–11 ppm, indicating the presence of the desired triazolium salts. The N*H* proton exhibited a chemical shift of 7.61 ppm in $[L^4H_2]Br_2$, whereas the corresponding signal was observed at 6.86 ppm in $[L^5H_2]Br_2$. These spectroscopic observations provided evidence for the successful synthesis of the bis(carbene) ligand precursors.

4. Experimental section

General information. The starting chemicals were obtained from suppliers and used as received without any additional purification. The solvents utilized in the reactions were purified using standard methods to remove any impurities. The reactions were carried out employing the standard Schlenk technique under a dry N_2 atmosphere to ensure an inert environment. NMR spectra, including ^1H and $^{13}C\{^1H\}$, were acquired using a Bruker AV-300 spectrometer operating at frequencies of 300.13 MHz and 75.47 MHz, respectively. Elemental analysis data, encompassing carbon, hydrogen, and nitrogen content, were obtained using a Thermo Flash 2000 CHN-O elemental analyzer. Pd(dba)(ma) (dba = *N*,*N*′-ditert-butylethane-1,2-diimine) was prepared according to a literature procedure.[1] These experimental procedures ensured the use of high-quality reagents, appropriate purification of solvents,

and suitable analytical techniques to obtain reliable and accurate results.

Synthesis of ligand precursor [L^4H_2]Br_2. A mixture of 3-*tert*-butylamino-1-*tert*-butyl-1,2,4-triazole (1.00 g, 5.09 mmol) and 1,2-dibromoethane (0.200 mL, 2.32 mmol) was combined with DMF (20 mL) in a Schlenk flask. The mixture was heated to 120 ºC and allowed to react for 48 h. After the reaction, the mixture was cooled, and the resulting white solid was collected on a frit. The collected solid was washed with THF and then dried under vacuum. Yield: 0.806 g (60%). M.p. = 294.3–294.8 °C. ^{1}H NMR ($CDCl_3$): δ 1.47 (s, 18H, C*H*$_3$), 1.64 (s, 18H, C*H*$_3$), 4.96 (s, 4H, C*H*$_2$), 7.61 (s, 2H, N*H*), 11.01 (s, 2H, NC*H*N). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 28.3, 28.4, 43.1 (*C*H$_2$), 54.0 (quaternary *C*), 62.7 (quaternary *C*), 137.2, 152.7 (quaternary *C*); HRMS (ESI) *m*/*z* calcd for $C_{22}H_{44}N_8$ [M–2Br]$^{2+}$ 210.1839; found 210.1843.

Synthesis of ligand precursor [L^5H_2]Br_2. To prepare the bis(carbene) ligand precursor, a similar procedure was followed as for [L^4H_2]Br_2. A mixture of 3-*tert*-butylamino-1-*tert*-butyl-1,2,4-triazole (1.00g, 5.09mmol) and 1,3-dibromopropan (0.236 mL, 2.32 mmol) were used. Yield: 0.48 g (38 %). M.p. = 225.0–225.7 °C. ^{1}H NMR ($CDCl_3$): δ 1.42 (s, 18H, C*H*$_3$), 1.56 (s, 18H, C*H*$_3$), 2.68 (br s, 2H, C*H*$_2$), 4.46 (t, 4H, *J* = 6.0 Hz, C*H*$_2$), 6.86 (s, 2H, N*H*), 10.11 (s, 2H, NC*H*N). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 28.3 (*C*H$_3$), 30.8 (*C*H$_2$), 41.7 (*C*H$_2$), 53.8 (quaternary *C*), 62.2 (quaternary *C*), 135.8, 152.3 (quaternary *C*); HRMS (ESI) *m*/*z* calcd for $C_{23}H_{46}N_8$ [M – 2Br]$^{2+}$ 217.1917; found 217.1921.

Synthesis of Pd(L^1)$_2$(ma) (1a). In a Schlenk flask, L^1 (100 mg, 0.32 mmol), Pd(dbd)(ma) (60 mg, 0.16 mmol) and DMF (10 mL) were combined. The mixture was stirred for 12 h at room temperature.

After the stirring period, the solvent was removed under vacuum, leaving behind a residue. The residue was then extracted twice with a mixture of dichloromethane and water. The organic extract was dried using anhydrous $MgSO_4$ and the solvent was evaporated under vacuum to yield a yellow solid. Diethyl ether was added to the solid, which was collected on a frit and dried under vacuum. Yield: 119 mg (90 %); mp 174.3–174.9 °C (dec.). Anal. Calc. for $C_{44}H_{34}N_8O_3Pd$: C, 63.73; H, 4.13; N, 13.51. Found: C, 63.52; H,4.51; N, 13.47%. ^{1}H NMR ($CDCl_3$): δ 3.19 (s, 2H, maleic *H*), 5.73 (s, 2H, N*H*), 7.01 (t, *J* = 9.0 Hz, 2H, Ar *H*), 7.13–7.19 (m, 10H, Ar *H*), 7.27–7.39 (m, 14H, Ar *H*), 7.70 (d, *J* = 6.0 Hz, 4H, Ar *H*). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 41.3 (maleic *C*), 117.4, 121.3, 122.8, 127.2, 127.6, 128.5, 129.3, 130.5, 130.6, 134.5, 138.2, 139.7, 149.9, 174.2 (*C*=O), 187.9 (Pd *C*).

Synthesis of Pd(L^2)$_2$(ma) (1b). The compound was prepared following a similar procedure as for **1a**. A mixture of **L$_2$** (80 mg, 0.27 mmol), Pd(dbd)(ma) (50 mg, 0.13 mmol), K_2CO_3 (37 mg, 0.27 mmol) and DMF (10 mL) was used. The solution was stirred at 80 ºC overnight. After the reaction, a yellow solid was obtained. Yield: 70.8 mg (84 %). M.p. 165.7–166.3 °C (dec.). Anal. Calc. for $C_{26}H_{46}N_8O_3Pd$: C, 49.95; H, 7.41; N, 17.92. Found: C, 49.86; H, 7.52; N, 18.25 %. ^{1}H NMR ($CDCl_3$): δ 1.34 (s, 18H, C*H*$_3$), 1.52 (s, 18H, C*H*$_3$), 3.44 (s, 2H, maleic *H*), 3.63 (s, 6H, NC*H*$_3$). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 28.7, 30.2, 33.6, 39.2 (maleic *C*), 52.3, 59.1, 150.8, 174.5 (*C*=O), 184.6 (Pd—*C*).

Synthesis of Pd(L^3)$_2$(ma) (1c). The compound was prepared following a similar procedure as for **1a**. A mixture of **L$_3$** (98 mg, 0.27 mmol), Pd(dbd)(ma) (50 mg, 0.13 mmol), K_2CO_3 (37 mg, 0.27 mmol) and DMF (10 mL) was used. The solution was stirred at 50 ºC overnight. After the reaction, a yellow

solid was obtained. Yield: 69 mg (66 %). M.p. 179.3–180.0 °C (dec.). Anal. Calc. for $C_{38}H_{54}N_8O_3Pd$: C, 58.71; H, 7.00; N, 14.41. Found: C, 59.09; H, 7.31; N, 13.96%. ^{1}H NMR ($CDCl_3$): δ 1.07 (s, 18H, C*H*$_3$), 1.60 (s, 18H, C*H*$_3$), 3.07 (s, 2H, N*H*), 3.51 (s, 2H, maleic *H*), 5.00 (d, *J* = 15 Hz, 2H, C*H*$_a$H$_b$), 5.77 (d, *J* = 18 Hz, 2H, CH$_a$*H*$_b$), 7.07 (d, *J* = 9.0 Hz, 4H, Ar *H*), 7.30-7.33 (m, 6H, Ar *H*). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 28.4, 30.5, 40.4 (maleic *C*), 50.9, 52.1 (*C*H$_2$), 59.7, 126.7, 128.3, 129.1, 134.7, 150.8, 173.9 (*C*=O), 185.6 (Pd—*C*).

Synthesis of Pd(L^4)(ma) (2). The compound was prepared, following a similar procedure as for **1a**. A mixture of **L4** (98 mg, 0.13 mmol), Pd(dbd)(ma) (50 mg, 0.13 mmol), K_2CO_3 (37 mg, 0.27 mmol) and DMF (10 mL) was used. The solution was stirred for 5 h at ambient temperature. After the reaction, an off-white solid was obtained. Yield: 83 mg (56 %). M.p. 221.8-222.1 °C (dec.). Anal. Calc. for $C_{26}H_{44}N_8O_3Pd$: C, 50.11; H, 7.11; N, 17.98. Found: C, 49.94; H, 7.53; N, 17.78 %. ^{1}H NMR ($CDCl_3$): δ 1.35 (s, 18H, C*H*$_3$), 1.66 (s, 18H, C*H*$_3$), 3.51 (s, 2H, maleic *H*), 4.07-4.11 (m, 2H, C*H*$_2$), 4.67 (s, 2H, N*H*), 4.72-4.76 (m, 2H, C*H*$_2$). ^{13}C{^{1}H} NMR ($CDCl_3$): δ 28.5, 30.5, 40.4 (maleic *C*), 43.5, 52.5, 59.4, 151.2, 174.4 (*C*=O), 177.9 (Pd—*C*).

Synthesis of Pd(L^5)(ma) (3). The compound was prepared, following a similar procedure as for **1a**. A mixture of **L5** (80 mg, 0.13 mmol), Pd(dbd)(ma) (50 mg, 0.13 mmol), K_2CO_3 (37 mg, 0.27 mmol) and DMF (10 mL) was used. The solution was stirred for 4 h at ambient temperature. After the reaction, a yellow solid was obtained. Yield: 85 mg (64 %). M.p. 157.9–158.6 °C (dec.). Anal. Calc. for $C_{27}H_{46}N_8O_3Pd$: C, 50.89; H, 7.27; N, 17.58. Found: C, 50.53; H, 7.37; N, 4.72, 17.23%. ^{1}H NMR

($CDCl_3$): δ 1.34 (s, 18H, C*H*$_3$), 1.64 (s, 18H, C*H*$_3$), 2.25–2.31 (m, 2H, C*H*$_2$), 3.52 (s, 2H, maleic *H*), 3.86–3.98 (m, 4H, N*H*, C*H*$_2$), 4.47–4.56 (m, 2H, C*H*$_2$). $^{13}C\{^1H\}$ NMR ($CDCl_3$): δ 28.8, 30.5, 40.3 (maleic *C*), 47.9, 52.5, 59.3, 151.3, 174.6 (*C*=O), 184.3 (Pd—*C*).

Synthesis of Pd(L^1)(py)I$_2$ (4). In a 20 mL Schlenk flask, nitron (100 mg, 0.32 mmol) and PdI_2 (115 mg, 0.32 mmol) were dissolved in pyridine (10 mL) under a nitrogen atmosphere. The solution was stirred at 100 ºC overnight. After cooling and drying under vacuum, the residue was extracted with dichloromethane and water twice. The organic extract was then dried over anhydrous $MgSO_4$ and evaporated to dryness under vacuum, resulting in the formation of a solid. Diethyl ether was added to the solid, and the resulting orange solid was collected on frit and dried under vacuum. Yield: 140 mg (58 %). M.p. 249.8–250.4 °C (dec.). ^1H NMR ($CDCl_3$): δ 6.00 (s, 1H, N*H*), 7.05 (t, 1H, *J* = 6.0 Hz, Ar *H*), 7.17 (t, 2H, *J* = 9.0 Hz, Ar *H*), 7.31 (t, 2H, *J* = 9.0 Hz, Ar *H*), 7.39–7.49 (m, 3H, Ar *H*, Py *H*), 7.56-7.73 (m, 6H, Ar *H,* Py *H*), 8.00 (d, 2H, *J* = 6.0 Hz, Ar *H*), 8.52 (d, 2H, *J* = 9.0 Hz, Py *H*), 8.63 (d, 2H, *J* = 3.0 Hz, Ar *H*). $^{13}C\{^1H\}$ NMR (DMSO-d_6): δ 117.7, 123.3, 124.5, 124.6, 128.7, 128.8, 129.4 (Py C), 129.5, 130.2, 131.0, 133.4, 137.6, 137.7 (Py *C*), 139.7 (Pd—*C*), 150.3 (N*C*N), 153.7 (py *C*). Elemental analysis calcd (%) for $C_{25}H_{21}N_5I_2Pd$: C, 39.95; H, 2.82; N, 9.32; found: C, 40.02; H, 3.00; N, 9.46 %.

A general procedure for Mizoroki−Heck reaction. In a typical reaction, an aryl halide (1 mmol), and styrene (1.4 mmol) were mixed with a base (1.1 equiv), a palladium catalyst (0.1–0.2 mol%), and TBAB (2 g). The mixture was stirred at 140 °C for an appropriate period of time, typically ranging

from 2−16 h. After the reaction was cooled, the product was extracted with ethyl ether (3×10 mL), and the organic layer was dried using anhydrous $MgSO_4$. The dried organic layer was then filtered, and the solvent was completely removed under high vacuum. The NMR yield was determined by using 1,3,5-trimethoxybenzene as an internal standard. The crude product was further purified by column chromatography.

Single-crystal X-ray diffraction studies. Crystals suitable for x-ray structural studies were obtained by employing different solvent combinations and allowing for slow evaporation. The solvent combinations used were DCM/toluene (**1a**), DCM/hexane (**1b**), DCM/hexane (**1c**), DCM/hexane (**2**), and chloroform/hexane (**4**).

The structural data for compounds **1a**, **1b**, and **4** were obtained using a Bruker APEX II X-ray diffractometer equipped with a CCD area detector. The data collection was performed at a temperature of 150(2) K. The data was acquired using MoKα radiation (λ = 0.71073 Å) from a sealed X-ray tube. The unit cell parameters were refined using the least-squares method and the data acquisition and reduction were carried out using the Bruker APEX and SAINT software packages.[2] Absorption corrections were performed using the multi-scan method implemented in SADABS.[3] For compounds **1c** and **2**, the structural data were obtained using a Rigaku XtaLab Synerg DW X-ray diffractometer equipped with a MicroMax-007 HF microfocus rotating anode that generated CuKα radiation (λ = 1.54184 Å) and a HyPix-Arc 150° curved hybrid photon counting X-ray detector. The data acquisition and reduction were carried out using the CrysAlisPro 1.171.42.51a software.[4] Empirical absorption

correction was performed using spherical harmonics implemented in SCALE3 ABSPACK.[4] The experiments were conducted at National Tsing Hua University, Hsinchu city, Taiwan

In the structural analysis of all the compounds, direct methods were initially used to solve the crystal structures. The obtained solutions were further refined using full-matrix least squares methods against F^2 with the SHELXL program.[5] Refinement of the non-hydrogen atoms was carried out using anisotropic refinement methods, taking into account the anisotropy of thermal motion. The positions of the hydrogen atoms were calculated and fixed at their respective calculated positions. Riding refinements were then performed for the hydrogen atoms. CCDC file numbers are 2277731 (**1a**), 2277757 (**1b**), 2277758 (**1c**), 2277759 (**2**), and 2277760 (**4**).

Computational studies. The calculations were conducted using the Gaussian 09W program.[6] Geometry optimizations and energy calculations for the free ligands were performed at the M06-2X/6-31G* level of theory. For the metal complexes, geometry optimizations were carried out at the B3LYP[7]/LANL2DZ[8] level of theory, based on the coordinates from the X-ray structural data. Energy calculations were performed using the M06-L functional with def2-TZVP[9] basis sets. The natural bond orbital (NBO) analysis was performed using the NBO 3.1 program within Gaussian 09W.[10] Charge decomposition analysis (CDA) was carried out using the Multiwfn 3.8 program based on M06-L/def2-TZVP and PBE1PBE/def2-TZVP levels of theory. To account for the solvent effects, the polarized continuum model (PCM) was employed to optimize all the geometries in DMF solvent.[11] This model considers the influence of the solvent on the molecular structure and properties during the optimization

process.

