Supporting Information

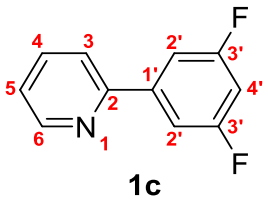
Contents

General considerations

2a-Au(OAc^F)$_2$,[1] **3b-AuOAc^F**,[2] **2a-Au(OAc)$_2$**,[3, 4] **2a-Au(CH$_2$=CHCH$_2$)Br**,[5] **2a-Au(C$_6$H$_5$)Br**,[1] **2a-Au(CH$_3$)Br**,[1] **2a-Au(CH$_3$)$_2$**,[1] 3,5-diethylphenylboronic acid[6, 7] and 3,5-diisopropylphenylboronic acid[6, 7] were synthesized according to literature procedures. $Au(OAc)_3$ was obtained from abcr. THF (unstabilized) and CH_2Cl_2 were dried using an MB SPS-800 solvent purifier system from MBraun. Hexanes and ethyl acetate were distilled before use. Deionized water was used. Other chemicals and solvents were used as received from commercial sources. TLC was performed using Merck 60 F254 plates. Flash chromatography was performed using silica gel from Merck (60, 0.040-0.063 mm). Microwave reactions were performed with a Milestone MicroSYNTH microwave reactor with a SK-10 rotor or, for reaction volumes smaller than 10 mL, in an Anton Paar GmbH Monowave 300 synthesis reactor equipped with an internal IR probe calibrated with a Ruby thermometer. NMR spectroscopy was performed using Bruker Avance DPX300, AVII400, AVIIIHD400, DRX500, AVI600, AVII600 or AVIIIHD800 operating at 300 MHz (^{1}H NMR), or 400 MHz (^{1}H NMR), 376 MHz (^{19}F NMR), 101 MHz (^{13}C NMR), or 500 MHz (^{1}H NMR), or 600 MHz (^{1}H NMR) and 151 MHz (^{13}C NMR), or 800 MHz (^{1}H NMR) and 201 MHz (^{13}C NMR) respectively. All spectra were recorded at room temperature. ^{1}H NMR and ^{13}C NMR spectra have been referenced relative to the residual solvent signals. Chemical shifts in ^{19}F NMR have been referenced to $CFCl_3$ by using C_6F_6 or C_6H_5F (−164.9 ppm and −116.1 ppm with respect to $CFCl_3$ at 0 ppm) as an internal standard, and are proton decoupled. Chemical shifts in ^{15}N NMR have been calibrated against CH_3NO_2 as an external standard (0.0 ppm). All ^{15}N NMR chemical shifts were obtained and assigned using ^{1}H-^{15}N HMBC experiments. The resonances in the ^{1}H NMR and ^{13}C NMR spectra were assigned using various 2D experiments (COSY, NOESY, HSQC and HMBC). MS (ESI and APPI) was recorded on a Bruker maXis II ETD spectrometer. All melting points are uncorrected and were obtained with a Stuart SMP10 melting point apparatus. Elemental analysis was performed by Mikroanalytisches Laboratorium Kolbe, Oberhausen, Germany.

Synthesis and characterization of arylpyridine ligands

General procedure for synthesis of arylpyridine ligands. 2-Bromopyridine or substituted 2-bromopyridine (5.00 mmol, 1.0 equiv.) and arylboronic acid (4.75-5.50 mmol, 0.95-1.1 equiv.) were dissolved in *n*-PrOH (10 mL). A solution of K_3PO_4 (10.0-11.5 mmol, 2.0-2.3 equiv.) in water (10 mL) was added, and the resulting biphasic mixture was degassed for 10 min by bubbling Ar through it. $Pd(OAc)_2$ (0.100 mmol, 2.0 mol-%) and PPh_3 (0.300 mmol, 6.0 mol-%) were added, and the reaction mixture was heated at reflux temperature for 3 h under Ar. After cooling to rt, CH_2Cl_2 (50 mL) and water (50 mL) were added. The phases were separated, and the CH_2Cl_2 solution was washed with 2M NaOH (aq) (2x 50 mL), brine (50 mL), and was dried over Na_2SO_4. The solvent was removed under reduced pressure. The obtained residue was purified by flash column chromatography (hexanes/EtOAc, hexanes/CH_2Cl_2 or hexanes/EtOAc/CH_2Cl_2 mixtures), furnishing the arylpyridine ligand.



1c

2-(3,5-Difluorophenyl)pyridine (1c). The general procedure was followed. 2-Bromopyridine (0.789 g, 4.99 mmol, 1.0 equiv.), 3,5-difluorophenylboronic acid (0.866 g, 5.48 mmol, 1.1 equiv.), K_3PO_4 (2.14 g, 10.1 mmol, 2.0 equiv.), $Pd(OAc)_2$ (0.0236 g, 0.105 mmol, 2.1 mol-%) and PPh_3 (0.0808 g, 0.308 mmol, 6.2 mol-%) were used. The crude product was purified by flash column chromatography (98 % hexanes/2 % EtOAc to 95 % hexanes/5 % EtOAc) yielding **1c** as a colorless solid.

Yield: 0.870 g, 4.55 mmol, 91 %.

M.p. 61-62 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.70 (d, $^3J_{H,H}$ = 4.8 Hz, 1H, **H^6**), 7.78 (ddd, $^3J_{H,H}$ = 7.8 Hz, $^3J_{H,H}$ = 7.7 Hz, $^4J_{H,H}$ = 1.8 Hz, 1H, **H^4**), 7.69 (d, $^3J_{H,H}$ = 7.9 Hz, 1H, **H^3**), 7.53-7.57 (m, 2H, **H$^{2'}$**), 7.29 (ddd, $^3J_{H,H}$ = 7.4 Hz, $^3J_{H,H}$ = 4.8 Hz, $^4J_{H,H}$ = 0.9 Hz, 1H, **H^5**), 6.85 ppm (m, 1H, **H$^{4'}$**).

^{13}C NMR (151 MHz, $CDCl_3$): δ 163.4 (dd, $^1J_{C,F}$ = 248.1 Hz, $^3J_{C,F}$ = 12.4 Hz, **C$^{3'}$**), 154.8 (m, **C^2**) 149.8 (**C^6**), 142.7 (m, **C$^{1'}$**), 137.0 (**C^4**), 123.2 (**C^5**), 120.5 (**C^3**), 109.6-109.8 (m, **C$^{2'}$**), 104.1 ppm (m, **C$^{4'}$**).

^{19}F NMR (376 MHz, $CDCl_3$): δ −112.8 ppm (Ar-**F**).

^{15}N{^{1}H} NMR (600 MHz, $CDCl_3$): δ −72.2 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 192.062 (100) $[M+H]^+$.

HRMS (ESI): Found 192.0619; calcd for $C_{11}H_8F_2N$ $[M+H]^+$: 192.0619.

The NMR data are in accordance with those reported in the literature.[8]

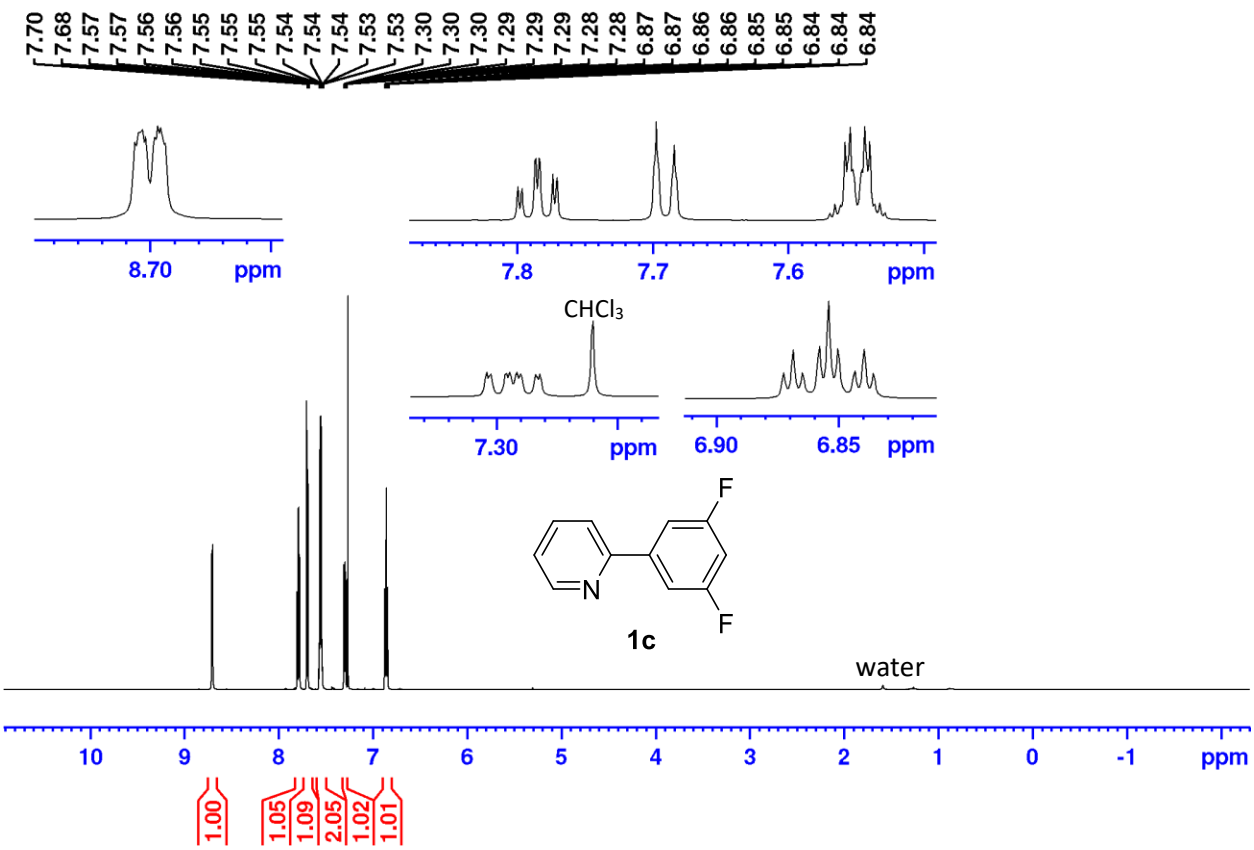


Figure S1. ^{1}H NMR (600 MHz, $CDCl_3$) of **1c**.

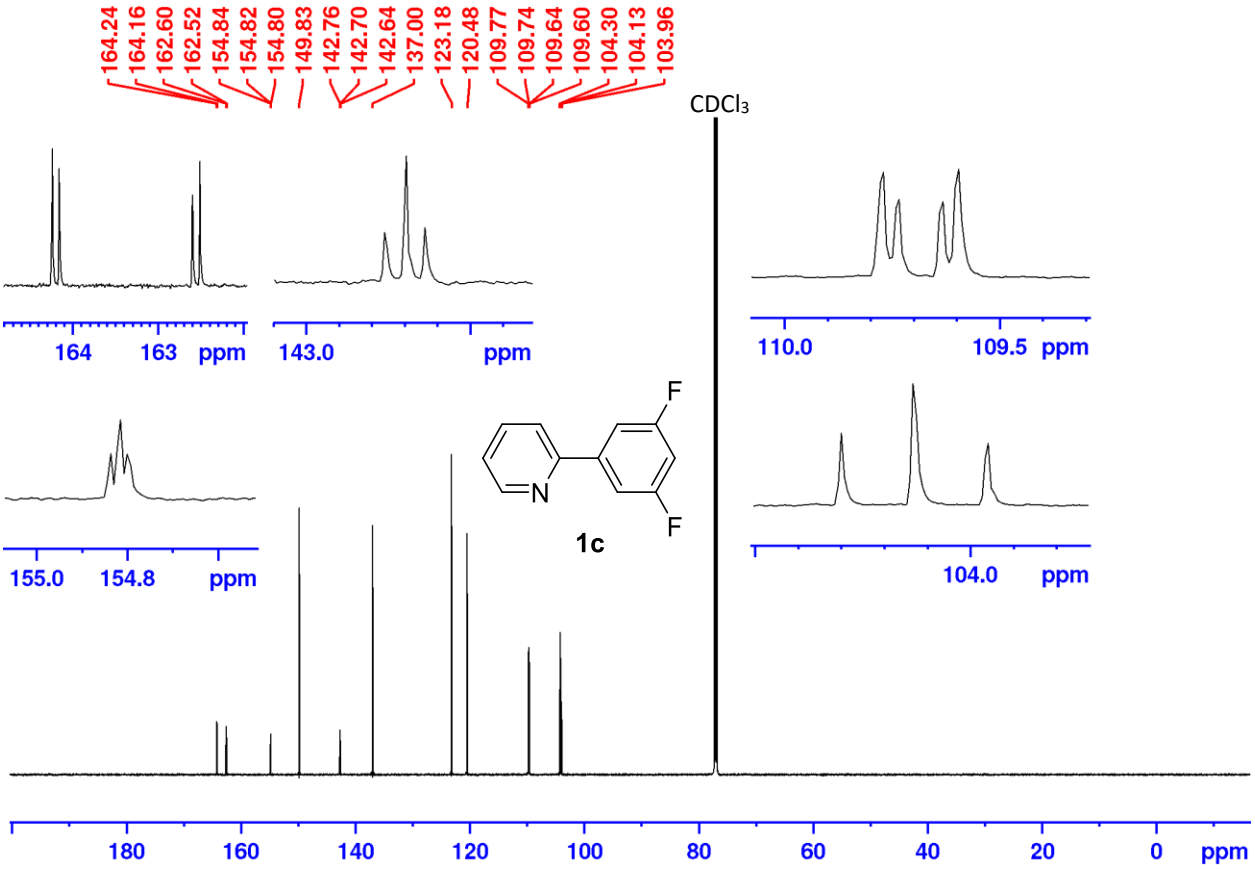


Figure S2. ^{13}C NMR (151 MHz, $CDCl_3$) of **1c**.

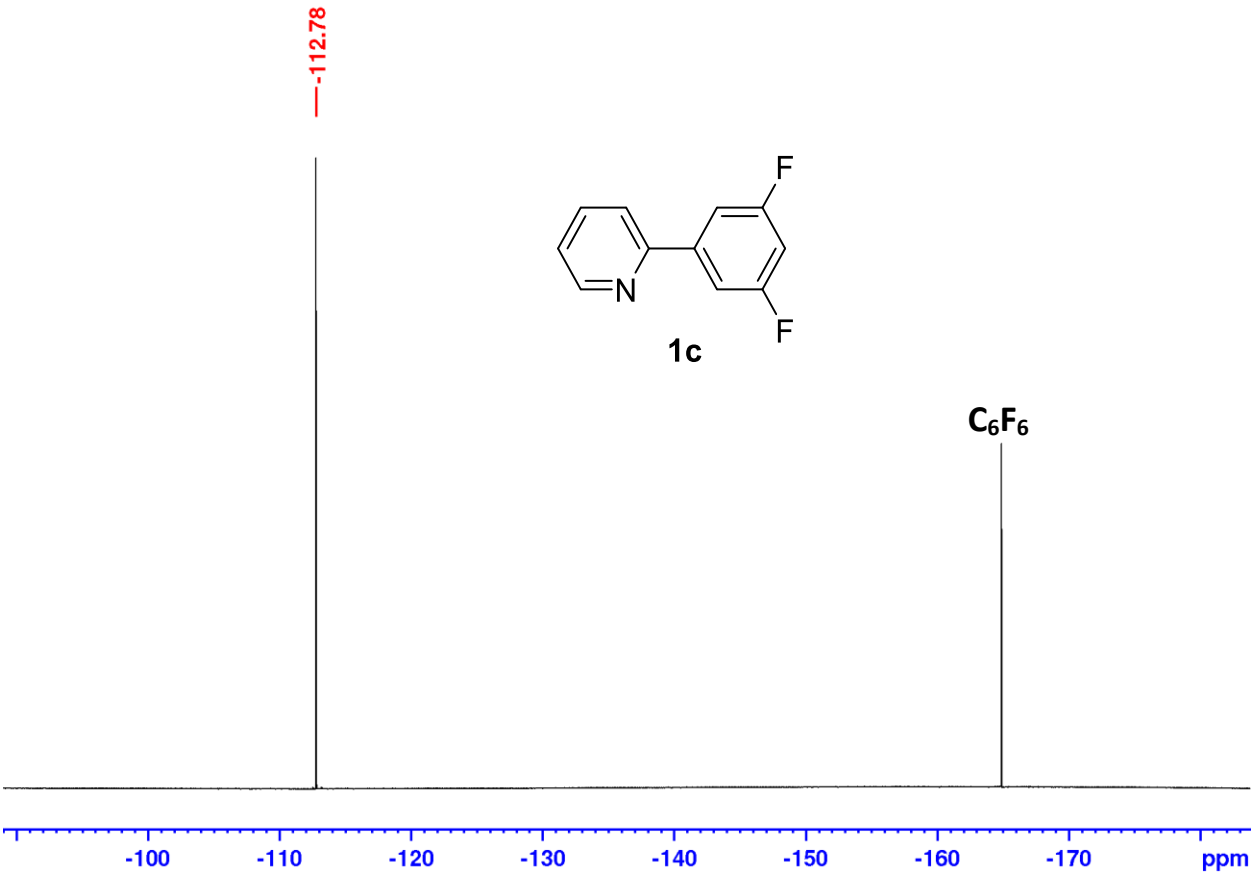


Figure S3. ^{19}F NMR (376 MHz, $CDCl_3$) of **1c**.

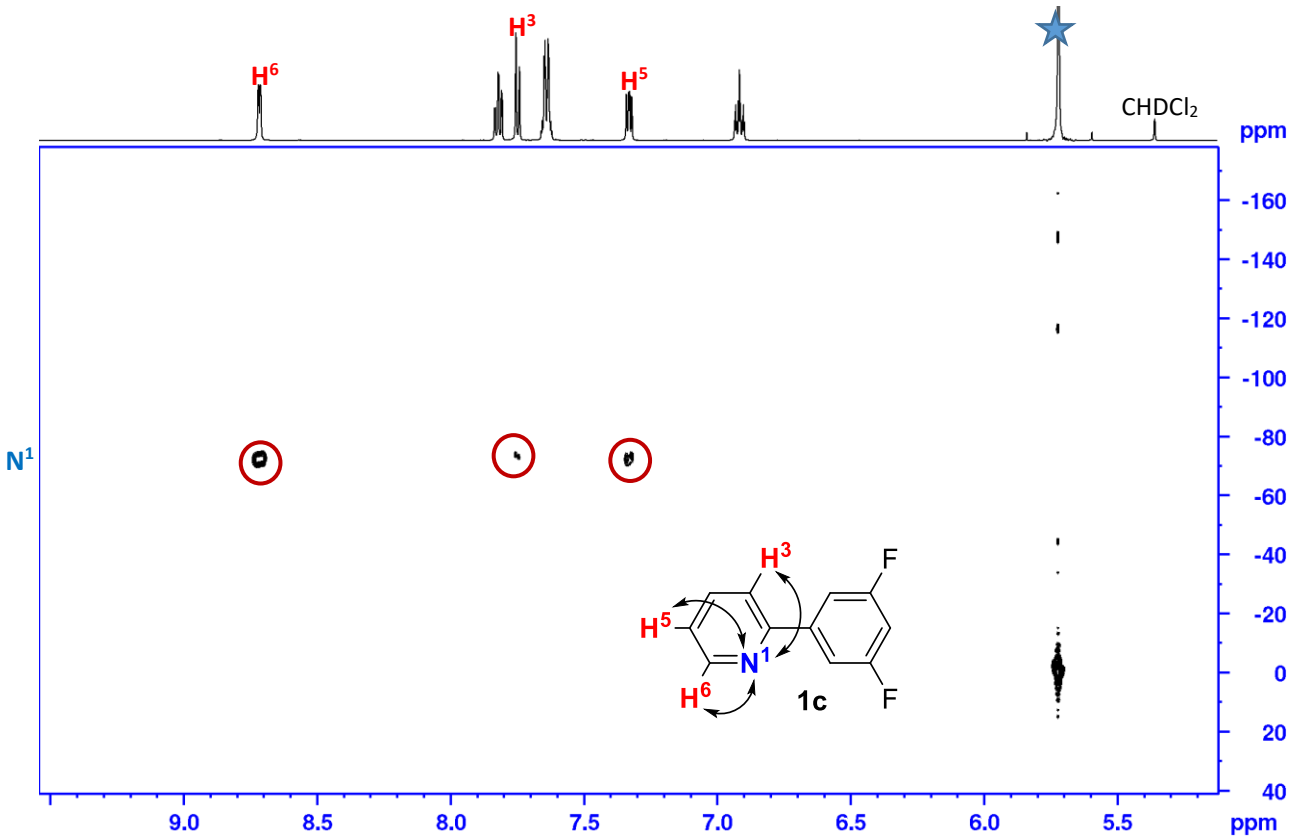
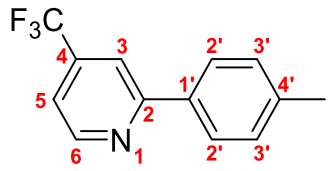


Figure S4. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1c**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1d

2-(4-Methylphenyl)-4-(trifluoromethyl)pyridine (1d). The general procedure was followed. 2-Bromo-4-(trifluoromethyl)pyridine (1.14 g, 5.04 mmol, 1.0 equiv.), 4-methylphenylboronic acid (0.790 g, 5.81 mmol, K_3PO_4 (2.15 g, 10.1 mmol, 2.0 equiv.), $Pd(OAc)_2$ (0.0230 g, 0.102 mmol, 2.0 mol-%) and PPh_3 (0.0808 g, 0.308 mmol, 6.1 mol-%) were used. The crude product was purified by flash column chromatography (99 % hexanes/1 % EtOAc to 98 % hexanes/2 % EtOAc) yielding **1d** as a pale yellow oil.

Yield: 1.03 g, 4.35 mmol, 86 %.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.84 (d, $^3J_{H,H}$ = 5.0 Hz, 1H, **H^6**), 7.93 (d, $^3J_{H,H}$ = 8.2 Hz, 2H, **H$^{2'}$**), 7.90 (s, 1H, **H^3**), 7.41 (d, $^3J_{H,H}$ = 4.7 Hz, 1H, **H^5**), 7.31 (d, $^3J_{H,H}$ = 8.0 Hz, 2H, **H$^{3'}$**), 2.42 ppm (s, 3H, C**H**$_3$).

^{13}C NMR (151 MHz, $CDCl_3$): δ 158.8 (**C^2**), 150.5 (**C^6**), 140.0 (**C$^{4'}$**), 139.0 (q, $^2J_{C,F}$ = 33.8 Hz, **C^4**), 135.3 (**C$^{1'}$**), 129.7 (**C$^{3'}$**), 126.9 (**C$^{2'}$**), 123.0 (q, $^1J_{C,F}$ = 273.3 Hz, **C**F$_3$), 117.2 (q, $^3J_{C,F}$ = 3.3 Hz, **C^5**), 115.7 (q, $^3J_{C,F}$ = 3.4 Hz, **C^3**), 21.3 ppm (**C**H$_3$).

^{19}F NMR (376 MHz, $CDCl_3$): δ −68.0 ppm (C**F**$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −64.9 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 238.084 (100) $[M+H]^+$.

HRMS (ESI): Found 238.0838; calcd for $C_{13}H_{11}F_3N$ $[M+H]^+$: 238.0838.

The NMR data are in accordance with those reported in the literature.[9]

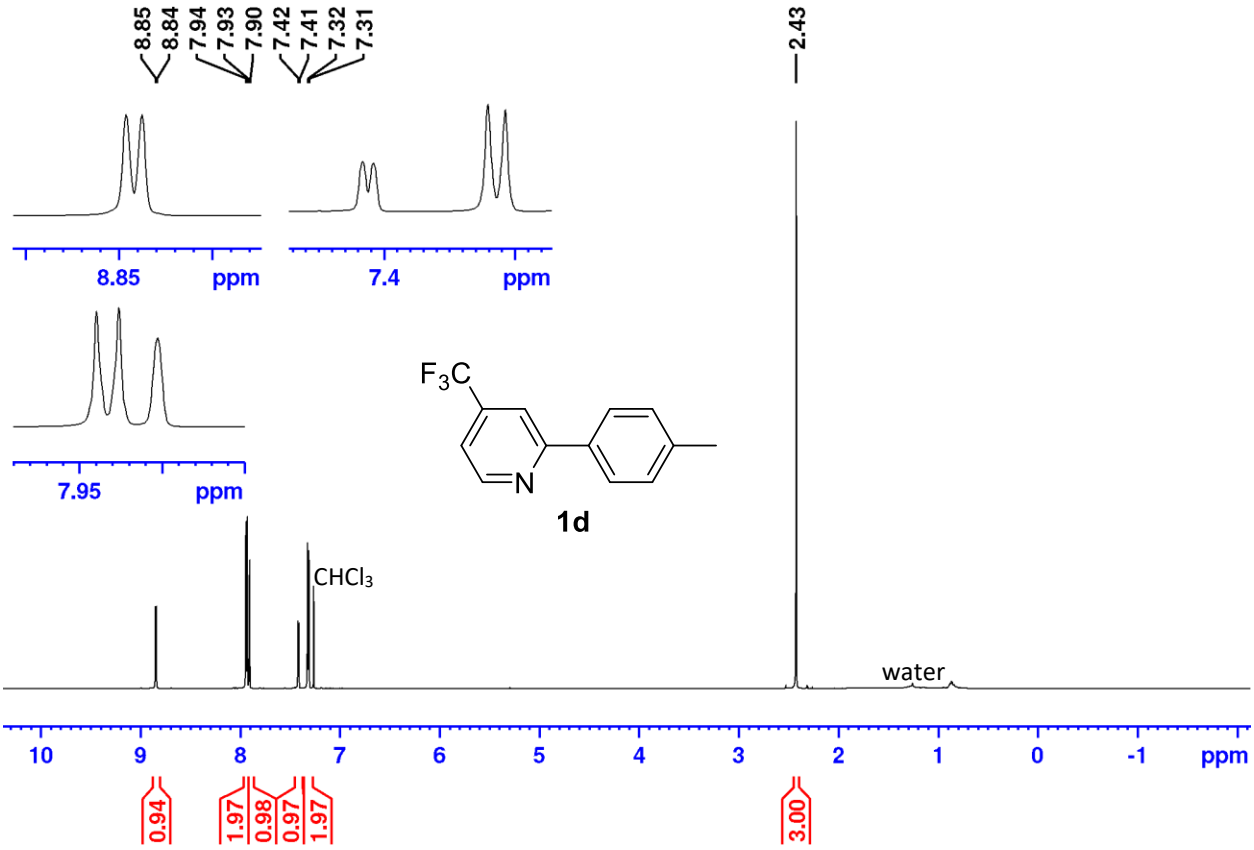


Figure S5. ^{1}H NMR (600 MHz, $CDCl_3$) of **1d**.

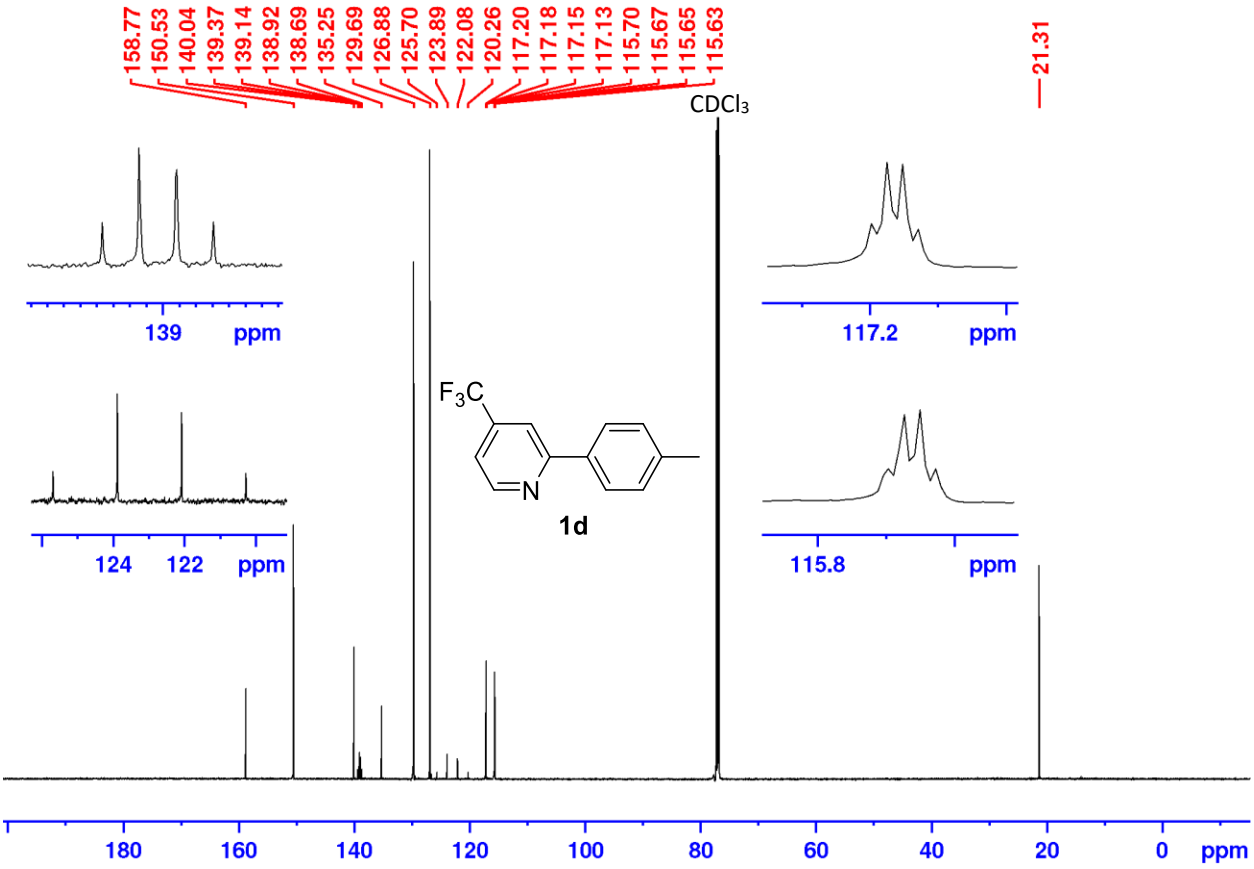


Figure S6. ^{13}C NMR (151 MHz, $CDCl_3$) of **1d**.

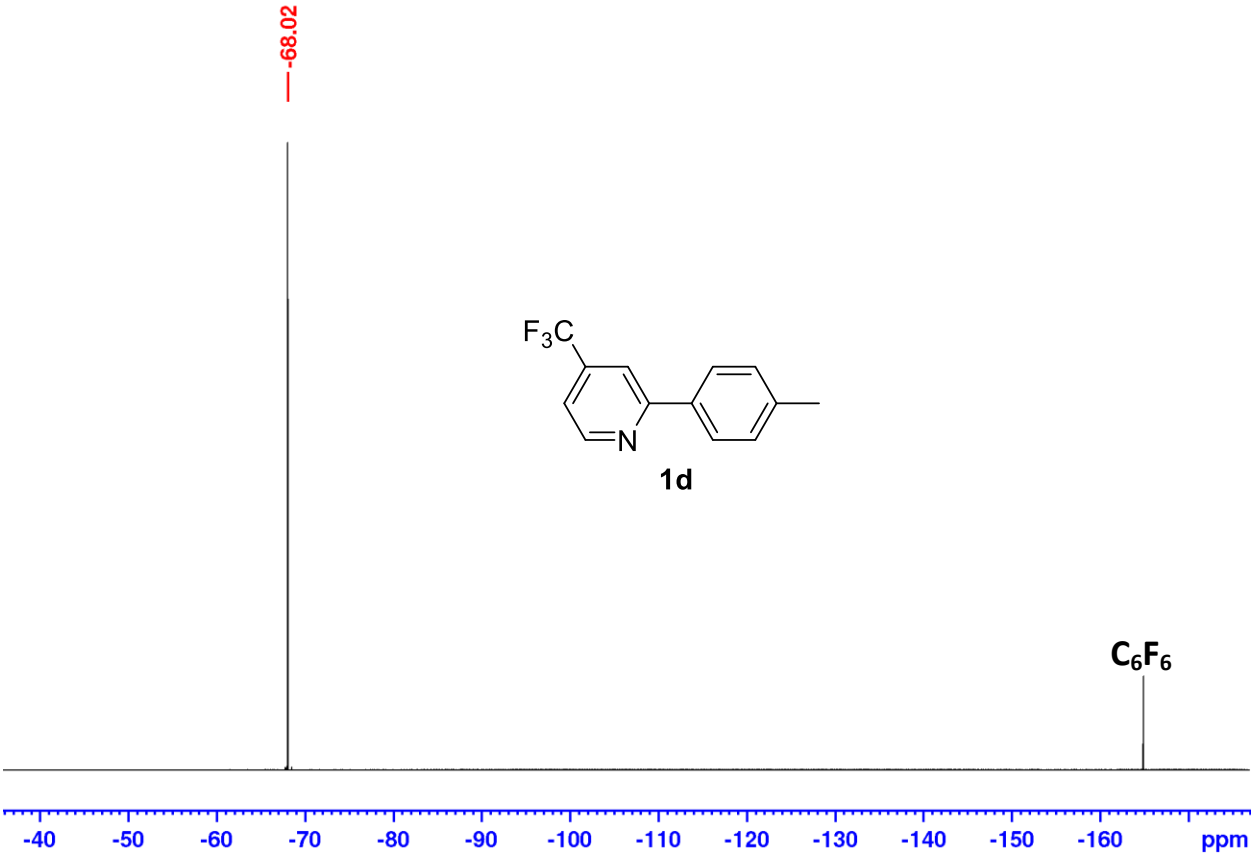


Figure S7. ^{19}F NMR (376 MHz, $CDCl_3$) of **1d**.

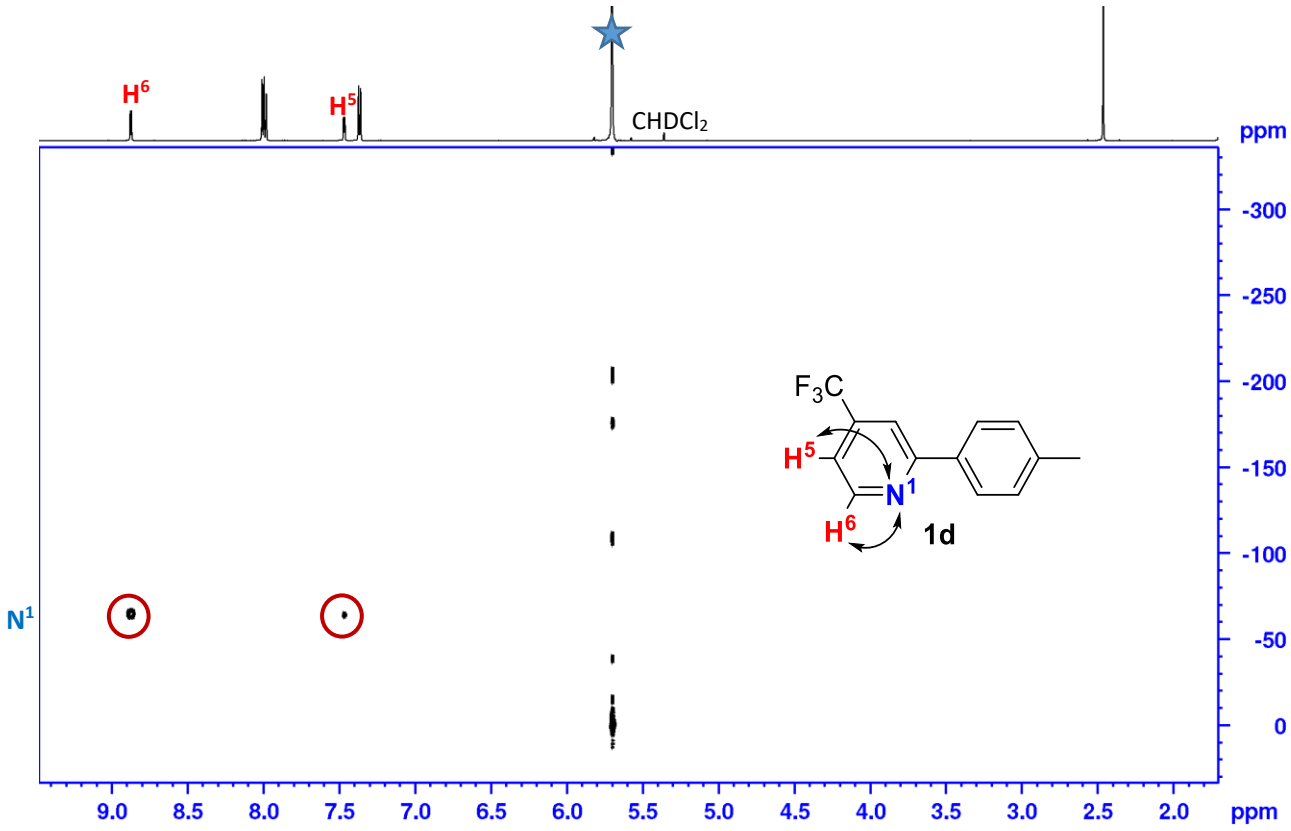
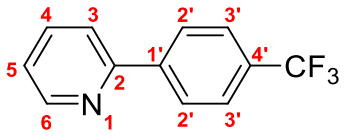


Figure S8. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1d**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1e

2-(4-(Trifluoromethyl)phenyl)pyridine (1e). The general procedure was followed. 2-Bromopyridine (0.802 g, 5.07 mmol, 1.0 equiv.), 4-(trifluoromethyl)phenylboronic acid (1.05 g, 5.52 mmol, 1.1 equiv.), K_3PO_4 (2.15 g, 10.1 mmol, 2.0 equiv.), $Pd(OAc)_2$ (0.0211 g, 0.0940 mmol, 1.8 mol-%) and PPh_3 (0.0783 g, 0.298 mmol, 5.9 mol-%) were used. The obtained crude product was purified by flash column chromatography (50 % hexanes/50 % CH_2Cl_2), furnishing **1e** as a colorless solid.