5. NMR spectra of ligand precursors

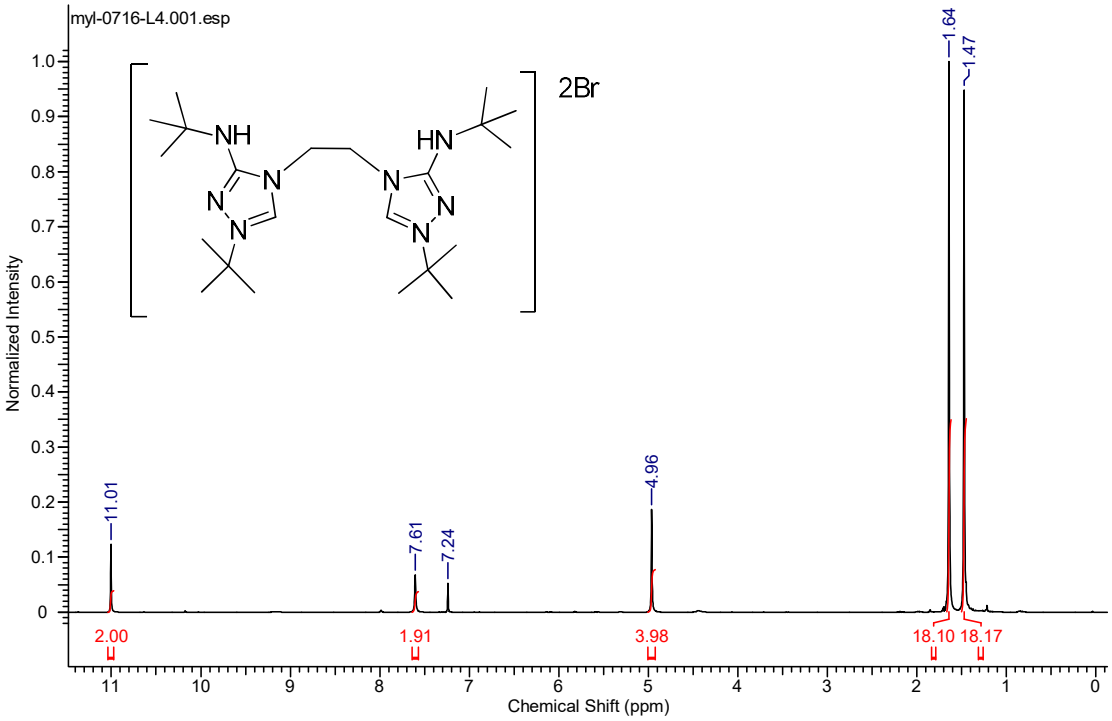


Figure S2. ^{1}H NMR spectrum of **[L^{4}H$_2$]Br$_2$**

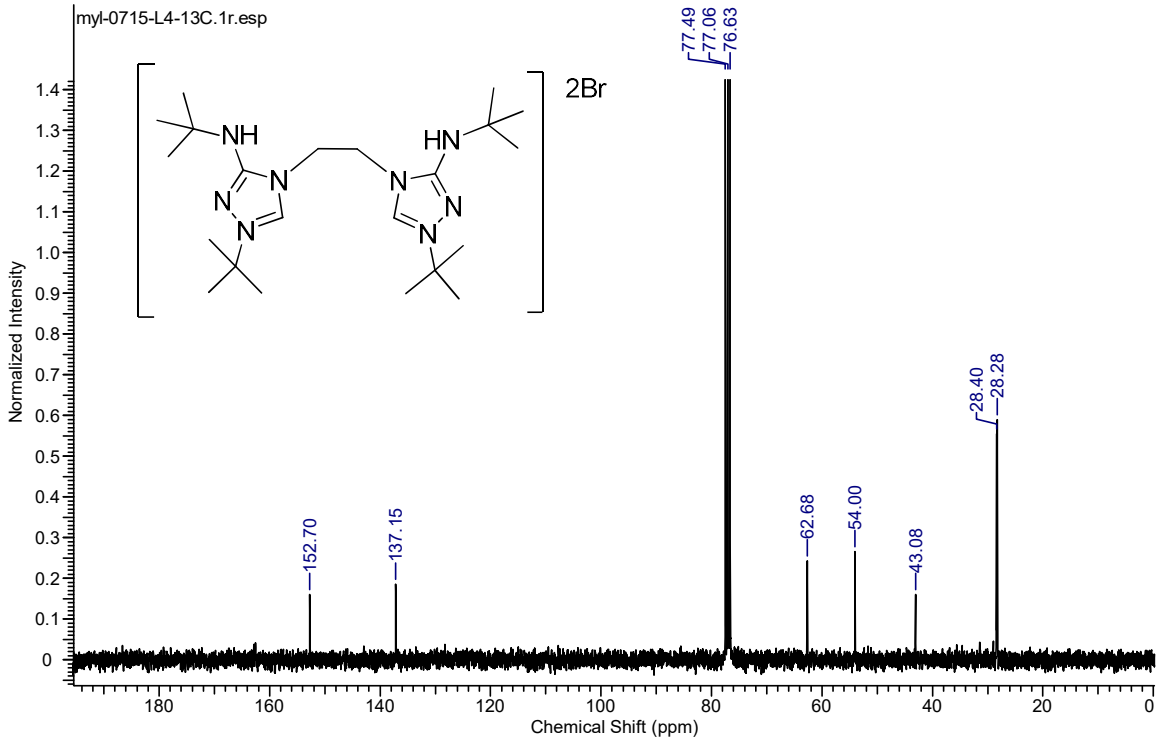


Figure S3. $^{13}C\{^{1}H\}$ NMR spectrum of **[L^{4}H$_2$]Br$_2$**

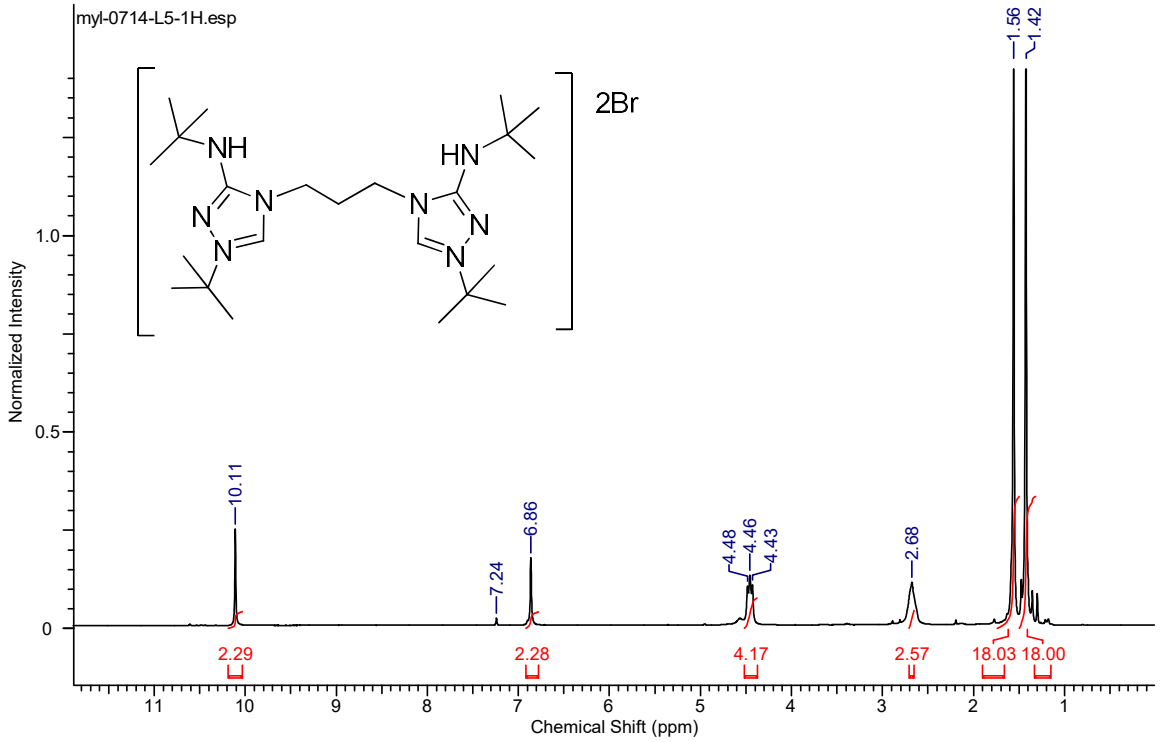


Figure S4. ^{1}H NMR spectrum of **[L^{5}H$_2$]Br$_2$**

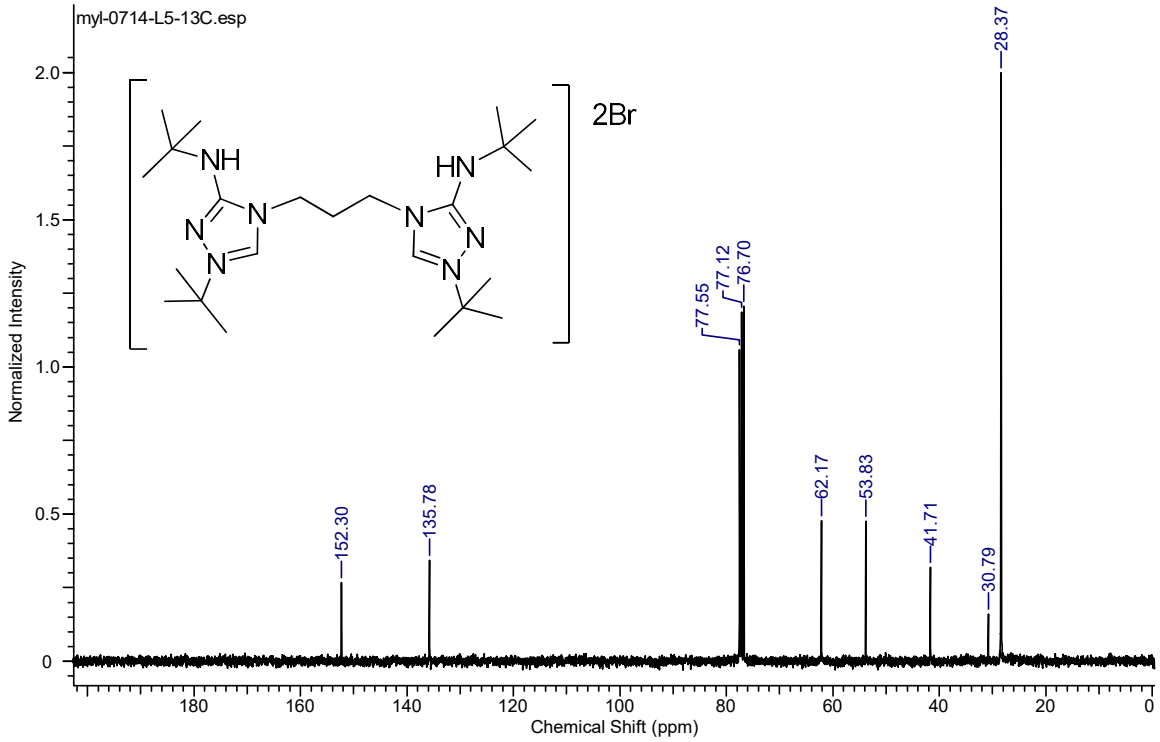


Figure S5. $^{13}C\{^{1}H\}$ NMR spectrum of **[L^{5}H$_2$]Br$_2$**

6. NMR spectra of metal complexes

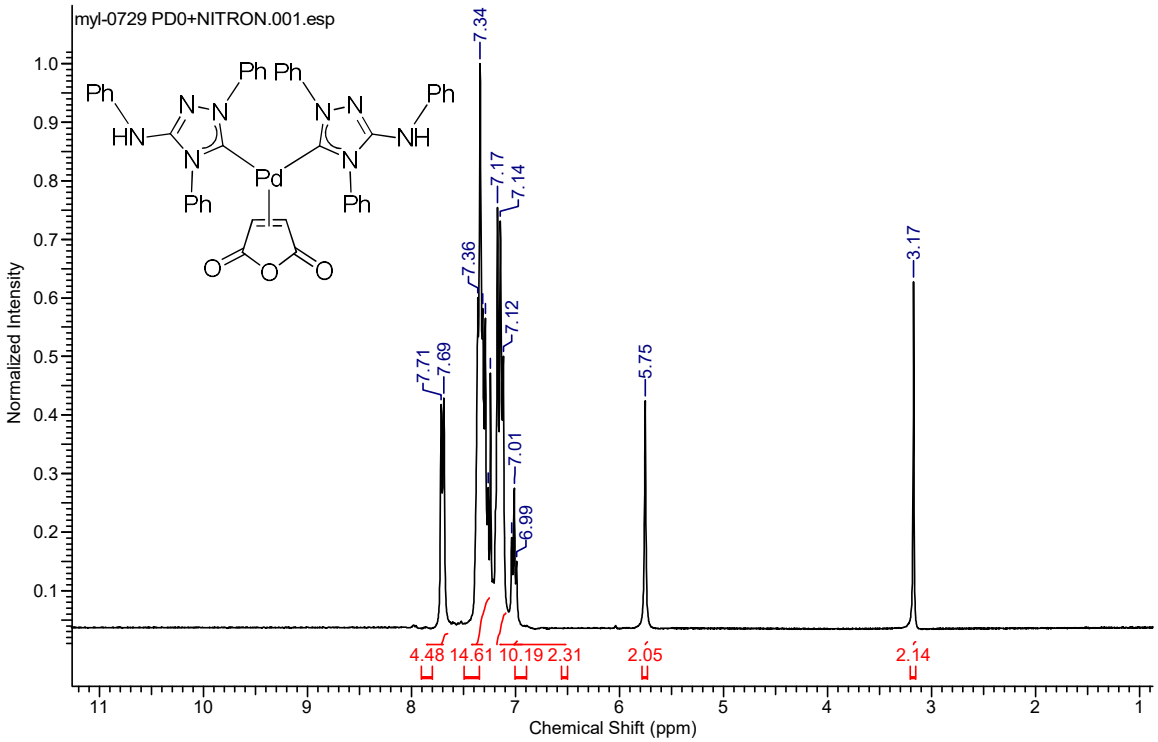


Figure S6. ^{1}H NMR spectrum of **1a**

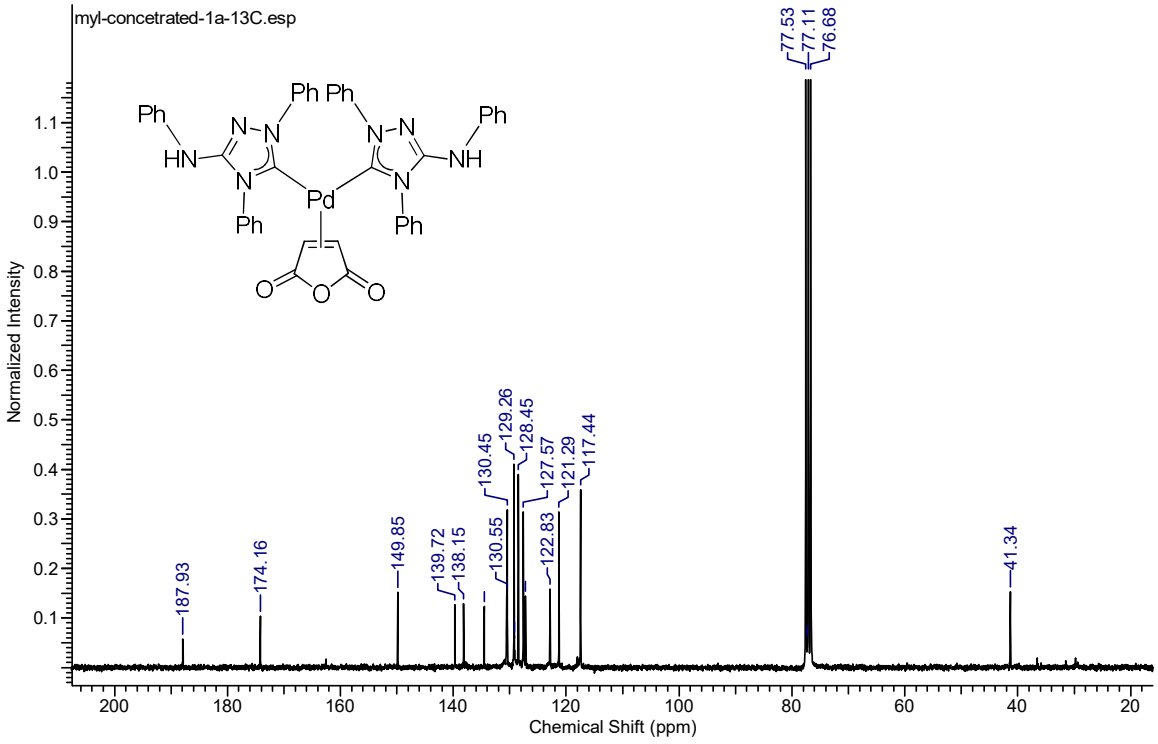


Figure S7. ^{13}C{^{1}H} NMR spectrum of **1a**

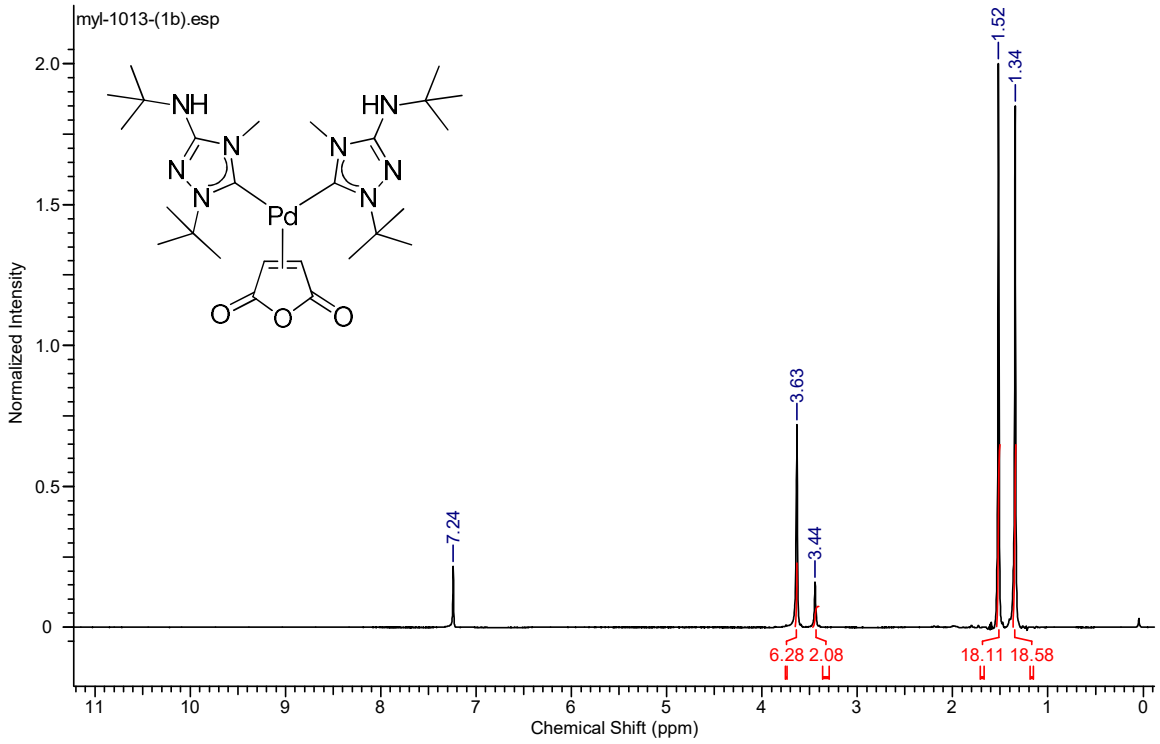


Figure S8. ^{1}H NMR spectrum of **1b**

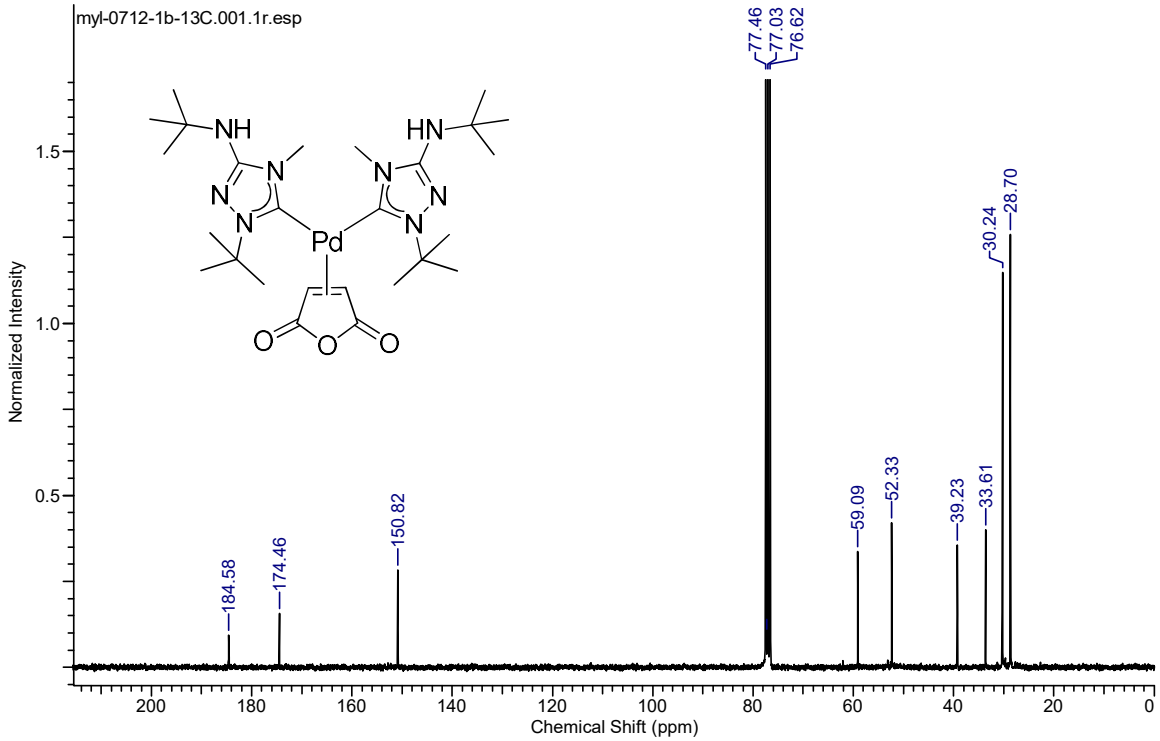


Figure S9. ^{13}C{^{1}H} NMR spectrum of **1b**

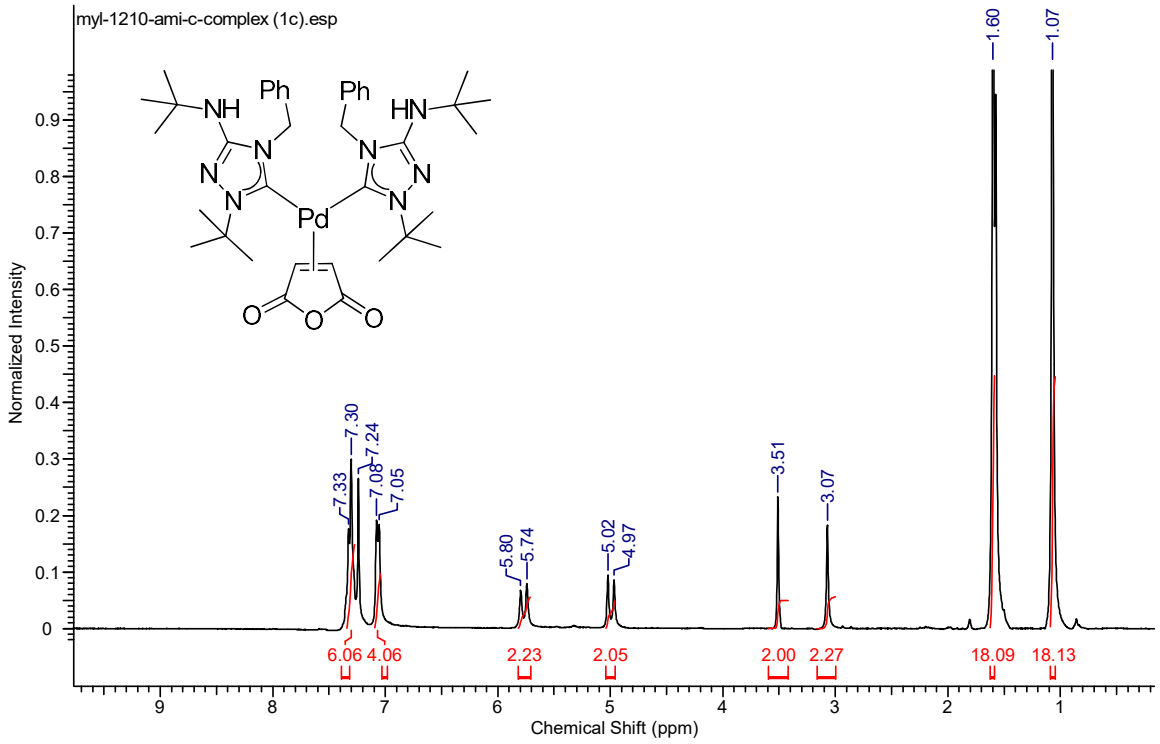


Figure S10. ^{1}H NMR spectrum of **1c**

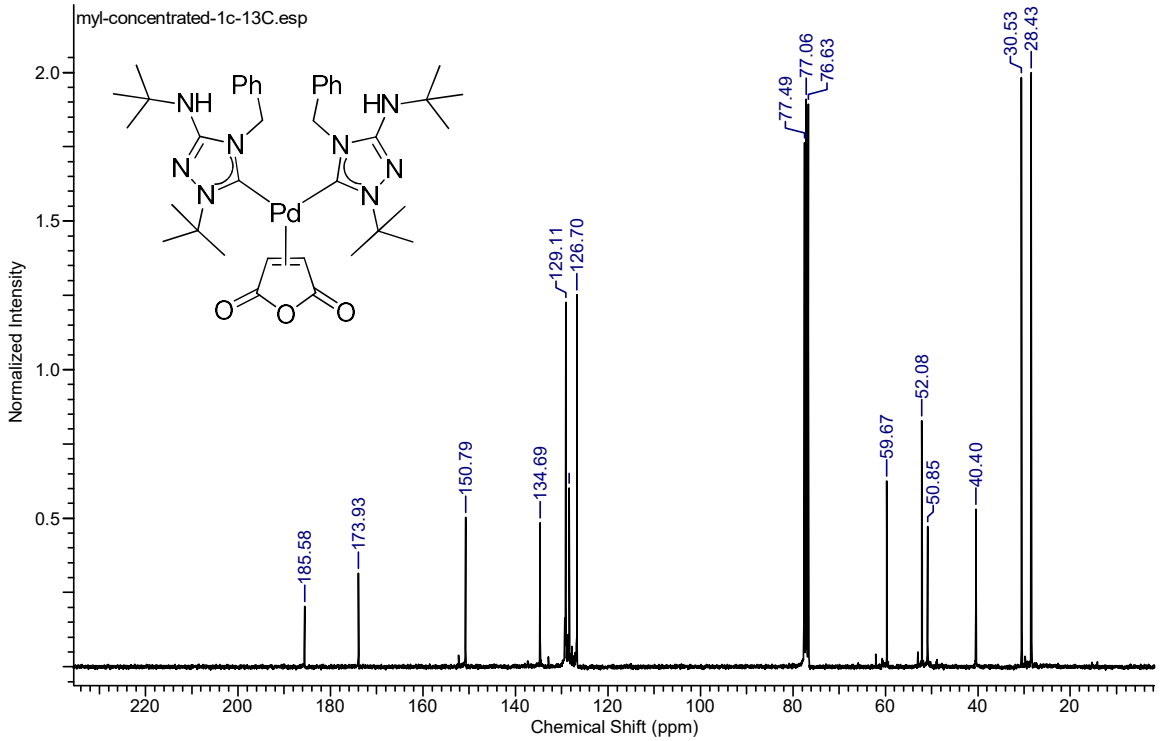


Figure S111. ^{13}C{^{1}H} NMR spectrum of **1c**

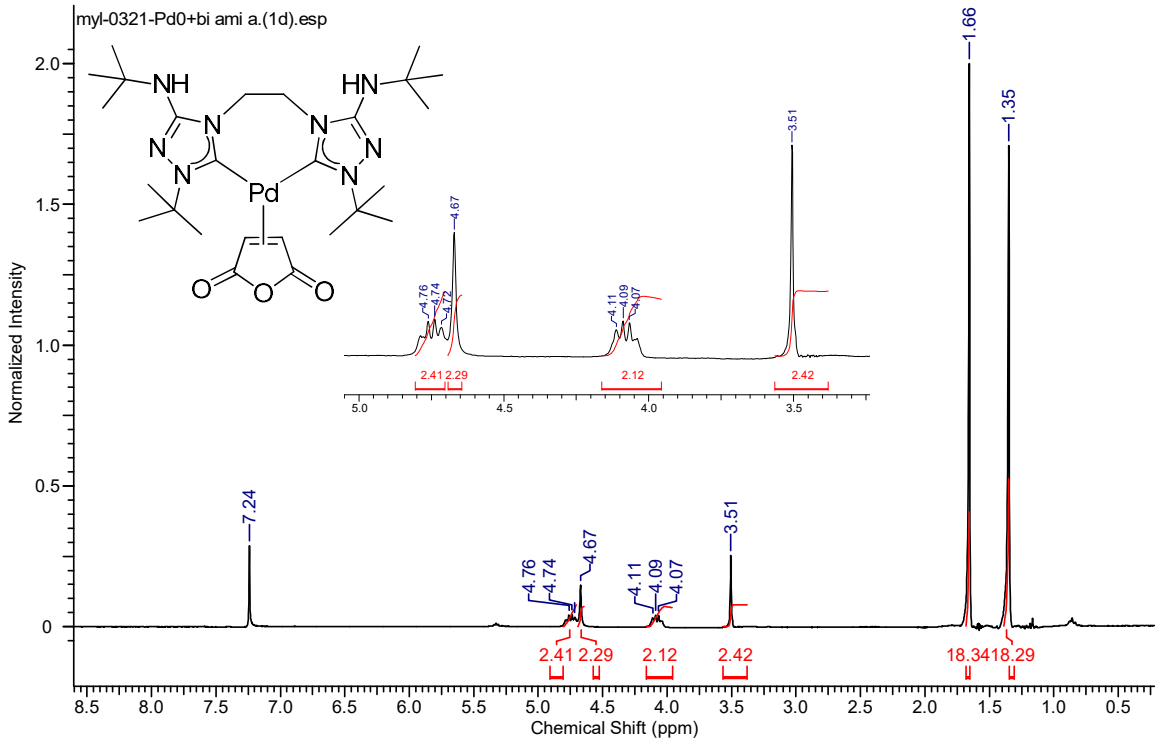


Figure S12. ^{1}H NMR spectrum of **2**

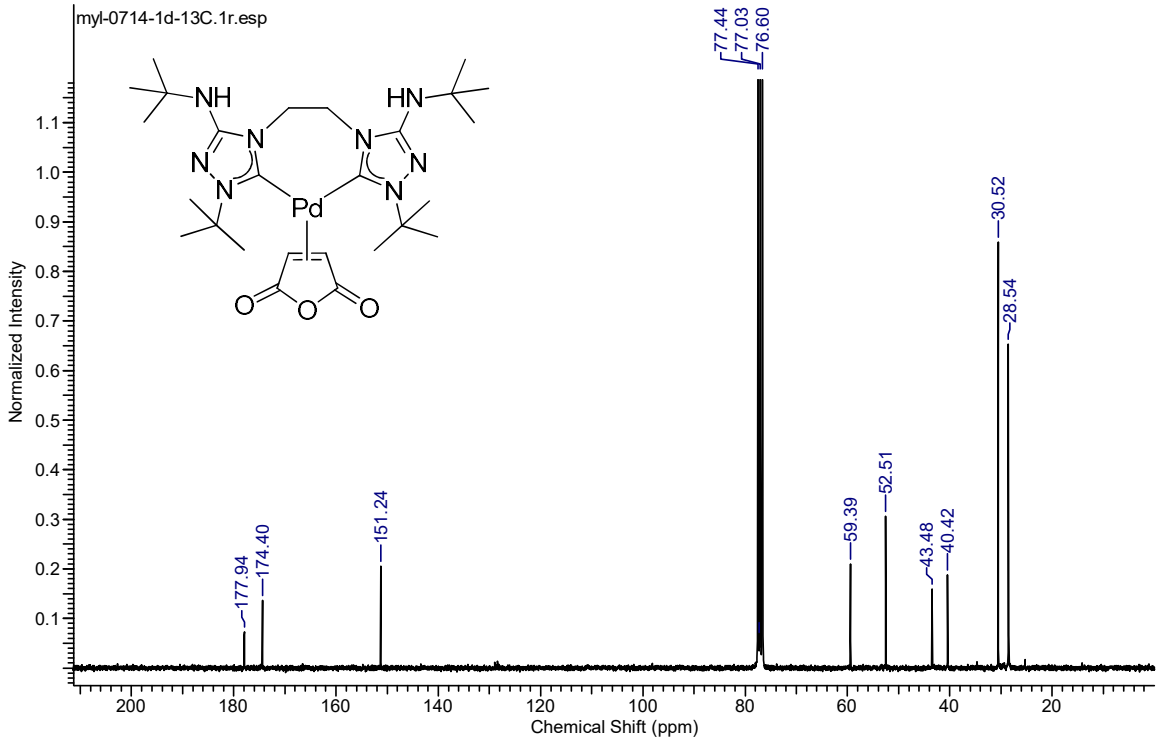


Figure S13. ^{13}C{^{1}H} NMR spectrum of **2**

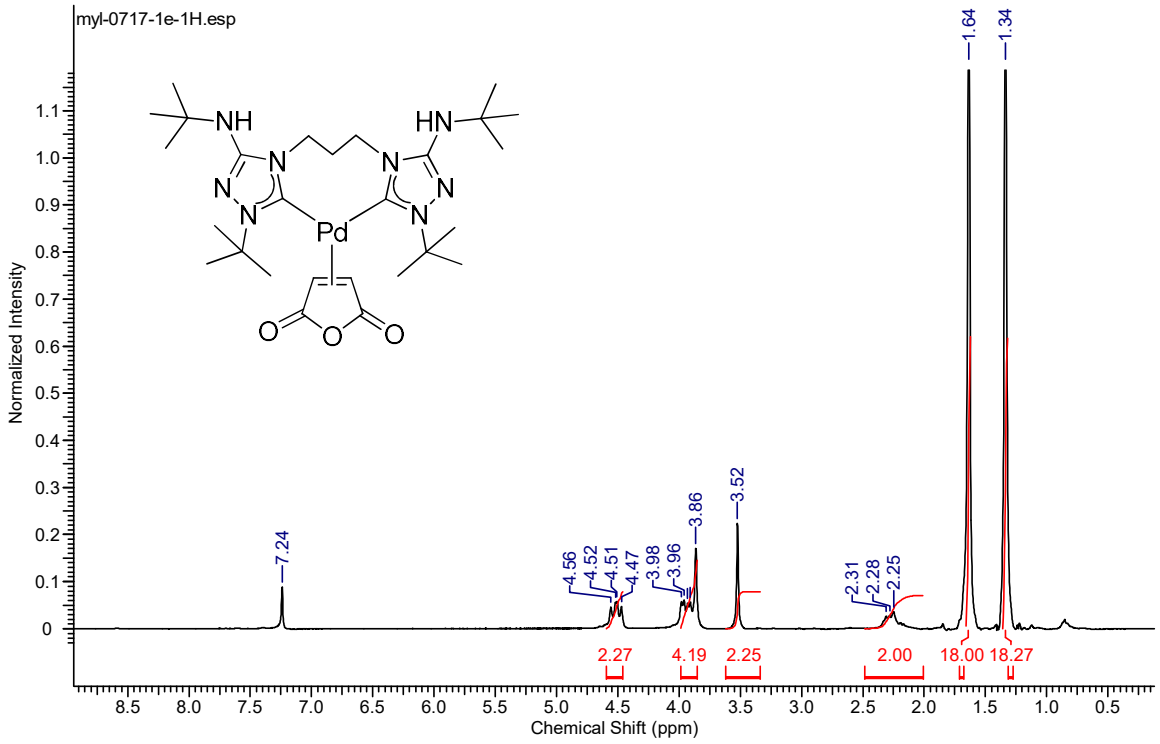


Figure S14. ^{1}H NMR spectrum of **3**

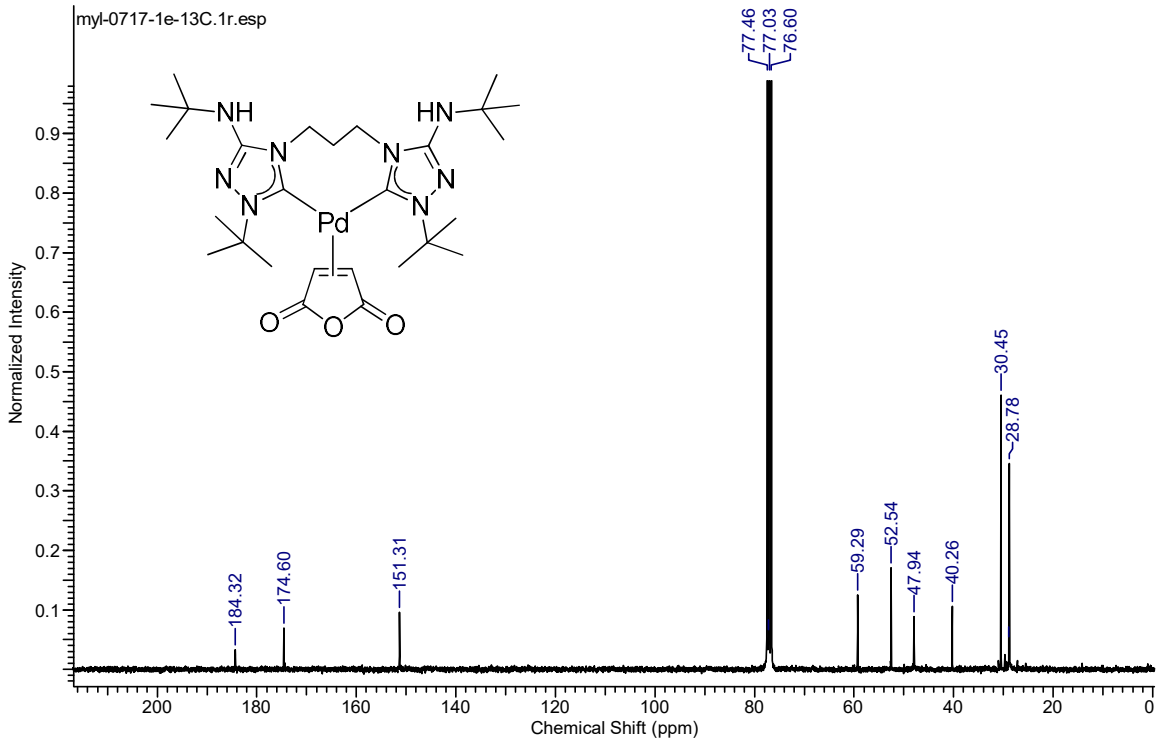


Figure S15. ^{13}C{^{1}H} NMR spectrum of **3**

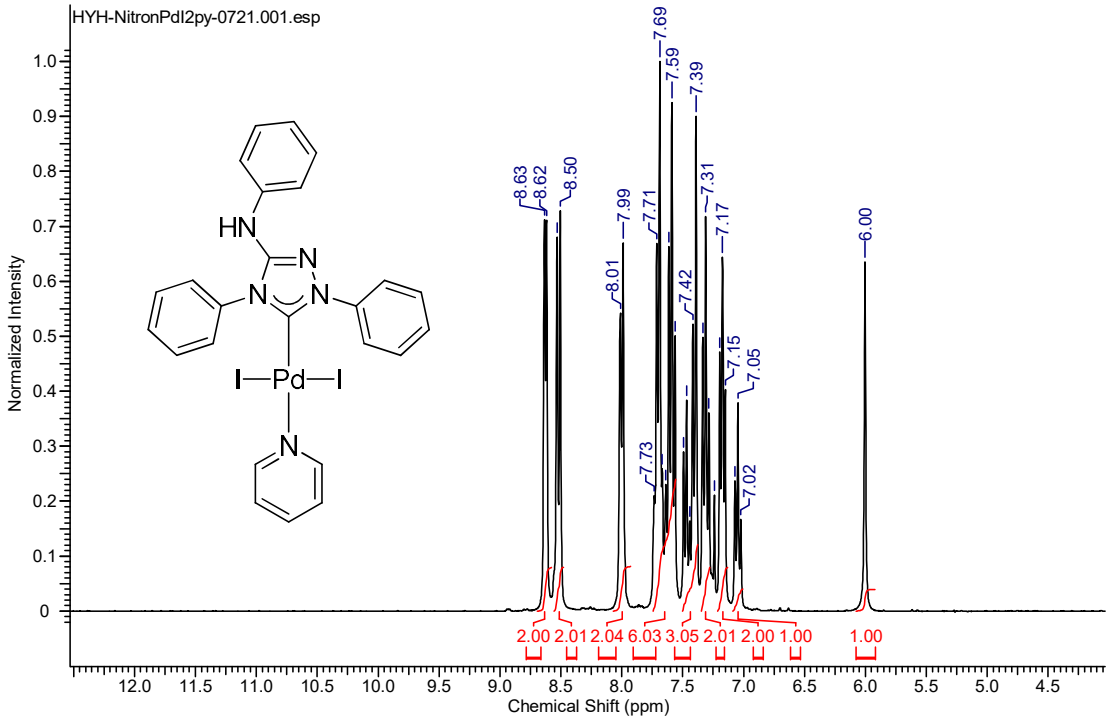


Figure S16. ^{1}H NMR spectrum of **4**

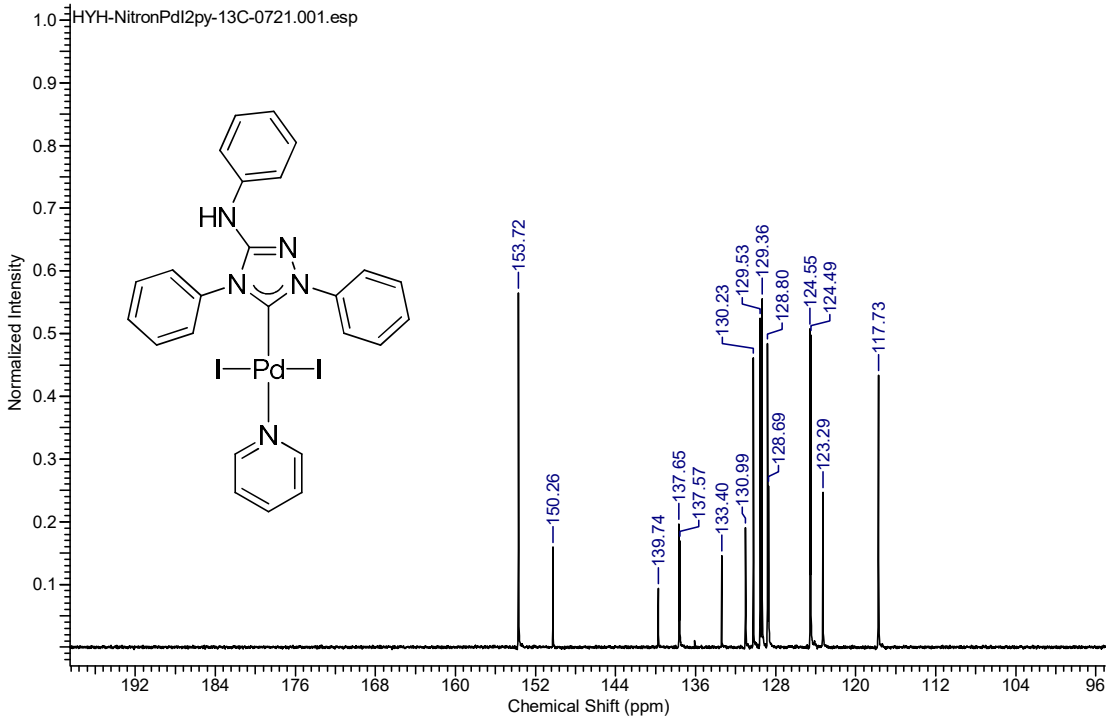


Figure S17. ^{13}C{^{1}H} NMR spectrum of **4**

7. NMR assignments of catalytic products

(*E*)-1-(4-Styrylphenyl)ethanone (5a).[12] ^{1}H NMR ($CDCl_3$): δ 2.59 (s, 3H, C*H*$_3$), 7.11 (d, 1H, *J* = 15.0 Hz, C*H*), 7.22 (d, 1H, *J* = 15.0 Hz, C*H*), 7.28-7.39 (m, 3H, Ar *H*), 7.51-7.58 (m, 4H, Ar *H*), 7.94 (d, 2H, *J* = 6.0 Hz, Ar *H*).

(*E*)-1-Nitro-4-styrylbenzene (5b).[13] ^{1}H NMR ($CDCl_3$): δ 7.12 (d, 1H, *J* = 18.0 Hz, C*H*), 7.26 (d, 1H, *J* = 9.0 Hz, C*H*), 7.32-7.41 (m, 3H, Ar *H*), 7.54 (d, 2H, *J* = 6.0 Hz, Ar *H*), 7.63 (d, 2H, *J* = 9.0 Hz, Ar *H*), 8.21 (d, 2H, *J* = 9.0 Hz, Ar *H*).

(*E*)-4-Styrylbenzonitrile (5c).[13] ^{1}H NMR ($CDCl_3$): δ 7.04 (d, 1H, *J* = 18.0 Hz, C*H*), 7.17 (d, 1H, *J* = 18.0 Hz, C*H*), 7.26-7.36 (m, 3H, Ar *H*), 7.47-7.60 (m, 6H, Ar *H*).

(*E*)-4-Styrylbenzaldehyde (5d).[14] ^{1}H NMR ($CDCl_3$): δ 7.12 (d, 1H, *J* = 15.0 Hz, C*H*), 7.25 (d, 1H, *J* = 18.0 Hz, C*H*), 7.28-7.32 (m, 1H, Ar *H*), 7.35-7.40 (t, 2H, *J* = 15.0 Hz, Ar *H*), 7.53 (d, 2H, *J* = 9.0 Hz, Ar *H*), 7.63 (d, 2H, *J* = 6.0 Hz, Ar *H*), 7.86 (d, 2H, *J* = 9.0 Hz, Ar *H*), 9.97 (s, 1H, CO*H*).

(*E*)-1-Styryl-4-(trifluoromethyl)benzene (5e).[13] ^{1}H NMR ($CDCl_3$): δ 7.10 (d, 1H, *J* = 15.0 Hz, C*H*), 7.19 (d, 1H, *J* = 15.0 Hz, C*H*), 7.27-7.40 (m, 3H, Ar *H*), 7.52 (d, 2H, *J* = 6.0 Hz, Ar *H*), 7.59 (s, 4H, Ar *H*).

(*E*)-Methyl-4-styrylbenzoate (5f).[15] ^{1}H NMR ($CDCl_3$): δ 3.91 (s, 3H, COOC*H*$_3$),δ 7.11 (d, 1H, *J* = 15.0 Hz, C*H*), 7.22 (d, 1H, *J* = 15.0 Hz, C*H*), 7.26-7.39 (m, 3H, Ar *H*), 7.54 (t, 4H, *J* = 8.0 Hz, Ar-*H*), 7.59 (d, 2H, *J* = 6.0 Hz, Ar *H*).

(*E*)-1,2-Diphenylethene (5g).[13] ^{1}H NMR ($CDCl_3$): δ 7.12 (s, 2H, C*H*), 7.26 (d, 2H, *J* = 9.0 Hz,

Ar *H*), 7.36 (t, 4H, *J* = 6.0 Hz, Ar *H*), 7.52 (d, 4H, *J* = 6.0 Hz, Ar *H*).

(*E*)-1-Methoxy-4-styrylbenzene (5h).[13] ^{1}H NMR ($CDCl_3$): δ 3.81 (s, 3H, OC*H*$_3$), 6.89 (d, 2H, *J* = 9.0 Hz, C*H*), 6.92-7.08 (m, 2*H*, Ar *H*), 7.19-7.24 (m, 1H, Ar *H*), 7.33 (t, *J* = 9.0 Hz , 2H , Ar *H*), 7.46 (t, *J* = 9.0 Hz, 4H, Ar *H*).

(*E*)-1-Methoxy-3-styrylbenzene (5i).[16] ^{1}H NMR ($CDCl_3$): δ 3.86 (s, 3H, OC*H*$_3$), 6.85 (d, 1H, *J* = 6.0 Hz, C*H*), 7.10-7.17 (m, 4*H*, C*H*, Ar *H*), 7.26-7.33 (m, 2H, Ar *H*), 7.54 (d, 2H, *J* = 6.0 Hz, Ar *H*).

(*E*)-1-Methoxy-2-styrylbenzene (5j).[17] ^{1}H NMR ($CDCl_3$): δ 3.98 (s, 3H, OC*H*$_3$), 7.01 (d, 1H, *J* = 8.0 Hz, C*H*) , 7.11 (t, 1H, *J* = 7.0 Hz, Ar *H*), 7.27 (d, 1H, *J* = 16.0 Hz, C*H*), 7.38 (t, 2H, *J* = 7.0 Hz, Ar *H*), 7.49 (t, 2H, *J* = 7.0 Hz, Ar *H*), 7.10-7.17 (m, 4*H*, C*H*, Ar *H*), 7.65-7.76 (m, 4H, Ar *H*).

1-[4-[(1*E*)-2-(4-Methoxyphenyl)ethenyl]phenyl]ethanone (5k).[18] ^{1}H NMR ($CDCl_3$): δ 2.58 (s, 3H, C*H*$_3$), 3.82 (s, 3H, OC*H*$_3$), 6.90 (d, 2H, *J* = 8.0 Hz, Ar *H*), 6.97 (d, 1H, *J* = 16.0 Hz, C*H*), 7.16 (d, 1H, *J* = 16.0 Hz, C*H*), 7.46 (d, 2H, *J* = 8.0 Hz, Ar *H*), 7.53 (d, 2H, *J* = 8.0 Hz, Ar *H*), 7.92 (d, 2H, *J* = 8.0 Hz, Ar *H*).

(*E*)-1-Methoxy-4-(4-nitrostyryl)benzene (5l).[19] ^{1}H NMR ($CDCl_3$): δ 3.83 (s, 3H, OC*H*$_3$), 6.90 (d, 2H, *J* = 8.0 Hz, Ar *H*), 6.99 (d, 1H, *J* = 16.0 Hz, C*H*), 7.21 (d, 1H, *J* = 16.0 Hz, C*H*), 7.48 (d, 2H, *J* = 8.0 Hz, Ar *H*), 7.58 (d, 2H, *J* = 8.0 Hz, Ar *H*), 8.18 (d, 2H, *J* = 8.0 Hz, Ar *H*).