Yield: 1.04 g, 4.66 mmol, 92 %.

M.p. 75-76 °C (Lit.[10]: 70-72 °C).

^{1}H NMR (800 MHz, $CDCl_3$): δ 8.73 (d, $^3J_{H,H}$ = 4.5 Hz, 1H, **H^6**), 8.12 (d, $^3J_{H,H}$ = 8.2 Hz, 2H, **H$^{2'}$**), 7.80 (ddd, $^3J_{H,H}$ = 7.6 Hz, $^3J_{H,H}$ = 7.6 Hz, $^4J_{H,H}$ = 1.8 Hz, 1H, **H^4**), 7.77 (d, $^3J_{H,H}$ = 7.9 Hz, 1H, **H^3**), 7.73 (d, $^3J_{H,H}$ = 8.2 Hz, 2H, **H$^{3'}$**), 7.30 ppm (ddd, $^3J_{H,H}$ = 7.3 Hz, $^3J_{H,H}$ = 4.8 Hz, $^4J_{H,H}$ = 1.2 Hz, 1H, **H^5**).

^{13}C NMR (201 MHz, $CDCl_3$): δ 155.9 (**C^2**), 149.9 (**C^6**), 142.7 (**C$^{1'}$**), 137.0 (**C^4**), 130.8 (q, $^2J_{C,F}$ = 32.5, **C$^{4'}$**), 127.2 (**C$^{2'}$**), 125.6-126.7 (m, **C$^{3'}$**), 124.2 (q, $^1J_{C,F}$ = 271.8 Hz, **C**F_3), 122.9 (**C^5**), 120.8 ppm (**C^3**).

^{19}F NMR (376 MHz, $CDCl_3$): δ −65.8 ppm (C**F**$_3$).

^{15}N{^{1}H} NMR (600 MHz, $CDCl_3$): δ −71.1 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 224.068 (100) $[M+H]^+$.

HRMS (ESI): Found 224.0681; calcd for $C_{12}H_9F_3N$ $[M+H]^+$: 224.0682.

The NMR data are in accordance with those reported in the literature.[10]

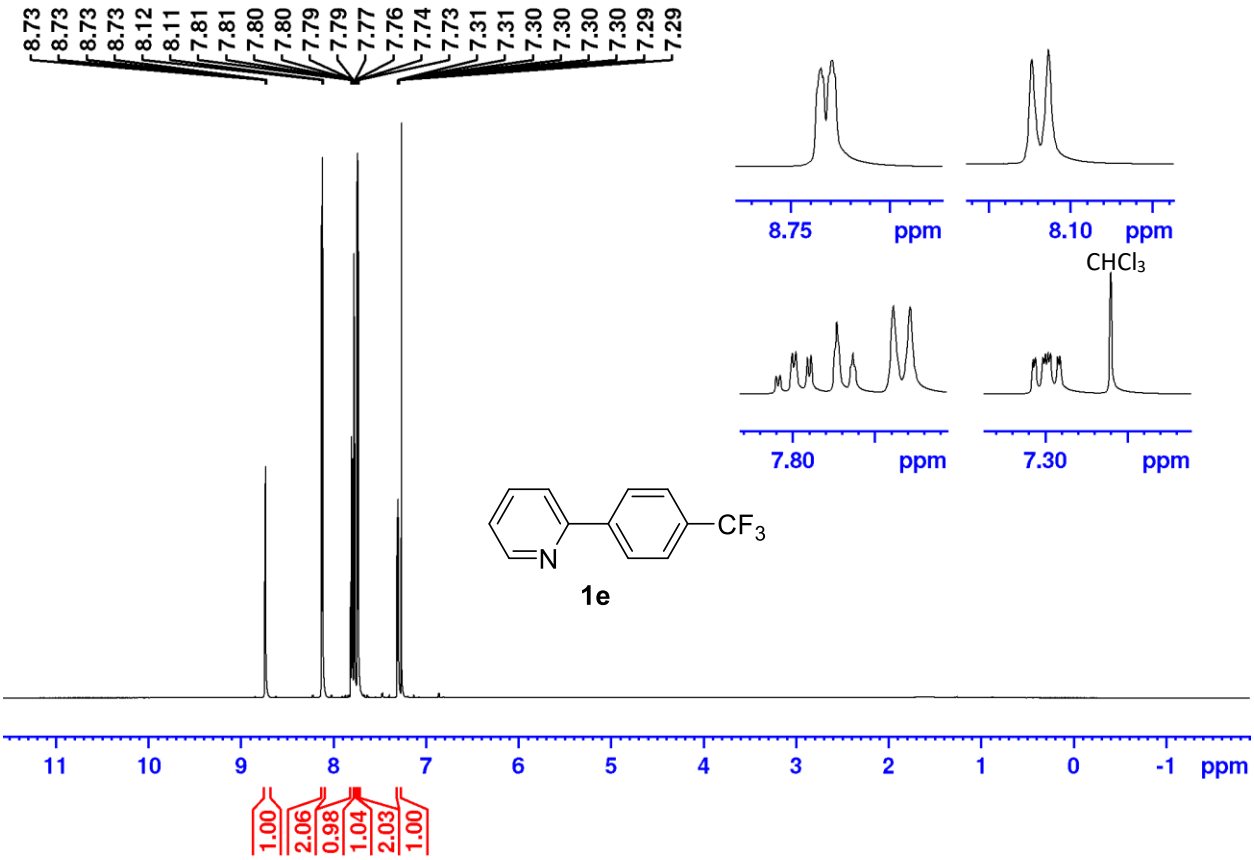


Figure S9. ^{1}H NMR (800 MHz, $CDCl_3$) of **1e**.

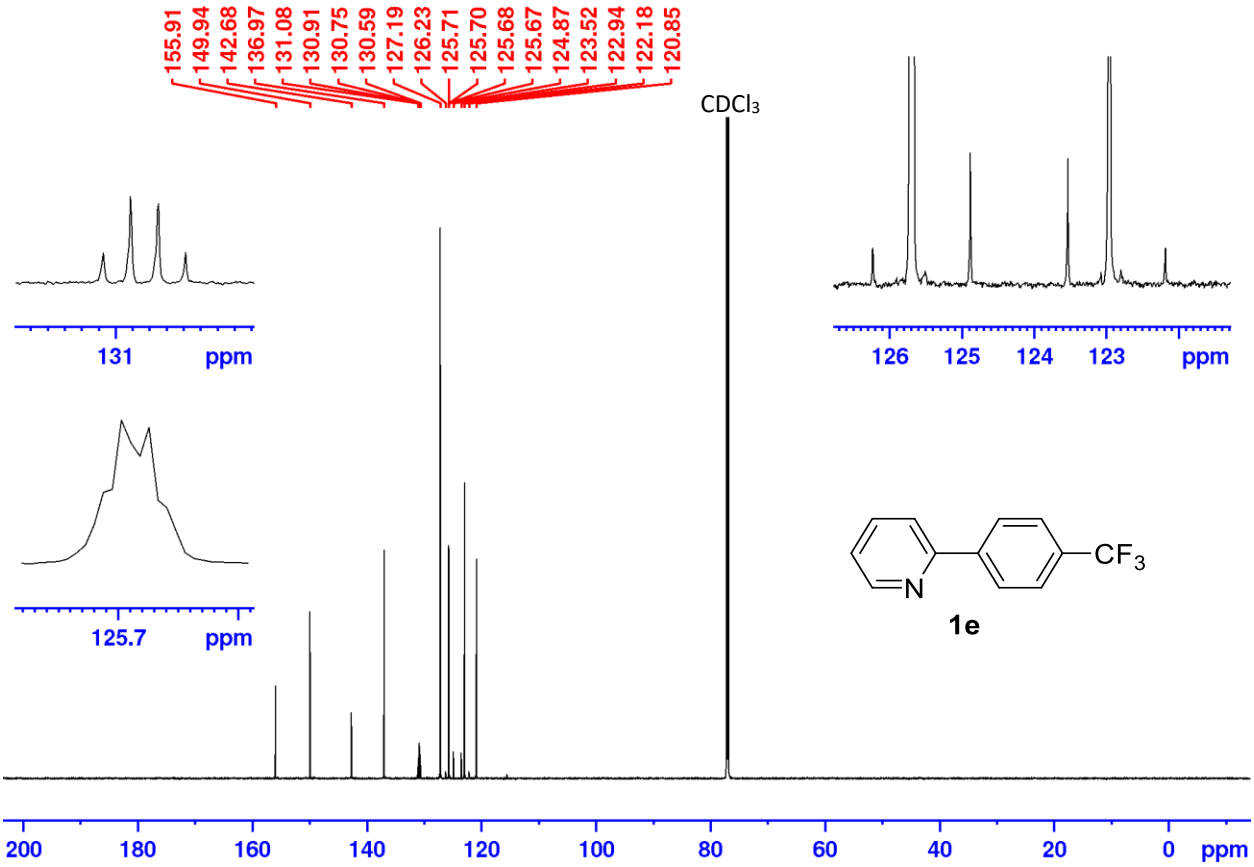


Figure S10. ^{13}C NMR (201 MHz, $CDCl_3$) of **1e**.

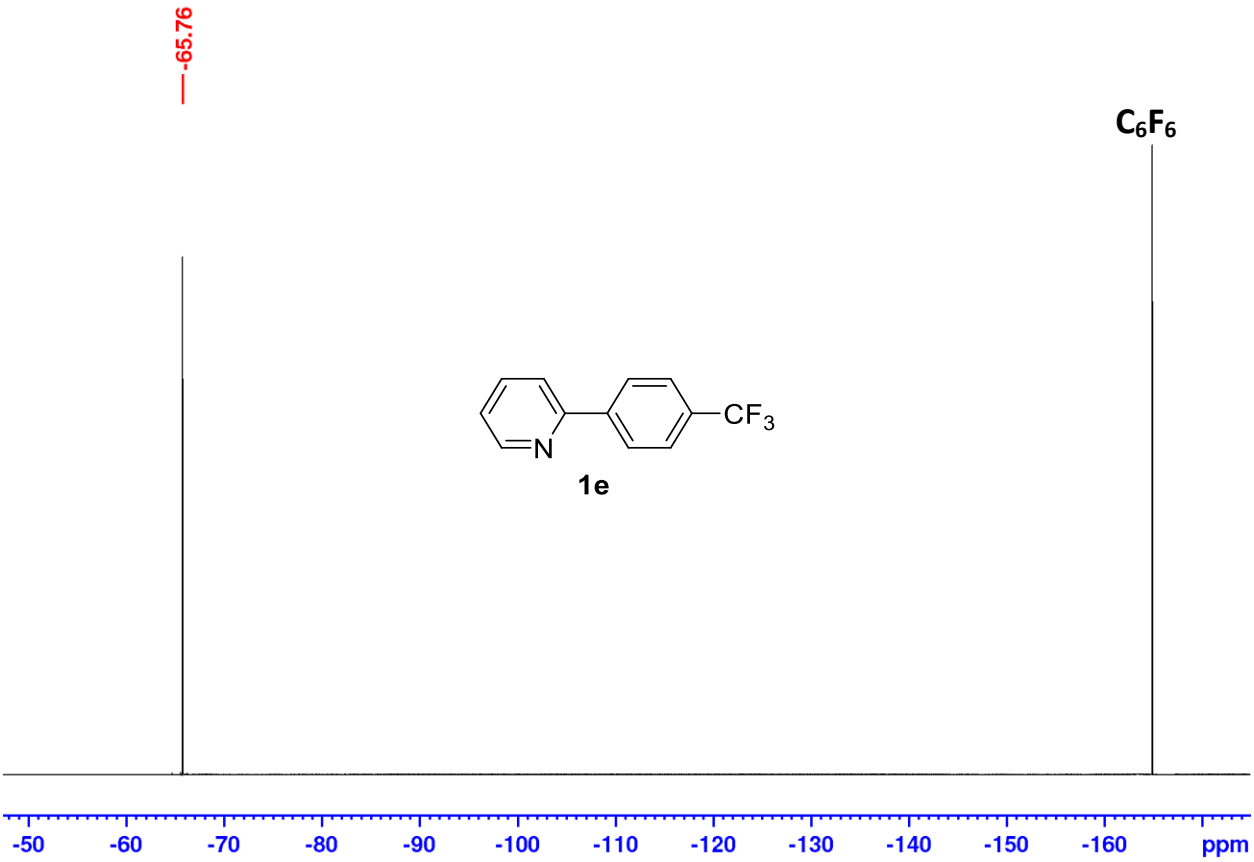


Figure S11. ^{19}F NMR (376 MHz, $CDCl_3$) of **1e**.

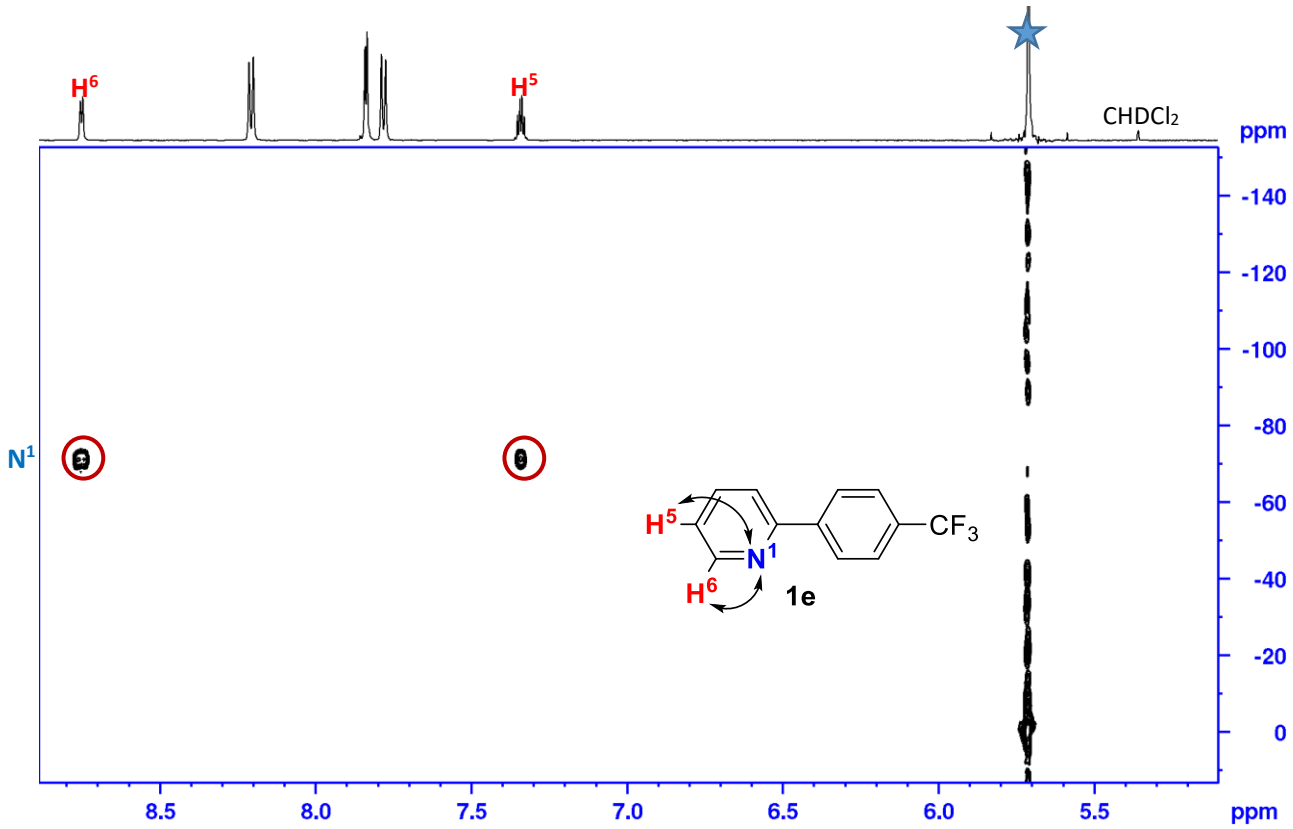
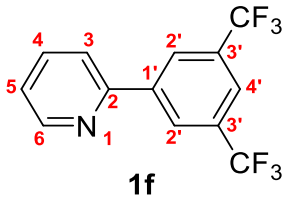


Figure S12. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1e**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1f

2-(3,5-Bis(trifluoromethyl)phenyl)pyridine (1f). The general procedure was followed. 2-Bromopyridine (1.58 g, 10.0 mmol, 1.0 equiv.), 3,5-bis(trifluoromethyl)phenylboronic acid (2.84 g, 11.0 mmol, 1.1 equiv.), K_3PO_4 (4.25 g, 20.0 mmol, 2.0 equiv.), $Pd(OAc)_2$ (0.0451 g, 0.201 mmol, 2.0 mol-%) and PPh_3 (0.158 g, 0.602 mmol, 6.0 mol-%) in *n*-PrOH (20 mL) and water (20 mL) were used. The crude product was purified by flash column chromatography (75 % hexanes/25 % CH_2Cl_2), furnishing **1f** as a colorless solid.

Yield: 2.70 g, 9.26 mmol, 92 %.

M.p. 48-49 °C (Lit.[11]: 45-46 °C).

^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.76 (d, $^3J_{H,H}$ = 4.8 Hz, **H^6**), 8.56 (s, 2H, **H$^{2'}$**), 7.96 (s, 1H, **H$^{4'}$**), 7.88-7.89 (m, 2H, **H^4** + **H^3**), 7.37-7.41 ppm (m, 1H, **H^5**).

^{13}C NMR (151 MHz, CD_2Cl_2): δ 154.2 (**C^2**), 150.5 (**C^6**), 141.8 (**C$^{1'}$**), 137.6 (**C^3** or **C^4**), 132.2 (q, $^2J_{C,F}$ = 33.3, **C$^{3'}$**), 127.3-127.4 (m, **C$^{2'}$**), 124.0 (**C^5**), 123.9 (q, $^1J_{C,F}$ = 272.7 Hz, **C**F_3), 122.7-122.8 (m, **C$^{4'}$**), 120.9 ppm (**C^3** or **C^4**).

^{19}F NMR (188 MHz, CD_2Cl_2): δ −65.4 ppm (**CF_3**).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −72.5 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 292.056 (100) $[M+H]^+$.

HRMS (ESI): Found 292.0555; calcd for $C_{13}H_8F_6N$ $[M+H]^+$: 292.0555.

The NMR data are in accordance with those reported in the literature.[11]

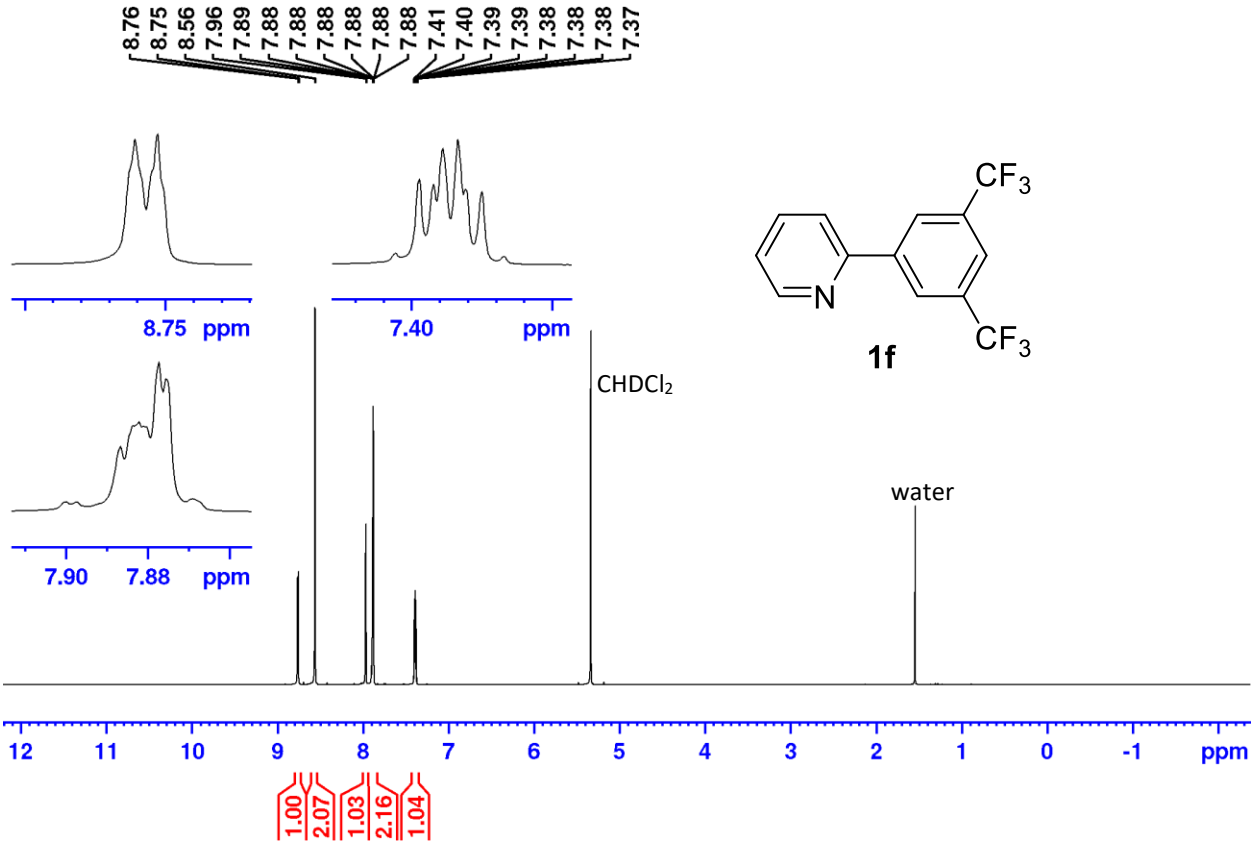


Figure S13. ^{1}H NMR (600 MHz, CD_2Cl_2) of **1f**.

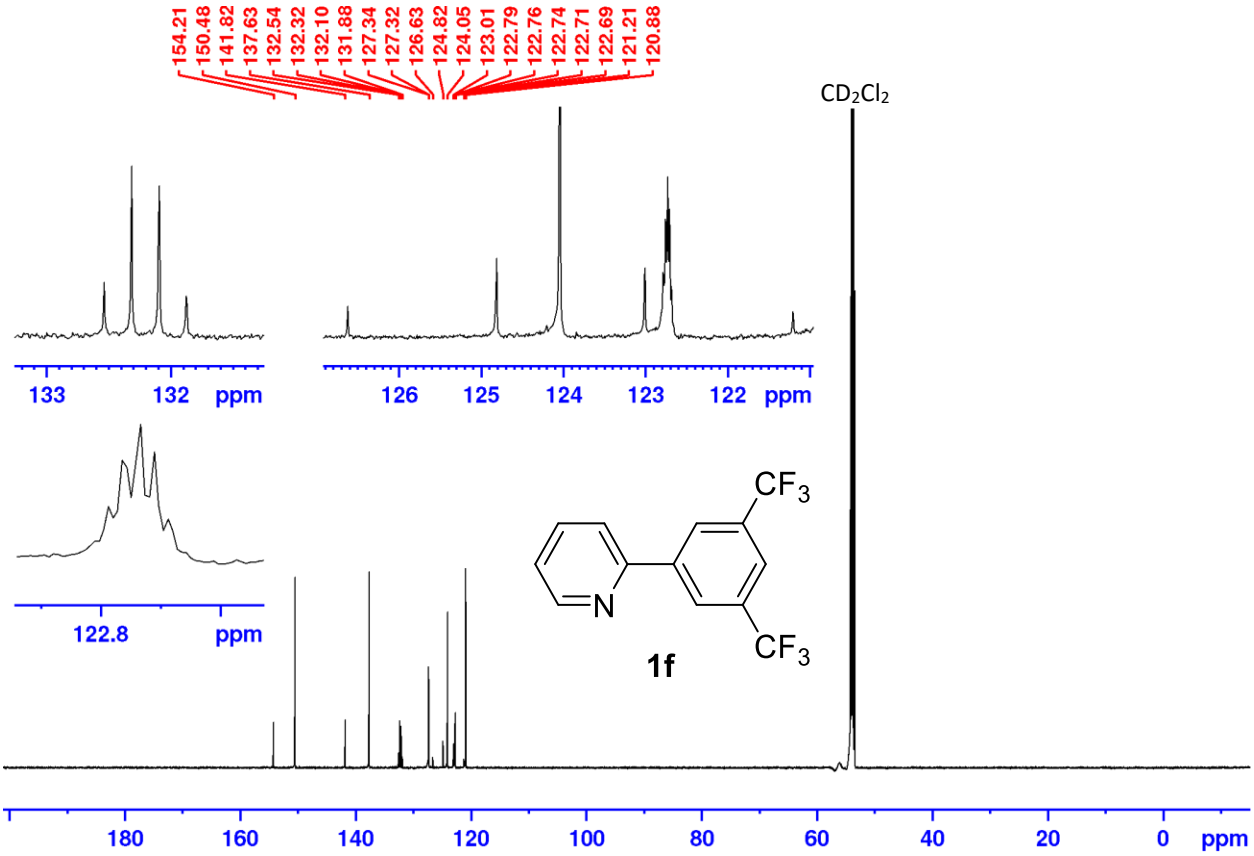


Figure S14. ^{13}C NMR (151 MHz, CD_2Cl_2) of **1f**.

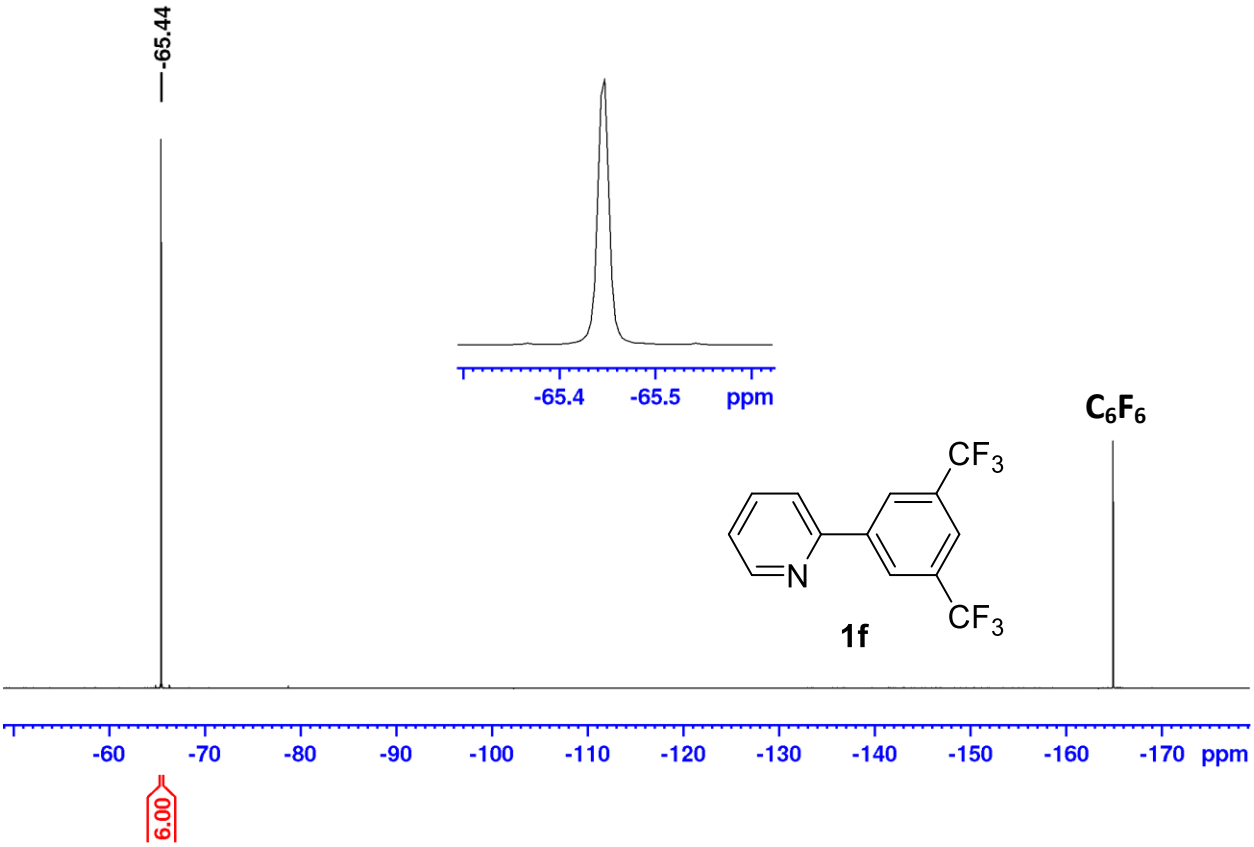


Figure S15. ^{19}F NMR (188 MHz, CD_2Cl_2) of **1f**.

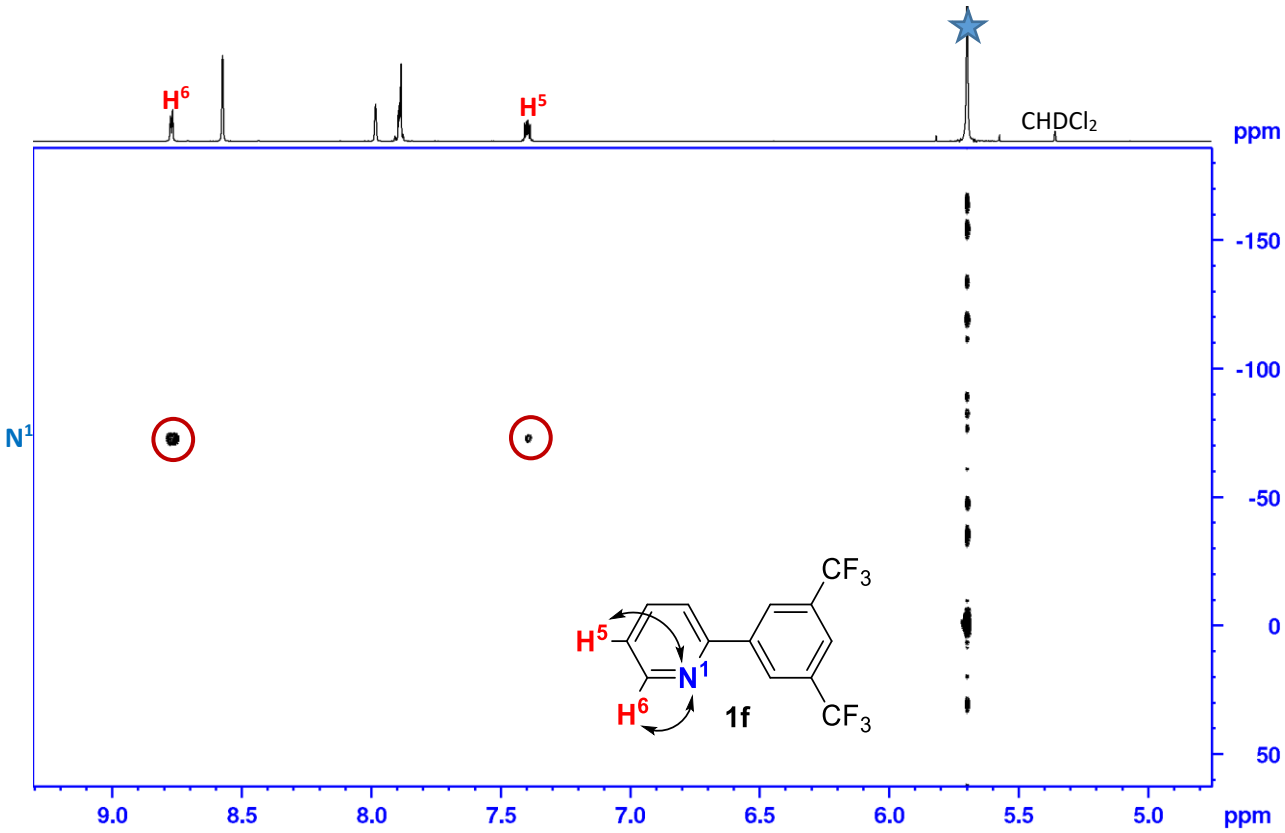
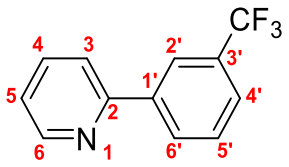


Figure S16. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1f**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1g

2-(3-(Trifluoromethyl)phenyl)pyridine (1g). The general procedure was followed. 2-Bromopyridine (0.673 g, 4.26 mmol, 1.0 equiv.), 3-(trifluoromethyl)phenylboronic acid (0.891 g, 4.69 mmol, 1.1 equiv.), K_3PO_4 (2.12 g, 10.0 mmol, 2.3 equiv.), $Pd(OAc)_2$ (0.0187 g, 0.0883 mmol, 2.0 mol-%) and PPh_3 (0.0664 g, 0.253 mmol, 6.0 mol-%) were used. The obtained crude product was purified by flash column chromatography (90 % hexanes/10 % EtOAc), furnishing **1g** as a pale yellow oil.

Yield: 0.801 g, 3.59 mmol, 84 %.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.73 (d, $^3J_{H,H}$ = 4.7 Hz, 1H, **H^6**), 8.29 (s, 1H, **H$^{2'}$**), 8.18 (d, $^3J_{H,H}$ = 7.8 Hz, 1H, **H$^{6'}$**), 7.78-7.81 (m, 1H, **H^4**), 7.76 (d, $^3J_{H,H}$ = 7.8 Hz, 1H, **H^3**), 7.67 (d, $^3J_{H,H}$ = 7.6 Hz, 1H, **H$^{4'}$**), 7.58-7.61 (m, 1H, **H$^{5'}$**), 7.28-7.30 ppm (m, 1H, **H^5**).

^{13}C NMR (151 MHz, $CDCl_3$): δ 155.8 (**C^2**), 149.9 (**C^6**), 140.1 (**C$^{1'}$**), 136.9 (**C^4**), 131.2 (q, $^2J_{C,F}$ = 32.1 Hz, **C$^{3'}$**), 130.0 (**C$^{6'}$**), 129.2 (**C$^{5'}$**), 125.5 (q, $^3J_{C,F}$ = 3.9 Hz, **C$^{4'}$**), 124.4 (q, $^1J_{C,F}$ = 272.5 Hz, **C**F_3), 123.8 (q, $^3J_{C,F}$ = 3.9 Hz, **C$^{2'}$**), 122.8 (**C^5**), 120.5 ppm (**C^3**).

^{19}F NMR (376 MHz, $CDCl_3$): δ −65.8 ppm (Ar-C**F**$_3$).

MS (ESI): *m/z* (rel. %): 246.050 (36) $[M+Na]^+$.

HRMS (ESI): Found 246.0501; calcd for $C_{12}H_8F_3NNa$ $[M+Na]^+$: 246.0501.