(*E*)-4-(4-Methoxystyryl)benzaldehyde (5m).[20] ^{1}H NMR ($CDCl_3$): δ 3.83 (s, 3H, OC*H*$_3$), 6.91 (d, 2H, *J* = 8.0 Hz, Ar *H*), 6.99 (d, 1H, *J* = 16.0 Hz, C*H*), 7.21 (d, 1H, *J* = 16.0 Hz, C*H*), 7.48 (d, 2H, *J* = 8.0 Hz, Ar *H*), 7.61 (d, 2H, *J* = 8.0 Hz, Ar *H*), 7.84 (d, 2H, *J* = 8.0 Hz, Ar *H*), 9.96 (s, 1H, CO*H*).

(*E*)-1,2-bis(4-methoxyphenyl)ethene (5n).[21] ^{1}H NMR ($CDCl_3$): δ 3.81 (s, 6H, OC*H*$_3$), 6.86-6.91 (m, 6H, C*H*, Ar *H*), 7.41 (d, 4H, *J* = 6.0 Hz, Ar *H*).

(*E*)-Butyl-3-(4-acetylphenyl)acrylate (5o).[22] ^{1}H NMR ($CDCl_3$): δ 0.87 (t, 3H, *J* = 9.0 Hz, C*H*$_3$), 1.34 (sext, 2H, *J* = 6.0 Hz, C*H*$_2$), 1.60 (quint, 2H, *J* = 6.0Hz, C*H*$_2$), 2.51 (s, 3H, C*H*$_3$), 4.12 (t, 2H, *J* = 6.0 Hz, C*H*$_2$), 6.43 (d, 1H, *J* = 18.0 Hz, C*H*), 7.51 (d, 2H, *J* = 9.0 Hz, Ar *H*), 7.59 (d, 1H, *J* = 18.0 Hz, C*H*),7.87 (d, 2H, *J* = 9.0 Hz, Ar *H*).

(*E*)-Butyl 3-(4-nitrophenyl)acrylate (5p).[23] ^{1}H NMR ($CDCl_3$): δ 0.95 (t, 3H, *J* = 9.0 Hz, C*H*$_3$), 1.42 (sext, 2H, *J* = 6.0 Hz, C*H*$_2$), 1.68 (quint, 2H, *J* = 6.0 Hz, C*H*$_2$), 4.21 (t, 2H, *J* = 6.0 Hz, C*H*$_2$), 6.55 (d, 1H, *J* = 18.0 Hz, C*H*), 7.64-7.71 (m, 3H, C*H*, Ar *H*), 8.23 (d, 2H, *J* = 9.0 Hz, Ar *H*).

(*E*)-Butyl 3-(4-cyanophenyl)acrylate (5q).[24] ^{1}H NMR ($CDCl_3$): δ 0.94 (t, 3H, *J* = 9.0 Hz, C*H*$_3$), 1.41 (sext, 2H, *J* = 6.0 Hz, C*H*$_2$), 1.67 (quint, 2H, *J* = 6.0 Hz, C*H*$_2$), 4.20 (t, 2H, *J* = 6.0 Hz, C*H*$_2$), 6.50 (d, 1H, *J* = 18.0 Hz, C*H*), 7.57-7.67 (m, 5H, C*H*, Ar *H*).

Butyl (*E*)-3-(4-formylphenyl)-2-propenoate (5r).[25] ^{1}H NMR ($CDCl_3$): δ 0.87 (t, 3H, *J* = 9.0 Hz, C*H*$_3$), 1.35 (sext, 2H, *J* = 6.0 Hz, C*H*$_2$), 1.60 (quint, 2H, *J* = 6.0Hz, C*H*$_2$), 4.13 (t, 2H, *J* = 6.0 Hz, C*H*$_2$), 6.46 (d, 1H, *J* = 18.0 Hz, C*H*), 7.64-7.71 (m, 3H, C*H*, Ar *H*), 7.80 (d, 2H, *J* = 9.0 Hz, Ar *H*), 9.97 (s, 1H, CO*H*).

Butyl (2*E*)-3-[4-(trifluoromethyl)phenyl]-2-propenoate (5s).[24] ^{1}H NMR ($CDCl_3$): δ 0.94 (t, 3H, *J* = 9.0 Hz, C*H*$_3$), 1.41 (sext, 2H, *J* = 6.0 Hz, C*H*$_2$), 1.67 (quint, 2H, *J* = 6.0 Hz, C*H*$_2$), 4.20 (t, 2H, *J* = 6.0 Hz, C*H*$_2$), 6.49 (d, 1H, *J* = 16.0 Hz, C*H*), 7.59 (m, 4H, Ar *H*), 7.66 (d, 1H, *J* = 16.0 Hz, C*H*).

Butyl (*E*)-3-phenylpropenoate (5t).[26] ^{1}H NMR ($CDCl_3$): δ 0.94 (t, 3H, *J*= 9.0 Hz, C*H*$_3$), 1.41 (sext, 2H, *J* = 6.0 Hz, C*H*$_2$), 1.67 (quint, 2H, *J* = 6.0Hz, C*H*$_2$), 4.19 (t, 2H, *J* = 6.0 Hz, C*H*$_2$), 6.43 (d, 1H, *J* = 16.0 Hz, C*H*), 7.36-7.37 (m, 3H, Ar *H*), 7.50-7.51 (m, 2H, Ar *H*) 7.67 (d, 1H, *J* = 16.0 Hz, C*H*).

(*E*)-Butyl 3-(4-methoxyphenyl)acrylate (5u).[27] ^{1}H NMR ($CDCl_3$): δ 0.94 (t, 3H, *J*= 9.0 Hz, C*H*$_3$), 1.41 (sext, 2H, *J* = 6.0 Hz, C*H*$_2$), 1.66 (quint, 2H, *J* = 6.0Hz, C*H*$_2$), 3.81 (s, 3H, OC*H*$_3$), 4.17 (t, 2H, *J* = 6.0 Hz, C*H*$_2$), 6.29 (d, 1H, *J* = 16.0 Hz, C*H*), 6.88 (d, 2H, *J* = 9.0 Hz, Ar *H*), 7.46 (d, 2H, *J* = 9.0 Hz, Ar *H*), 7.62 (d, 1H, *J* = 16.0 Hz, C*H*)

8. NMR spectra of catalytic products

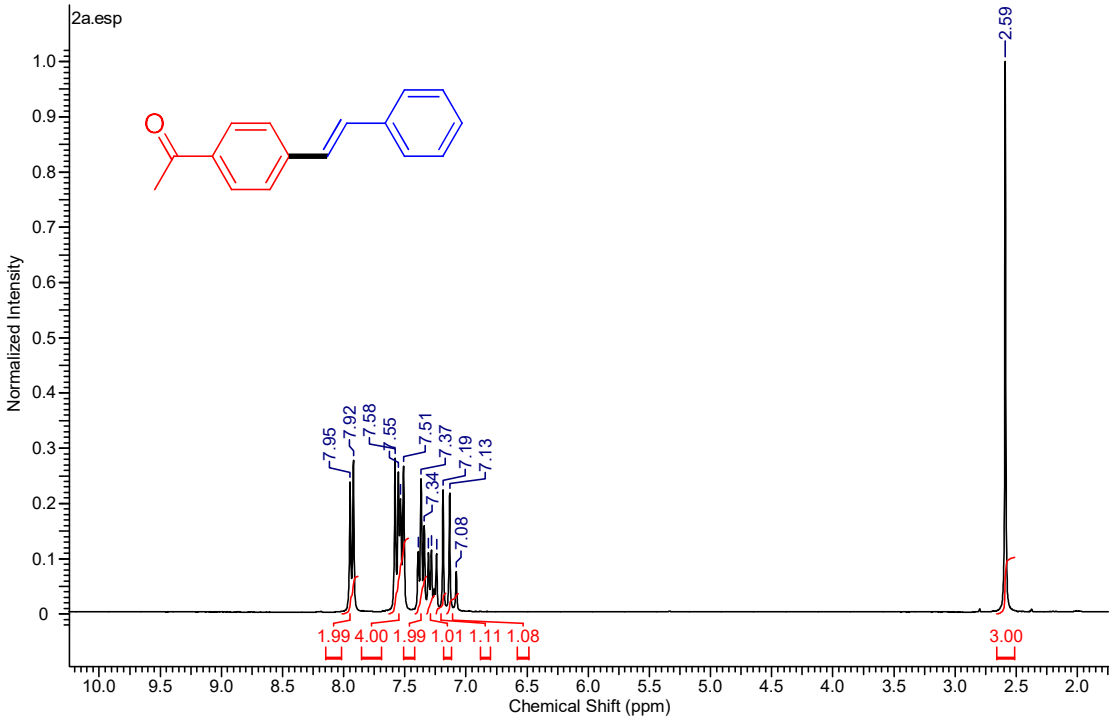


Figure S18. ^{1}H NMR spectrum of **5a**

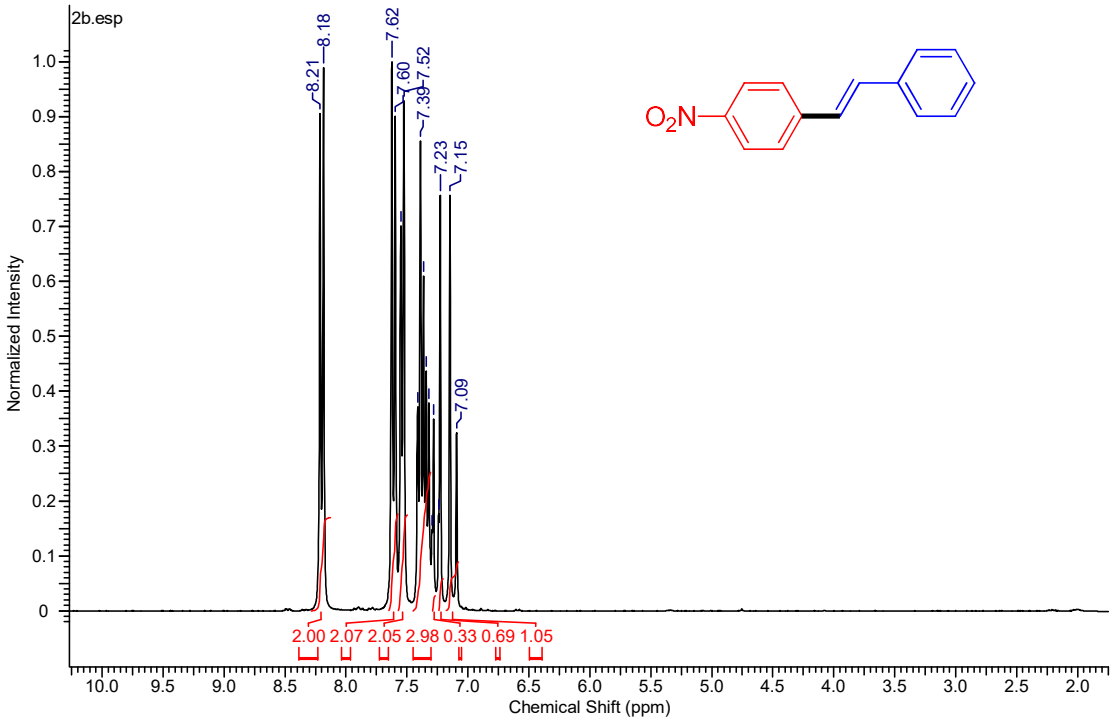


Figure S19. ^{1}H NMR spectrum of **5b**

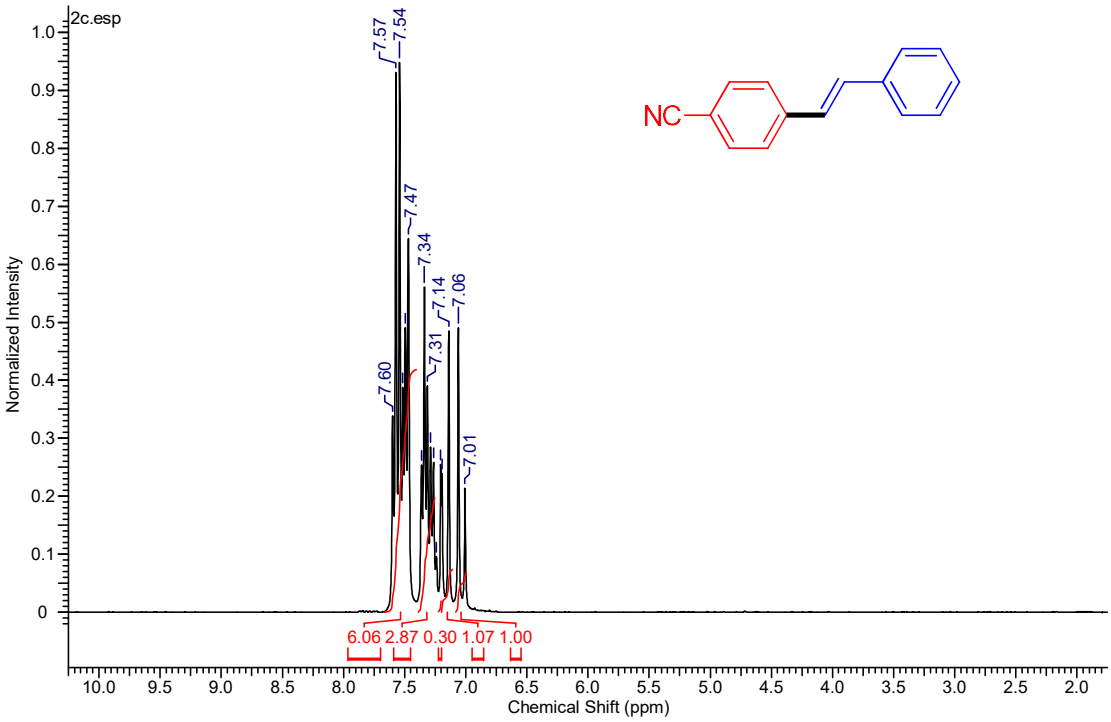


Figure S20. ^{1}H NMR spectrum of **5c**

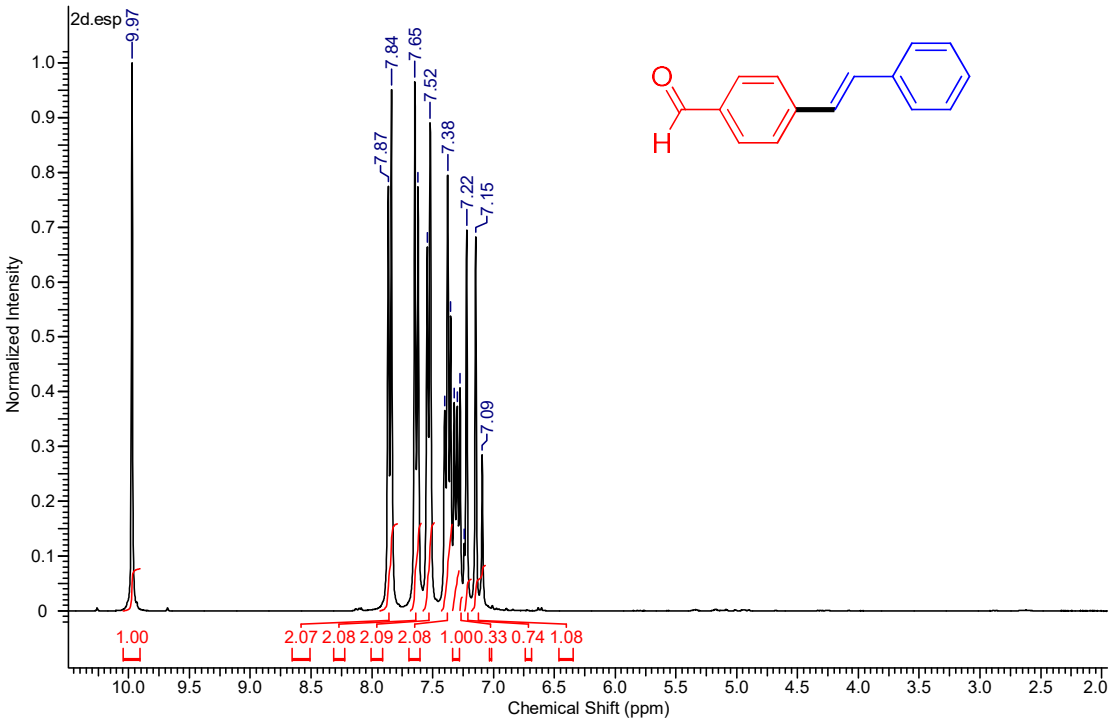


Figure S21. ^{1}H NMR spectrum of **5d**

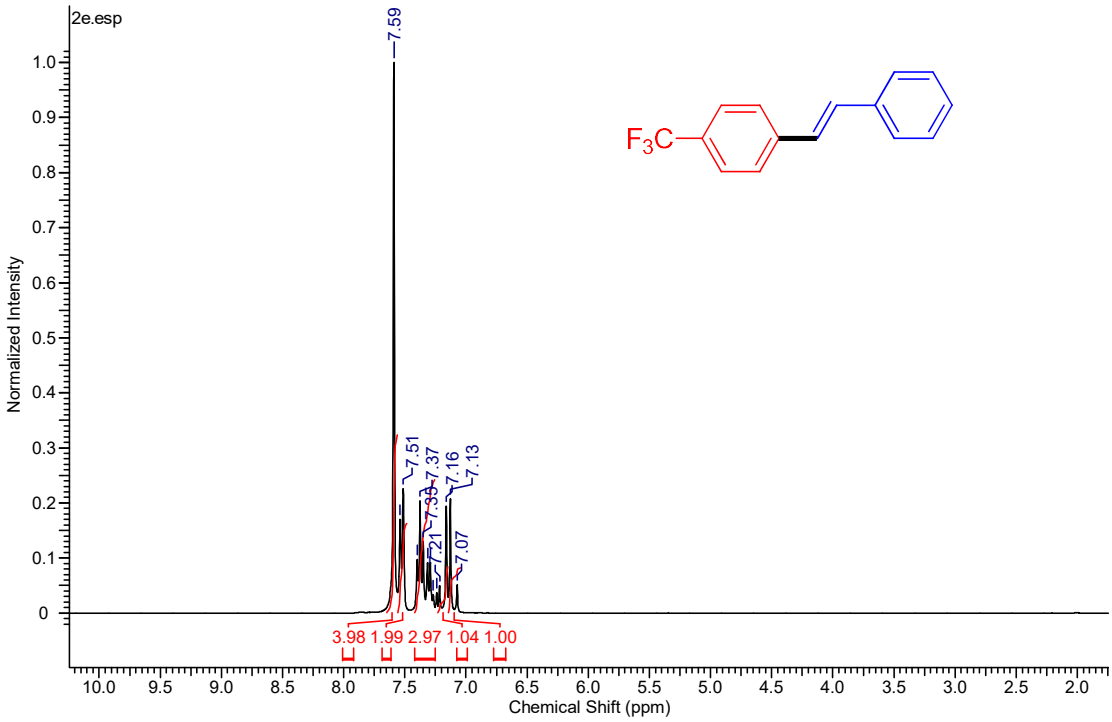


Figure S22. ^{1}H NMR spectrum of **5e**

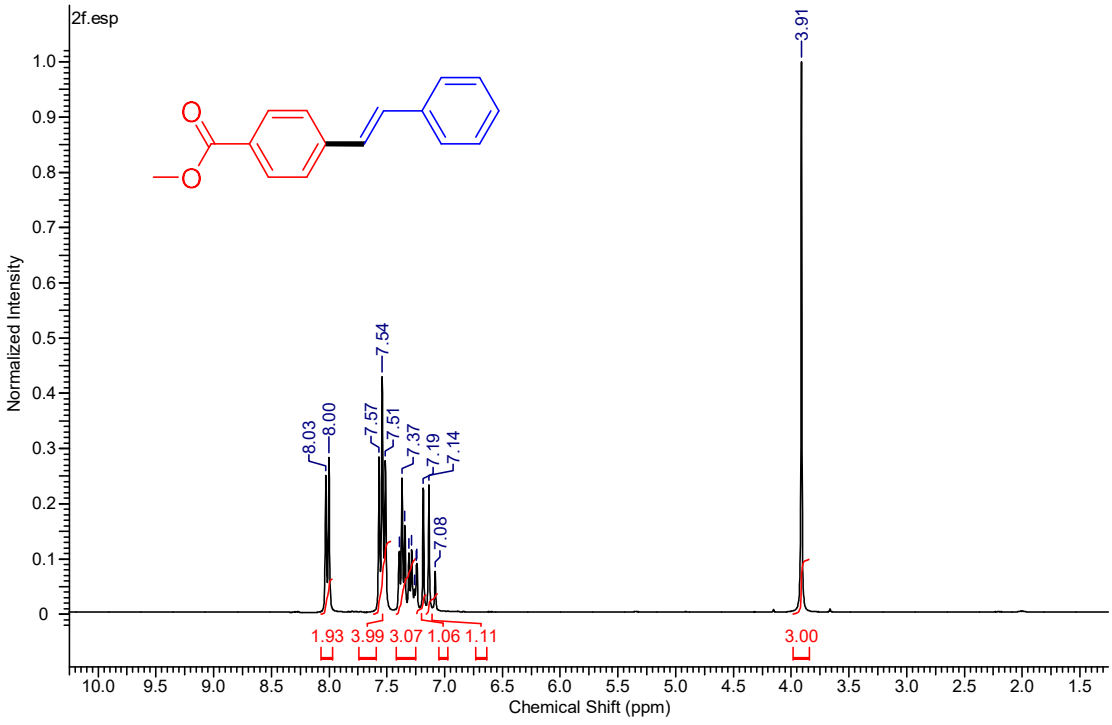


Figure S23. ^{1}H NMR spectrum of **5f**

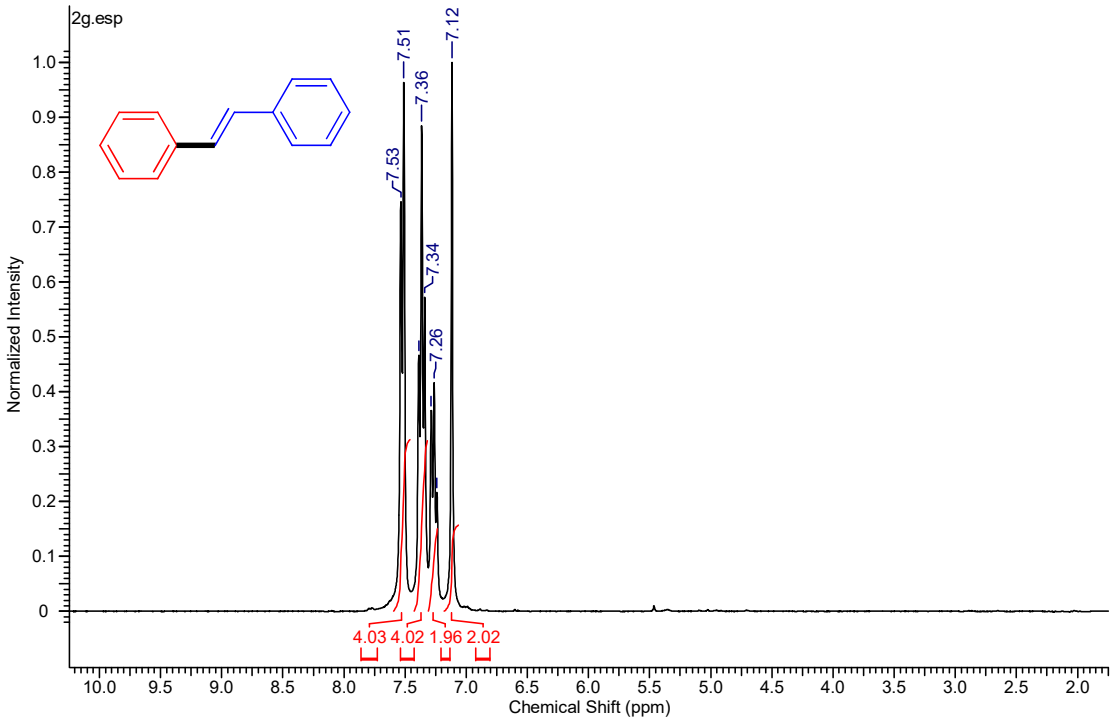


Figure S24. ^{1}H NMR spectrum of **5g**

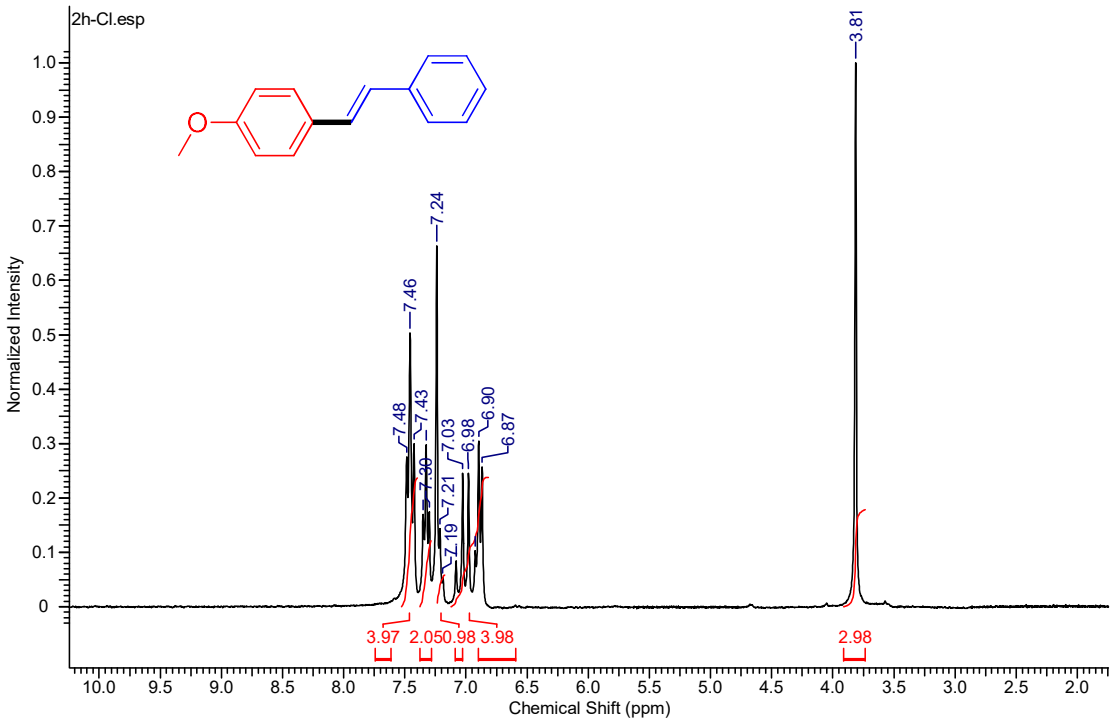


Figure S25. ^{1}H NMR spectrum of **5h**

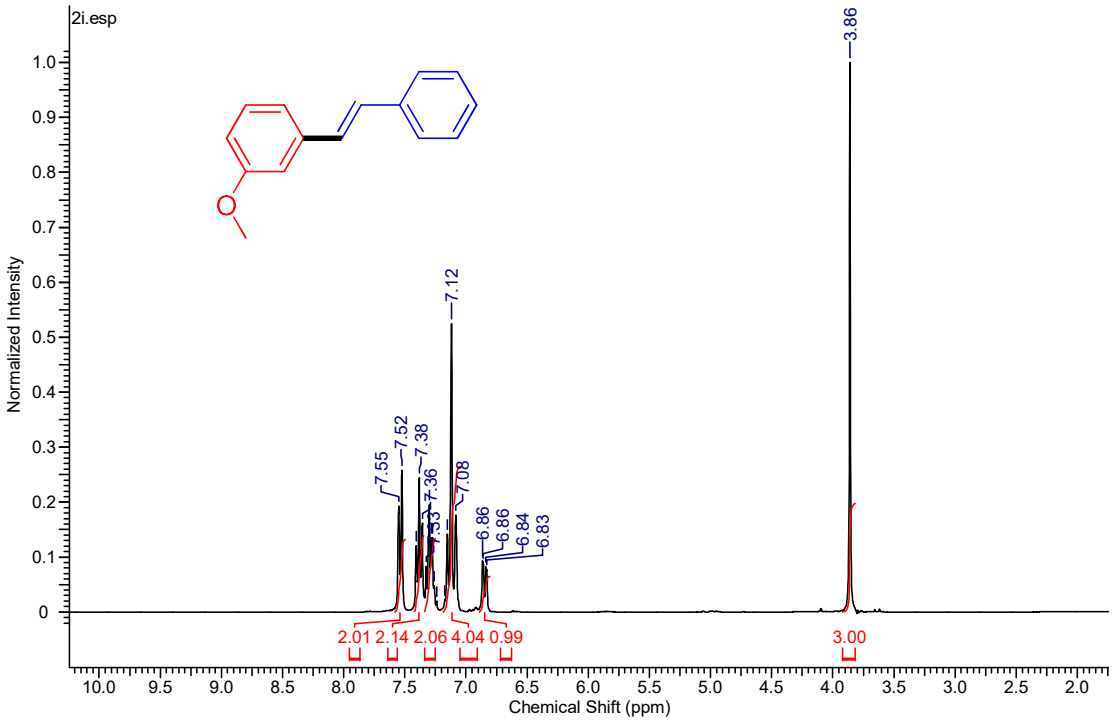


Figure S26. ^{1}H NMR spectrum of **5i**

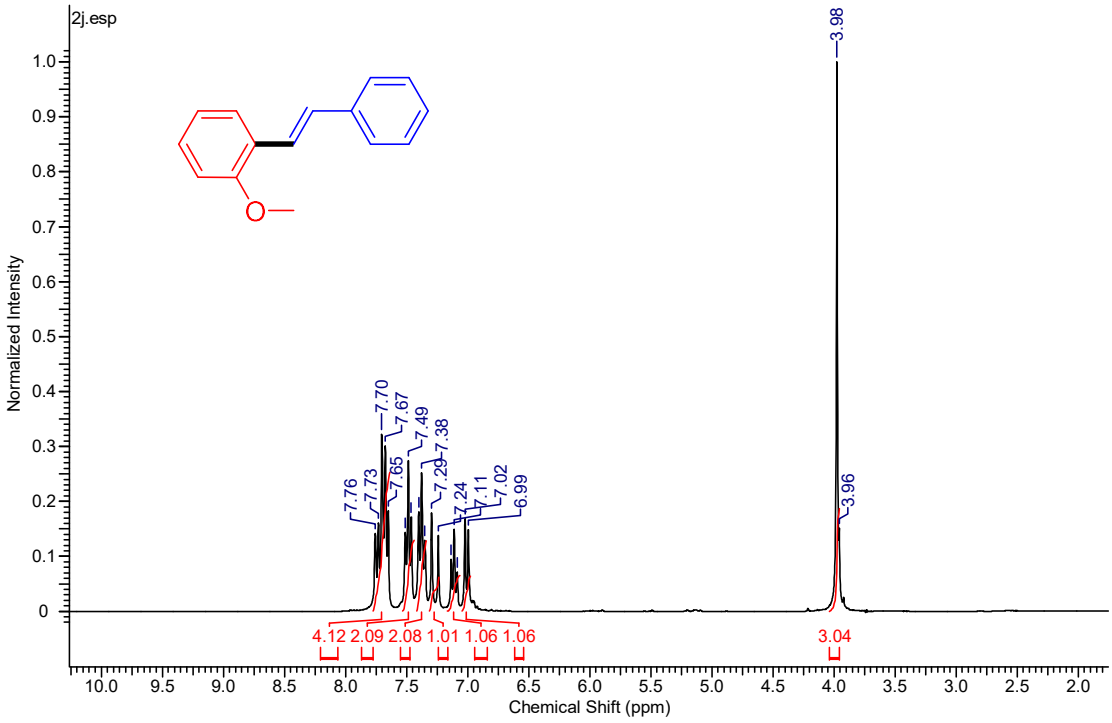


Figure S27. 1H NMR spectrum of **5j**

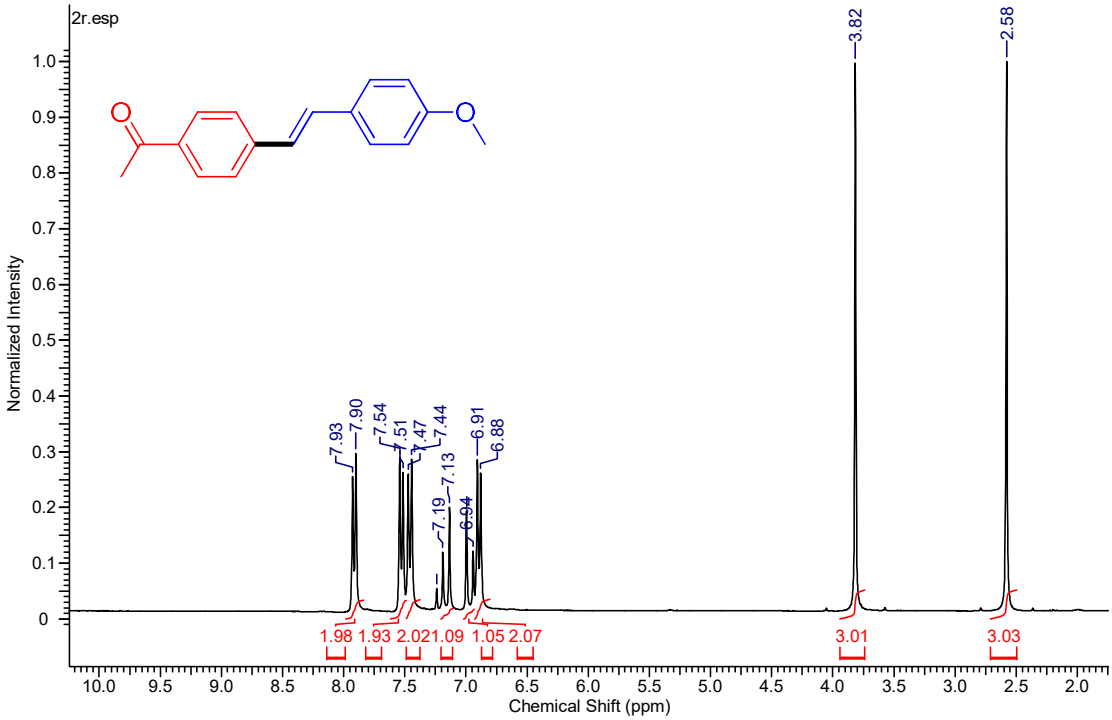


Figure S28. ^{1}H NMR spectrum of **5k**

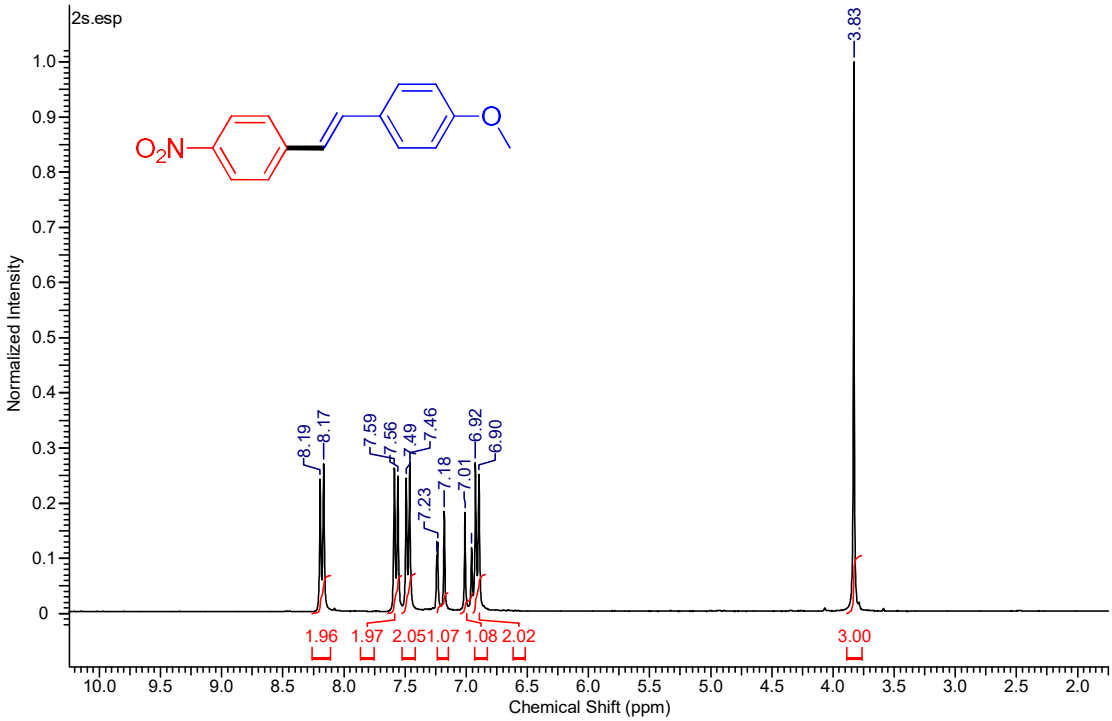


Figure S29. ^{1}H NMR spectrum of **5l**

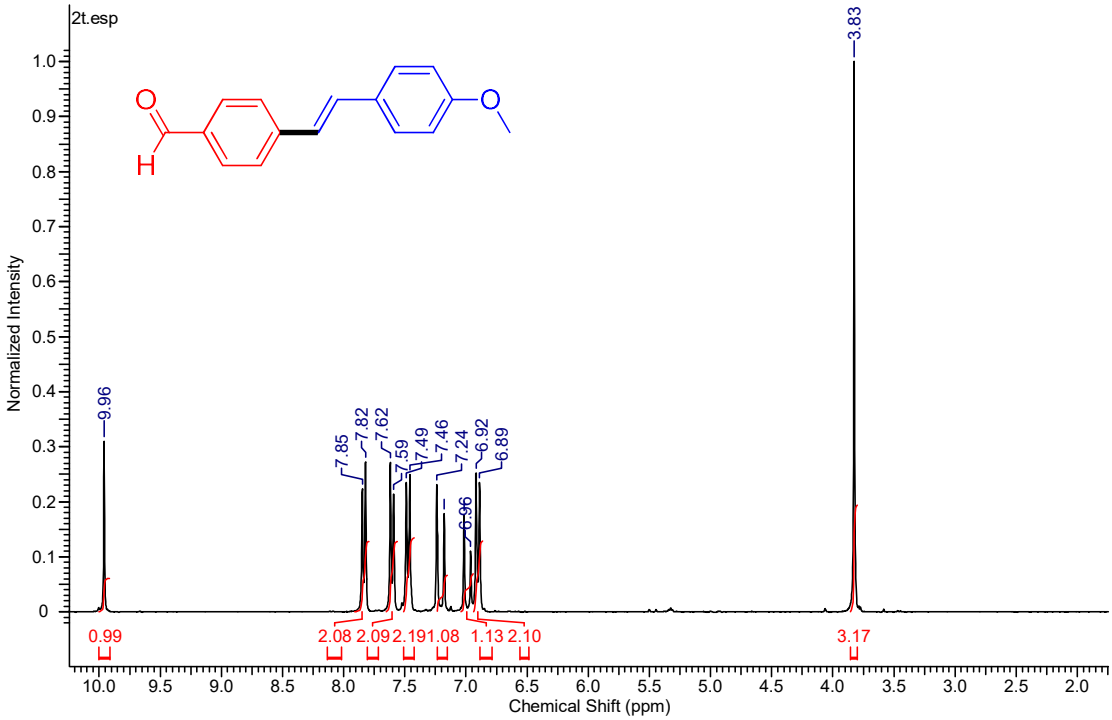


Figure S30. ^{1}H NMR spectrum of **5m**

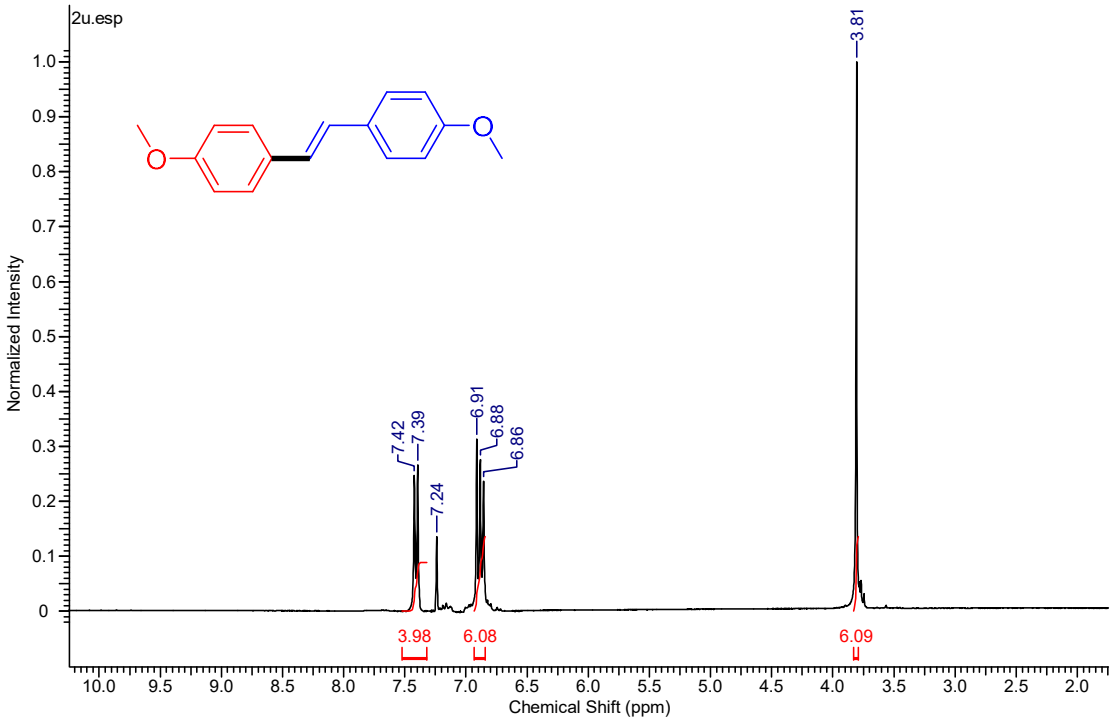