The NMR data are in accordance with those reported in the literature.[11]

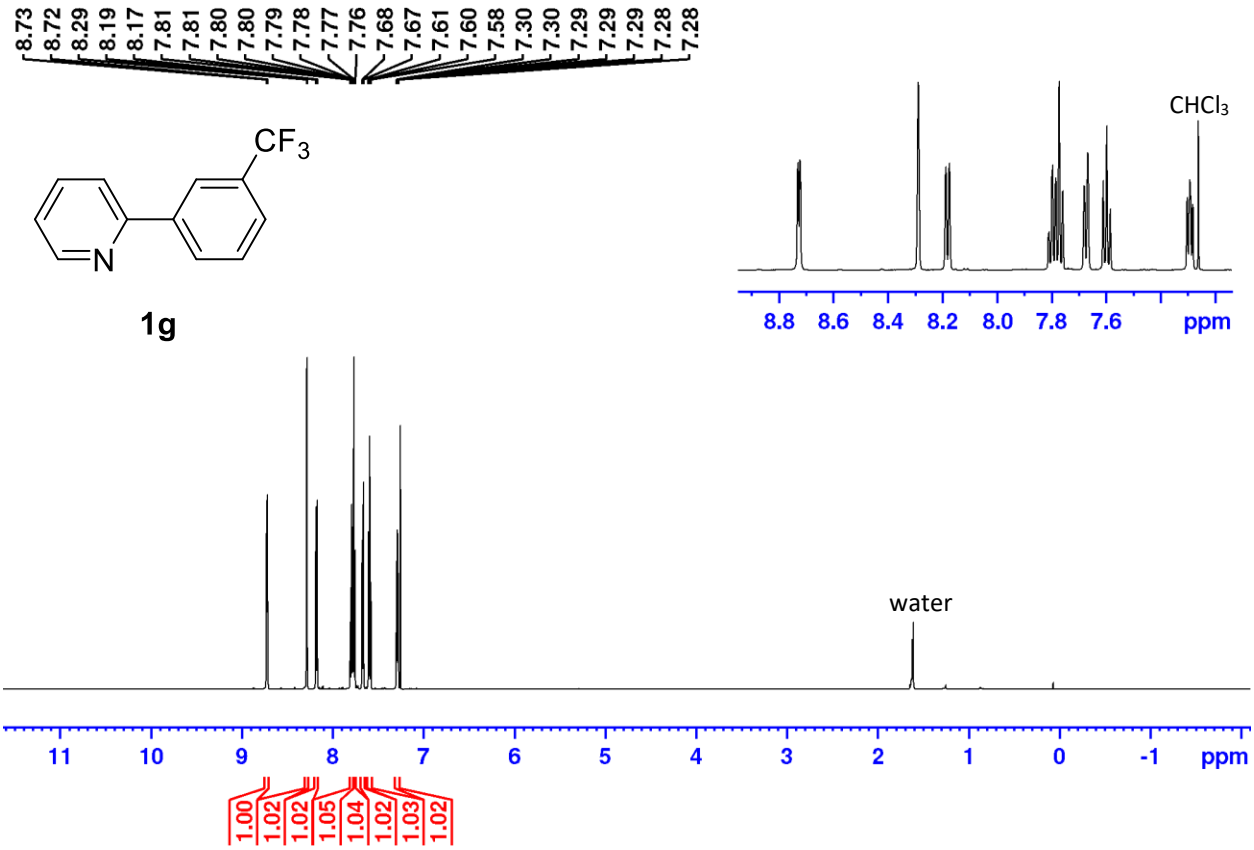


Figure S17. ^{1}H NMR (600 MHz, $CDCl_3$) of **1g**.

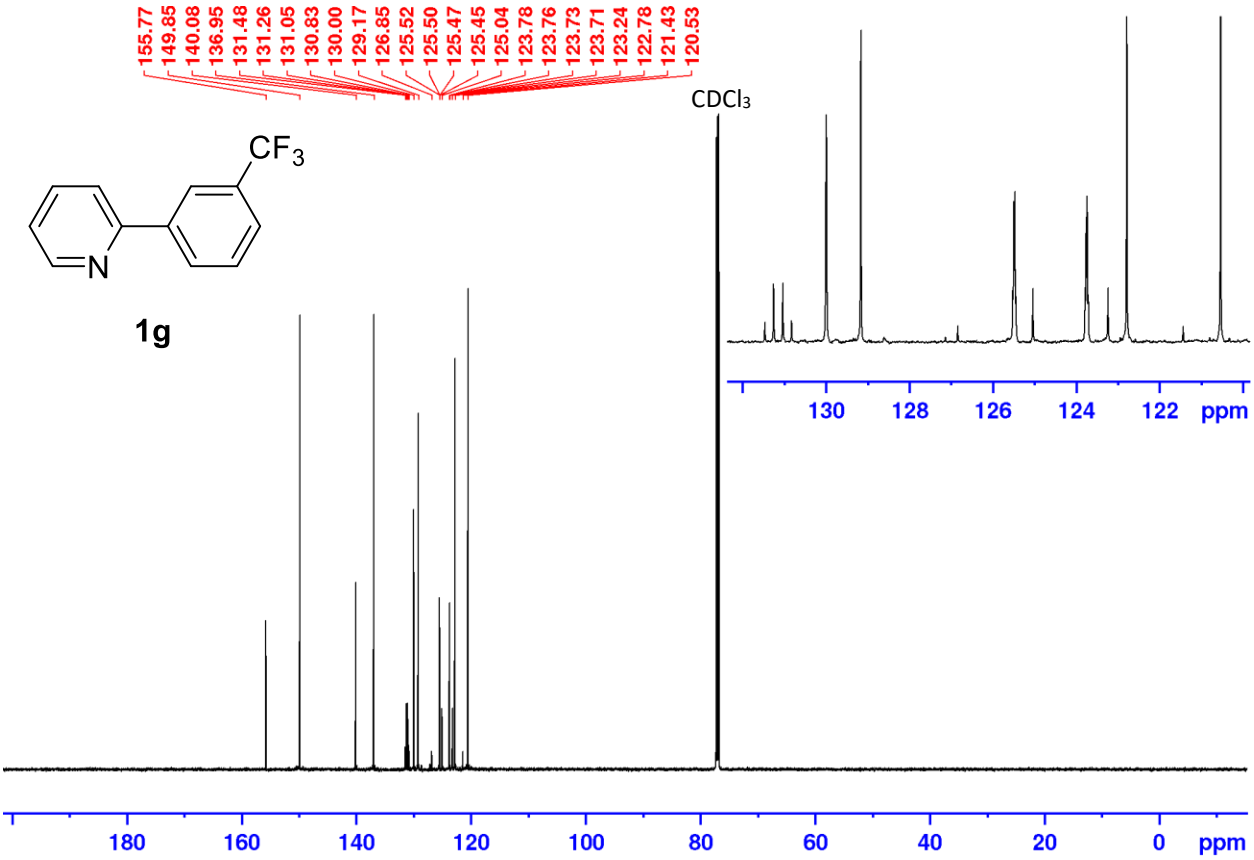


Figure S18. ^{13}C NMR (151 MHz, $CDCl_3$) of **1g**.

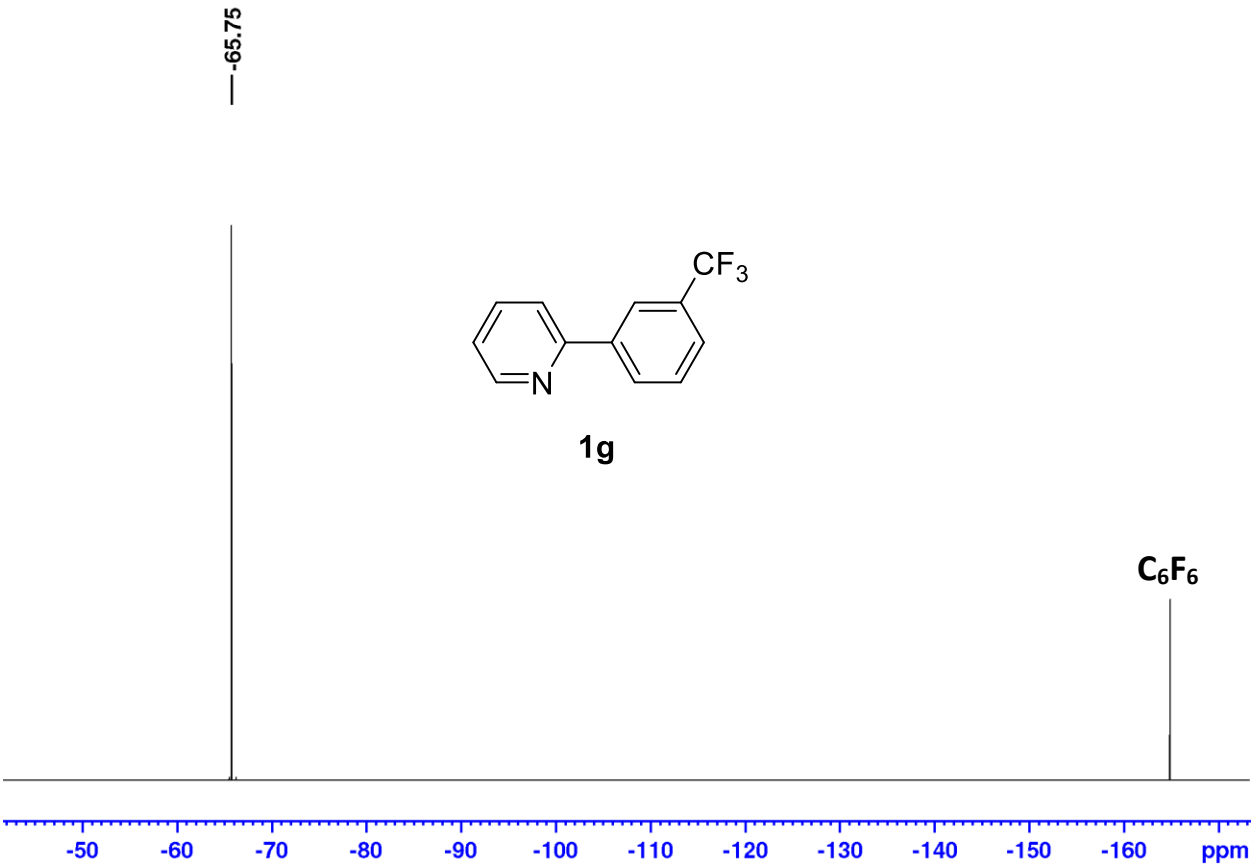
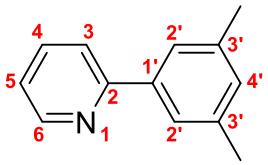


Figure S19. ^{19}F NMR (376 MHz, $CDCl_3$) of **1g**.



1h

2-(3,5-Dimethylphenyl)pyridine (1h). The general procedure was followed. 2-Bromopyridine (0.816 g, 5.16 mmol, 1.0 equiv.), 3,5-dimethylphenylboronic acid (0.867 g, 5.67 mmol, 1.1 equiv.), K_3PO_4 (2.16 g, 10.2 mmol, 2.0 equiv.), $Pd(OAc)_2$ (0.0241 g, 0.107 mmol, 2.0 mol-%) and PPh_3 (0.0830 g, 0.316 mmol, 6.1 mol-%) were used.The crude product was purified by flash column chromatography (1:1 CH_2Cl_2:95 % hexanes/5 % EtOAc), furnishing **1h** as a pale yellow oil.

Yield: 0.875 g, 4.77 mmol, 93 %.

^{1}H NMR (400 MHz, $CDCl_3$): δ 8.68 (d, $^3J_{H,H}$ = 4.8 Hz, 1H, **H^6**), 7.69-7.75 (m, 2H, **H^3** + **H^4**), 7.60 (s, 2H, **H$^{2'}$**), 7.21 (ddd, $^3J_{H,H}$ = 6.3 Hz, $^3J_{H,H}$ = 4.8 Hz, $^4J_{H,H}$ = 2.2 Hz, 1H, **H^5**), 7.06 (s, 1H, **H$^{4'}$**), 2.40 (s, 6H, C**H**$_3$).

^{13}C NMR (101 MHz, $CDCl_3$): δ 157.8 (**C^2**), 149.5 (**C^6**), 139.3 (**C$^{1'}$**), 138.3 (**C$^{3'}$**), 136.6 (**C^3** or **C^4**), 130.6 (**C$^{4'}$**), 124.7 (**C$^{2'}$**), 121.9 (**C^5**), 120.6 (**C^3** or **C^4**), 21.4 (**C**H_3).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −72.6 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 184.112 (100) $[M+H]^+$.

HRMS (ESI): Found 184.1120; calcd for $C_{13}H_{14}N$ $[M+H]^+$: 184.1121.

The NMR data are in accordance with those reported in the literature.[12]

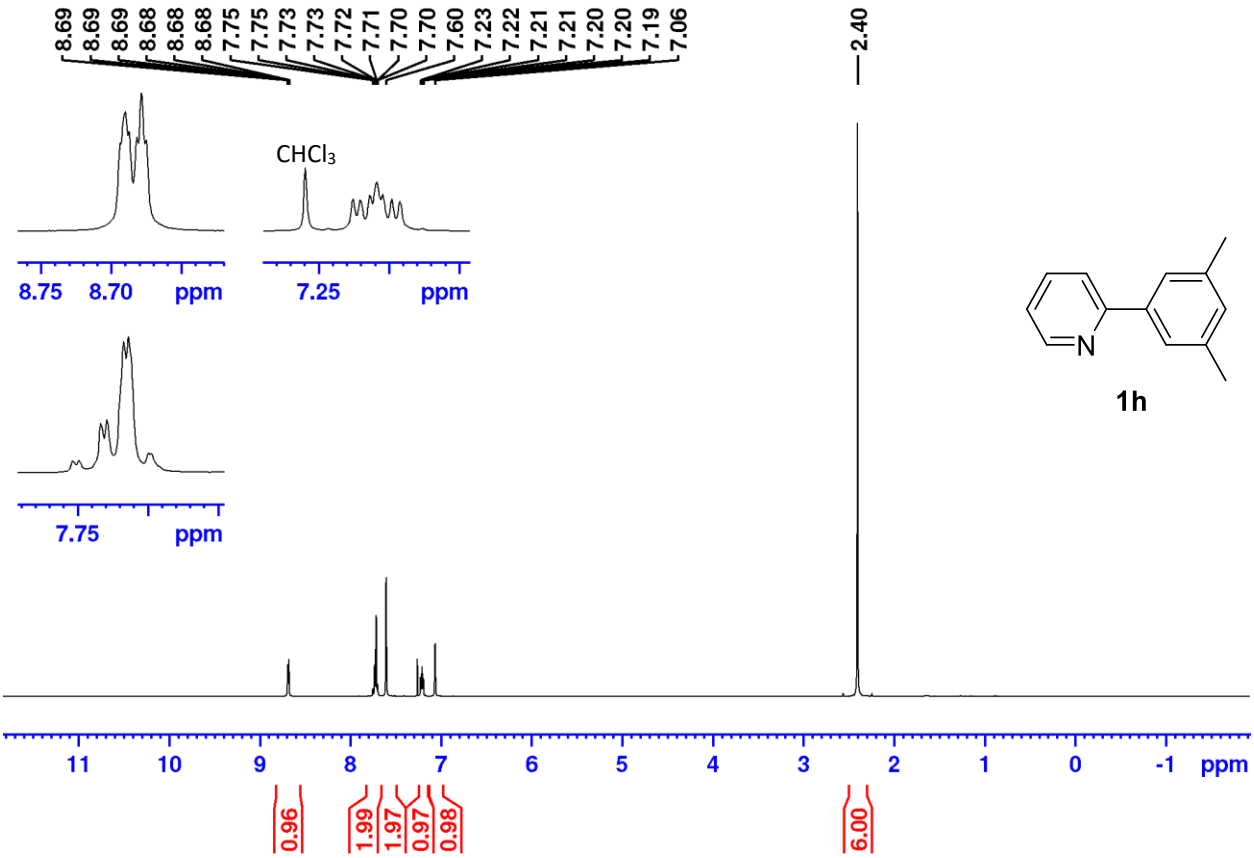


Figure S20. ^{1}H NMR (400 MHz, $CDCl_3$) of **1h**.

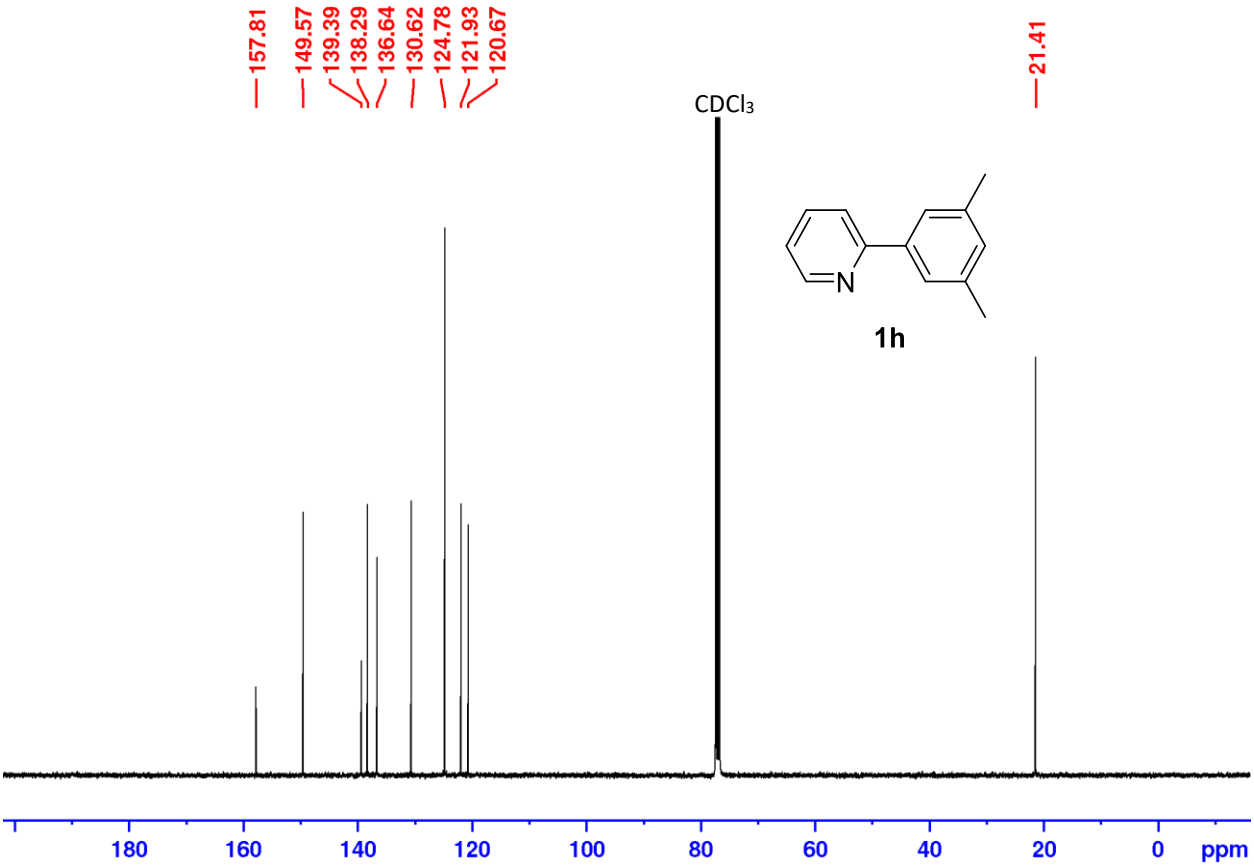


Figure S21. ^{13}C NMR (101 MHz, $CDCl_3$) of **1h**.

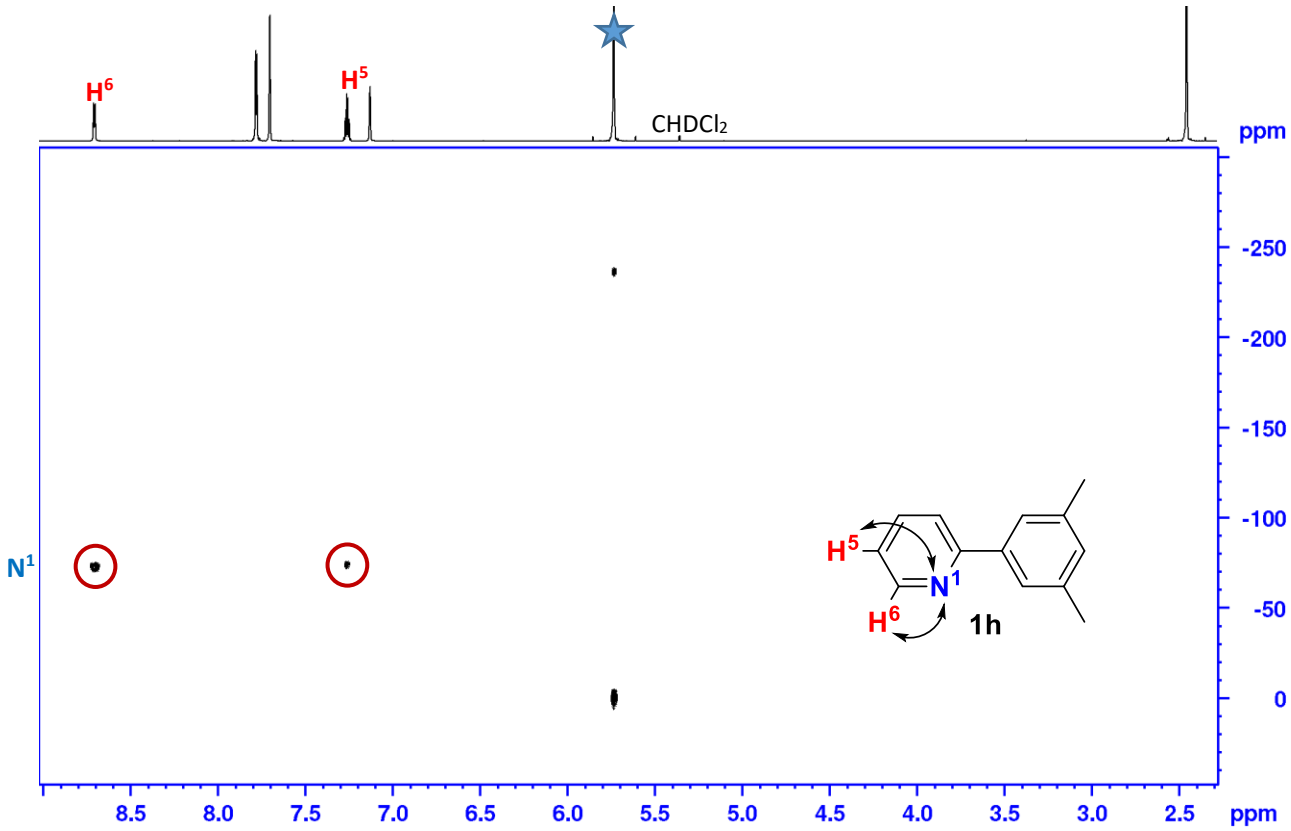
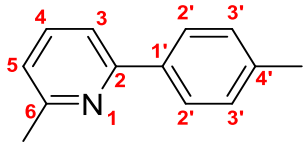


Figure S22. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1h**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1i

6-Methyl-2-(4-methylphenyl)pyridine (1i). The general procedure was followed. 2-Bromo-6-methylpyridine (0.737 g, 4.26 mmol, 1.0 equiv.), 4-methylphenylboronic acid (0.638 g, 4.69 mmol, 1.1 equiv.), K_3PO_4 (2.12 g, 10.0 mmol, 2.3 equiv.), $Pd(OAc)_2$ (0.0187 g, 0.0883 mmol, 2.0 mol-%) and PPh_3 (0.0664 g, 0.253 mmol, 5.9 mol-%) were used. The obtained crude product was purified by flash column chromatography (1:2 CH_2Cl_2:95 % hexanes/5 % EtOAc), furnishing **1i** as a colorless oil.

Yield: 0.717 g, 3.91 mmol, 92 %.

^{1}H NMR (600 MHz, $CDCl_3$): δ 7.89 (d, $^3J_{H,H}$ = 8.3 Hz, 2H, **H$^{2'}$**), 7.59-7.62 (m, 1H, **H^4**), 7.49 (d, $^3J_{H,H}$ = 7.9 Hz, 1H, **H^3**), 7.27 (d, $^3J_{H,H}$ = 8.3 Hz, 2H, **H$^{3'}$**), 7.06 (d, $^3J_{H,H}$ = 8.3 Hz, 1H, **H^5**), 2.62 (s, 3H, pyr-C**H**$_3$), 2.40 ppm (s, 3H, Ar-C**H**$_3$).

^{13}C NMR (151 MHz, $CDCl_3$): δ 158.2 (**C^6**), 156.9 (**C^2**), 138.6 (**C$^{4'}$**), 137.0 (**C$^{1'}$**), 136.7 (**C^4**), 129.4 (**C$^{3'}$**), 126.8 (**C$^{2'}$**), 121.2 (**C^5**), 117.2 (**C^3**), 24.8 (pyr-**C**H$_3$), 21.2 ppm (Ar-**C**H$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −73.5 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 184.112 (100) $[M+H]^+$.

HRMS (ESI): Found 184.1121; calcd for $C_{13}H_{14}N$ $[M+H]^+$: 184.1121.

The NMR data are in accordance with those reported in the literature.[13]

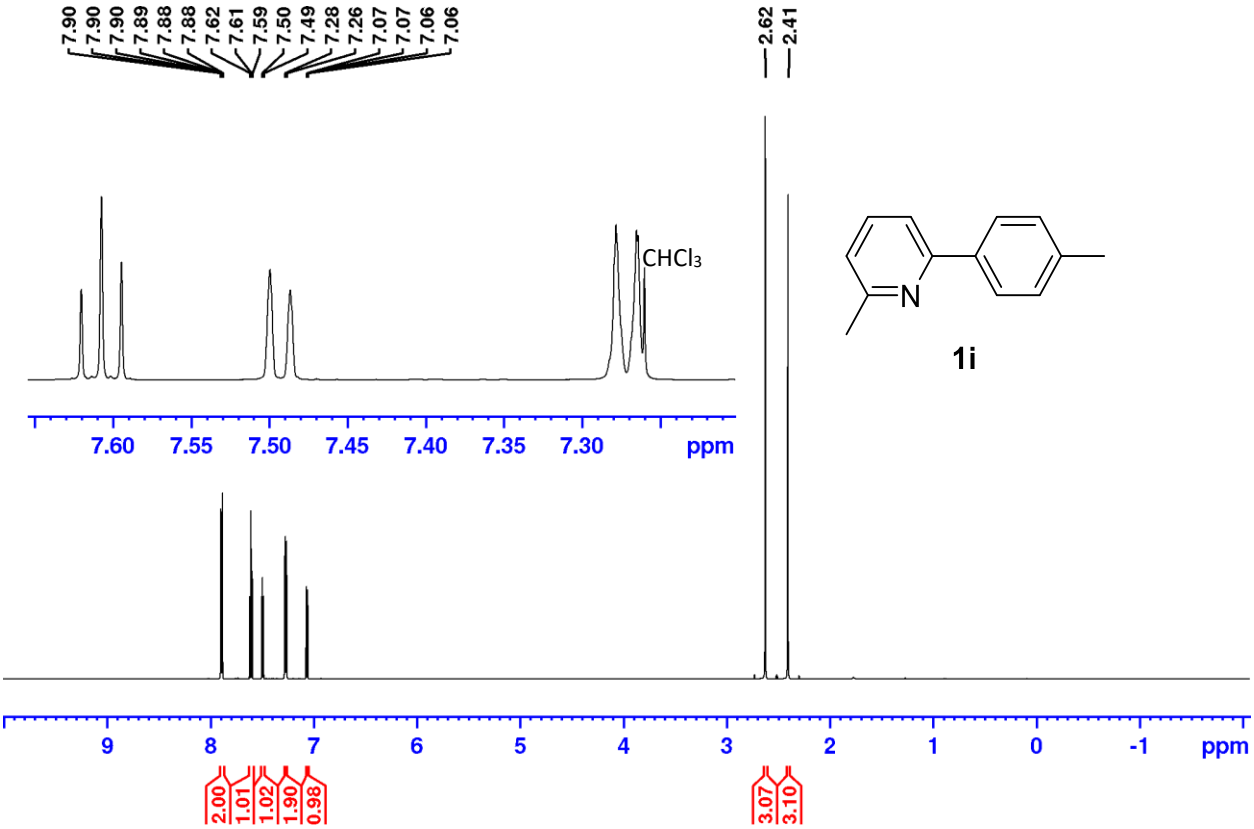


Figure S23. ^{1}H NMR (600 MHz, $CDCl_3$) of **1i**.

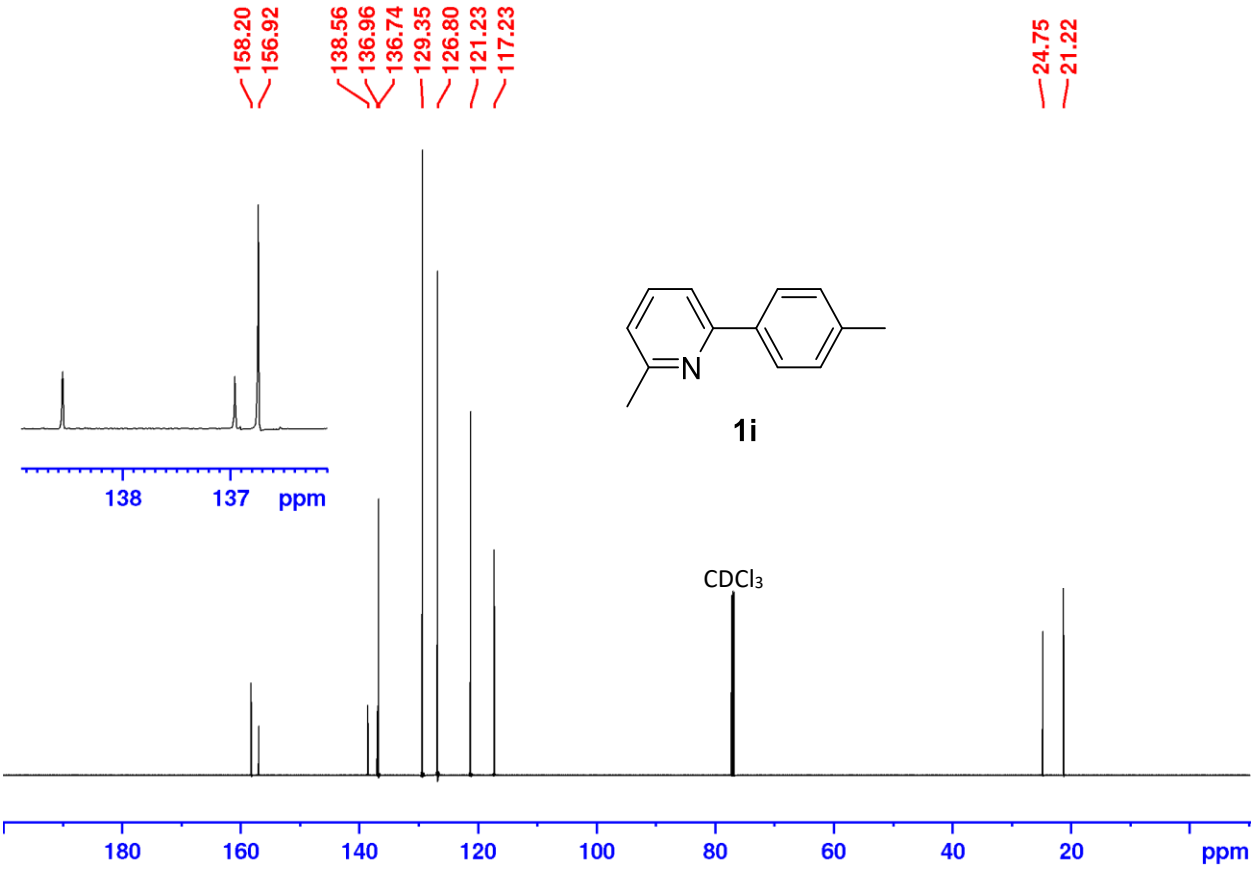


Figure S24. ^{13}C NMR (151 MHz, $CDCl_3$) of **1i**.

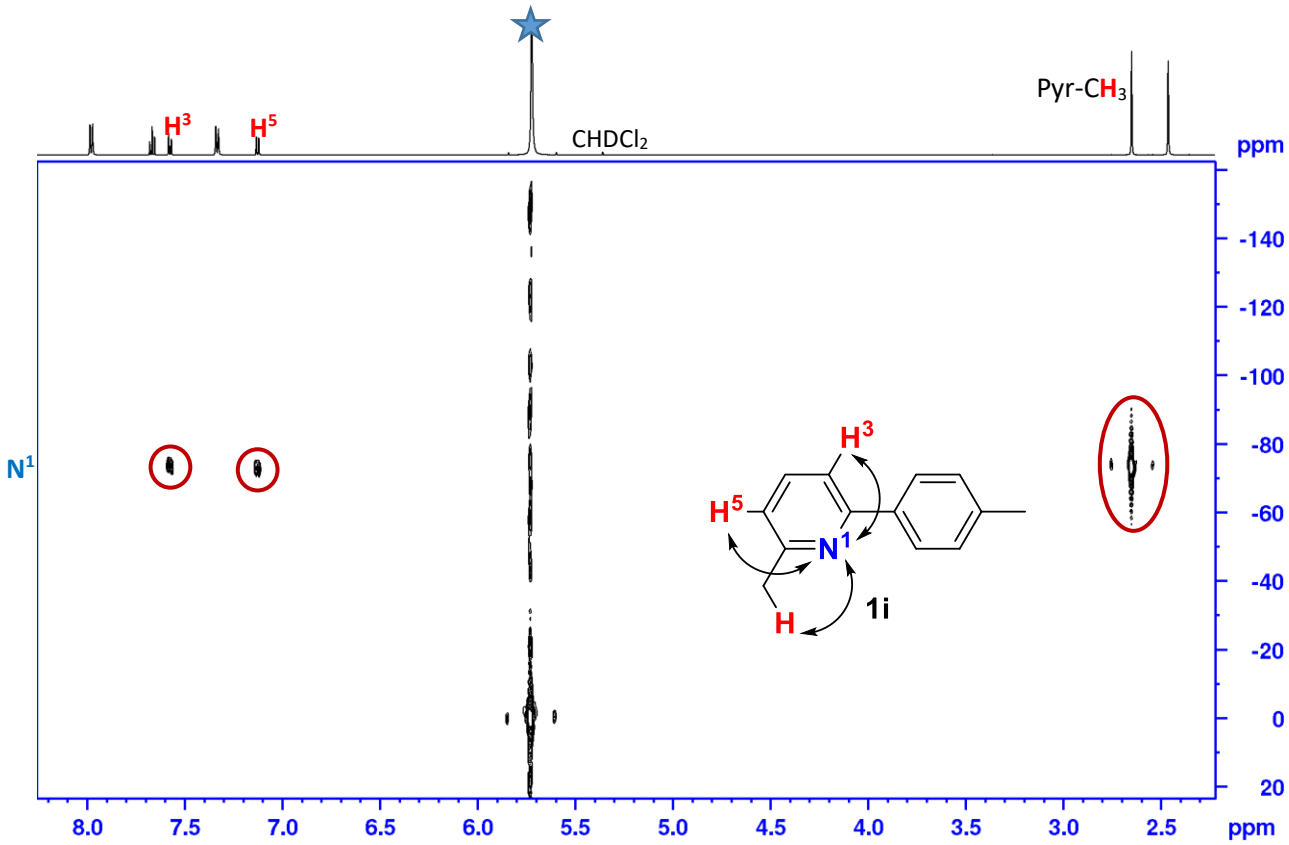
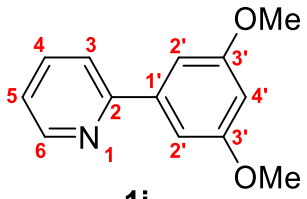


Figure S25. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1i**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1j

2-(3,5-Dimethoxyphenyl)pyridine (1j). The general procedure was followed. 2-Bromopyridine (0.781 g, 4.94 mmol, 1.0 equiv.), 3,5-dimethoxyphenylboronic acid (0.998 g, 5.48 mmol, 1.1 equiv.), K_3PO_4 (2.13 g, 10.0 mmol, 2.0 equiv.), $Pd(OAc)_2$ (0.0225 g, 0.100 mmol, 2.0 mol-%) and PPh_3 (0.0788 g, 0.300 mmol, 6.0 mol-%) were used. The crude product was purified by flash column chromatography (80 % hexanes/20 % EtOAc), yielding **1j** as a pale yellow oil.

Yield: 0.923 g, 4.29 mmol, 87 %.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.68-8.69 (m, 1H, **H^6**), 7.75 (dd, ^3J = 7.9 Hz, $^3J_{H,H}$ = 7.5 Hz, $^4J_{H,H}$ = 1.9 Hz, 1H, **H^4**), 7.69-7.71 (m, 1H, **H^3**), 7.24 (ddd, ^3J = 7.3 Hz, $^3J_{H,H}$ = 4.9 Hz, $^4J_{H,H}$ = 1.2 Hz, 1H, **H^5**), 7.15 (d, $^4J_{H,H}$ = 2.3 Hz, 1H, **H$^{2'}$**), 6.53 (m, 1H, **H$^{4'}$**), 3.87 ppm (s, 6H, OC**H**$_3$).