Figure S31. ^{1}H NMR spectrum of **5n**

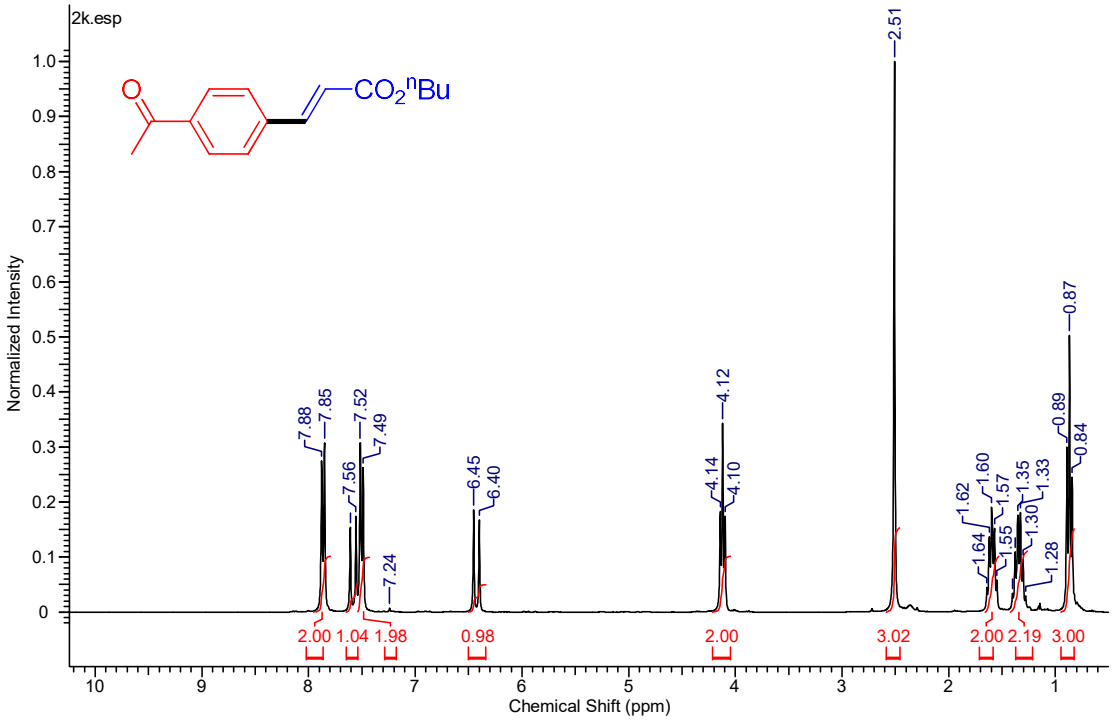


Figure S32. ^{1}H NMR spectrum of **5o**

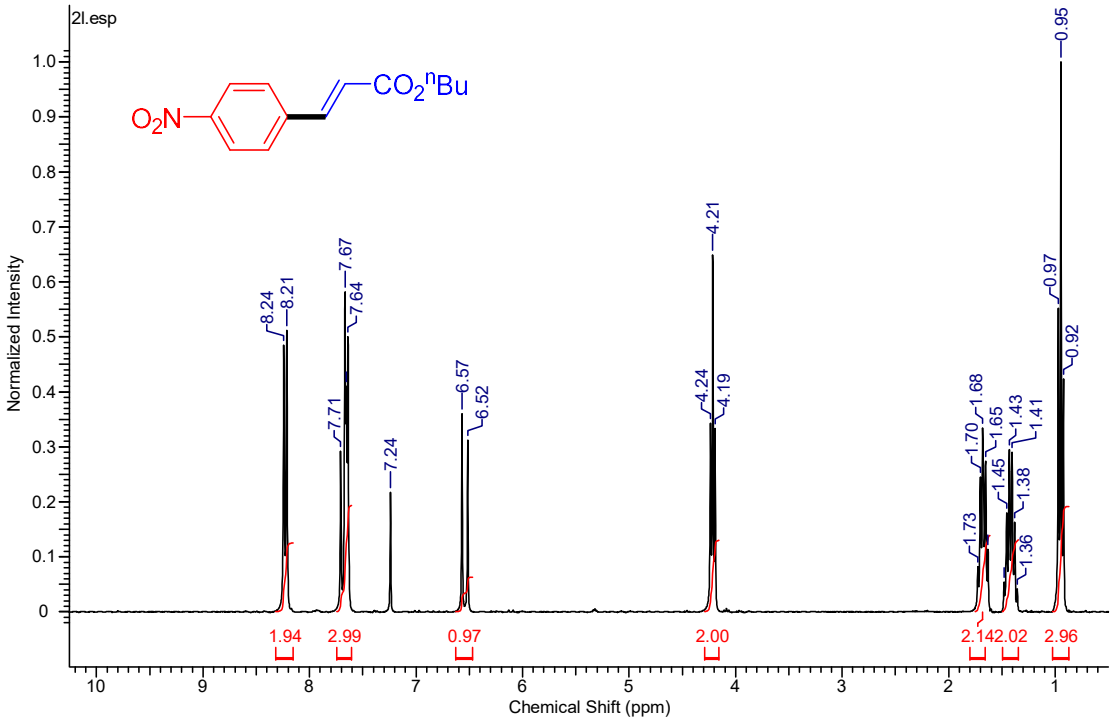


Figure S33. ^{1}H NMR spectrum of **5p**

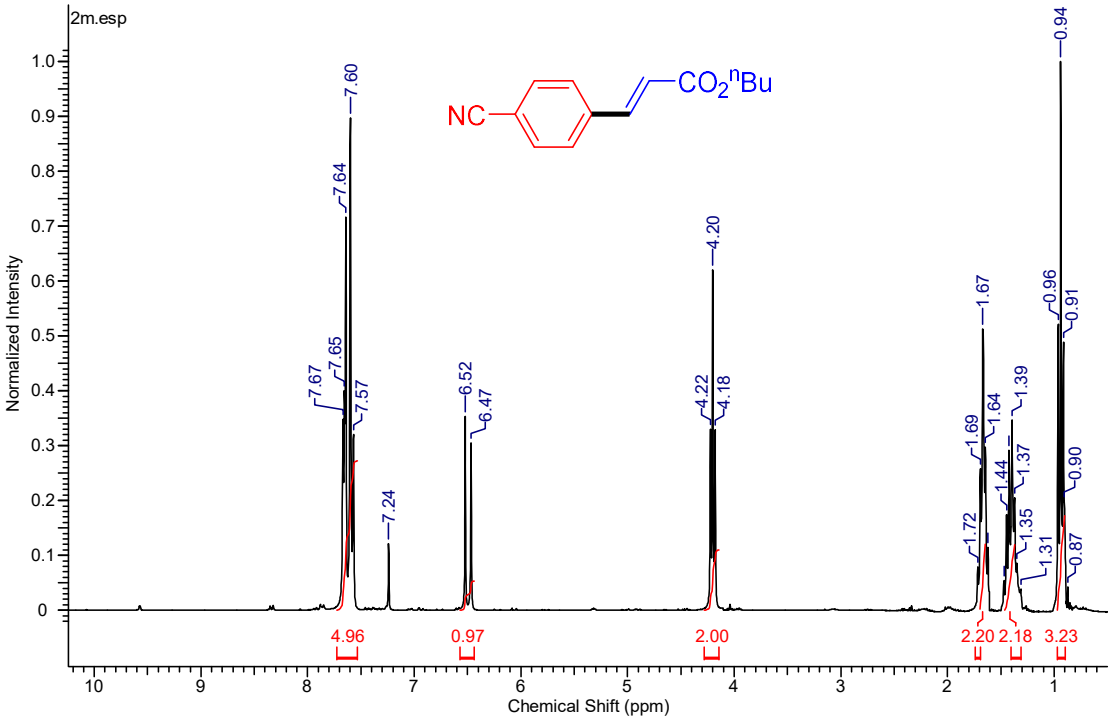


Figure S34. ^{1}H NMR spectrum of **5q**

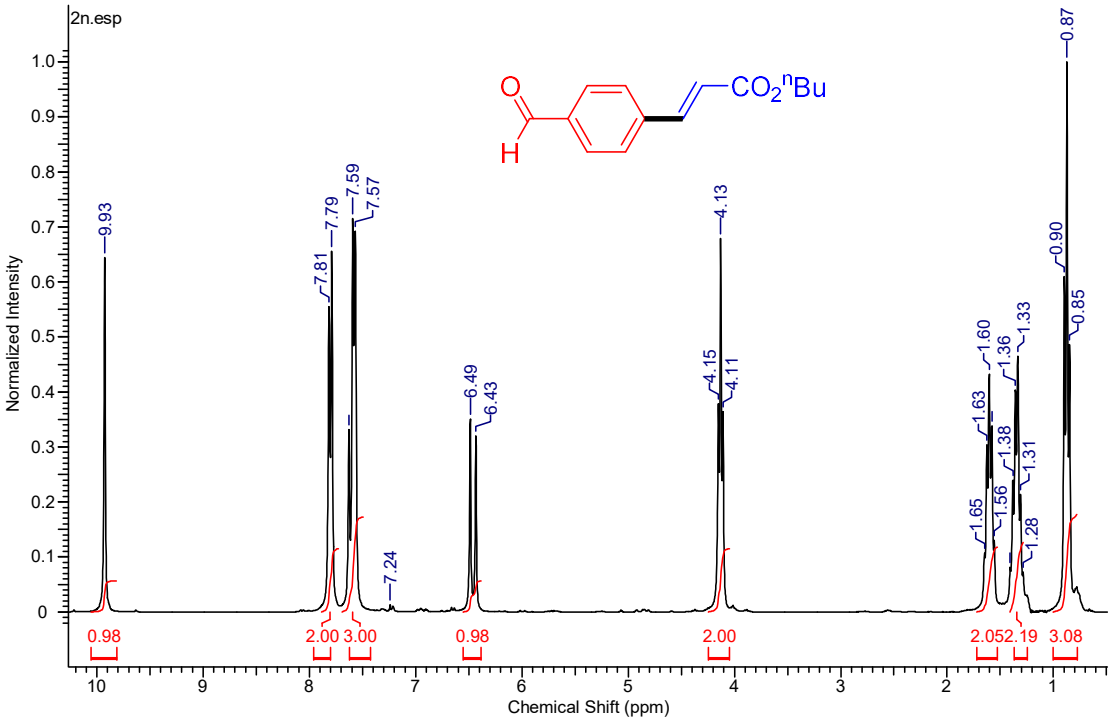


Figure S35. ^{1}H NMR spectrum of **5r**

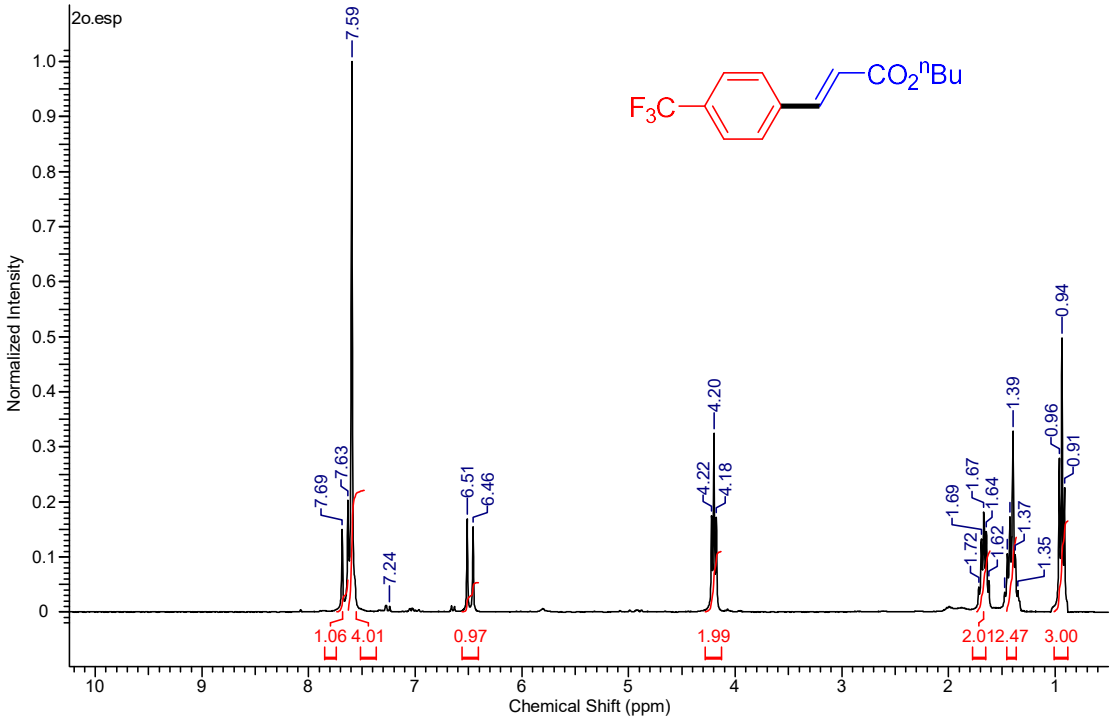


Figure S36. [1]H NMR spectrum of **5s**

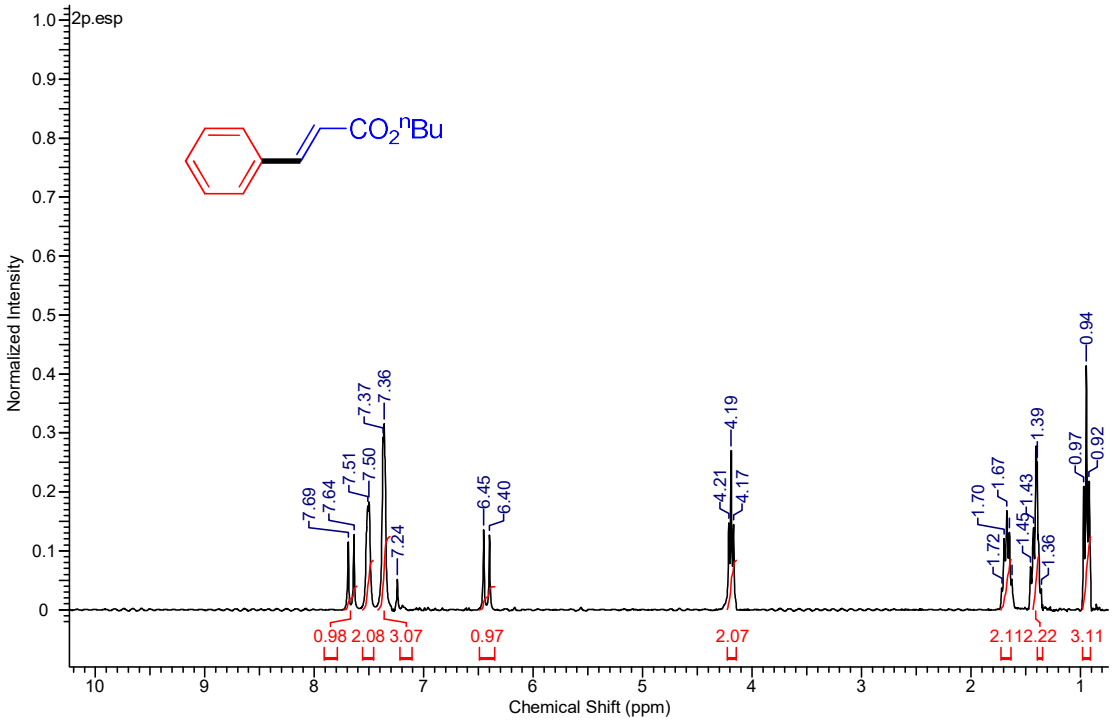


Figure S37. 1H NMR spectrum of **5t**

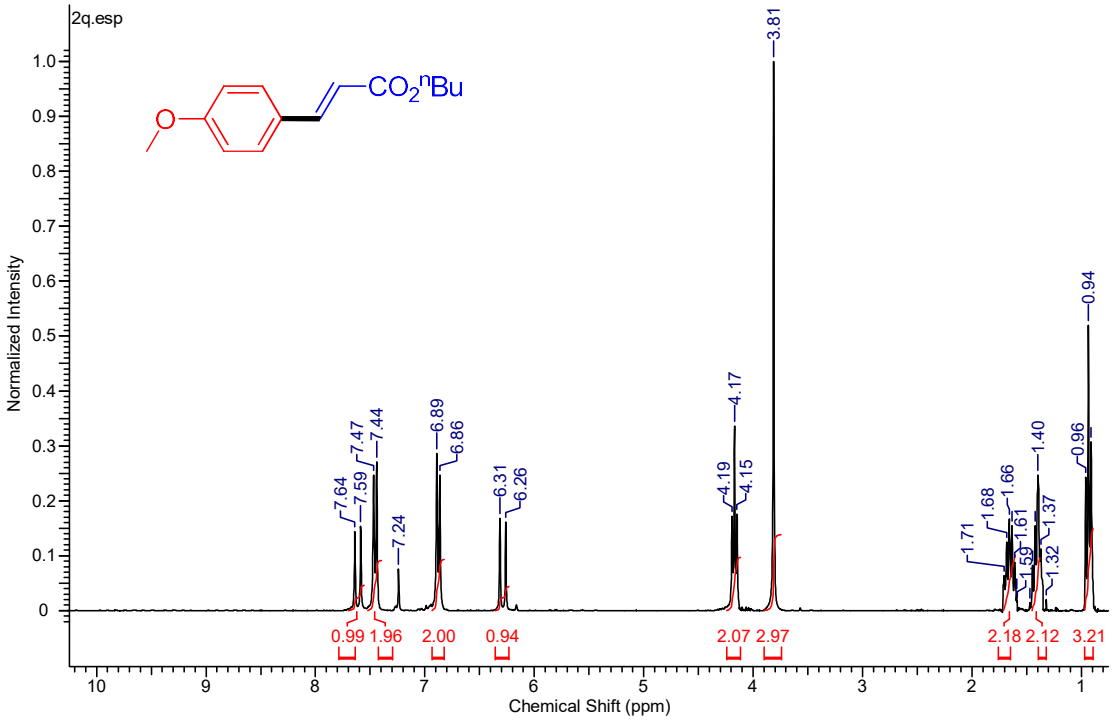


Figure S38. ^{1}H NMR spectrum of **5u**

9. XPS spectra

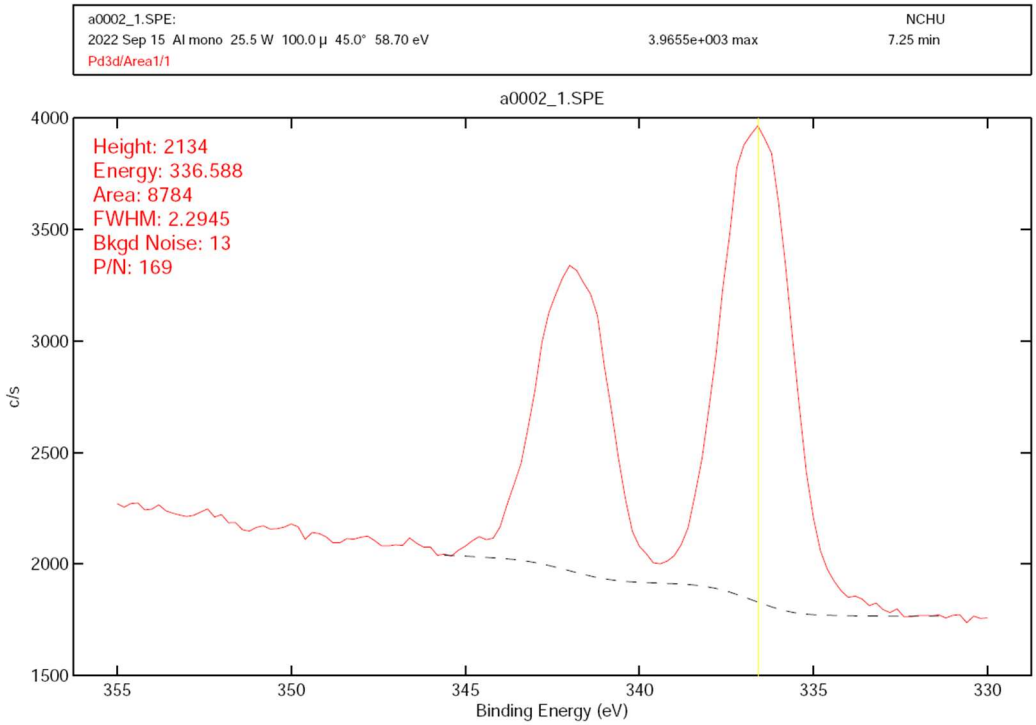


Figure S39. XPS spectrum of **1a**

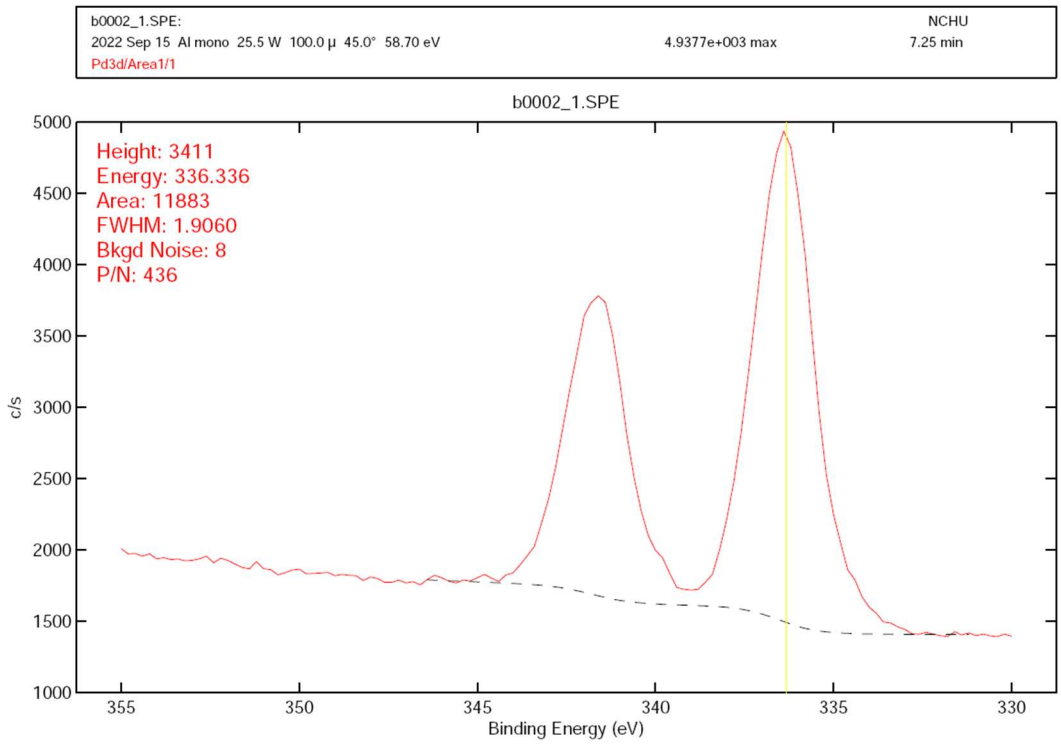


Figure S40. XPS spectrum of **1b**

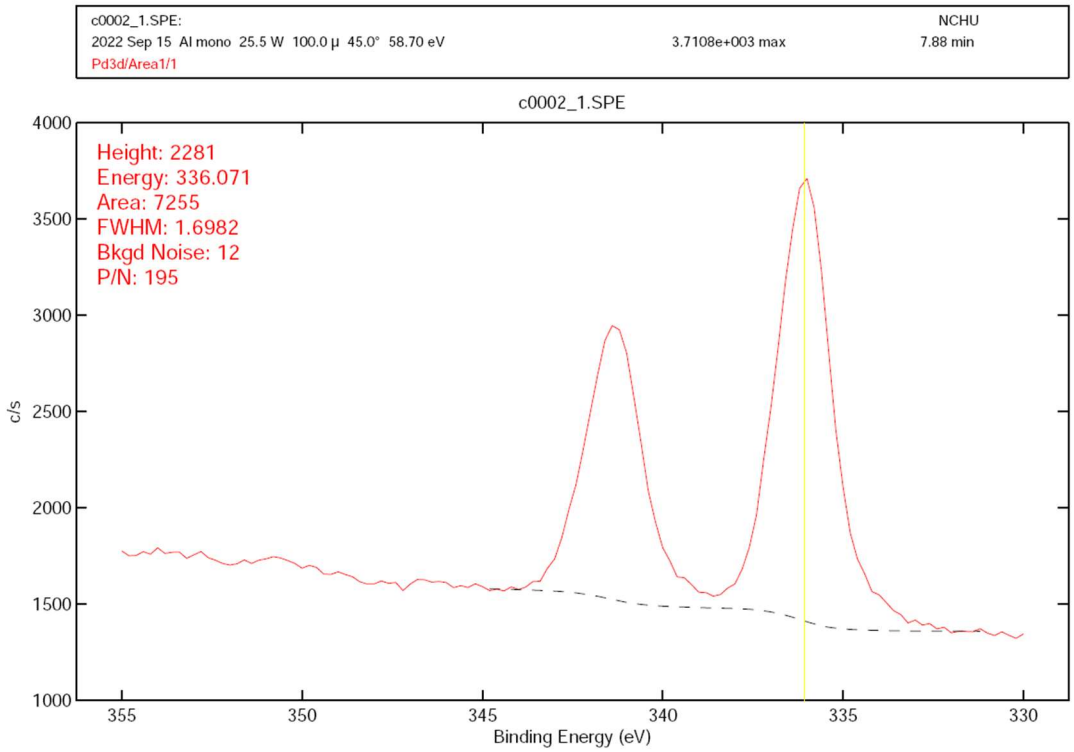


Figure S41. XPS spectrum of **1c**

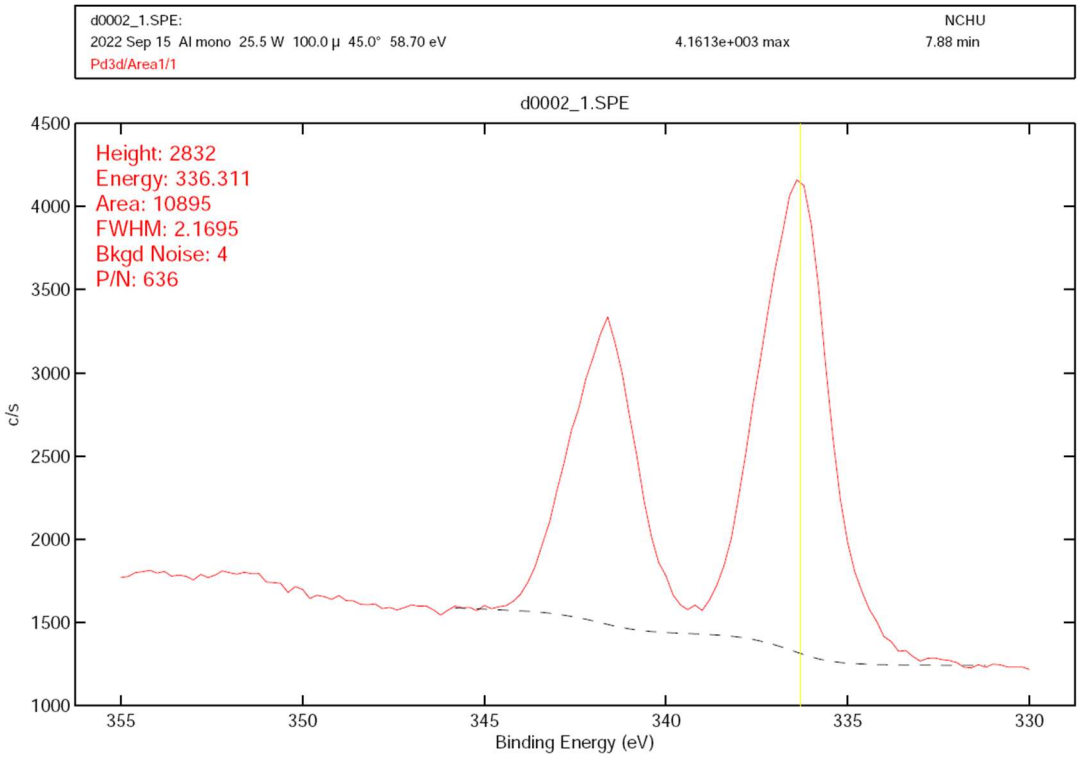


Figure S42. XPS spectrum of **2**

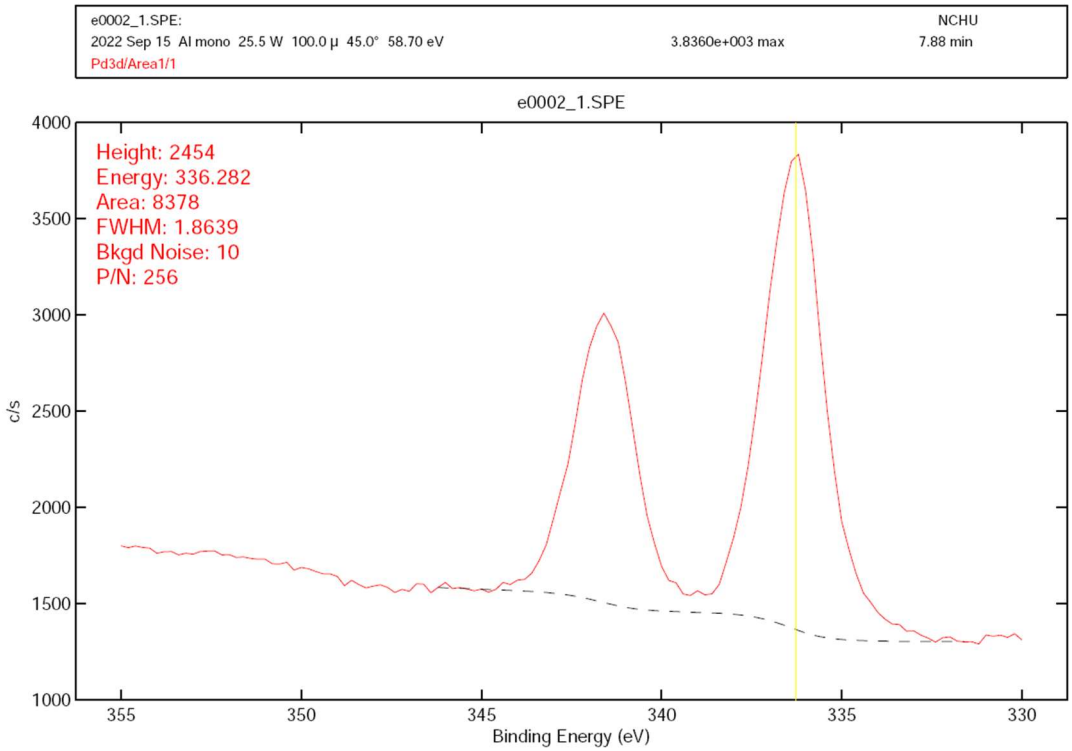


Figure S43. XPS spectrum of **3**

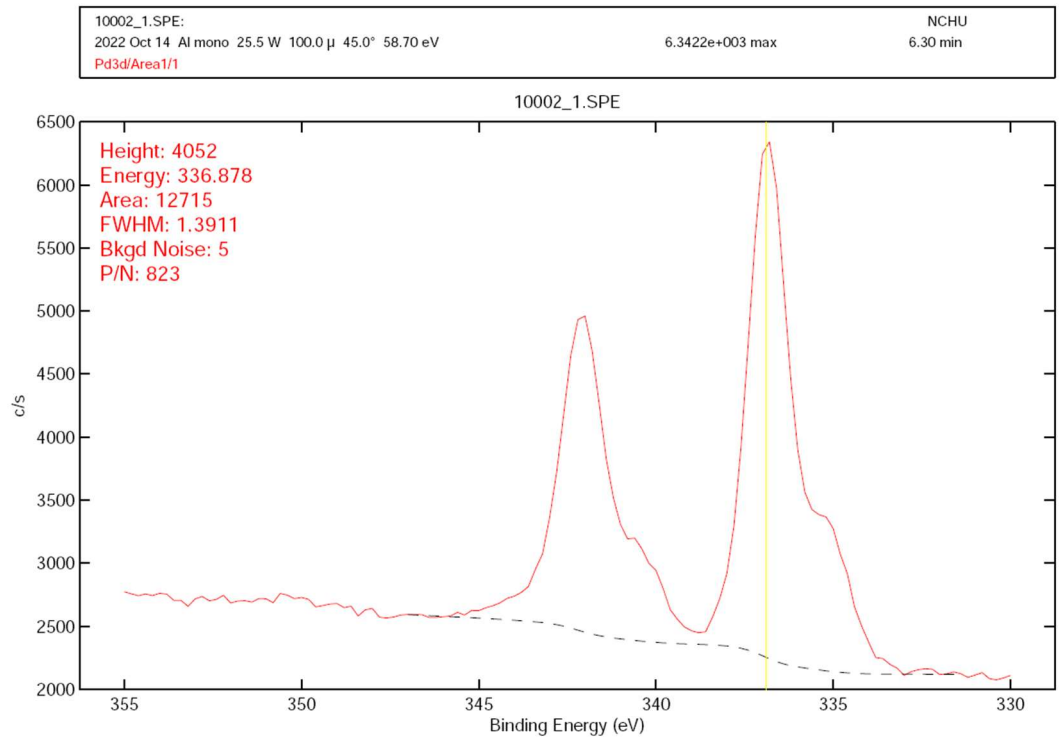


Figure S44. XPS spectrum of **4**

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11. Optimized geometries.

Nitron

N	-0.80502974	0.64260052	-0.05865041
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C	-3.07059727	-0.17586478	0.00652746
C	1.29492834	-2.25467957	0.03484579
C	-3.97019053	-1.23617724	-0.11704938
C	-5.33556815	-0.98133473	-0.06719119
C	-5.80964260	0.31979351	0.09964756
C	-4.90215804	1.36869435	0.21693185
C	-3.53068752	1.12944069	0.17202809