^{13}C NMR (151 MHz, $CDCl_3$): δ 161.0 (**C$^{3'}$**), 157.1 (**C^2**), 149.5 (**C^6**), 141.5 (**C$^{1'}$**), 136.8 (**C^4**), 122.4 (**C^5**), 120.8 (**C^3**), 104.8 (**C$^{2'}$**), 101.3 (**C$^{4'}$**), 55.5 ppm (O**C**H$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −72.3 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 216.102 (100) $[M+H]^+$, 238.084 (100) $[M+Na]^+$.

HRMS (ESI): Found 216.1019; calcd for $C_{13}H_{14}NO_2$ $[M+H]^+$: 216.1019.

HRMS (ESI): Found 238.0838; calcd for $C_{13}H_{13}NNaO_2$ $[M+Na]^+$: 238.0838.

The NMR data are in accordance with those reported in the literature.[14]

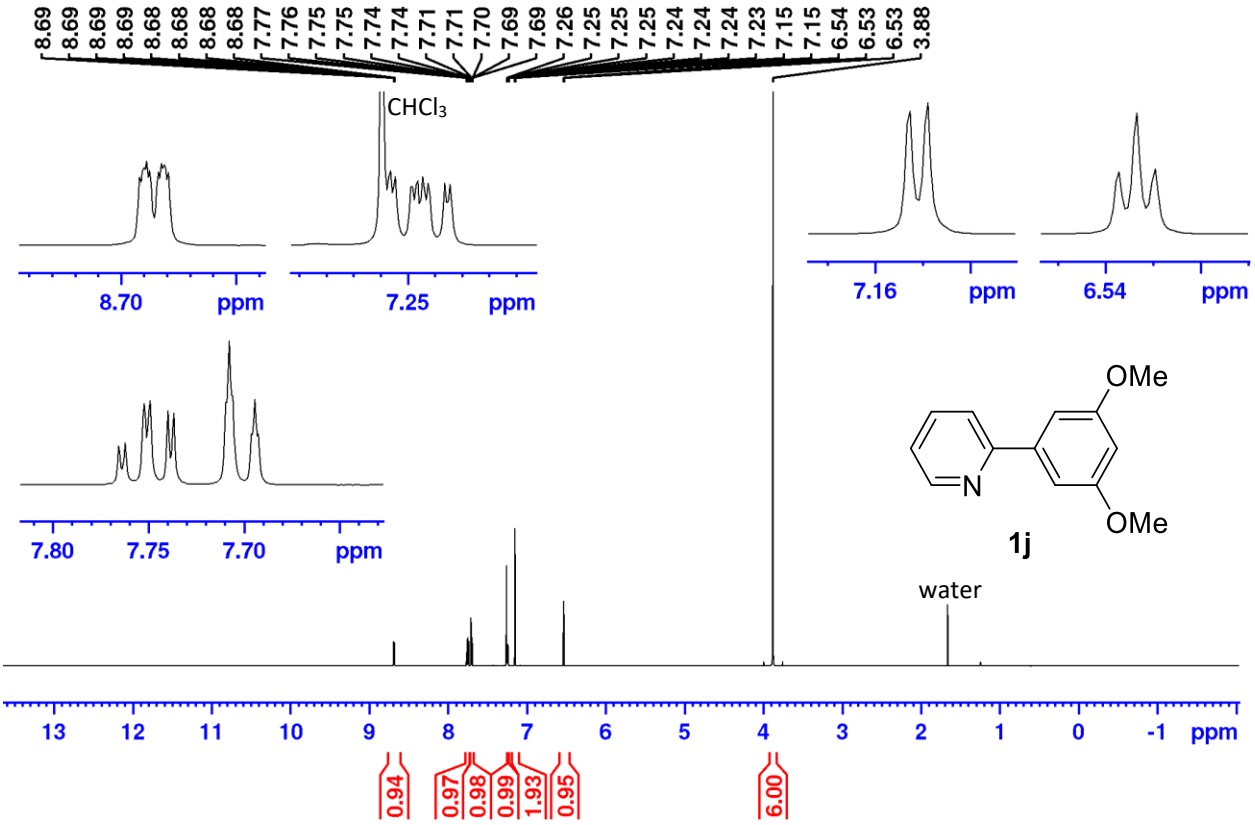


Figure S26. ^{1}H NMR (600 MHz, $CDCl_3$) of **1j**.

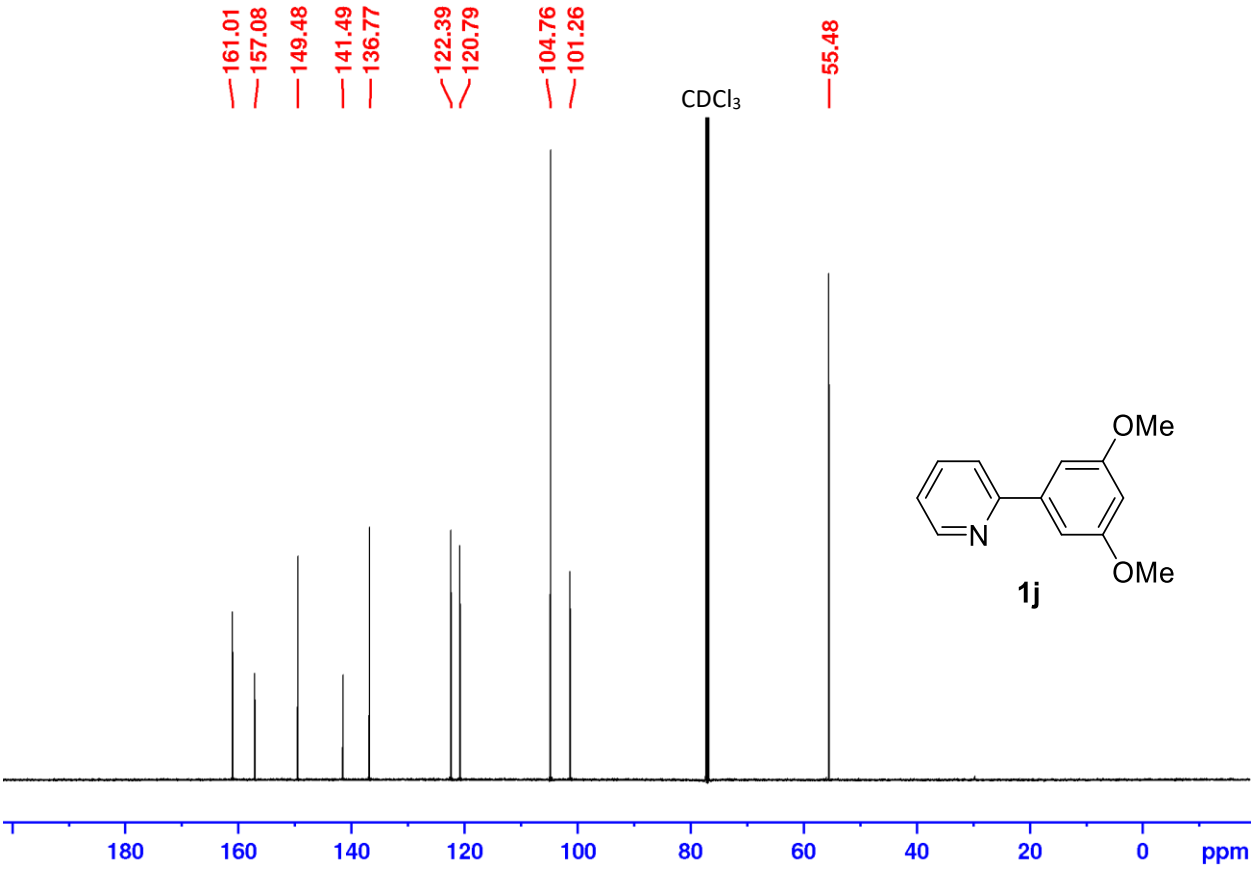


Figure S27. ^{13}C NMR (151 MHz, $CDCl_3$) of **1j**.

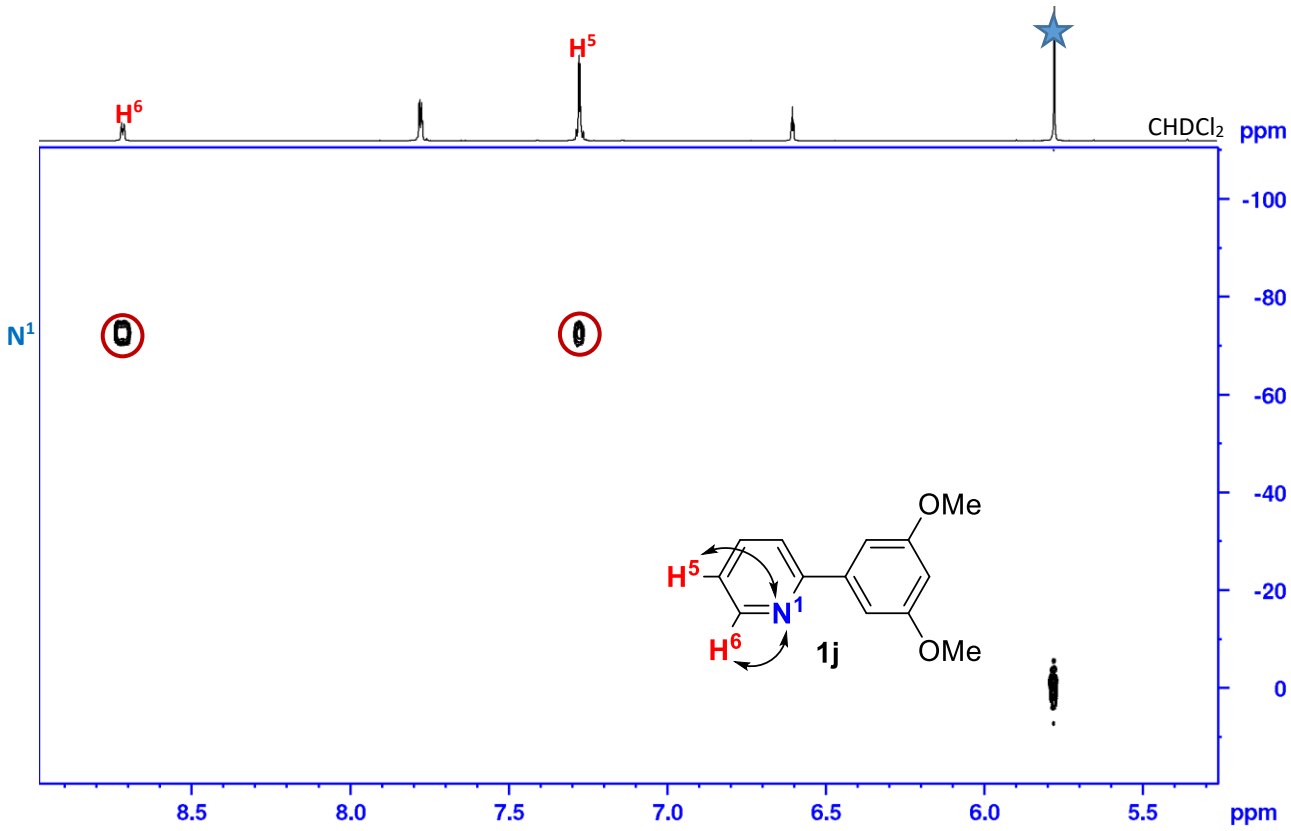
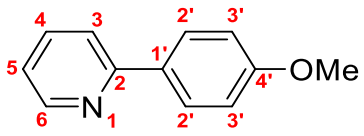


Figure S28. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1j**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1k

2-(4-Methoxyphenyl)pyridine (1k). The general procedure was followed. 2-Bromopyridine (0.673 g, 4.26 mmol, 1.0 equiv.), 4-methoxyphenylboronic acid (0.713 g, 4.69 mmol, 1.1 equiv.), K_3PO_4 (2.12 g, 10.0 mmol, 2.3 equiv.), $Pd(OAc)_2$ (0.0187 g, 0.0883 mmol, 2.0 mol-%) and PPh_3 (0.0664 g, 0.253 mmol, 6.0 mol-%) were used. The obtained crude product was purified by flash column chromatography (70 % hexanes/30 % EtOAc), furnishing **1k** as a pale yellow solid.

Yield: 0.666 g, 3.60 mmol, 85 %.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.65 (m, 1H, **H^6**), 7.95 (d, $^3J_{H,H}$ = 8.8 Hz, 2H, **H$^{2'}$**), 7.71 (ddd, $^3J_{H,H}$ = 7.9 Hz, $^3J_{H,H}$ = 7.3 Hz, $^4J_{H,H}$ = 1.8 Hz, 1H, **H^4**), 7.67 (d, $^3J_{H,H}$ = 7.9 Hz, 1H, **H^3**), 7.17 (ddd, $^3J_{H,H}$ = 7.3 Hz, $^3J_{H,H}$ = 4.8 Hz, $^4J_{H,H}$ = 1.1 Hz, 1H, **H^5**), 7.00 (d, $^3J_{H,H}$ = 8.8 Hz, 2H, **H$^{3'}$**), 3.86 ppm (s, 3H, Ar-OC**H**$_3$).

^{13}C NMR (151 MHz, $CDCl_3$): δ 160.4 (**C$^{4'}$**), 157.1 (**C^2**), 149.5 (**C^6**), 135.6 (**C^4**), 132.0 (**C$^{1'}$**), 128.1 (**C$^{2'}$**), 121.3 (**C^5**), 119.7 (**C$^{3'}$**), 114.1 (**C^3**), 55.3 ppm (Ar-O**C**H$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −74.6 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 186.091 (100) $[M+H]^+$.

HRMS (ESI): Found 186.0913; calcd for $C_{12}H_{12}NO$ $[M+H]^+$: 186.0913.

The NMR data are in accordance with those reported in the literature.[15]

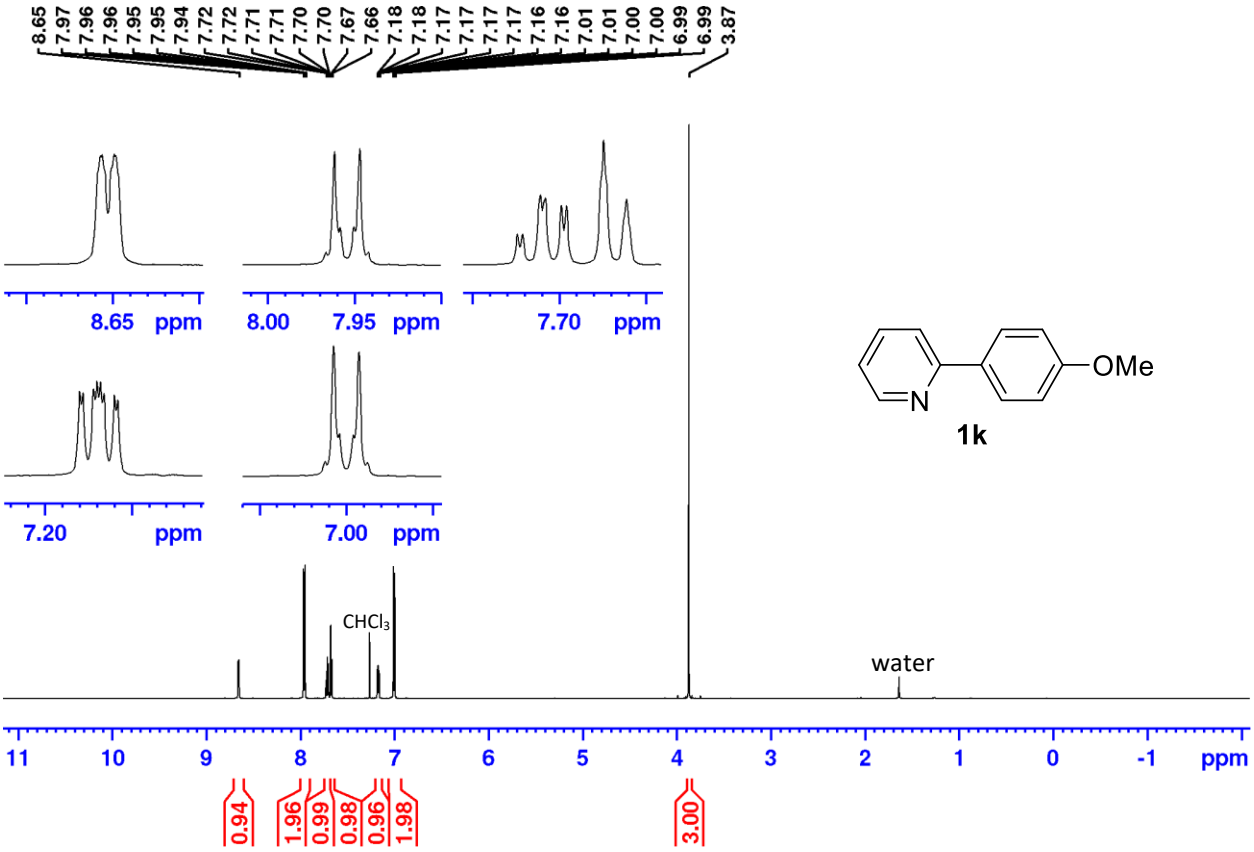


Figure S29. ^{1}H NMR (600 MHz, $CDCl_3$) of **1k**.

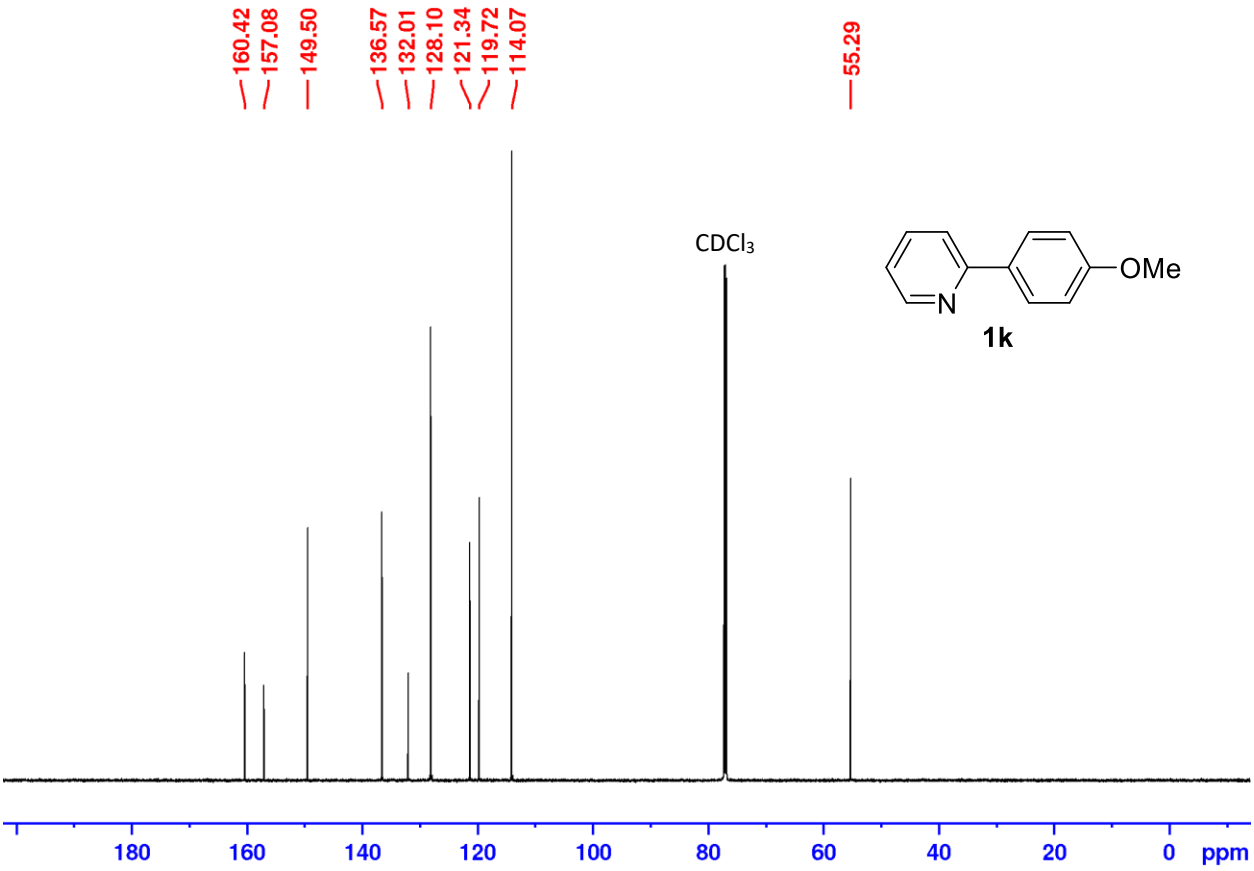


Figure S30. ^{13}C NMR (151 MHz, $CDCl_3$) of **1k**.

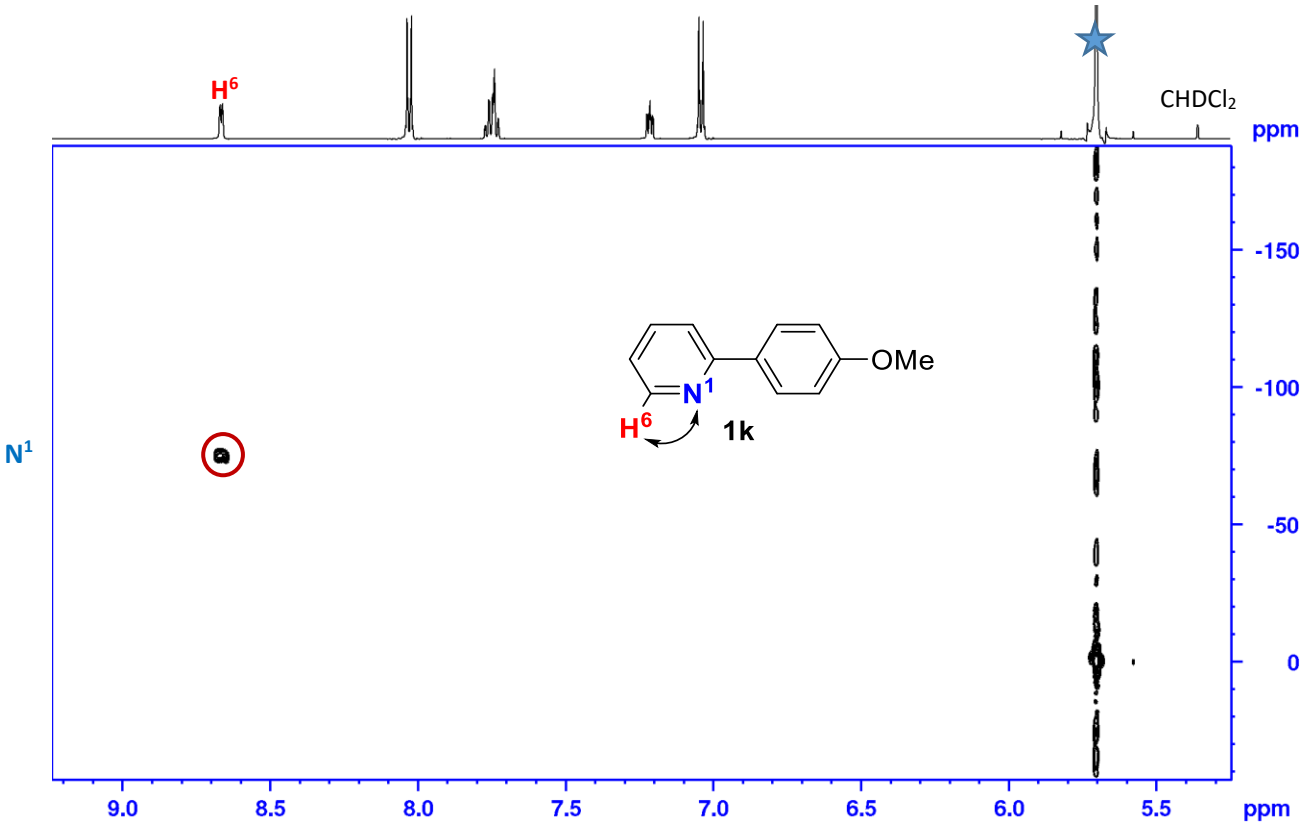
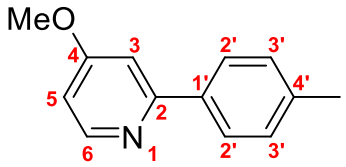


Figure S31. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1k**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1l

4-Methoxy-2-(4-methylphenyl)pyridine (1l). The general procedure was followed. 2-Bromo-4-methoxypyridine (0.968 g, 5.15 mmol, 1.0 equiv.), 4-methylphenylboronic acid (0.782 g, 5.75 mmol, 1.1 equiv.), K_3PO_4 (2.19 g, 10.3 mmol, 2.0 equiv.), $Pd(OAc)_2$ (0.0236 g, 0.105 mmol, 2.0 mol-%) and PPh_3 (0.0824 g, 0.314 mmol, 6.1 mol-%) were used. The crude product was purified by flash column chromatography (CH_2Cl_2), furnishing **1l** as a pale yellow solid.

Yield: 0.912 g, 4.58 mmol, 89 %.

M.p. 58-59 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.50 (d, $^3J_{H,H}$ = 5.7 Hz, 1H, **H^6**), 7.86 (d, $^3J_{H,H}$ = 8.1 Hz, 2H, **H$^{2'}$**), 7.27 (d, $^3J_{H,H}$ = 8.0 Hz, 2H, **H$^{3'}$**), 7.21 (d, $^4J_{H,H}$ = 2.4 Hz, 1H, **H^3**), 6.75 (dd, $^3J_{H,H}$ = 5.7 Hz, $^4J_{H,H}$ = 2.4 Hz, 1H, **H^5**), 3.90 (s, 3H, OC**H**$_3$), 2.40 ppm (s, 3H, C**H**$_3$).

^{13}C NMR (151 MHz, $CDCl_3$): δ 166.3 (**C^4**), 159.1 (**C^2**), 150.8 (**C^6**), 139.0 (**C$^{4'}$**), 136.5 (**C$^{1'}$**), 129.4 (**C$^{3'}$**), 126.7 (**C$^{2'}$**), 107.8 (**C^5**), 106.4 (**C^3**), 55.1 (O**C**H$_3$), 21.3 ppm (**C**H$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −94.2 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 200.107 (100) $[M+H]^+$.

HRMS (ESI): Found 200.1070; calcd for $C_{13}H_{14}NO$ $[M+H]^+$: 200.1070.

The NMR data are in accordance with those reported in the literature.[16]

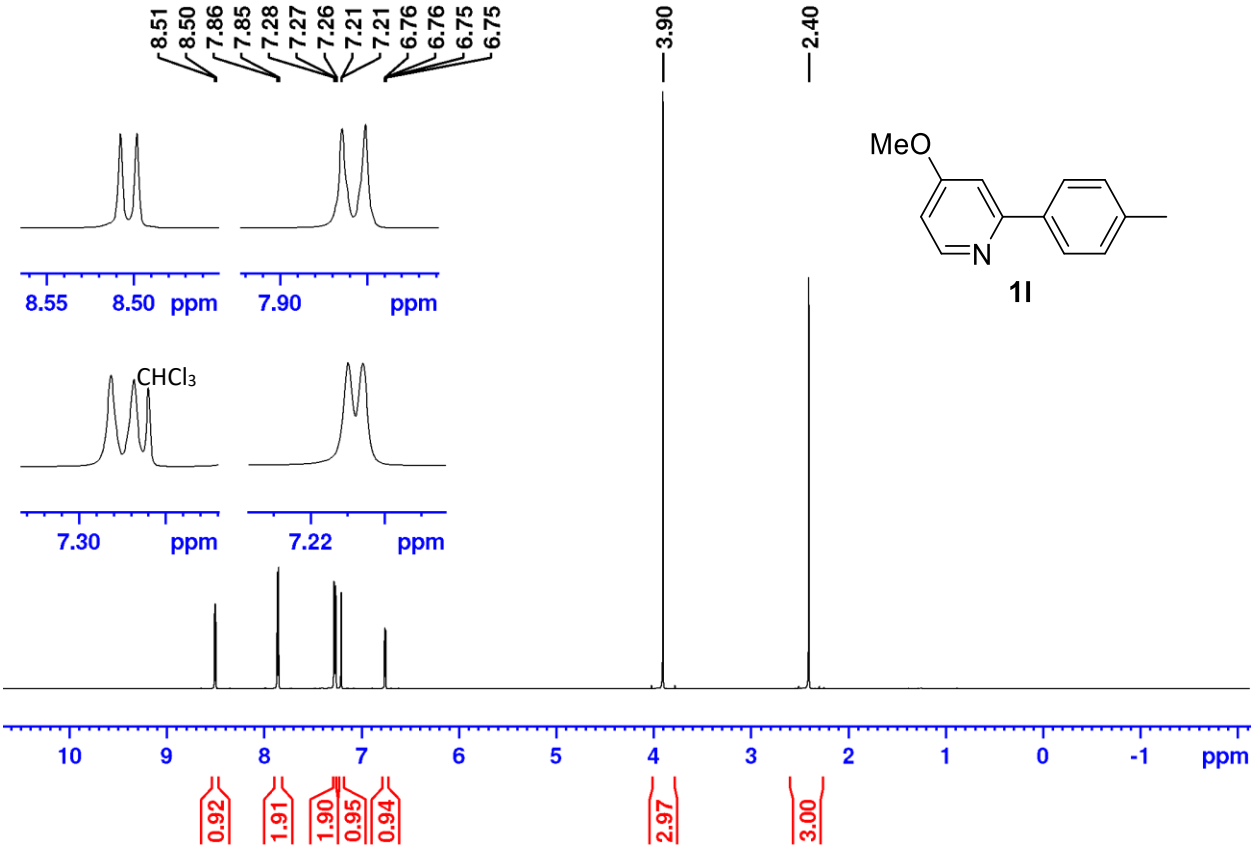


Figure S32. ^{1}H NMR (600 MHz, $CDCl_3$) of **1l**.

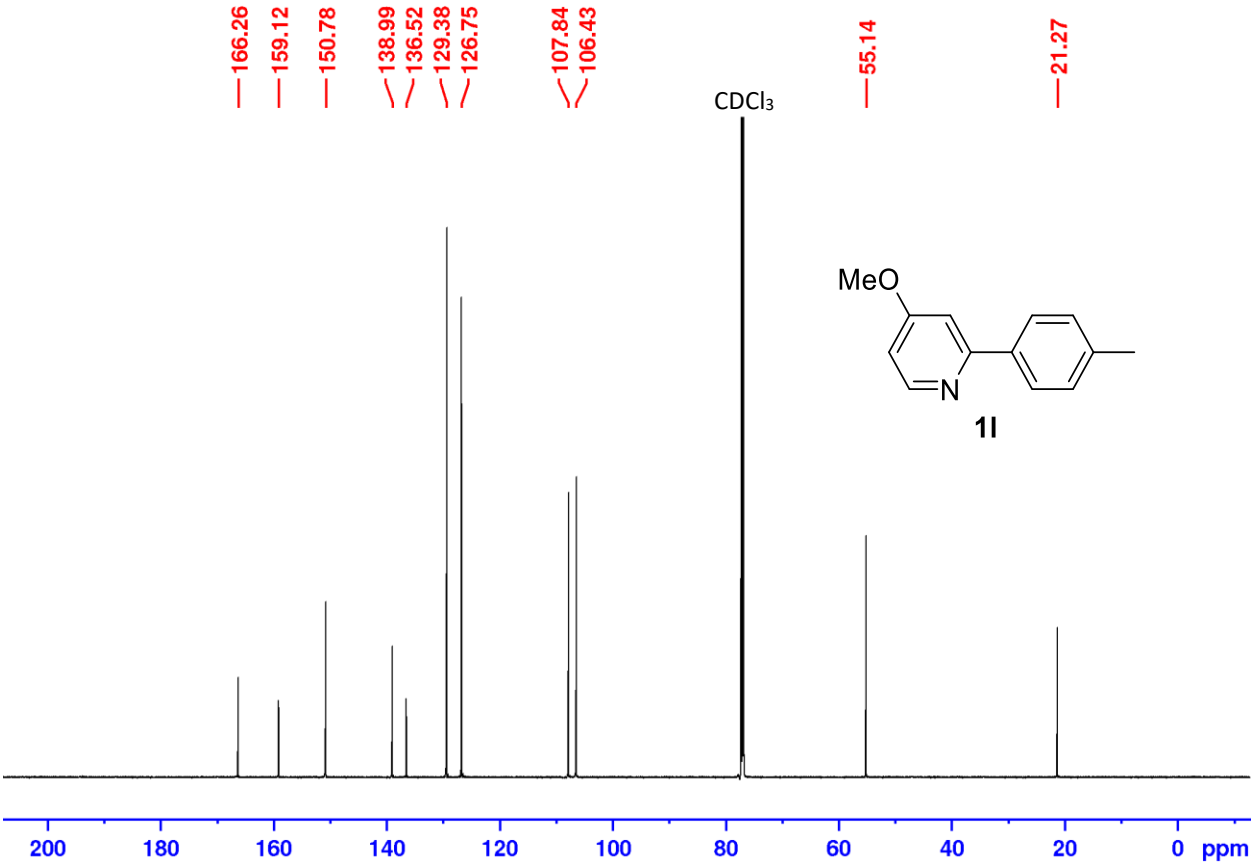


Figure S33. ^{13}C NMR (151 MHz, $CDCl_3$) of **1l**.

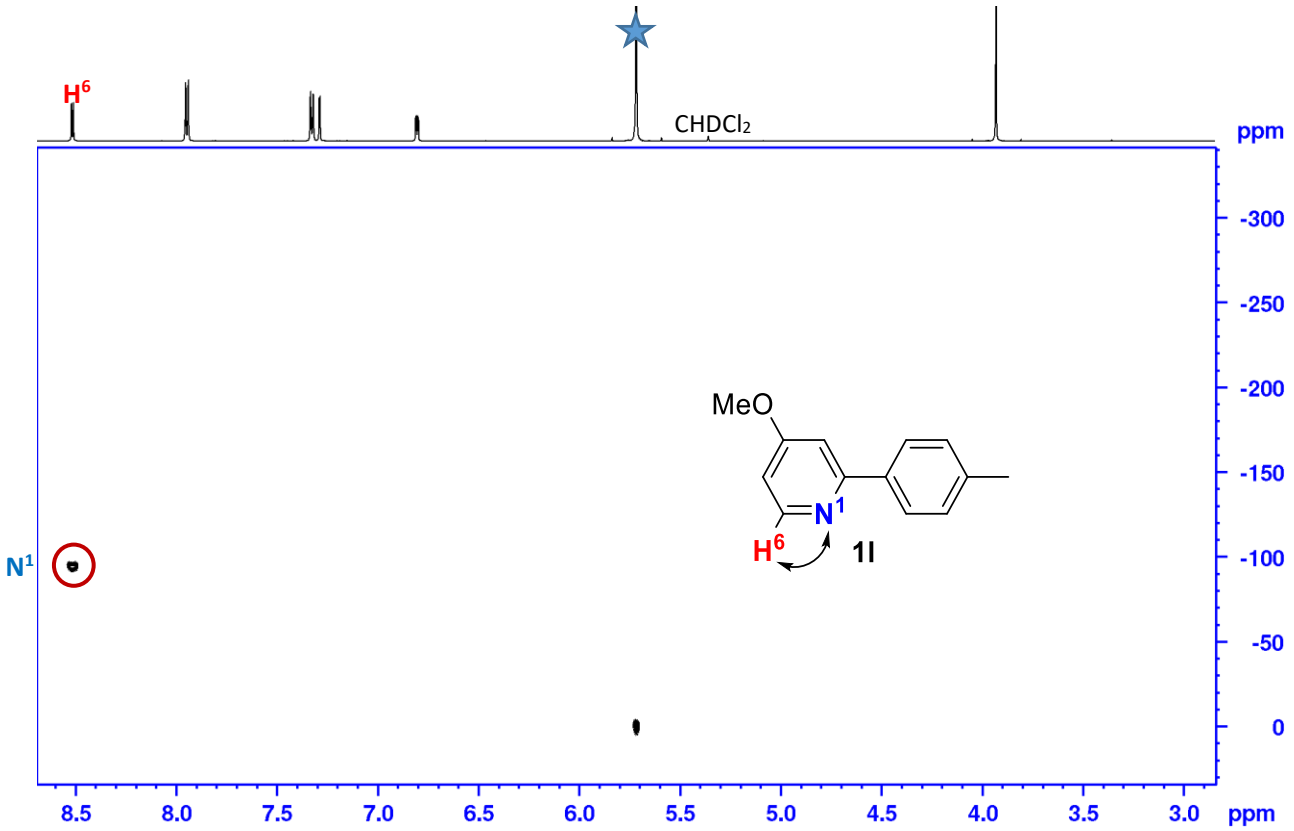
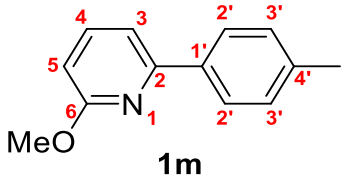


Figure S34. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1l**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1m

6-Methoxy-2-(4-methylphenyl)pyridine (1m). The general procedure was followed. 2-Bromo-6-methoxypyridine (0.803 g, 4.27 mmol, 1.0 equiv.), 4-methylphenylboronic acid (0.638 g, 4.69 mmol, 1.1 equiv.), K_3PO_4 (2.12 g, 10.0 mmol, 2.3 equiv.), $Pd(OAc)_2$ (0.0187 g, 0.0883 mmol, 2.0 mol-%) and PPh_3 (0.0664 g, 0.253 mmol, 5.9 mol-%) were used. The obtained crude product was purified by flash column chromatography (98 % hexanes/2 % EtOAc), furnishing **1m** as a colorless oil.

Yield: 0.697 g, 3.50 mmol, 82 %.

^{1}H NMR (400 MHz, $CDCl_3$): δ 7.95 (d, $^3J_{H,H}$ = 8.2 Hz, 2H, **H$^{2'}$**), 7.59-7.63 (m, 1H, **H^4**), 7.32 (d, $^3J_{H,H}$ = 7.4 Hz, 1H, **H^3**), 7.25-7.28* (m, 2H, **H$^{3'}$**), 6.66 (d, $^3J_{H,H}$ = 8.2 Hz, 1H, **H^5**), 4.04 (s, 3H, OC**H**$_3$), 2.41 ppm (s, 3H, Ar-C**H**$_3$).

*The resonance was found to partially overlap with the resonance corresponding to residual $CHCl_3$ in the NMR solvent.

^{13}C NMR (101 MHz, $CDCl_3$): δ 163.6 (**C^6**), 154.7 (**C^2**), 139.07 (**C^4**), 138.77 (**C$^{4'}$**), 136.3 (**C$^{1'}$**), 129.3 (**C$^{3'}$**), 126.6 (**C$^{2'}$**), 112.4 (**C^3**), 108.8 (**C^5**), 53.1 (O**C**H$_3$), 21.2 ppm (Ar-**C**H$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −121.5 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 222.089 (100) $[M+Na]^+$.

HRMS (ESI): Found 222.0887; calcd for $C_{13}H_{13}NNaO$ $[M+Na]^+$: 222.0889.

The NMR data are in accordance with those reported in the literature.[17]

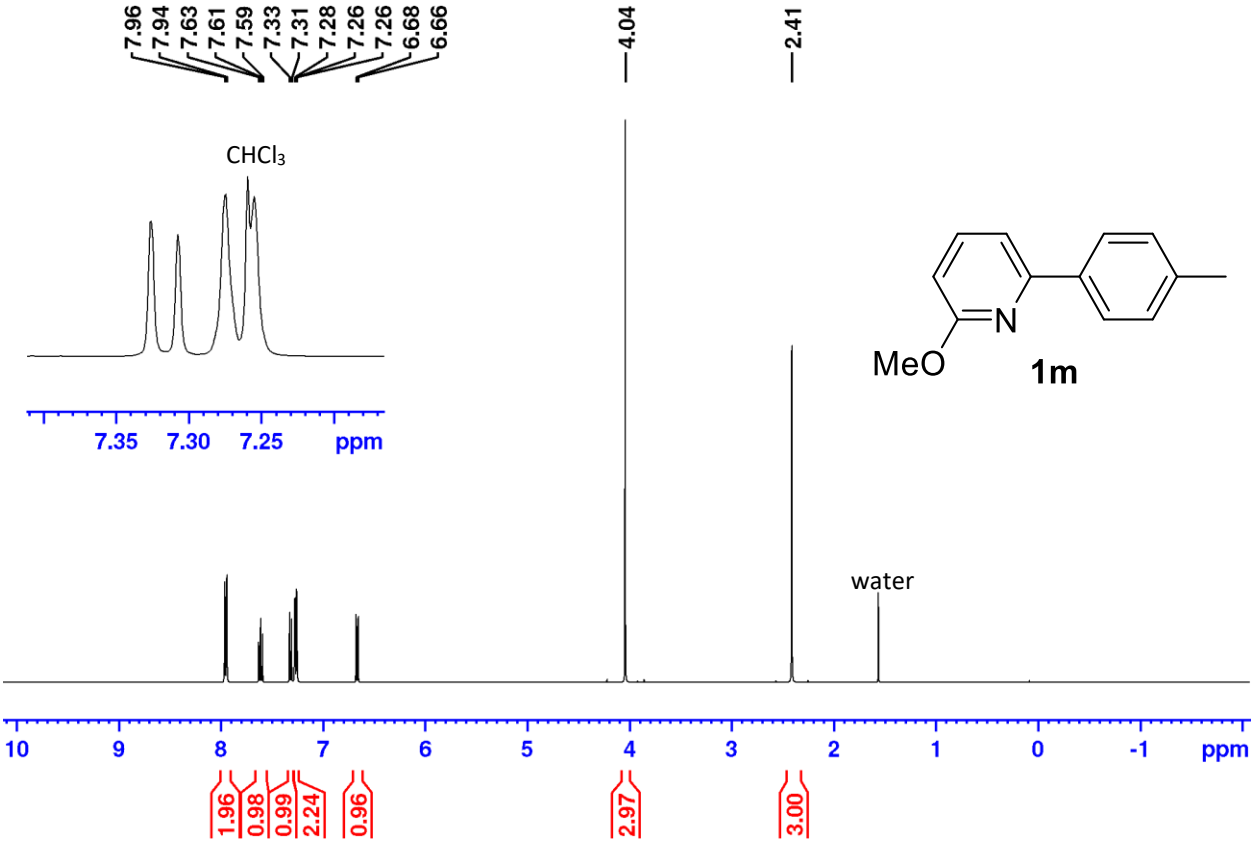


Figure S35. ^{1}H NMR (400 MHz, $CDCl_3$) of **1m**.

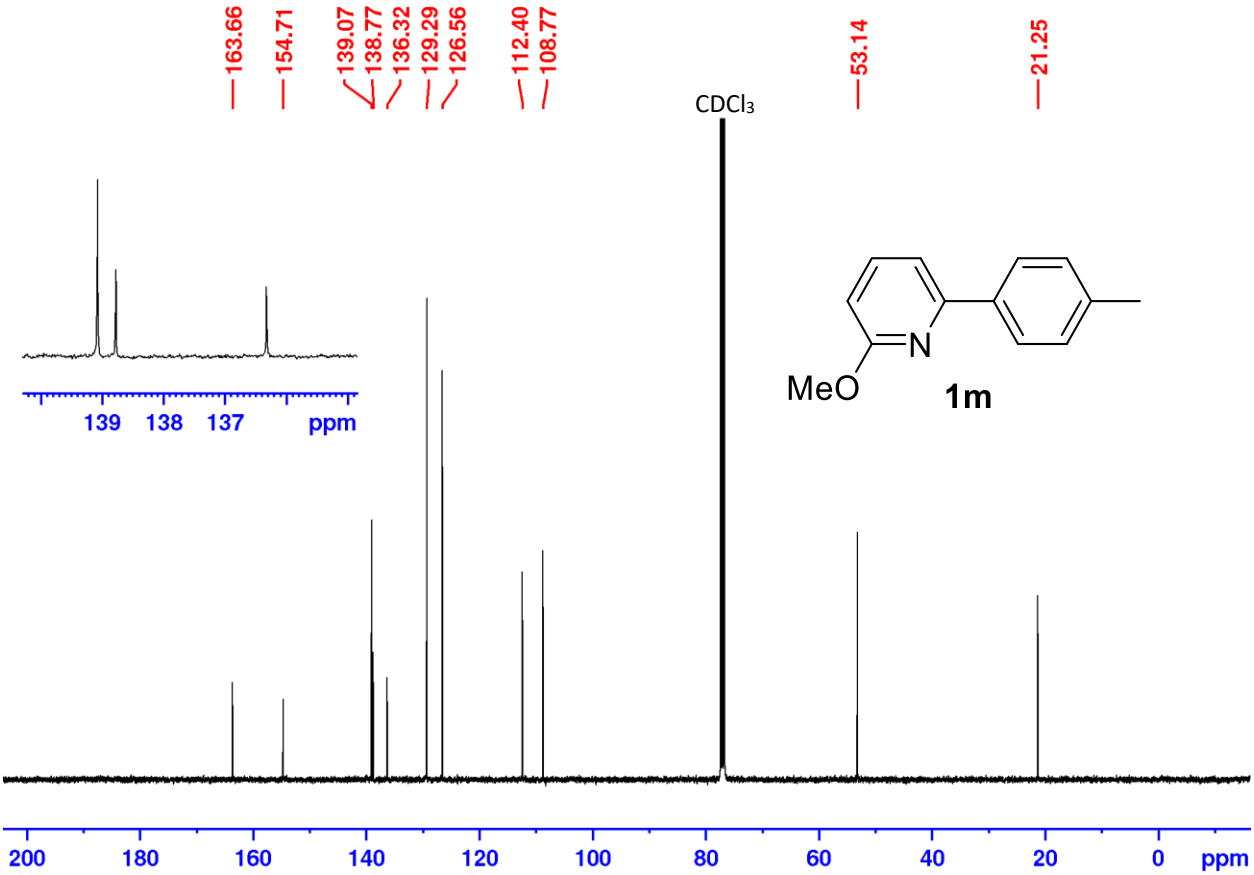


Figure S36. ^{13}C NMR (101 MHz, $CDCl_3$) of **1m**.

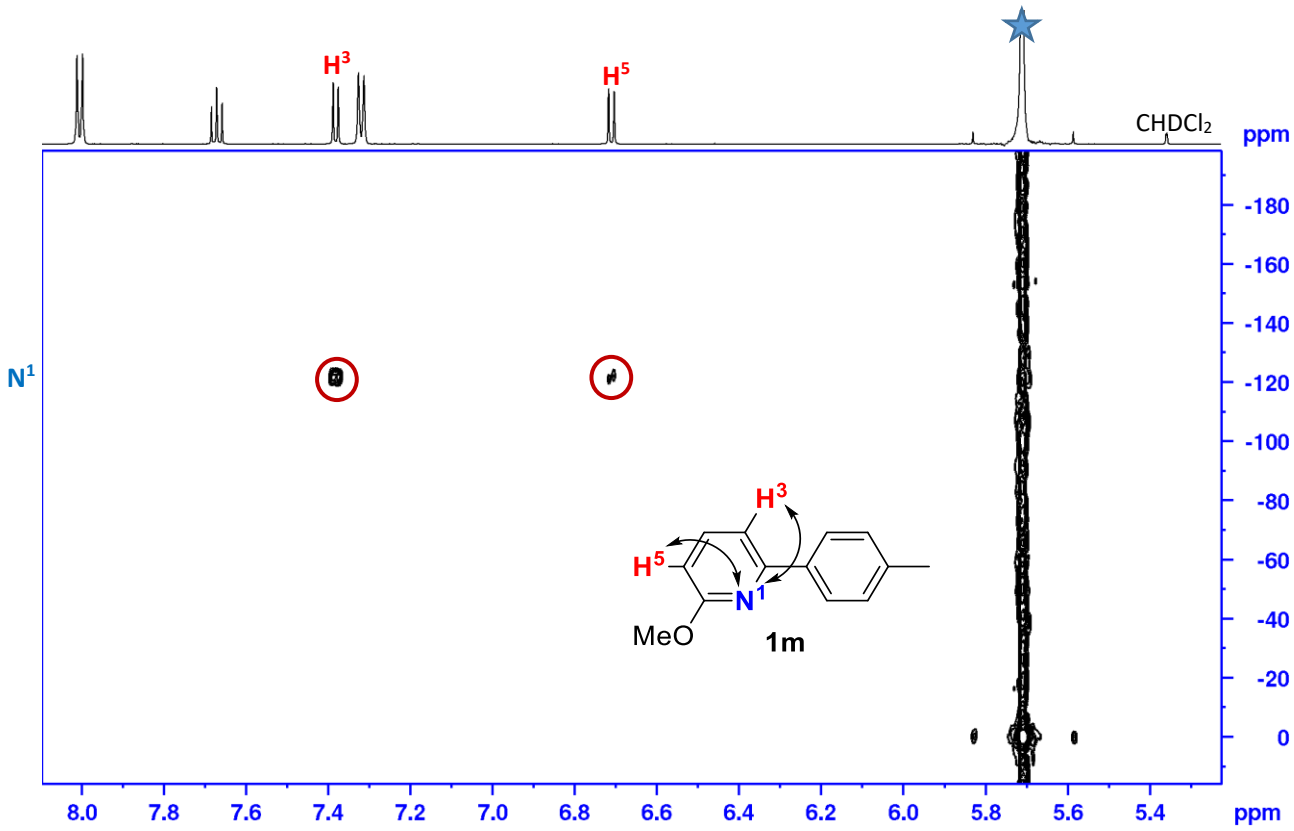
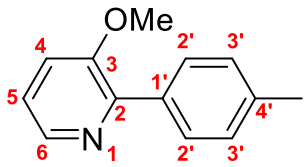


Figure S37. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1m**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1n

3-Methoxy-2-(4-methylphenyl)pyridine (1n). The general procedure was followed. 2-Bromo-3-methoxypyridine (1.88 g, 10.0 mmol, 1.0 equiv.), 4-methylphenylboronic acid (1.36 g, 10.0 mol, 1.0 equiv.), K_3PO_4 (4.25 g, 20.0 mmol, 2.0 equiv.), $Pd(OAc)_2$ (0.0451 g, 0.201 mmol, 2.0 mol-%) and PPh_3 (0.158 g, 0.602 mmol, 6.0 mol-%) in *n*-PrOH (20 mL) and water (20 mL) were used. The crude product was purified by flash column chromatography (85 % hexanes/15 % EtOAc), furnishing **1n** as a yellow oil.

Yield: 1.47 g, 7.36 mmol, 74 %.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.31 (dd, $^3J_{H,H}$ = 4.6 Hz, $^4J_{H,H}$ = 1.3 Hz, 1H, **H^6**), 7.83 (d, $^3J_{H,H}$ = 8.2 Hz, 2H, **H$^{2'}$**), 7.26-7.28 (m, 3H, **H^4** + **H$^{3'}$**), 7.21 (dd, $^3J_{H,H}$ = 8.3 Hz, $^3J_{H,H}$ = 4.6 Hz, 1H, **H^5**), 3.85 (s, 3H, OC**H**$_3$), 2.42 ppm (s, 3H, Ar-C**H**$_3$).

^{13}C NMR (151 MHz, $CDCl_3$): δ 153.4 (**C^3**), 148.2 (**C^2**), 141.2 (**C^6**), 138.1 (**C$^{4'}$**), 134.8 (**C$^{1'}$**), 129.2 (**C$^{2'}$**), 128.6 (**C$^{3'}$**), 122.5 (**C^5**), 118.3 (**C^4**), 55.4 (O**C**H$_3$), 21.3 ppm (Ar-**C**H$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −63.9 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 200.107 (100) $[M+H]^+$.

HRMS (ESI): Found 200.1069; calcd for $C_{13}H_{14}NO$ $[M+H]^+$: 200.1070.

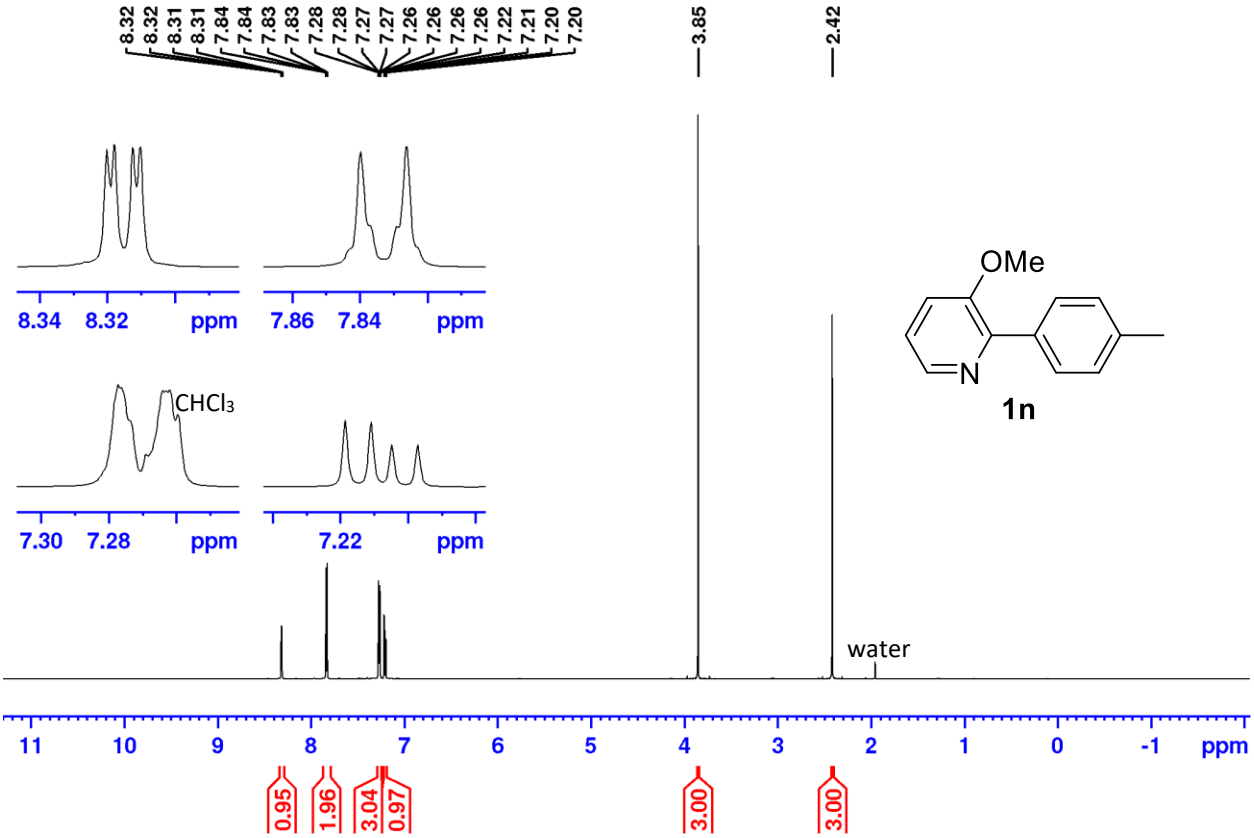


Figure S38. ^{1}H NMR (600 MHz, $CDCl_3$) of **1n**.

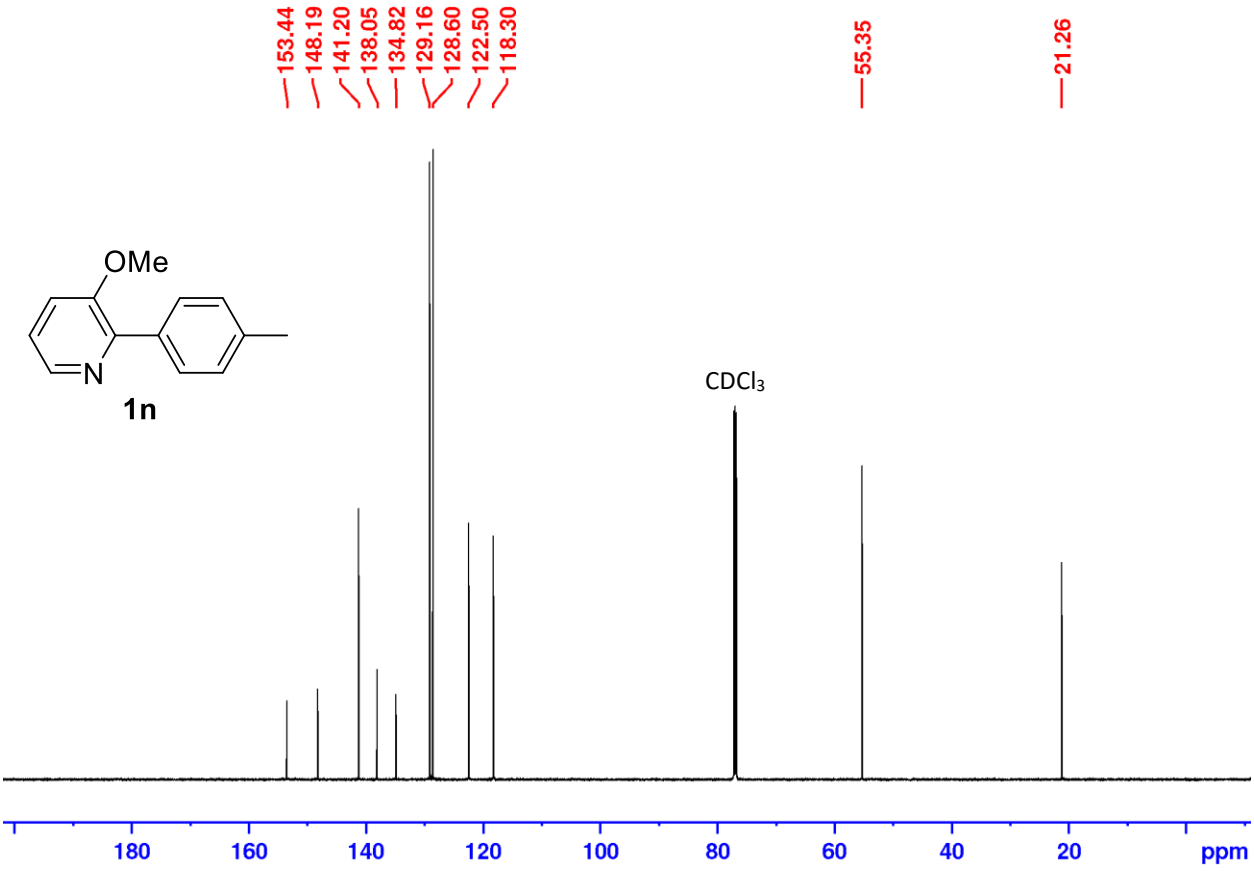


Figure S39. ^{13}C NMR (151 MHz, $CDCl_3$) of **1n**.

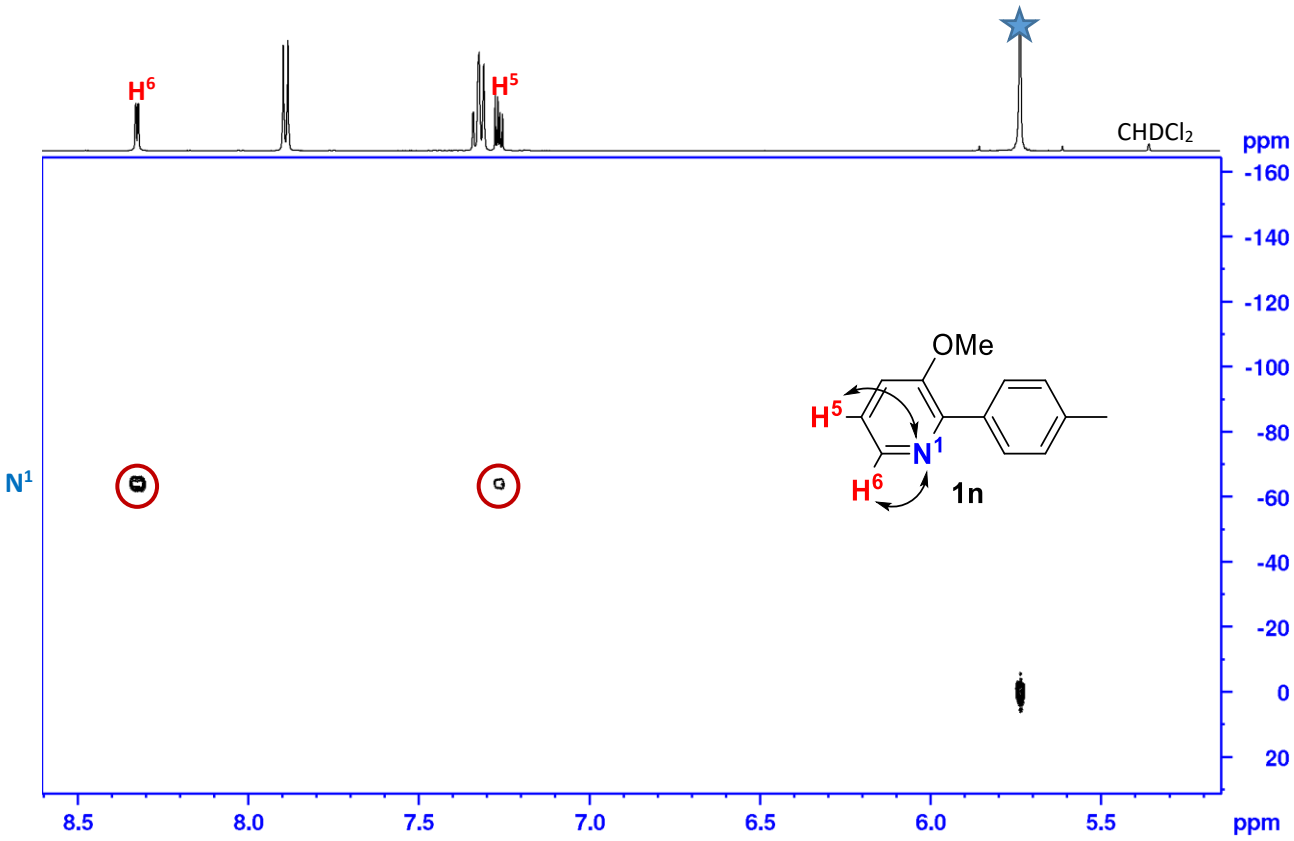
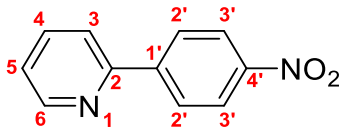


Figure S40. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1n**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1o

2-(4-Nitrophenyl)pyridine (1o). A suspension of 2-bromopyridine (0.795 g, 5.03 mmol, 1.0 equiv.), 4-nitrophenylboronic acid (0.919 g, 5.51 mmol, 1.1 equiv.) and $KF{\cdot}2H_2O$ (1.60 g, 17.0 mmol, 3.4 equiv.) in THF (10 mL) was bubbled with Ar for 15 min. Pd_2dba_3 (0.121 g, 0.132 mmol, 2.6 mol-%) and $HBF_4{\cdot}P(t\text{-}Bu)_3$ (0.0865 g, 0.298 mmol, 5.9 mol-%) were added under a flow of Ar, and the resulting suspension was heated at reflux temperature for 1 h under Ar. After cooling to rt, CH_2Cl_2 (50 mL in total) was added to the reaction mixture, and the solution was transferred to a round bottom flask, leaving insoluble inorganics behind. The solvent was removed under reduced pressure. The obtained residue was purified by flash column chromatography (1:2 CH_2Cl_2:95 % hexanes/5 % EtOAc, to 1:1 CH_2Cl_2:95 % hexanes/5 % EtOAc), yielding **1o** as a pale yellow solid.

Yield: 0.636 g, 3.18 mmol, 63 %.

M.p. 131-132 °C (Lit.[18]: 130-131 °C).

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.75 (d, $^3J_{H,H}$ = 4.6 Hz, 1H, **H^6**), 8.33 (d, $^3J_{H,H}$ = 8.8 Hz, 1H, **H$^{3'}$**), 8.18 (d, $^3J_{H,H}$ = 8.8 Hz, 1H, **H$^{2'}$**), 7.81-7.85 (m, 2H, **H^3** + **H^4**), 7.34 ppm (ddd, $^3J_{H,H}$ = 6.8 Hz, $^3J_{H,H}$ = 4.8 Hz, $^4J_{H,H}$ = 1.7 Hz, 1H, **H^5**).

^{13}C NMR (151 MHz, $CDCl_3$): δ 154.8 (**C^2**), 150.1 (**C^6**), 148.1 (**C$^{4'}$**), 145.2 (**C$^{1'}$**), 137.1 (**C^4**), 127.7 (**C$^{2'}$**), 124.0 (**C$^{3'}$**), 123.5 (**C^5**), 121.2 ppm (**C^3**).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −11.6 (**N**O_2), −71.0 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 201.066 (100) $[M+H]^+$.

HRMS (ESI): Found 201.0658; calcd for $C_{11}H_9N_2O_2$ $[M+H]^+$: 201.0659.

The NMR data are in accordance with those reported in the literature.[19]

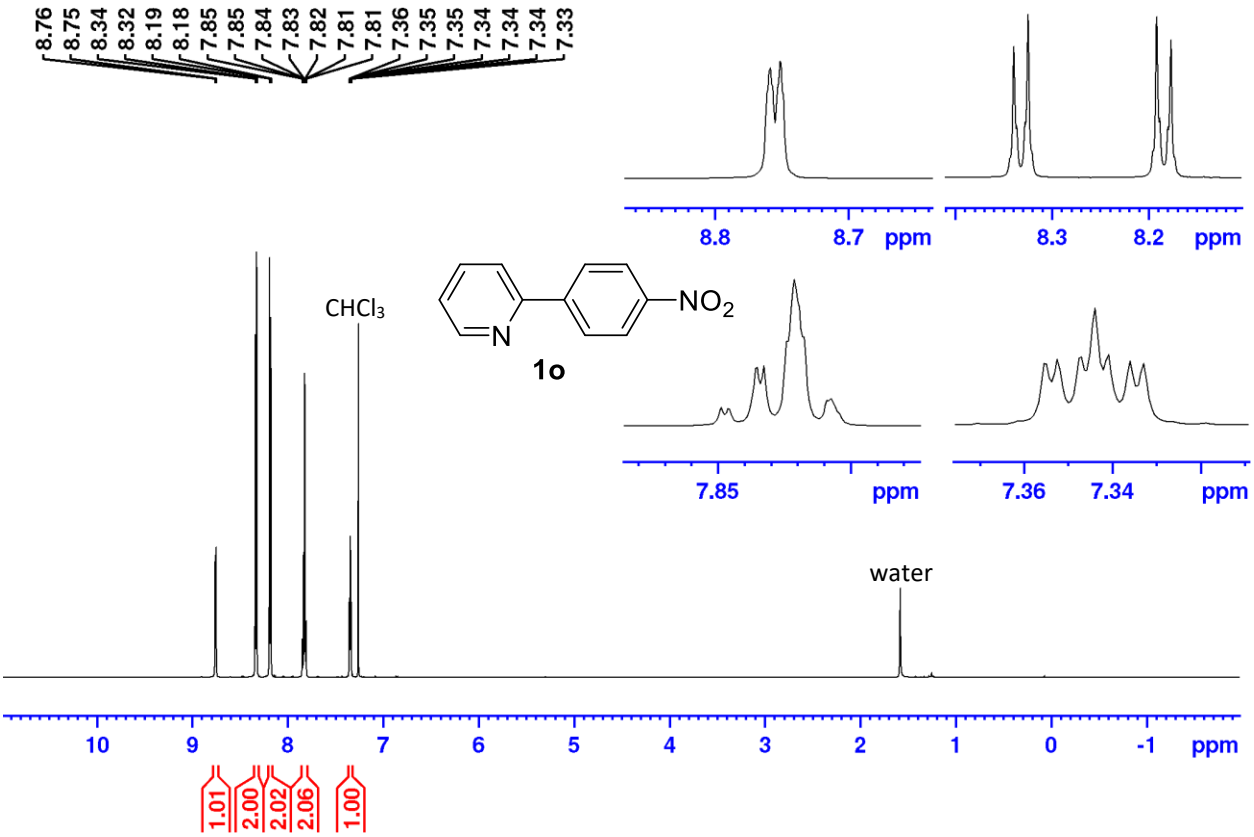


Figure S41. ^{1}H NMR (600 MHz, $CDCl_3$) of **1o**.

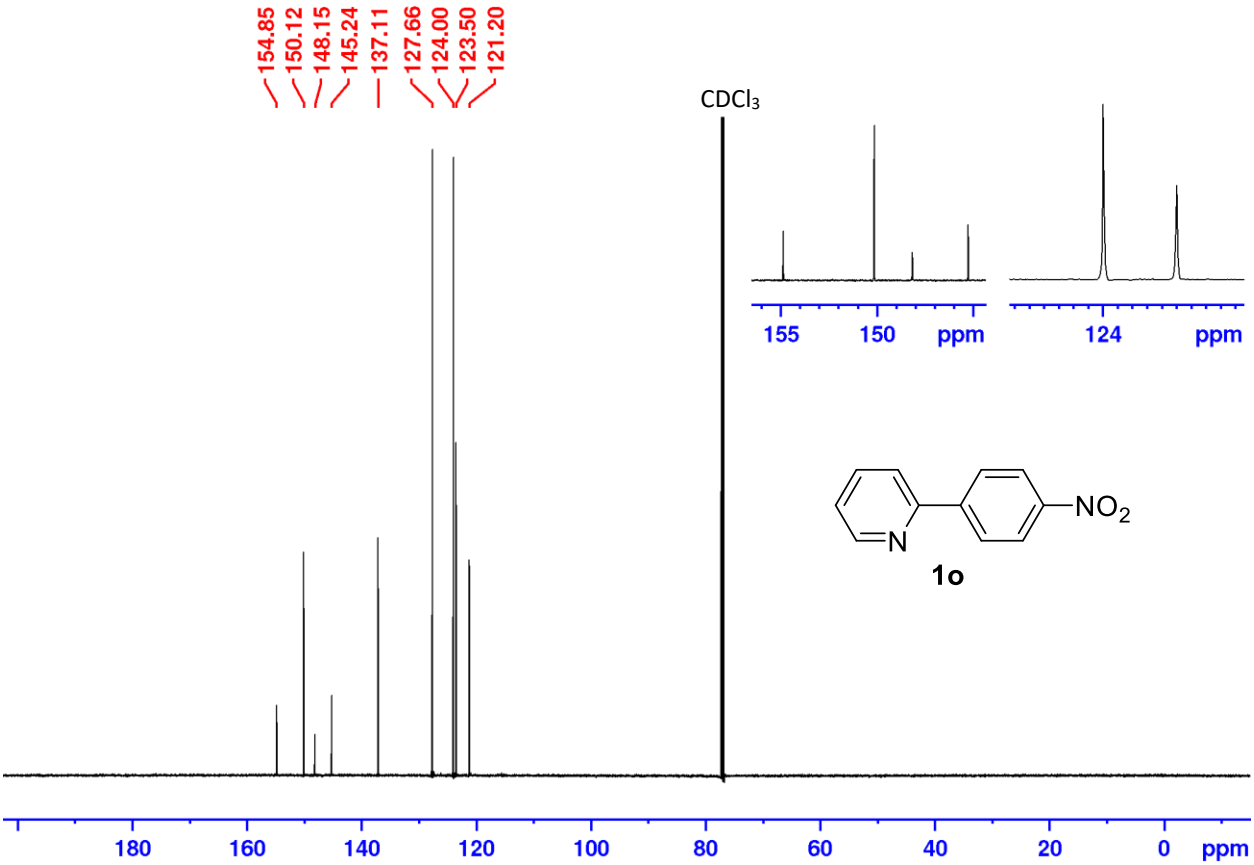


Figure S42. ^{13}C NMR (151 MHz, $CDCl_3$) of **1o**.