C	1.34172787	-3.29077016	-0.89489560
C	2.37809783	-4.21701195	-0.82864156
C	3.36625789	-4.09942898	0.14835349
C	3.31020056	-3.06008677	1.07361559
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N	1.58831232	0.66626118	-0.09746615
C	1.88819369	2.03721945	-0.10381623
C	3.23627877	2.39230342	-0.25117322
C	3.61284459	3.72791367	-0.24781910
C	2.65602050	4.73203536	-0.09852171
C	1.31962282	4.37464836	0.04700797
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H	-6.87684743	0.51265585	0.13698328
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H	3.98643604	1.61445154	-0.36723164
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H	-0.12062534	2.77634200	0.15930319

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IPr

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H	1.73733513	-2.50164719	0.48936904
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H	1.20150509	-1.96988815	-1.87302214
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1a

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C	1.60941294	0.40568584	0.18257152
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H	-4.65692235	-1.80005914	1.65178813
H	-2.37567918	-2.94355723	1.77026713
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H	-2.63099220	2.61090920	-1.92932115
H	2.22993717	3.24676225	-1.59741212

4

I	-1.43572663	-0.77058159	2.65481363
Pd	-1.43835956	-0.02068113	0.00847488
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C	-5.35627274	-1.83380489	-0.58624086
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C	-5.77621098	0.45122993	0.10689745