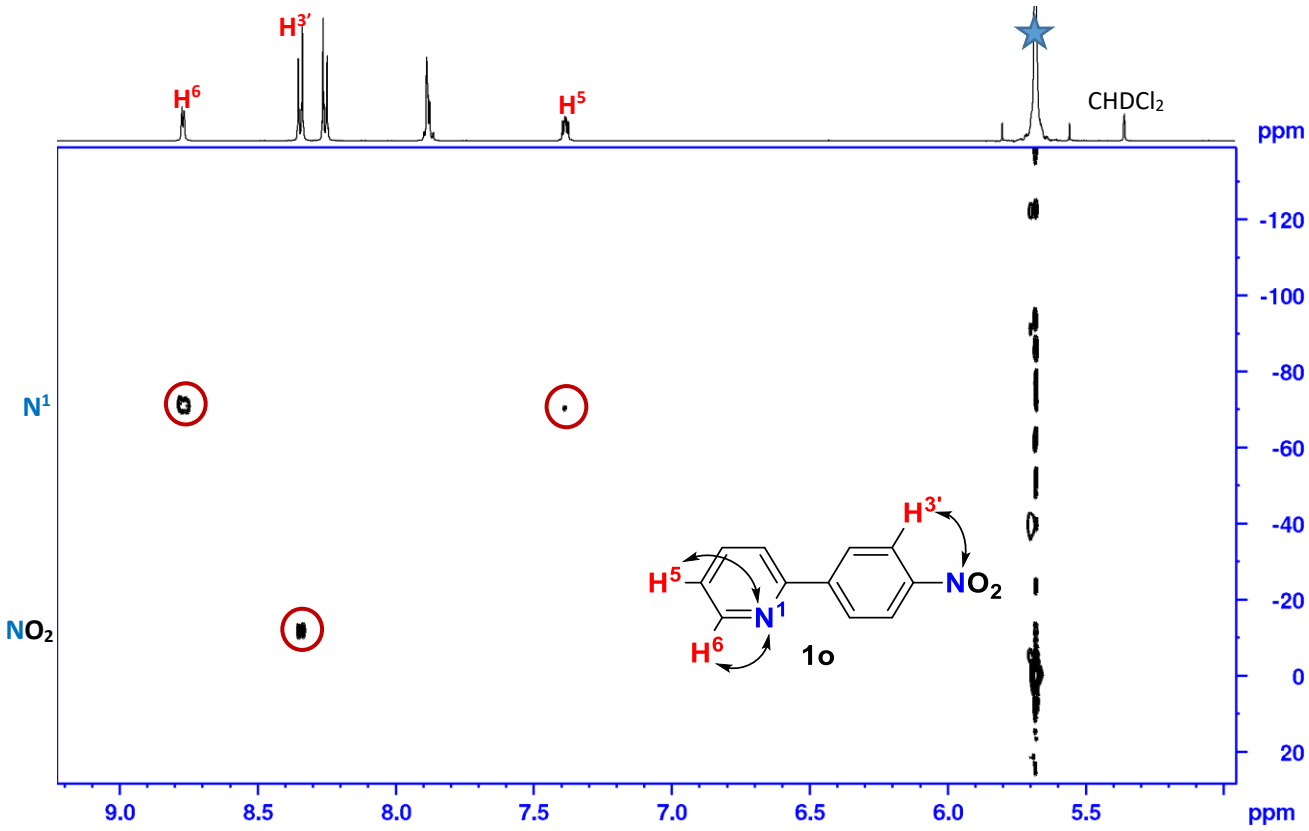
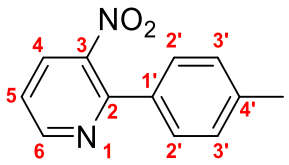


Figure S43. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1o**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1p

3-Nitro-2-(4-methylphenyl)pyridine (1p). A suspension of 2-chloro-3-nitropyridine (4.03 g, 25.5 mmol, 1.0 equiv.), 4-methylphenylboronic acid (5.18 g, 38.1 mmol, 1.5 equiv.) and KF·2H_2O (11.4 g, 121 mmol, 4.7 equiv.) in THF (50 mL) was bubbled with Ar for 15 min. Pd_2dba_3 (1.19 g, 1.31 mmol, 5.1 mol-%) and HBF_4·P(*t*-Bu)$_3$ (0.913 g, 3.15 mmol, 12 mol-%) were added under a flow of Ar. The reaction mixture was heated at reflux temperature for 90 min under Ar. After cooling to rt, CH_2Cl_2 (100 mL) was added to the reaction mixture, and the suspension was filtered through Celite. The Celite was washed with additional CH_2Cl_2 (200 mL). The CH_2Cl_2/THF solution was washed with 2M NaOH (aq) (4x 100 mL), water (100 mL), brine (100 mL), and dried over Na_2SO_4. The solvent was removed under reduced pressure. The obtained residue was purified by flash column chromatography, (1:2 CH_2Cl_2:95 % hexanes/5 % EtOAc), furnishing **14** as a pale yellow solid.

Yield: 3.67 g, 17.2 mmol, 67 %.

M.p. 63-64 °C.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.84 (dd, $^3J_{H,H}$ = 4.6 Hz, $^4J_{H,H}$ = 1.4 Hz, 1H, **H^6**), 8.11 (dd, $^3J_{H,H}$ = 8.1 Hz, $^4J_{H,H}$ = 1.4 Hz, 1H, **H^4**), 7.47 (d, $^3J_{H,H}$ = 7.9 Hz, 2H, **H$^{2'}$**), 7.41 (dd, $^3J_{H,H}$ = 8.1 Hz, $^3J_{H,H}$ = 4.6 Hz, 1H, **H^5**), 7.27 (d, $^3J_{H,H}$ = 7.9 Hz, 2H, **H$^{3'}$**), 2.42 ppm (s, 3H, C**H**$_3$).

^{13}C NMR (151 MHz, $CDCl_3$): δ 152.8 (**C^2**), 152.1 (**C^6**), 146.2 (**C^3**), 140.1 (**C$^{4'}$**), 133.3 (**C$^{1'}$**), 132.1 (**C^4**), 129.5 (**C$^{3'}$**), 128.0 (**C$^{2'}$**), 122.0 (**C^5**), 21.4 ppm (**C**H$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −6.6 (**N**O_2), −59.4 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 215.082 (100) $[M+H]^+$.

HRMS (ESI): Found 215.0815; calcd for $C_{12}H_{11}N_2O_2$ $[M+H]^+$: 215.0815.

The NMR data are in accordance with those reported in the literature.[20]

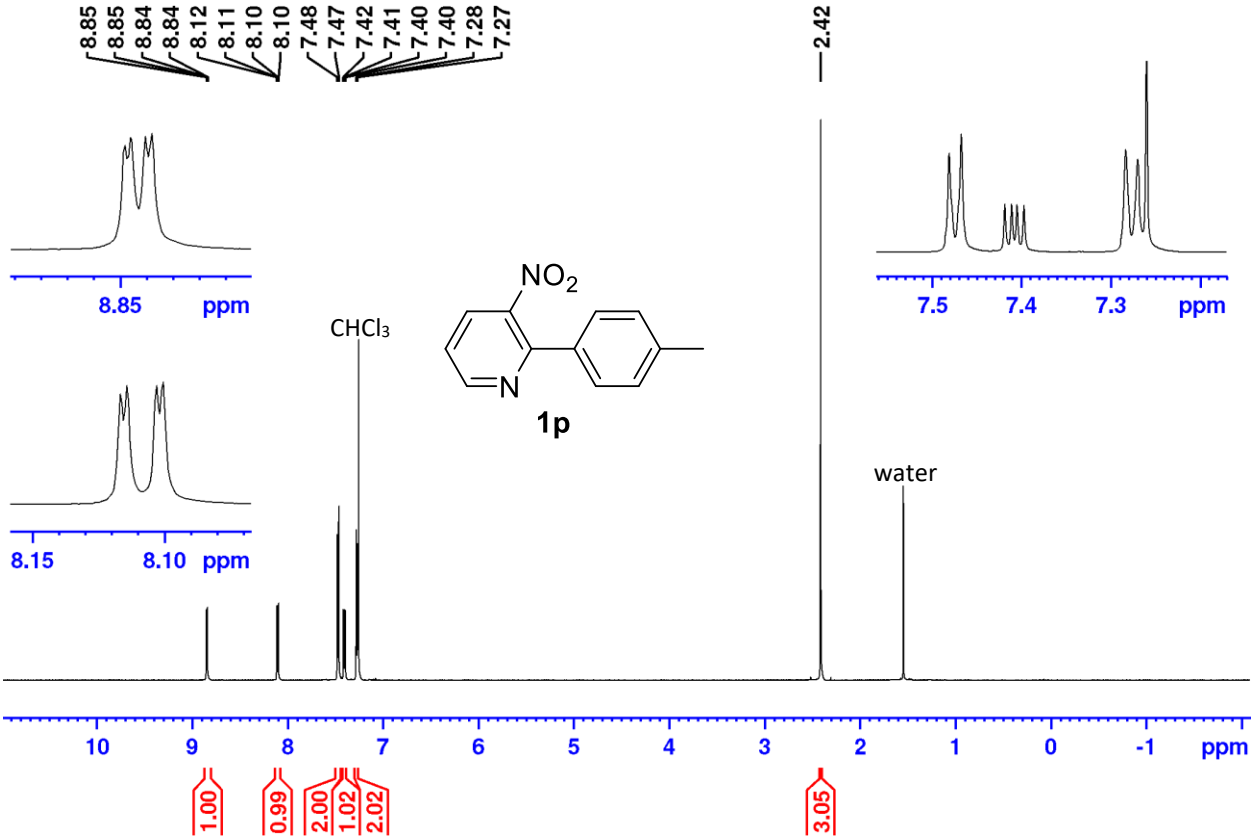


Figure S44. ^{1}H NMR (600 MHz, $CDCl_3$) of **1p**.

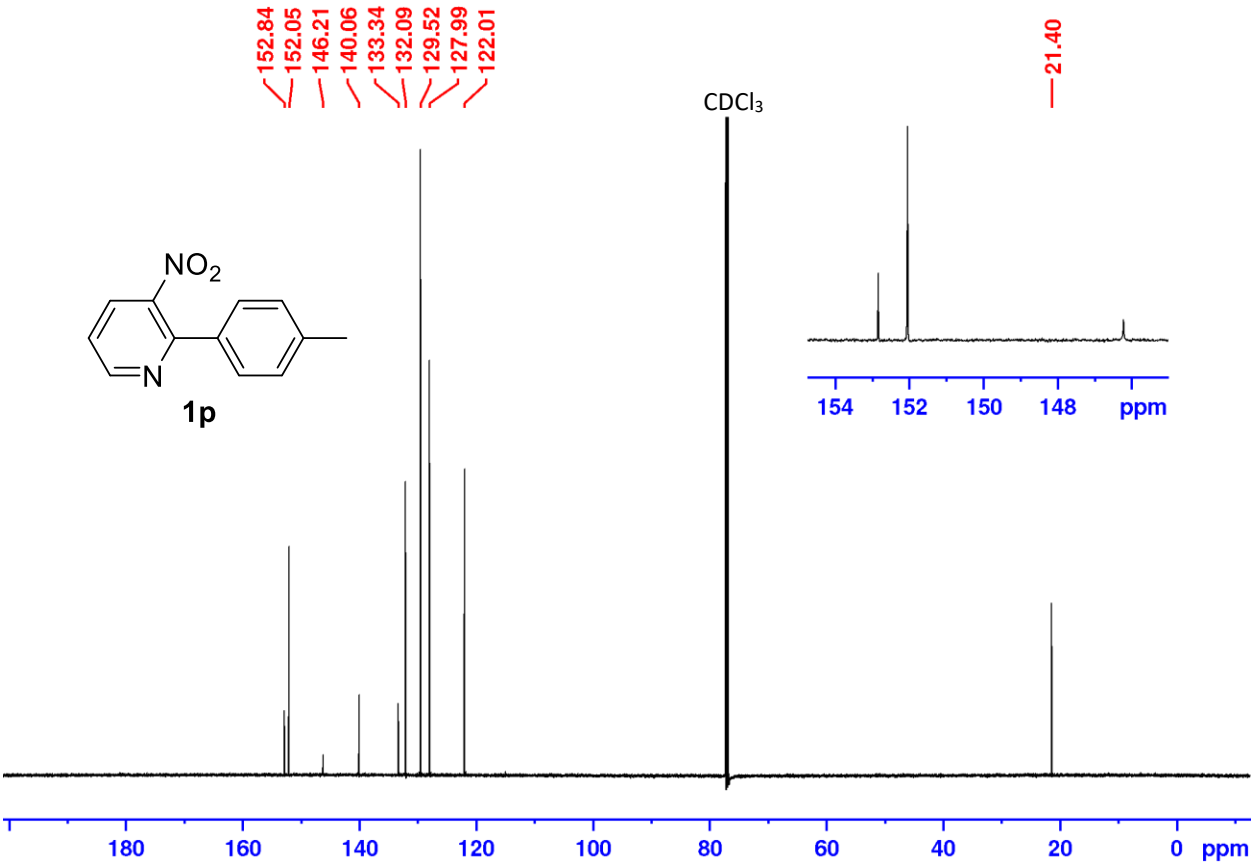


Figure S45. ^{13}C NMR (151 MHz, $CDCl_3$) of **1p**.

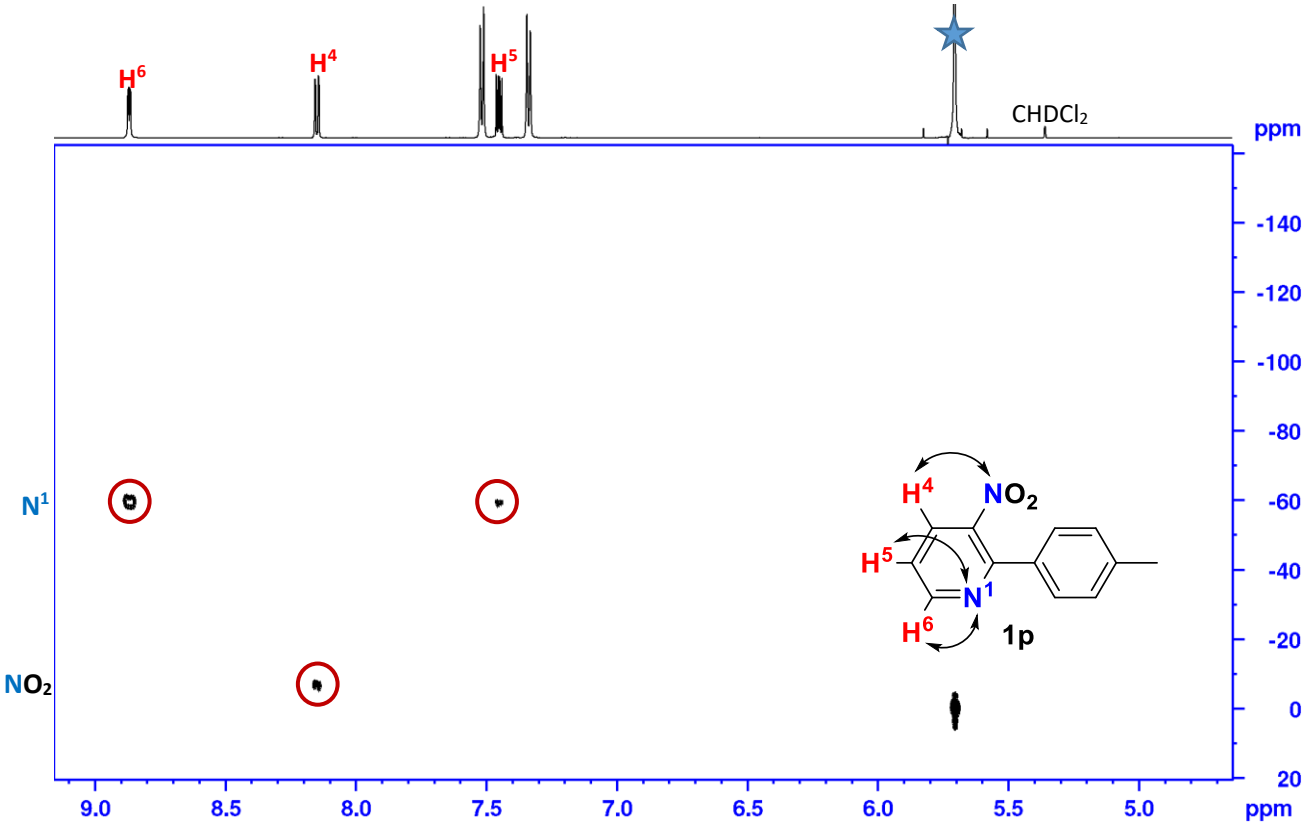
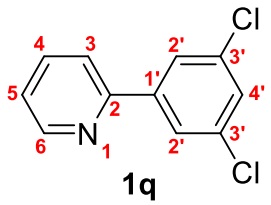


Figure S46. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1p**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1q

2-(3,5-dichlorophenyl)pyridine (1q). The general procedure was followed. 2-Bromopyridine (3.95 g, 25.0 mmol, 1.0 equiv.), 3,5-dichlorophenylboronic acid (4.53 g, 23.8 mmol, 0.95 equiv.), K_3PO_4 (10.6 g, 49.9 mmol, 2.0 equiv.), $Pd(OAc)_2$ (0.112 g, 0.501 mmol, 2.0 mol-%) and PPh_3 (0.396 g, 1.51 mmol, 6.0 mol-%) in *n*-PrOH (50 mL) and water (50 mL) were used. The reaction mixture was refluxed for 75 min. The obtained crude product was purified by flash column chromatography (85 % hexanes/15 % EtOAc), furnishing **1q** as a colorless solid.

Yield: 5.20 g, 23.2 mmol, 98 %.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.69 (d, $^3J_{H,H}$ = 4.8 Hz, 1H, **H^6**), 7.89 (d, $^4J_{H,H}$ = 1.9 Hz, 2H, **H$^{2'}$**), 7.76-7.78 (m, 1H, **H^4**), 7.68 (d, $^3J_{H,H}$ = 7.9 Hz, 1H, **H^3**), 7.38-7.39 (m, 1H, **H$^{4'}$**), 7.28 ppm (ddd, $^3J_{H,H}$ = 7.6 Hz, $^3J_{H,H}$ = 4.8 Hz, $^4J_{H,H}$ = 0.6 Hz, 1H, **H^5**).

^{13}C NMR (151 MHz, $CDCl_3$): δ 154.5 (**C^2**), 149.9 (**C^6**), 142.2 (**C$^{1'}$**), 137.0 (**C^4**), 135.4 (**C$^{3'}$**), 128.7 (**C$^{4'}$**), 125.3 (**C$^{2'}$**), 123.2 (**C^5**), 120.6 ppm (**C^3**).

MS (ESI, MeCN): *m/z* (rel. %): 224.003 (100) $[M+H]^+$.

HRMS (ESI, MeCN): Found 224.0028; calcd for $C_{11}H_8Cl_2N$ $[M+H]^+$: 224.0028.

The NMR data are in accordance with those reported in the literature.[21]

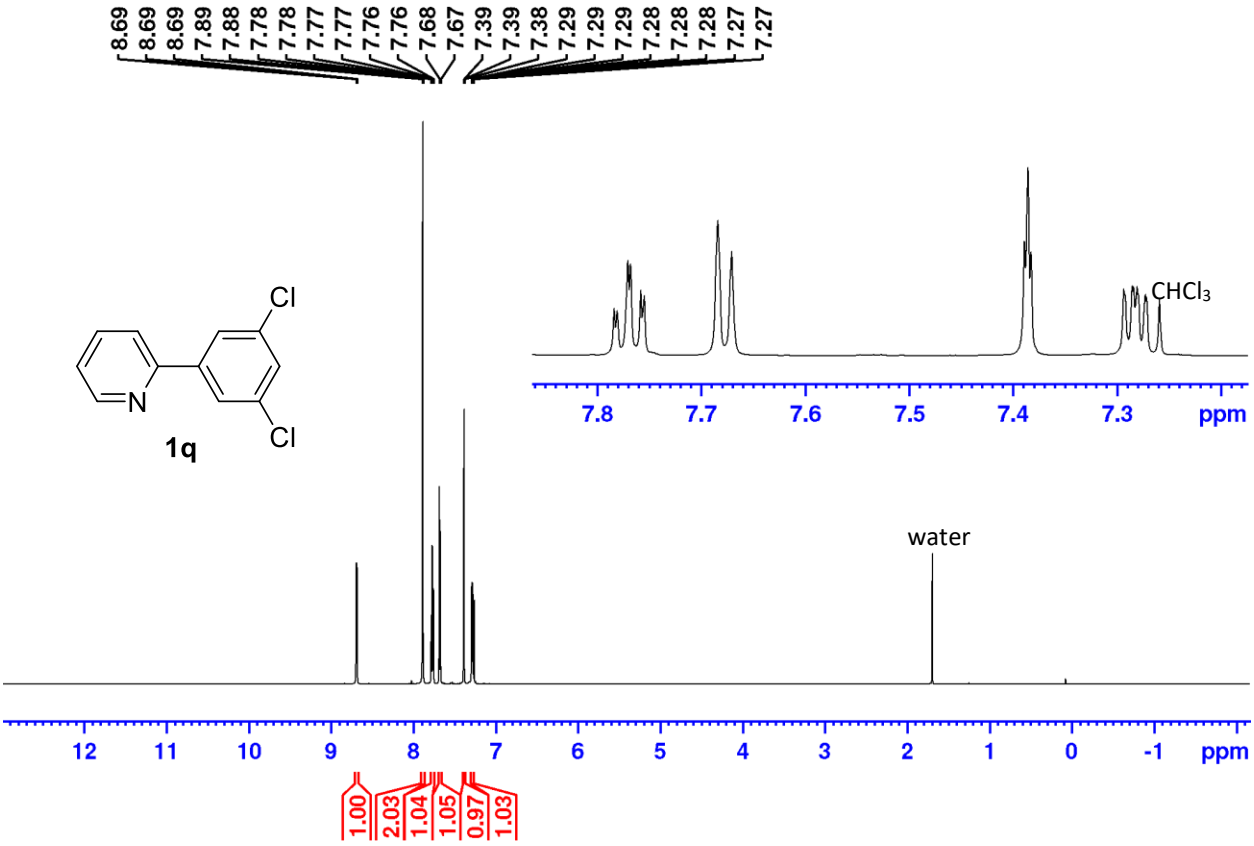


Figure S47. ^{1}H NMR (600 MHz, $CDCl_3$) of **1q**.

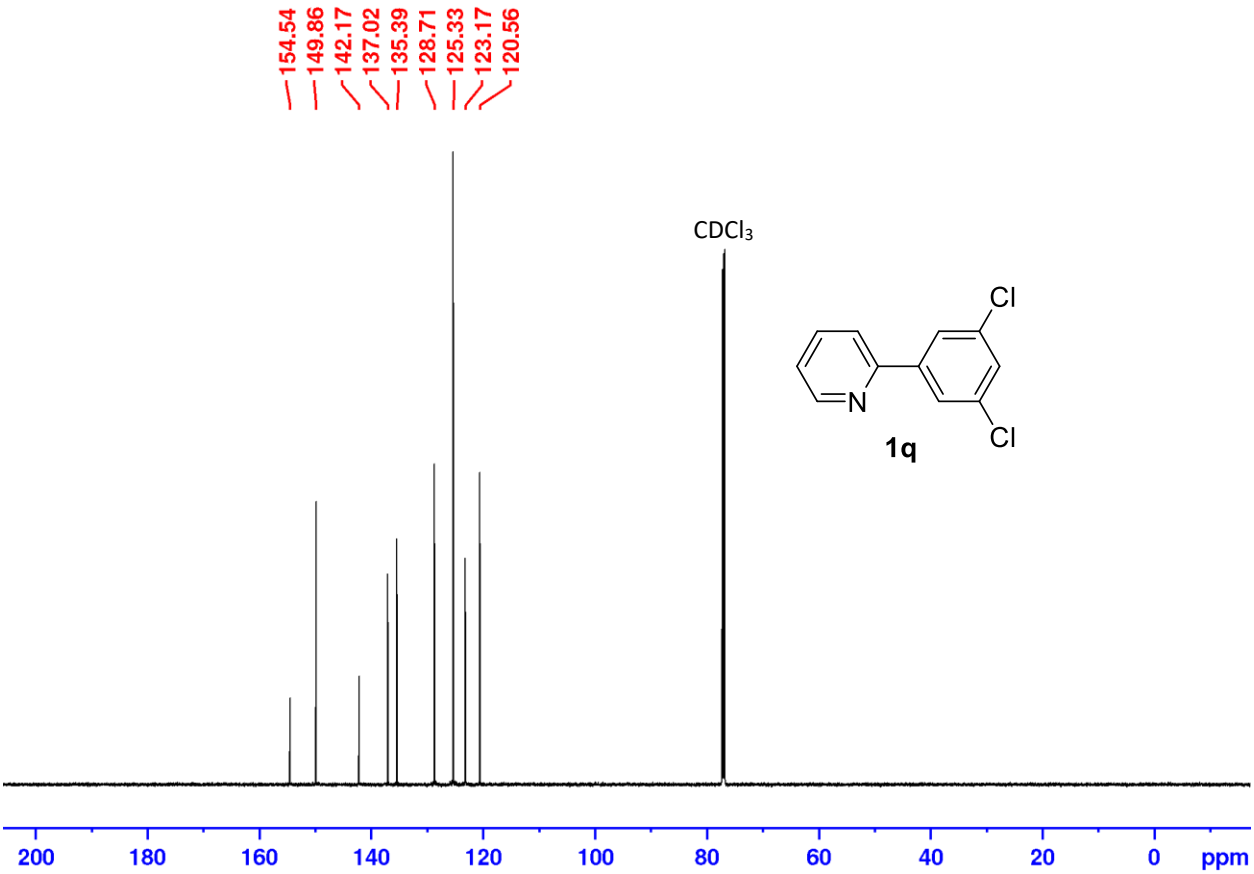
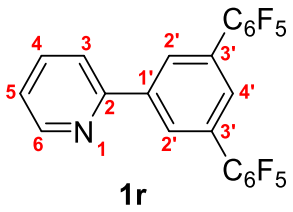


Figure S48. ^{13}C NMR (151 MHz, $CDCl_3$) of **1q**.



1r

2-(2,2'',3,3'',4,4'',5,5'',6,6''-decafluoro-[1,1':3',1''-terphenyl]-5'-yl)pyridine (1r). The synthesis of **1r** was adapted from a literature procedure.[22] K_2CO_3 (1.11 g, 8.00 mmol, 4.0 equiv.), $Pd(OAc)_2$ (0.0225 g, 0.100 mmol, 5.0 mol-%) and S-Phos (0.0821 g, 0.200 mmol, 10 mol-%) were added to a Schlenk flask, and flushed with Ar for 15 min. Pentafluorobenzene (1.00 g, 6.00 mmol, 3.0 equiv.) and *i*-PrOAc (4 mL) were added, followed by a solution of **1q** (0.448 g, 2.00 mmol, 1.0 equiv.) in *i*-PrOAc (2 mL). After flushing with Ar, the reaction flask was sealed and stirred at 80 °C for 14 h. After cooling to rt, insoluble material was separated from the reaction mixture by filtration. The solids were washed with additional *i*-PrOAc, and the washings were combined with the original filtrate. The solvent was removed under reduced pressure, and the obtained solid was purified by flash column chromatography (85 % hexanes/15 % EtOAc), followed by two-fold recrystallization from EtOH. **1r** was obtained as a colorless fluffy solid.

Yield: 0.356 g, 0.730 mmol, 37 %.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.72-8.73 (m, 1H, **H^6**), 8.18 (s, 2H, **H$^{2'}$**), 7.78-7.83 (m, 2H, **H^4** + **H^3**), 7.54 (s, 1H, **H$^{4'}$**), 7.31 ppm (ddd, $^3J_{H,H}$ = 7.8 Hz, $^3J_{H,H}$ = 4.8 Hz, $^4J_{H,H}$ = 1.4 Hz, 1H, **H^5**).

^{13}C NMR (201 MHz, $CDCl_3$): δ 155.5 (**C^2**), 150.0 (**C^6**), 144.3 (d, $^1J_{C,F}$ = 248.5 Hz, Ar-**C**-F), 140.80 (d, $^1J_{C,F}$ = 254.8 Hz, Ar-**C**-F), 140.74 (**C$^{1'}$**), 137.9 (d, $^1J_{C,F}$ = 251.3 Hz, Ar-**C**-F), 137.1 (**C^4**), 132.0 (**C$^{4'}$**), 129.5 (**C$^{2'}$**), 127.6 (**C$^{3'}$**), 123.0 (**C^5**), 120.6 (**C^3**), 114.87-115.05 ppm (m, Ar-**C**-C-F).

^{19}F NMR (376 MHz, $CDCl_3$): δ −145.6 (dd, $^3J_{F,F}$ = 22.6 Hz, $^4J_{F,F}$ = 6.0 Hz, 4F, C_6**F**$_5$), −157.4 (dd, $^3J_{F,F}$ = 21.0 Hz, $^3J_{F,F}$ = 20.9 Hz, 2F, C_6**F**$_5$), −164.6 ppm (m, 4F, C_6**F**$_5$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −73.0 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 510.031 (100) $[M+Na]^+$.

HRMS (ESI): Found 510.0311; calcd for $C_{23}H_7F_{10}NNa$ $[M+Na]^+$: 510.0311.

Elemental Analysis: Anal. calcd. For $C_{23}H_7F_{10}N$: C, 56.69; H, 1.45; N. 2.87. Found: C, 56.68; H, 1.44; N, 2.88.

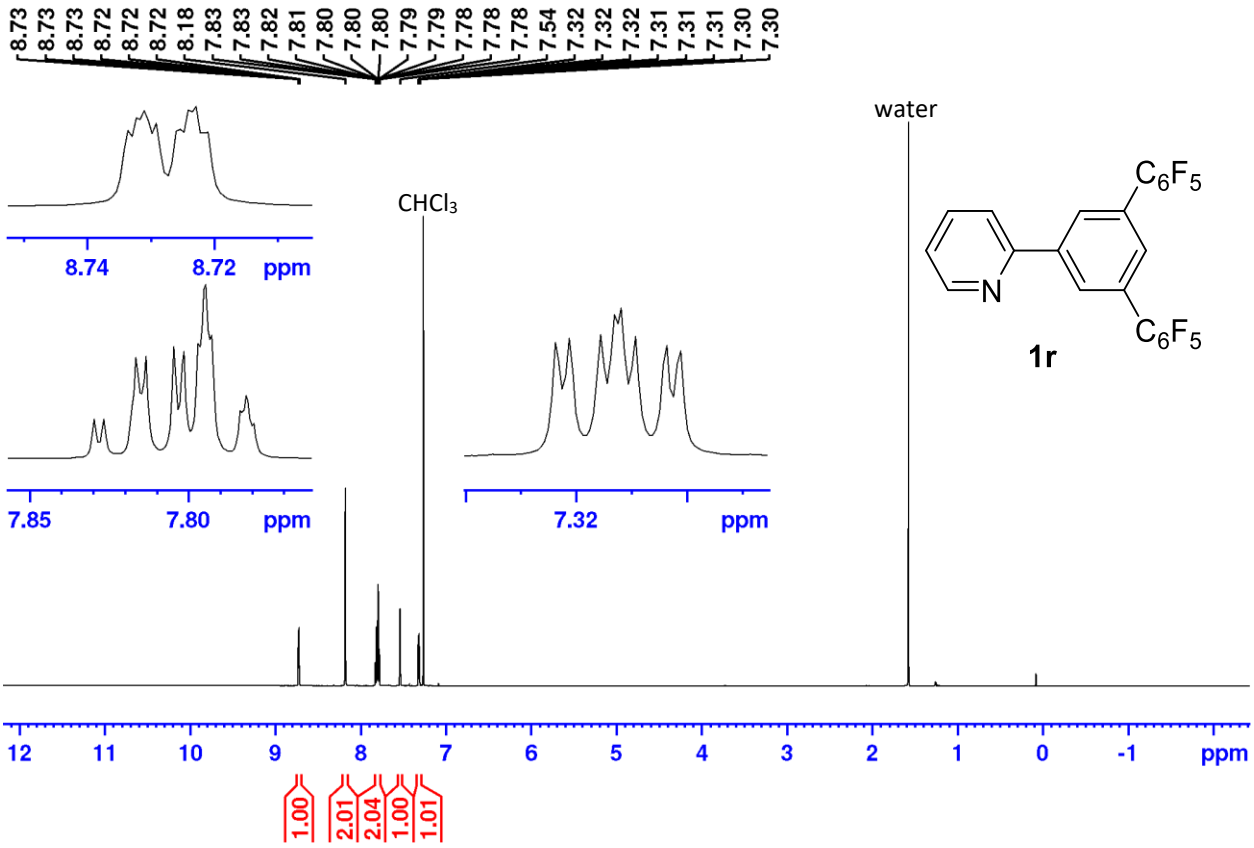


Figure S49. ^{1}H NMR (600 MHz, $CDCl_3$) of **1r**.

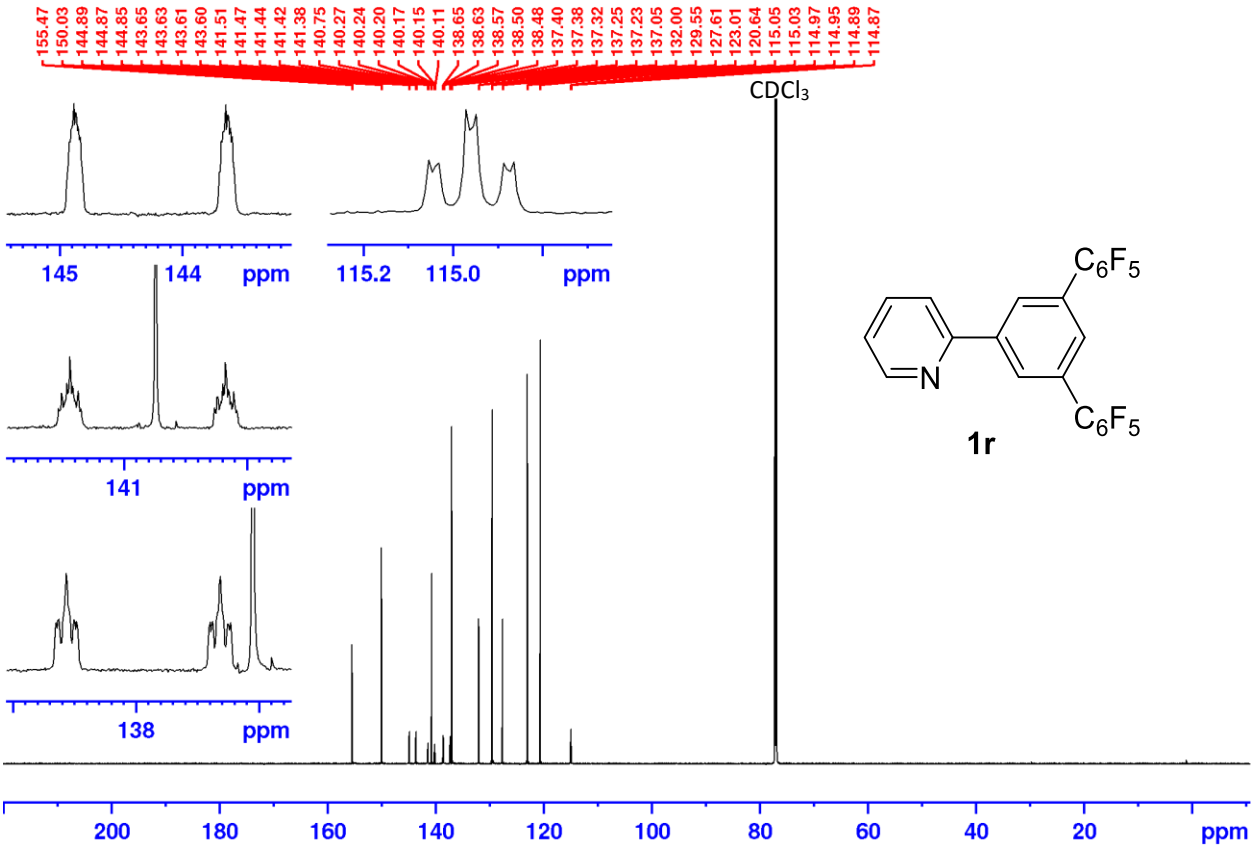


Figure S50. ^{13}C NMR (201 MHz, $CDCl_3$) of **1r**.

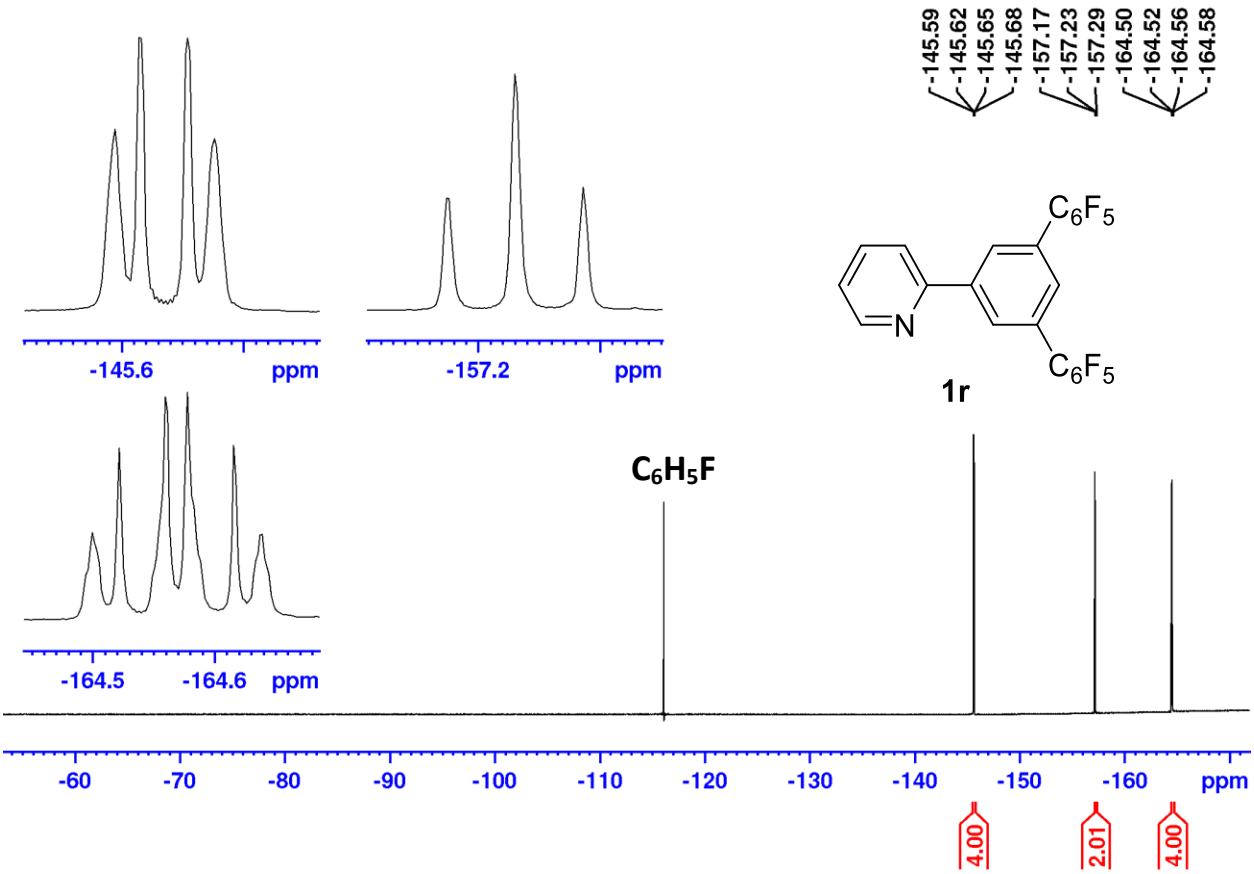
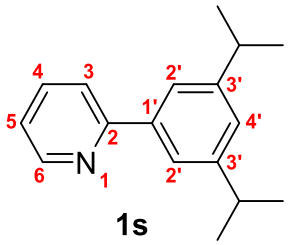


Figure S51. ^{19}F NMR (376 MHz, $CDCl_3$) of **1r**.



1s

2-(3,5-diisopropylphenyl)pyridine (1s). The general procedure was followed. 2-Bromopyridine (0.924 g, 5.85 mmol, 1.0 equiv.), 3,5-diisopropylphenylboronic acid (1.20 g, 5.84 mmol, 1.0 equiv.), K_3PO_4 (2.48 g, 11.7 mmol, 2.0 equiv.), $Pd(OAc)_2$ (0.0273 g, 0.122 mmol, 2.1 mol-%) and PPh_3 (0.0921 g, 0.352 mmol, 6.0 mol-%) were used. The crude product was purified twice by flash column chromatography (first 85 % hexanes/15 % EtOAc, then CH_2Cl_2), yielding **1s** as a colorless oil.

Yield: 0.847 g, 3.54 mmol, 61 %.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.70 (d, $^3J_{H,H}$ = 4.8 Hz, 1H, **H^6**), 7.72-7.75 (m, 2H, **H^3** + **H^4**), 7.66 (s, 2H, **H$^{2'}$**), 7.21 (ddd, $^3J_{H,H}$ = 6.1 Hz, $^3J_{H,H}$ = 4.8 Hz, $^4J_{H,H}$ = 2.5 Hz, 1H, **H^5**), 7.15 (s, 1H, **H$^{4'}$**), 2.99 (sp, $^3J_{H,H}$ = 7.0 Hz, 2H, C**H**$(CH_3)_2$), 1.31 ppm (d, $^3J_{H,H}$ = 7.0 Hz, 12H, CH(C**H**$_3)_2$).

^{13}C NMR (151 MHz, $CDCl_3$): δ 158.2 (**C^2**), 149.6 (**C^6**), 149.3 (**C$^{3'}$**), 139.4 (**C$^{1'}$**), 136.6 (**C^4**), 125.4 (**C$^{4'}$**), 122.7 (**C$^{2'}$**), 121.8 (**C^5**), 120.8 (**C^3**), 34.3 (**C**H$(CH_3)_2$), 24.1 ppm (CH(**C**H$_3)_2$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −73.6 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 240.175 (100) $[M+H]^+$.

HRMS (ESI): Found 240.1746; calcd for $C_{17}H_{22}N$ $[M+H]^+$: 240.1747.

Elemental Analysis: Anal. calcd. For $C_{17}H_{21}N$: C, 85.30; H, 8.84; N. 5.85. Found: C, 85.27; H, 8.87; N, 5.85.

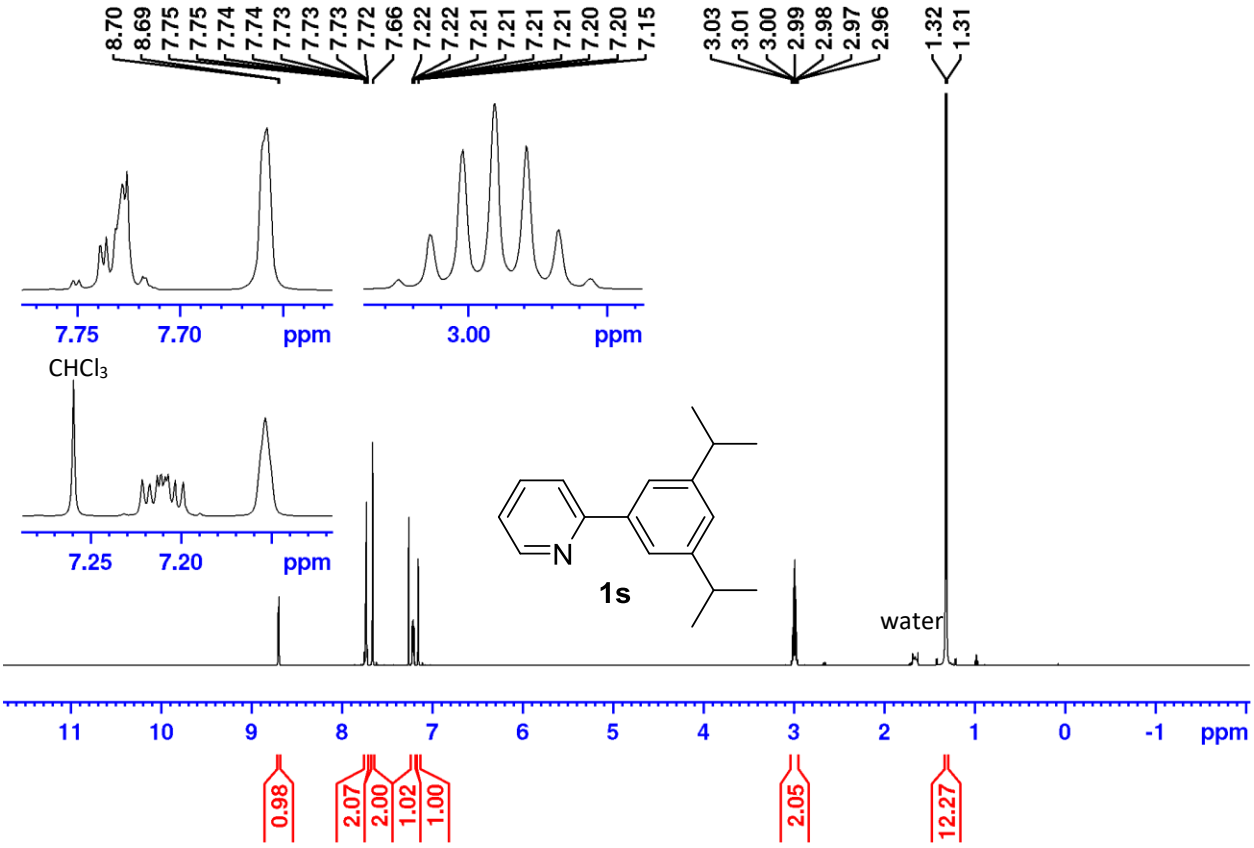


Figure S52. ^{1}H NMR (600 MHz, $CDCl_3$) of **1s**.

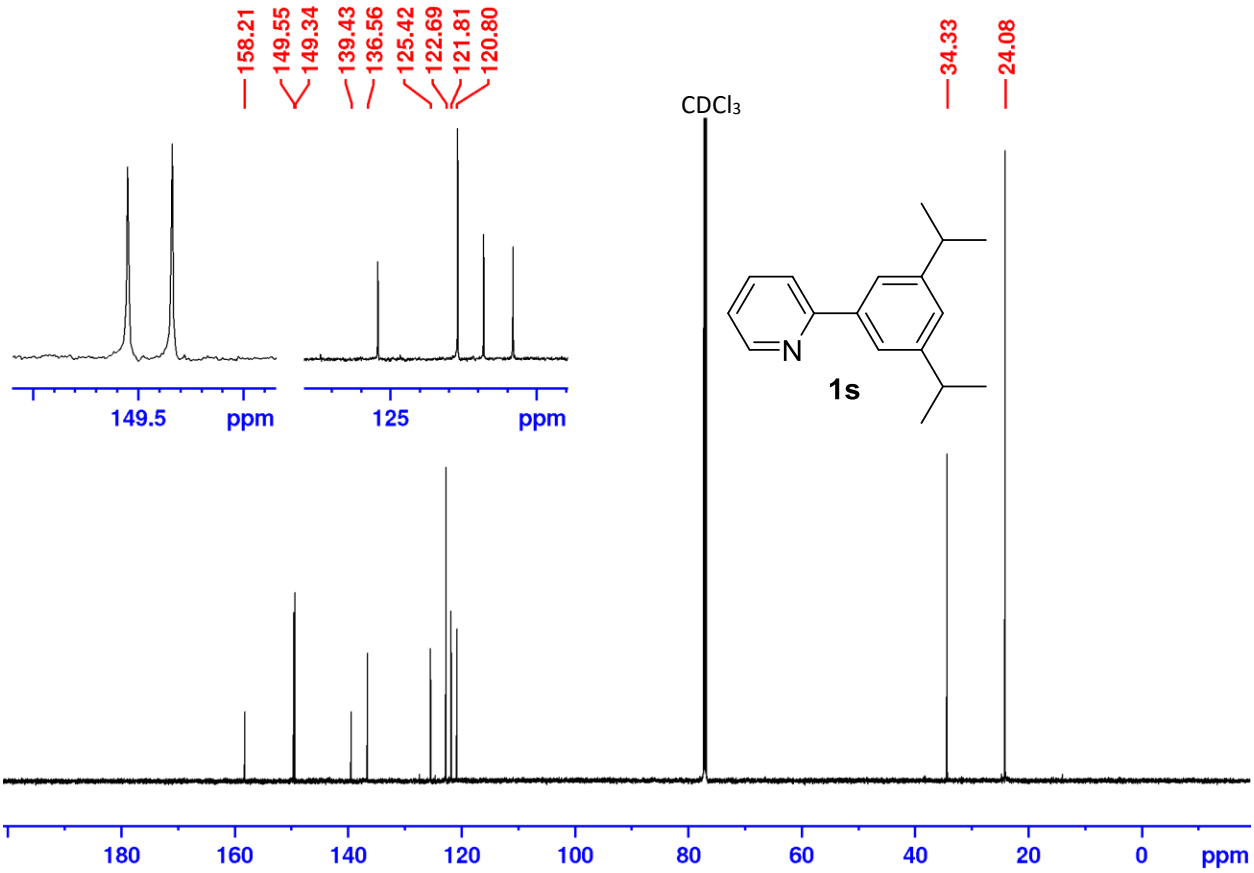


Figure S53. ^{13}C NMR (151 MHz, $CDCl_3$) of **1s**.

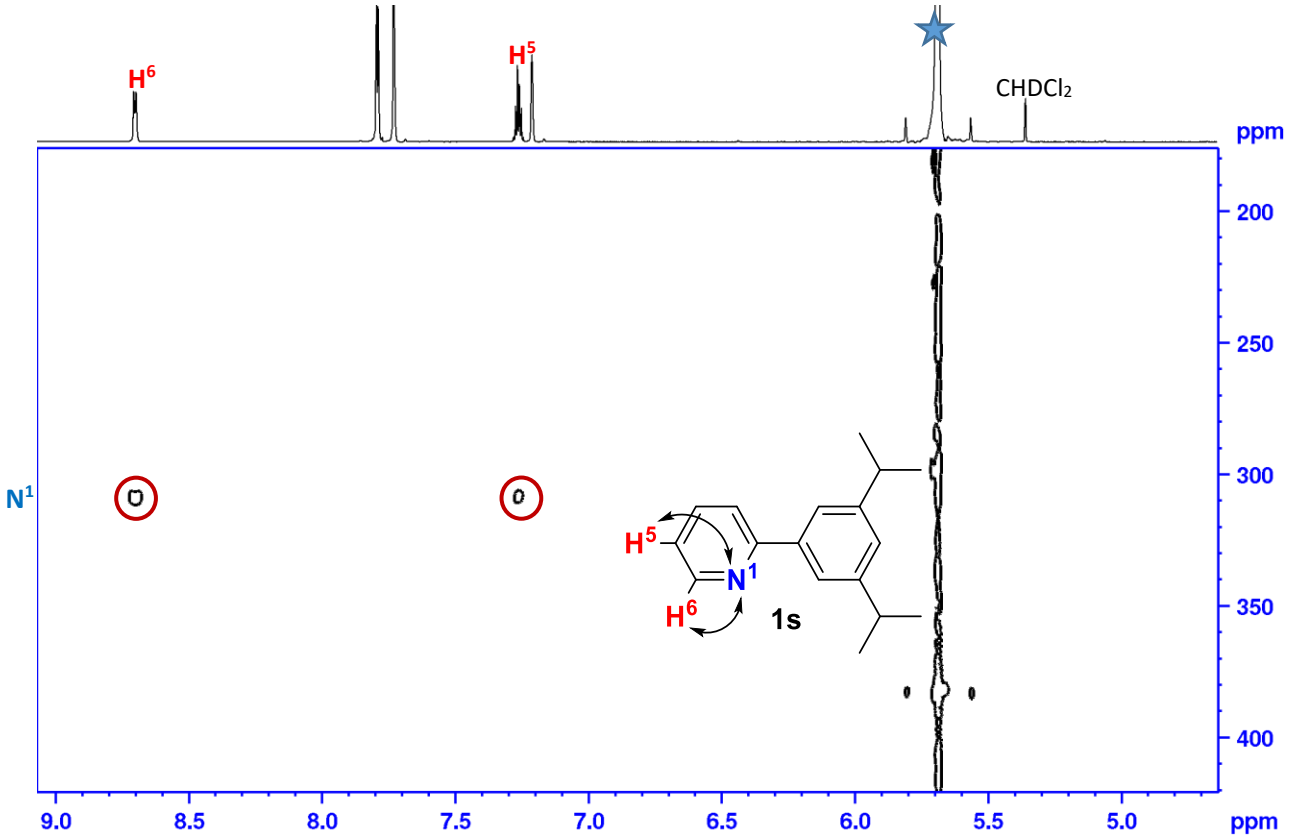
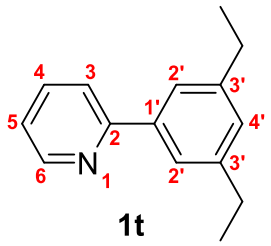


Figure S54. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1s**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1t

2-(3,5-diethylphenyl)pyridine (1t). The general procedure was followed. 2-Bromopyridine (0.670 g, 4.26 mmol, 1.0 equiv.), 3,5-diethylphenylboronic acid (0.670 g, 4.26 mmol, 1.0 equiv.), K_3PO_4 (1.81 g, 8.52 mmol, 2.0 equiv.), $Pd(OAc)_2$ (0.0187 g, 0.0831 mmol, 2.0 mol-%) and PPh_3 (0.0664 g, 0.253 mmol, 6.0 mol-%) were used. The crude product was purified by flash column chromatography (85 % hexanes/15 % EtOAc), yielding **1t** as a colorless oil.

Yield: 0.438 g, 2.070 mmol, 49 %.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.69-8.71 (ddd, $^3J_{H,H}$ = 4.7 Hz, $^4J_{H,H}$ = 1.3 Hz, $^5J_{H,H}$ = 1.3 Hz, 1H, **H^6**), 7.72-7.74 (m, 2H, **H^3** + **H^4**), 7.65 (d, $^4J_{H,H}$ = 1.2 Hz, 2H, **H$^{2'}$**), 7.20-7.22 (m, 1H, **H^5**), 7.11 (s, 1H, **H$^{4'}$**), 2.73 (q, $^3J_{H,H}$ = 7.6 Hz, 4H, C**H**$_2$CH$_3$), 1.30 ppm (t, $^3J_{H,H}$ = 7.6 Hz, 6H, CH$_2$C**H**$_3$).

^{13}C NMR (151 MHz, $CDCl_3$): δ 158.0 (**C^2**), 149.5 (**C^6**), 144.7 (**C$^{3'}$**), 139.4 (**C$^{1'}$**), 136.6 (**C^4**), 128.3 (**C$^{4'}$**), 123.9 (**C$^{2'}$**), 121.8 (**C^5**), 120.7 (**C^3**), 28.6 (**C**H$_2$CH$_3$), 15.6 ppm (CH$_2$**C**H$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −73.6 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 212.143 (100) $[M+H]^+$.

HRMS (ESI): Found 212.1433; calcd for $C_{15}H_{18}N$ $[M+H]^+$: 212.1434.

Elemental Analysis: Anal. calcd. For $C_{15}H_{17}N$: C, 85.26; H, 8.11; N. 6.63. Found: C, 85.19; H, 8.07; N, 6.59.

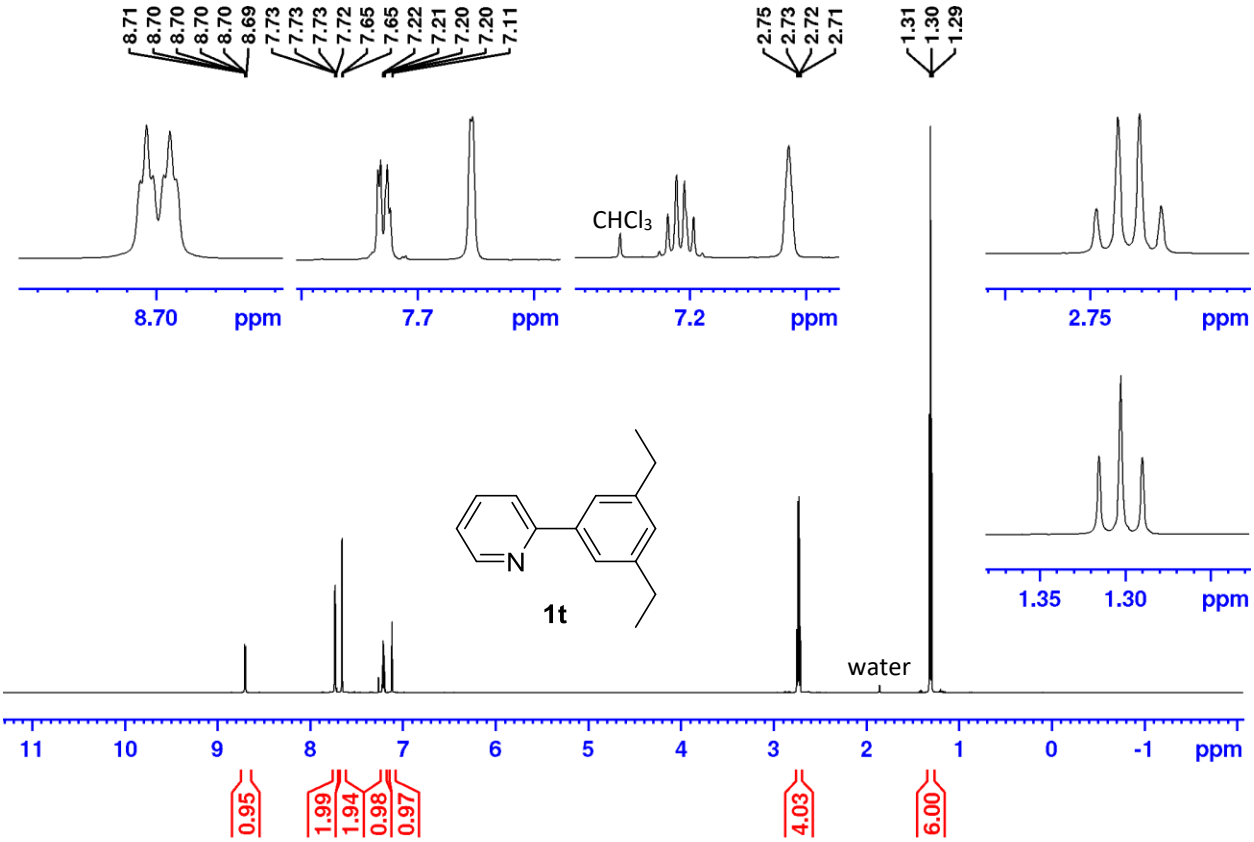


Figure S55. ^{1}H NMR (600 MHz, $CDCl_3$) of **1t**.

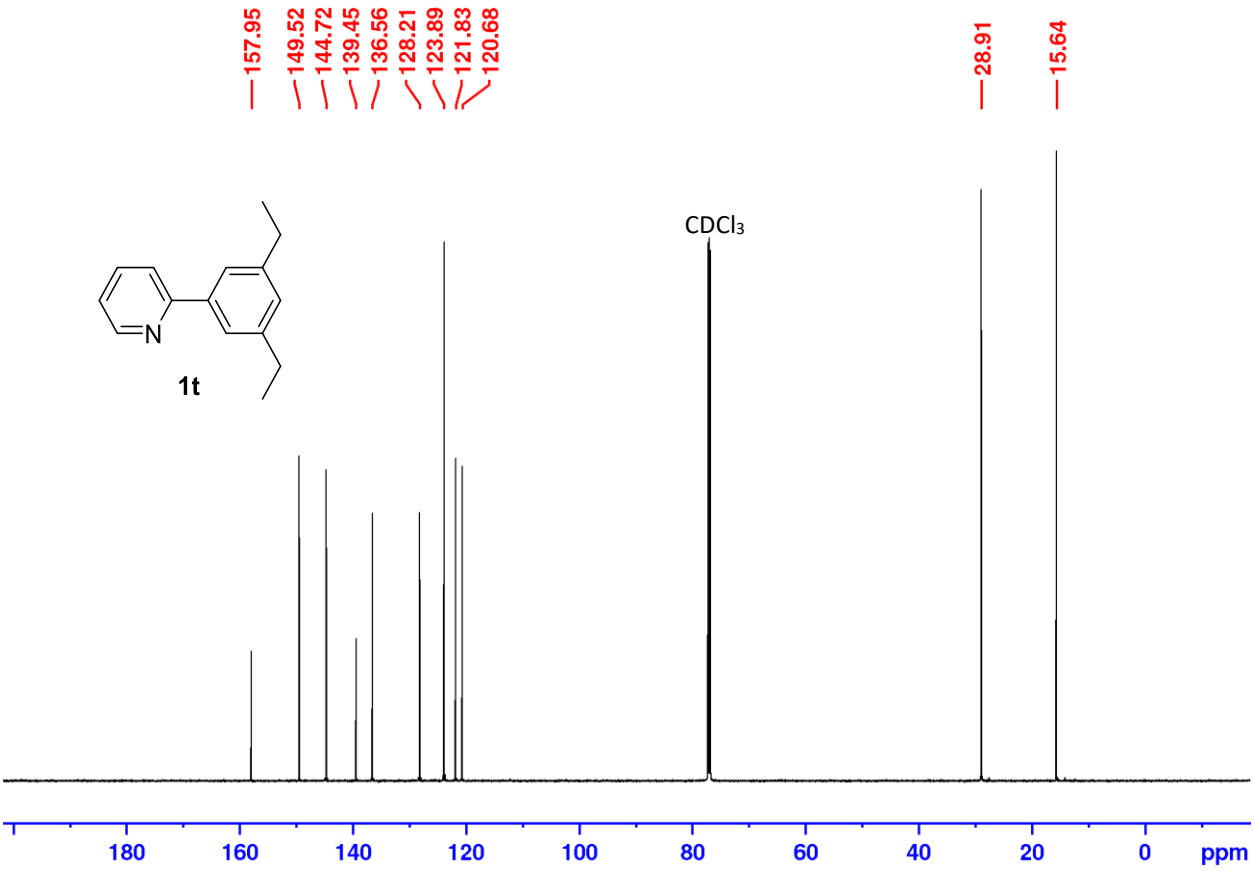


Figure S56. ^{13}C NMR (151 MHz, $CDCl_3$) of **1t**.

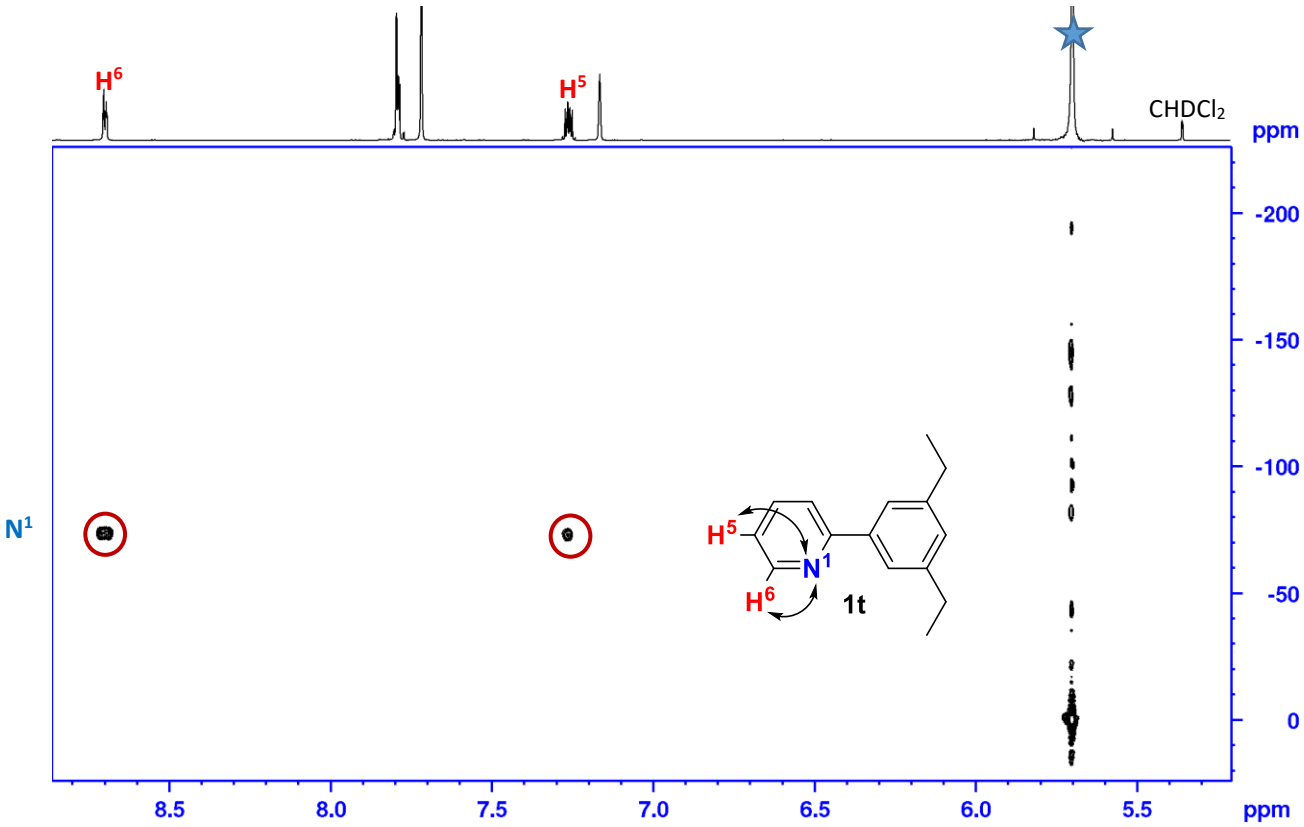
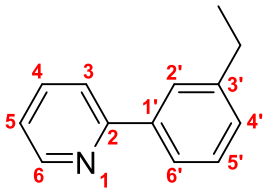


Figure S57. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1t**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



1u

2-(3,5-diethylphenyl)pyridine (1u). The general procedure was followed. 2-bromopyridine (0.670 g, 4.26 mmol, 1.0 equiv.), 3-ethylphenyboronic acid (0.703 g, 4.690 mmol, 1.1 equiv.), K_3PO_4 (2.12 g, 10.0 mmol, 2.3 equiv.), $Pd(OAc)_2$ (0.0187 g, 0.0883 mmol, 2.0 mol-%) and PPh_3 (0.0664 g, 0.253 mmol, 5.9 mol-%) were used. The obtained crude product was purified by flash column chromatography (80 % hexanes/20 % EtOAc), furnishing **1u** as a colorless oil.

Yield: 0.684 g, 3.730 mmol, 88 %.

^{1}H NMR (600 MHz, $CDCl_3$): δ 8.69-8.70 (m, 1H, **H^6**), 7.86 (s, 1H, **H$^{2'}$**), 7.77 (d, $^3J_{H,H}$ = 7.8 Hz, 1H, **H$^{6'}$**), 7.72-7.76 (m, 2H, **H^3** + **H^4**), 7.38-7.41 (m, 1H, **H$^{5'}$**), 7.26-7.27 (m, 1H, **H$^{4'}$**), 7.22 (ddd, $^3J_{H,H}$ = 6.5 Hz, $^3J_{H,H}$ = 4.8 Hz, $^4J_{H,H}$ = 2.1 Hz, 1H, **H^5**), 2.75 (q, $^3J_{H,H}$ = 7.6 Hz, 2H, C**H**$_2$CH$_3$), 1.30 ppm (t, $^3J_{H,H}$ = 7.6 Hz, 3H, CH$_2$C**H**$_3$).

^{13}C NMR (151 MHz, $CDCl_3$): δ 157.7 (**C^2**), 149.6 (**C^6**), 144.8 (**C$^{3'}$**), 139.4 (**C$^{1'}$**), 136.6 (**C^4**), 128.7 (**C$^{5'}$**), 128.5 (**C$^{4'}$**), 126.5 (**C$^{6'}$**), 124.2 (**C$^{2'}$**), 121.9 (**C^5**), 120.6 (**C^3**), 29.0 (**C**H$_2$CH$_3$), 15.6 ppm (CH$_2$**C**H$_3$).

MS (ESI, MeCN): *m/z* (rel. %): 184.112 (100) $[M+H]^+$.

HRMS (ESI, MeCN): Found 184.1120; calcd for $C_{13}H_{14}N$ $[M+H]^+$: 184.1121.

The compound is known,[23] but spectral data have not been reported.

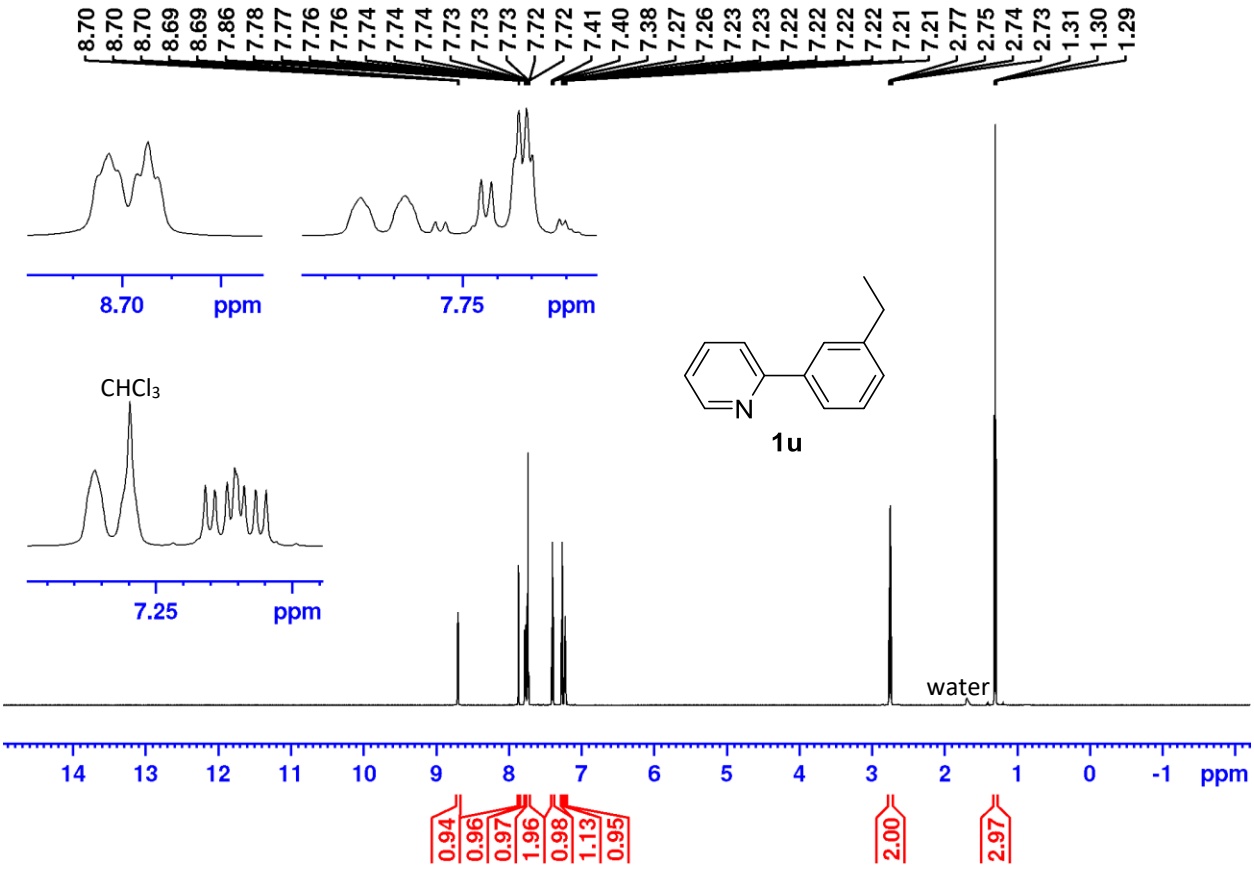


Figure S58. ^{1}H NMR (600 MHz, $CDCl_3$) of **1u**.

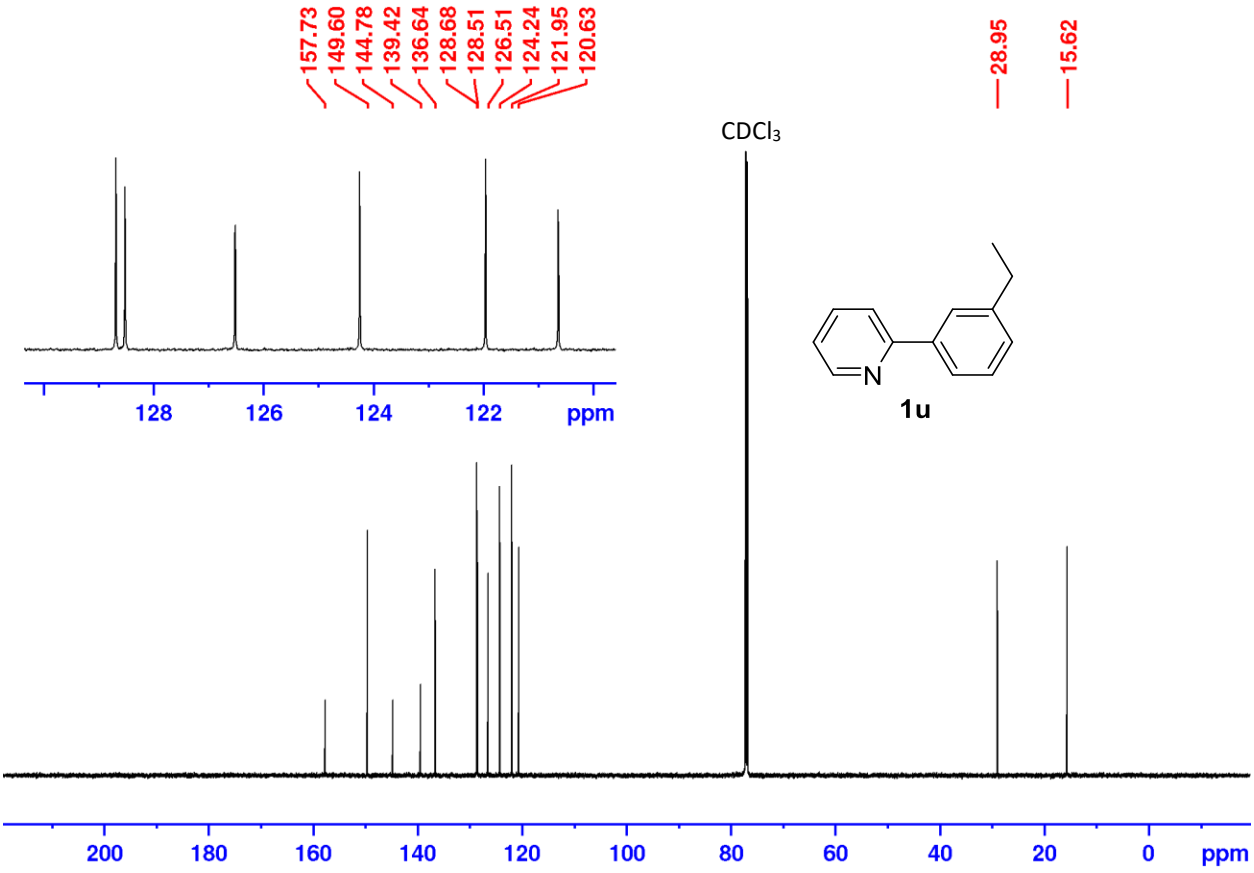
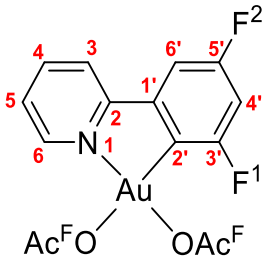


Figure S59. ^{13}C NMR (151 MHz, $CDCl_3$) of **1u**.