C	-4.38911862	0.64437495	0.18236017
C	0.54080920	0.25625087	0.10090216
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C	1.21615905	-2.15084953	-0.30726173
C	0.52194395	-3.93096735	-1.80271394
C	0.75737689	-4.87358788	-0.78106517
C	1.22364802	-4.44803856	0.47912036

C	1.45259370	-3.08087743	0.72292566
C	2.77035686	-0.18066371	0.01364598
C	5.25191973	-0.52402442	-0.09432394
C	6.23646416	-1.52200043	-0.29356391
C	7.59834176	-1.18316215	-0.26806633
C	7.99871790	0.15115655	-0.04423174
C	7.01511705	1.13864695	0.15308548
C	5.64466127	0.81551109	0.13068479
N	1.28532553	1.37787165	0.28814848
C	0.86750799	2.74017742	0.48176623
C	-0.39330127	3.03631290	1.03463300
C	-0.77603277	4.37871959	1.20242888
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C	1.75292133	3.77576111	0.11992433
H	0.57930181	-1.82656133	-2.34931181
H	3.73725695	-1.93140815	-0.30101677
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H	-3.24396496	-2.33256944	-0.71319862
H	-5.69244195	-2.81890263	-0.89092918
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H	-6.44416729	1.27044384	0.34959088
H	-3.96666970	1.59684927	0.47901546
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H	0.57894823	-5.92947500	-0.96519742
H	1.40175930	-5.17192708	1.26908770
H	1.79147760	-2.74127889	1.69717325
H	5.93678420	-2.55327520	-0.46802554
H	8.34397277	-1.95874808	-0.42256495
H	9.05321190	0.41194398	-0.02482243
H	7.31007706	2.17069189	0.32650667
H	4.89777561	1.58332450	0.28360968
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H	-0.20412976	6.45869818	0.97106360
H	2.72407419	3.53297465	-0.29452782