Synthesis and characterization of Au(III) complexes



2c-Au(OAc^F)$_2$

2c-Au(OAc^F)$_2$. A microwave vessel was charged with $Au(OAc)_3$ (0.373 g, 0.999 mmol, 1.00 equiv.) and **1c** (0.193 g, 1.01 mmol, 1.01 equiv.) in a 1:1 mixture of $HOAc^F$ and water (30 mL). The reaction mixture was heated at 120 °C for 30 min in a microwave. After cooling to room temperature, $HOAc^F$ (30 mL) was added to dissolve partially precipitated product, and the resulting solution was filtered. Water (50 mL) was added to the filtrate, resulting in the precipitation of a solid. After cooling on an ice-water bath for 15 min, the precipitate was filtered off, washed with water (3x5 mL) and Et_2O (5 mL), and dried under a stream of air for ca. 3 h, furnishing **2c-Au(OAc^F)$_2$** as a colorless solid.

Yield: 0.527 g, 0.860 mmol, 85 %.

^{1}H NMR (800 MHz, CD_2Cl_2): δ 8.62 (dd, $^3J_{H,H}$ = 6.0 Hz, $^4J_{H,H}$ = 1.0 Hz, **H^6**), 8.33 (ddd, $^3J_{H,H}$ = 7.9 Hz, $^3J_{H,H}$ = 7.8 Hz, $^4J_{H,H}$ = 1.4 Hz, **H^4**), 7.95 (d, $^3J_{H,H}$ = 8.1 Hz, **H^3**), 7.66 (ddd, $^3J_{H,H}$ = 7.6 Hz, $^3J_{H,H}$ = 6.0 Hz, $^4J_{H,H}$ = 1.3 Hz, **H^5**), 7.28 (dd, $^3J_{H,F}$ = 7.8 Hz, $^4J_{H,H}$ = 2.4 Hz, **H$^{6'}$**), 6.87 ppm (ddd, $^3J_{H,F}$ = 9.1 Hz, $^3J_{H,F}$ = 9.1 Hz, $^4J_{H,H}$ = 2.5 Hz, **H$^{4'}$**).

^{13}C NMR (201 MHz, CD_2Cl_2): δ 164.1 (**C^2**), 164.0 (dd, $^1J_{C,F}$ = 251.5 Hz, $^3J_{C,F}$ = 12.0 Hz, **C$^{3'}$** or **C$^{5'}$**), 162.8 (dd, $^1J_{C,F}$ = 253.4 Hz, $^3J_{C,F}$ = 12.1 Hz, **C$^{3'}$** or **C$^{5'}$**), 161.1 (q, $^2J_{C,F}$ = 38.2 Hz, O**C**OCF$_3$), 161.0 (q, $^2J_{C,F}$ = 39.5 Hz, O**C**OCF$_3$), 148.2 (**C^6**), 145.4 (**C^4**), 145.1 (dd, $^3J_{C,F}$ = 9.9 Hz, $^3J_{C,F}$ = 9.6 Hz, **C$^{1'}$**), 126.4 (**C^5**), 122.9 (**C^3**), 118.8 (dd, $^2J_{C,F}$ = 25.3 Hz, $^4J_{C,F}$ = 3.6 Hz, **C$^{2'}$**), 118.0 (q, $^1J_{C,F}$ = 288.6 Hz, OCO**C**F$_3$), 115.5 (q, $^1J_{C,F}$ = 287.8 Hz, OCO**C**F$_3$), 109.2-109.5 ppm (m, **C$^{4'}$** + **C$^{6'}$**).

^{19}F NMR (188 MHz, CD_2Cl_2): δ −75.5 (d, $^7J_{F,F}$ = 4.0 Hz, 3F, OCOC**F$_3$** (*trans*-N)), −77.0 (s, 3F, OCOC**F$_3$** (*cis*-N)), −102.46 - −102.53 (m, 1F, Ar**F^1**), −109.2 ppm (d, $^4J_{F,F}$ = 10.0 Hz, 1F, Ar**F^2**).

MS (ESI): m/z (rel. %): 499.998 (90) $[M–OCOCF_3]^+$.

HRMS (ESI): Found: 499.9979; calcd for $C_{13}H_6AuF_5NO_2$ $[M–OCOCF_3]^+$: 499.9979.

Elemental Analysis: Anal. calcd. For $C_{15}H_6AuF_8NO_4$: C, 29.38; H, 0.99; N. 2.28. Found: C, 29.37; H, 1.01; N, 2.27.

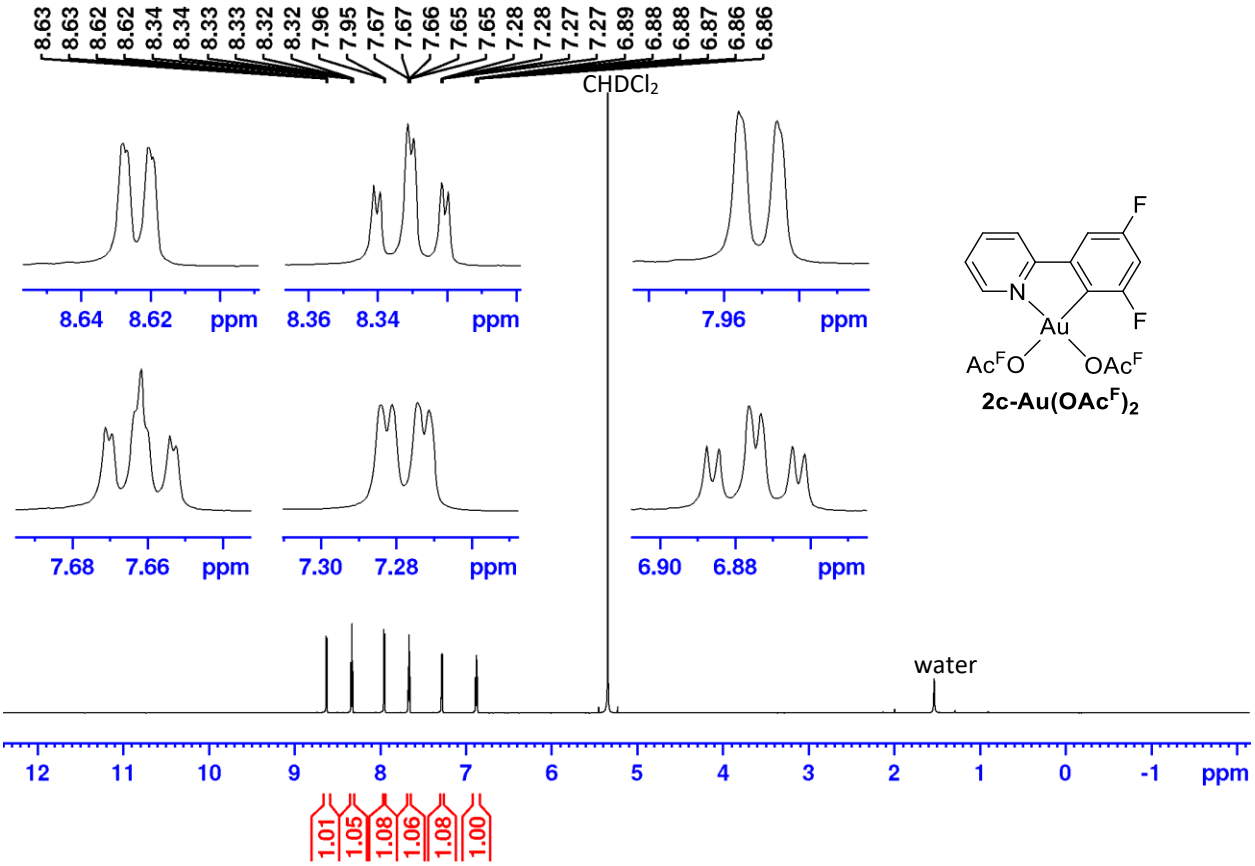


Figure S60. ^{1}H NMR (800 MHz, CD_2Cl_2) of **2c-Au(OAc^F)$_2$**.

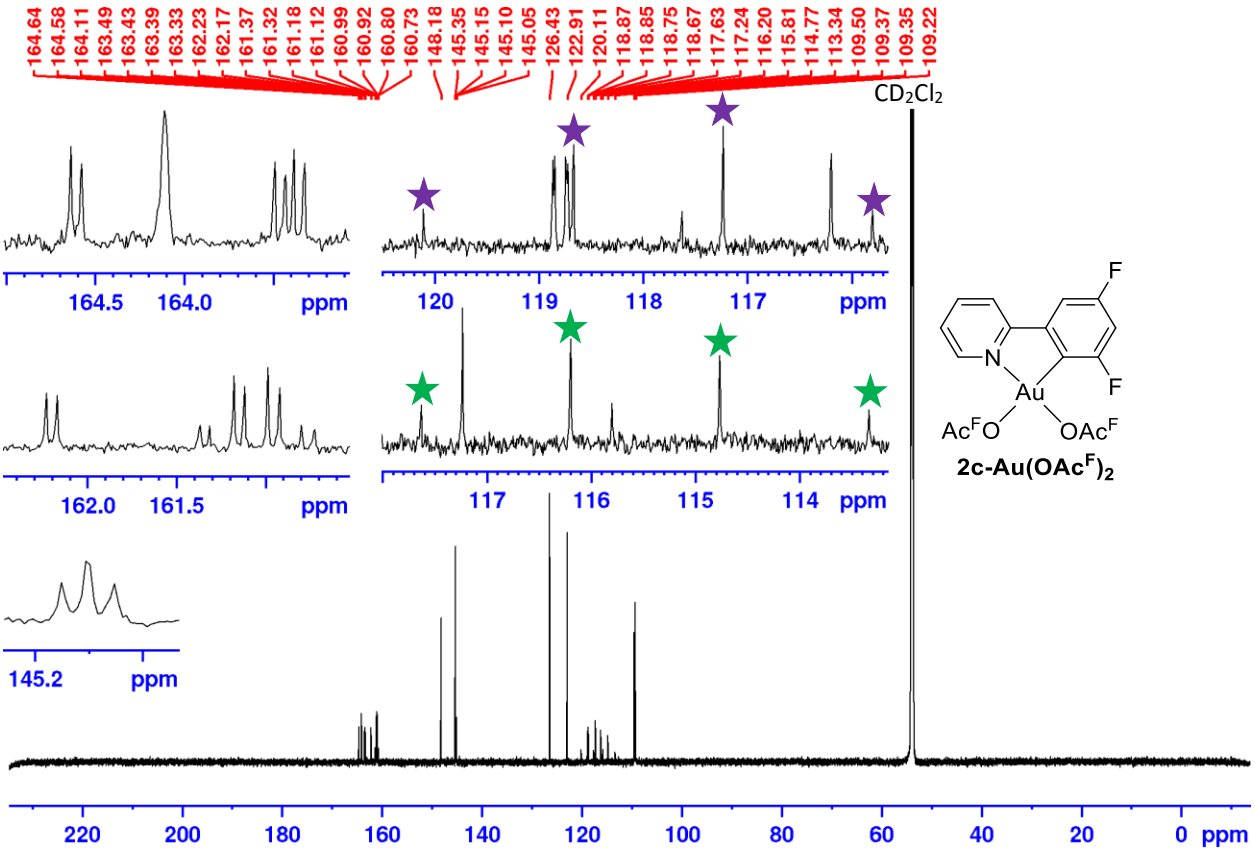


Figure S61. ^{13}C NMR (201 MHz, CD_2Cl_2) of **2c-Au(OAc^F)$_2$**. The quartets corresponding to the two **C**F_3 carbons of the trifluoroacetate ligands are indicated by purple and green stars in the inserts.

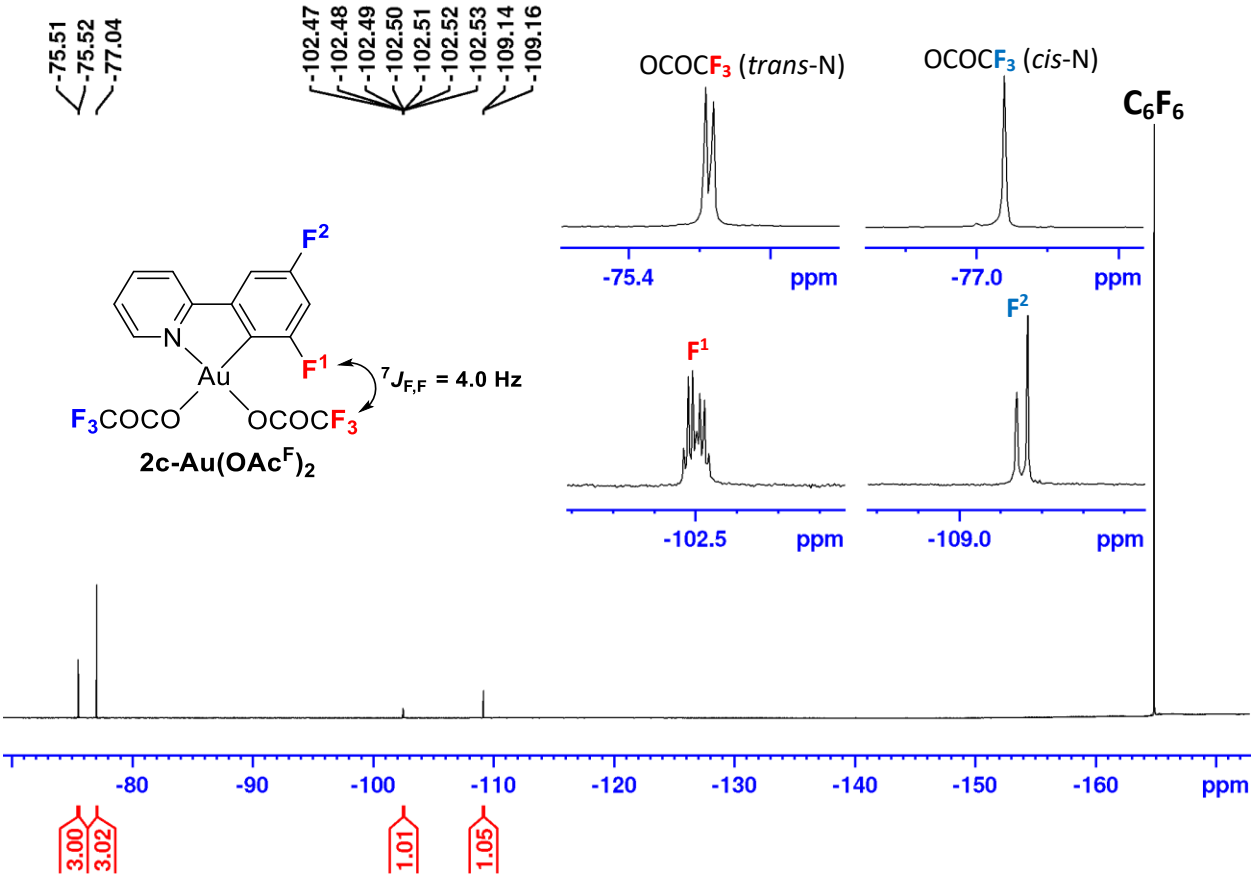
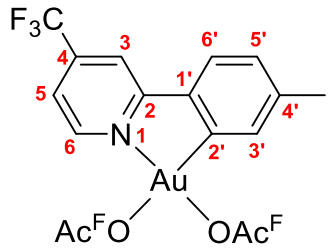


Figure S62. ^{19}F NMR (376 MHz, CD_2Cl_2) of **2c-Au(OAc^F)$_2$**.



2d-Au(OAc^F)$_2$

2d-Au(OAc^F)$_2$. A microwave vessel was charged with $Au(OAc)_3$ (0.375 g, 1.00 mmol, 1.00 equiv.) and **1d** (0.242 g, 1.02 mmol, 1.02 equiv.) in a 1:1 mixture of $HOAc^F$ and water (30 mL). The reaction mixture was heated at 120 °C for 30 min in a microwave. After cooling to room temperature, $HOAc^F$ (30 mL) was added to dissolve partially precipitated product, and the resulting solution was filtered. Water (50 mL) was added to the filtrate, resulting in the precipitation of a solid. After cooling on an ice-water bath for 15 min, the precipitate was filtered off, washed with water (3x5 mL) and pentane (5 mL), and dried under a stream of air for ca. 3 h. The obtained solid was twice recrystallized from a mixture of $HOAc^F$ and water (1:2 and then 1:1), yielding **2d-Au(OAc^F)$_2$** as a pale yellow solid.

Yield: 0.421 g, 0.640 mmol, 64 %.

^{1}H NMR (800 MHz, CD_2Cl_2): δ 8.78 (d, $^3J_{H,H}$ = 6.2 Hz, 1H, **H^6**), 8.10 (d, $^4J_{H,H}$ = 1.1 Hz, 1H, **H^3**), 7.71 (dd, $^3J_{H,H}$ = 6.2 Hz, $^4J_{H,H}$ = 1.7 Hz, 1H, **H^5**), 7.51 (d, $^3J_{H,H}$ = 7.8 Hz, 1H, **H$^{6'}$**), 7.35 (d, $^3J_{H,H}$ = 7.8 Hz, **H$^{5'}$**), 6.93 (s, 1H, **H$^{3'}$**), 2.47 ppm (s, 3H, Ar-C**H**$_3$).

^{13}C NMR (201 MHz, CD_2Cl_2): δ 167.1 (**C^2**), 161.4 (d (q expected), $^2J_{C,F}$ = 37.8 Hz, O**C**OCF$_3$), 160.7 (q, $^2J_{C,F}$ = 40.1 Hz, O**C**OCF$_3$), 149.7 (**C^6**), 146.3 (**C$^{4'}$**), 145.5 (q, $^2J_{C,F}$ = 36.3 Hz, **C^4**), 142.9 (**C$^{2'}$**), 137.5 (**C$^{1'}$**), 131.8 (**C$^{5'}$**), 129.6 (**C$^{3'}$**), 126.7 (**C$^{6'}$**), 121.6 (q, $^1J_{C,F}$ = 276.4 Hz, pyr-**C**F$_3$), 121.0 (**C^5**), 118.2 (d (q expected), $^1J_{C,F}$ = 288.9 Hz, OCO**C**F$_3$), 118.1 (**C^3**), 115.9 (q, $^1J_{C,F}$ = 286.9 Hz, OCO**C**F$_3$), 22.6 ppm (Ar-**C**H$_3$).

^{19}F NMR (188 MHz, CD_2Cl_2): δ –68.1 (3F, pyr-C**F**$_3$), −76.1 (3F, OCOC**F**$_3$), −77.1 ppm (3F, OCOC**F**$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ –160.4 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 603.978 (40) $[M–OCOCF_3+NaCl]^+$.

HRMS (ESI): Found: 603.9784; calcd for $C_{15}H_9AuClF_6NNaO_2$ $[M–OCOCF_3+NaCl]^+$: 499.9979.

Elemental Analysis: Anal. calcd. For $C_{17}H_9AuF_9NO_4$: C, 30.97; H, 1.38; N. 2.12. Found: C, 30.81; H, 1.47; N, 2.01.

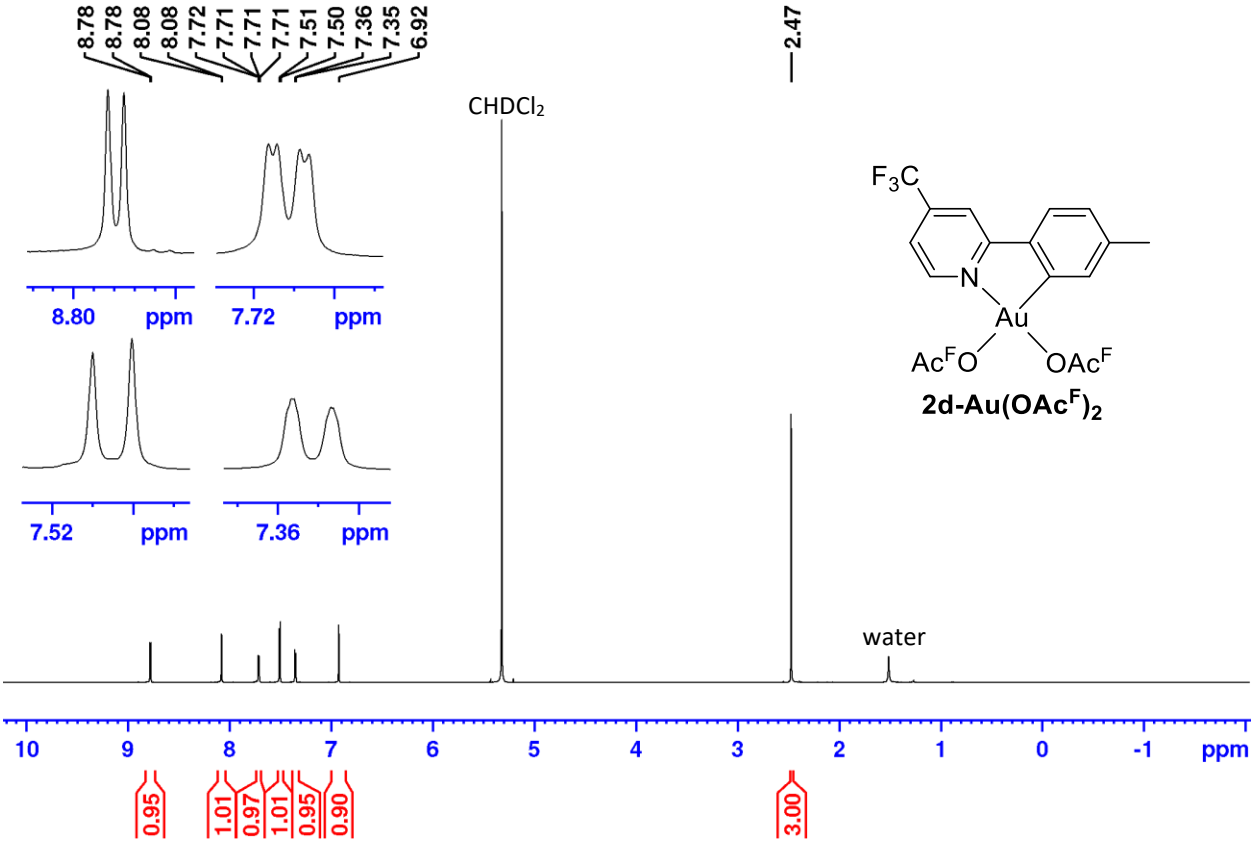


Figure S63. ^{1}H NMR (800 MHz, CD_2Cl_2) of **2d-Au(OAc^{F})$_2$**.

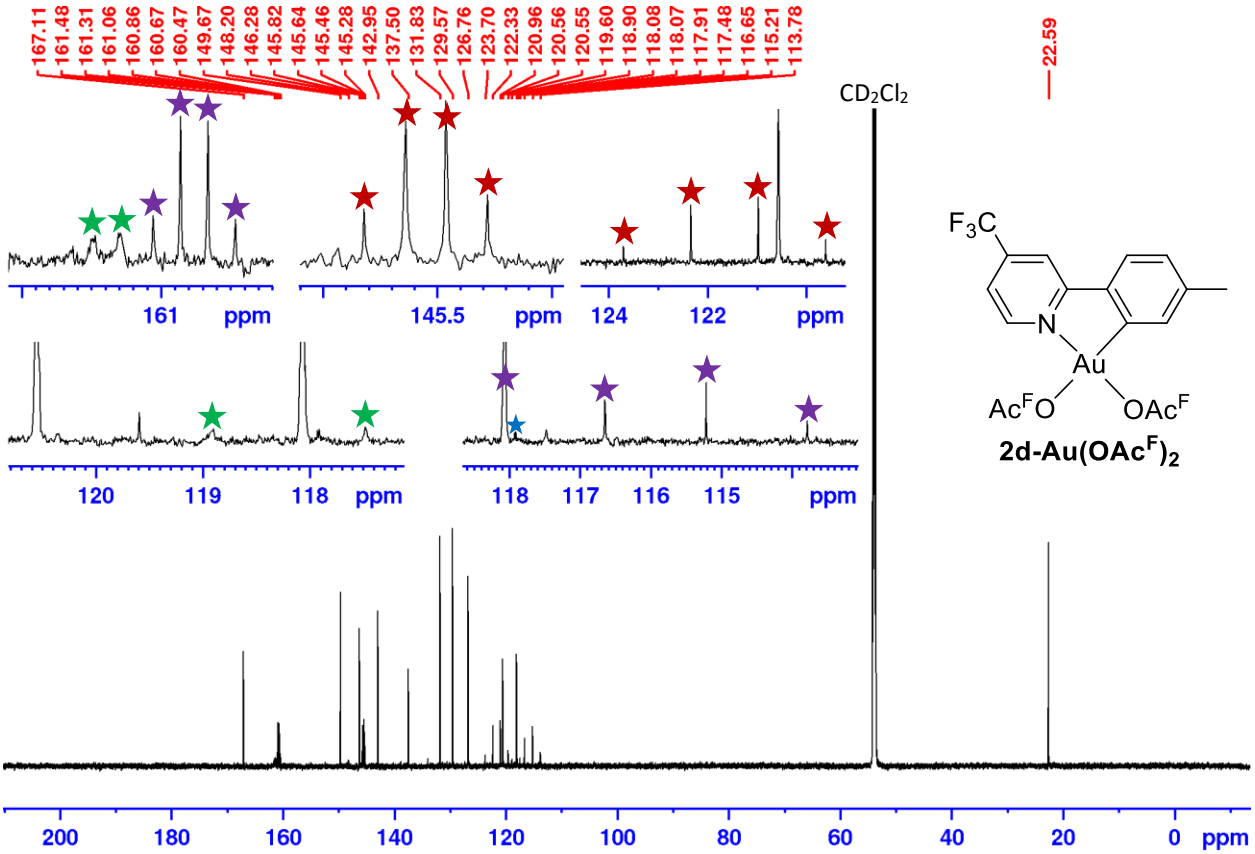


Figure S64. ^{13}C NMR (201 MHz, CD_2Cl_2) of **2d-Au(OAc^F)$_2$**. The quartets (or doublets) corresponding to the three **C**F_3 carbons of the trifluoroacetate ligands and the trifluoromethyl group in the pyridine ring are indicated by red, purple and green stars in the inserts. For the quartet labeled with purple stars, one of the lines was found to overlap with the resonance at δ 118.1. The quartets (or doublets) corresponding to the carbonyl carbons of the trifluoroacetate ligands and the C-**C**F_3 carbon of the pyridine ring are indicated by the same colors. The resonance labeled with a blue star is an unidentified impurity in the sample.

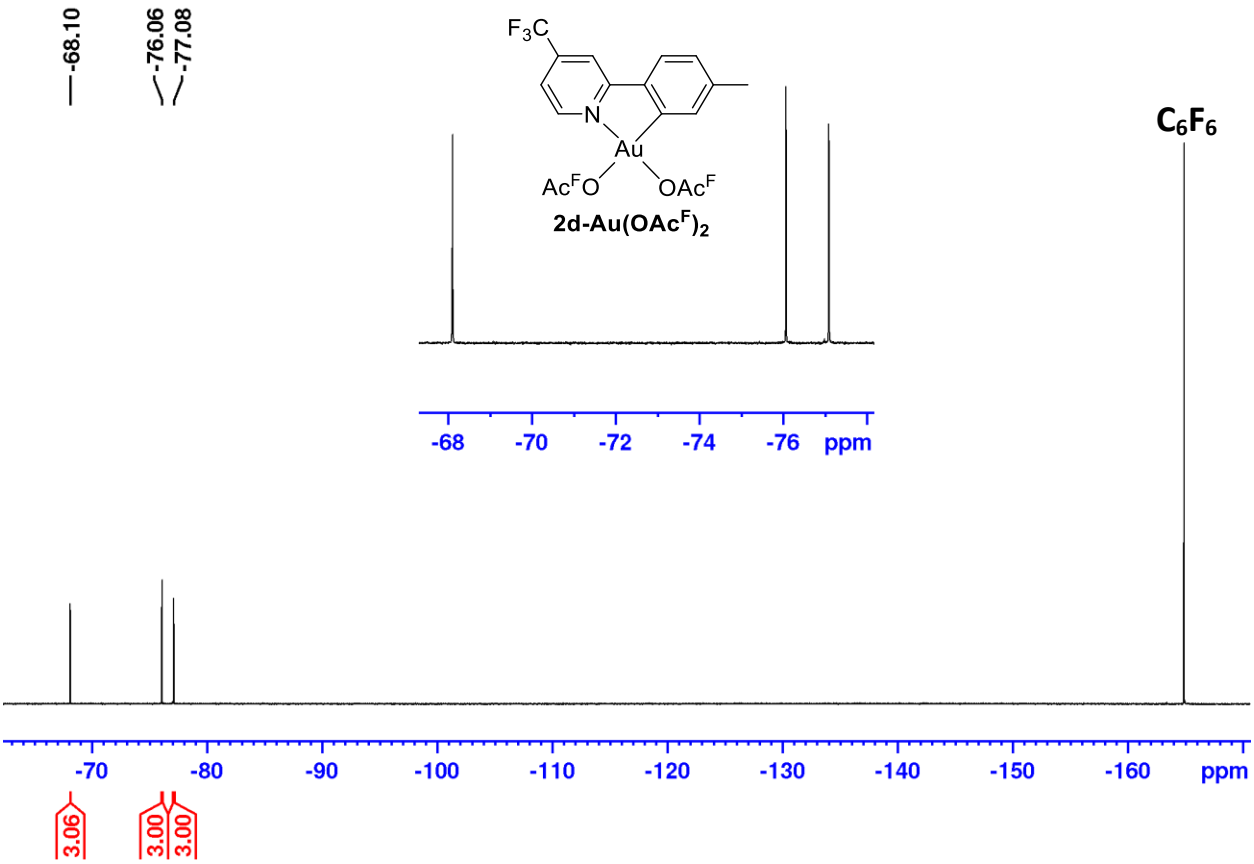


Figure S65. ^{19}F NMR (188 MHz, CD_2Cl_2) of **2d-Au(OAc^F)$_2$**.

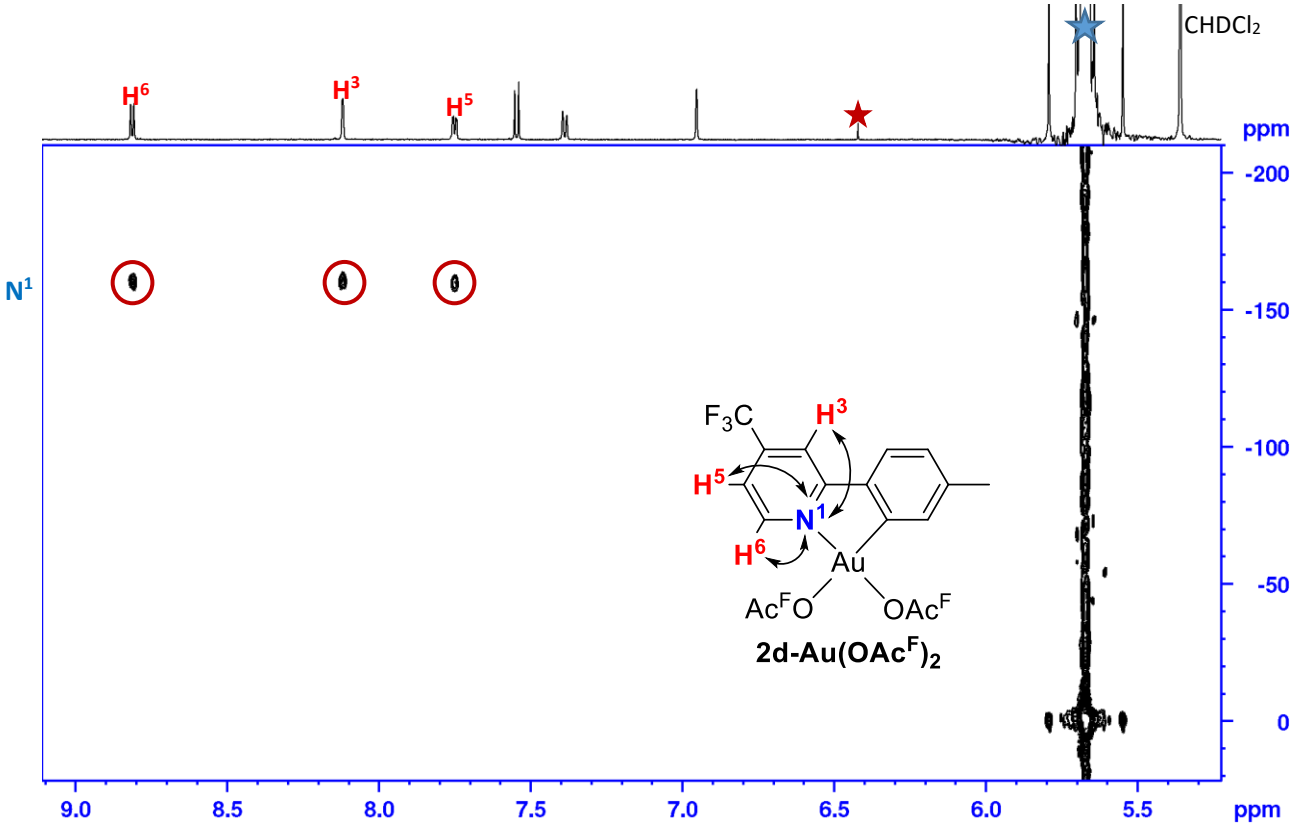
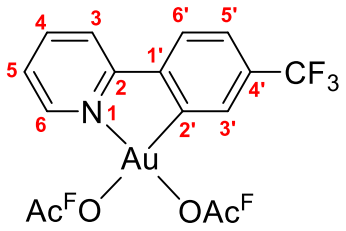


Figure S66. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **2d-Au(OAc^F)$_2$**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection). The signal marked with a red star is an unidentified impurity in CH_3NO_2.



2e-Au(OAc^F)$_2$

2e-Au(OAc^F)$_2$. A microwave vessel was charged with $Au(OAc)_3$ (0.390 g, 1.04 mmol, 1.00 equiv.) and **1e** (0.230 g, 1.03 mmol, 1.00 equiv.) in a 1:1 mixture of $HOAc^F$ and water (30 mL). The reaction mixture was heated at 120 °C for 30 min in a microwave. After cooling to room temperature, $HOAc^F$ (30 mL) was added to dissolve partially precipitated product, and the resulting solution was filtered. Water (50 mL) was added to the filtrate, resulting in the precipitation of a solid. After cooling on an ice-water bath for 15 min, and then at 4-8 °C overnight, the precipitate was filtered off, washed with water (3x5 mL) and pentane (3x5 mL), and dried under a stream of air for ca. 3 h, yielding **2e-Au(OAc^F)$_2$** as a white solid (0.182 g, 0.282 mmol, 27 %). A second crop of product (0.112 g, 0.173 mmol, 17 %) could be obtained from the filtrate, after addition of more water (50 mL), followed by filtration.

Yield: 0.293 g, 0.454 mmol, 44 %.

^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.66 (dd, 1H, $^3J_{H,H}$ = 6.0 Hz, $^4J_{H,H}$ = 1.2 Hz, **H^6**), 8.33 (ddd, 1H, $^3J_{H,H}$ = 7.8, $^3J_{H,H}$ = 7.8, $^4J_{H,H}$ = 1.4 Hz, **H^4**), 8.04 (dd, 1H, $^3J_{H,H}$ = 8.1, $^4J_{H,H}$ = 0.9 Hz, **H^3**), 7.78 (dd, 1H, $^3J_{H,H}$ = 8.1, $^4J_{H,H}$ = 0.8 Hz, **H$^{5'}$**), 7.72 (d, 1H, $^3J_{H,H}$ = 8.0 Hz, **H$^{6'}$**), 7.68 (ddd, 1H, $^3J_{H,H}$ = 7.6, $^3J_{H,H}$ = 6.1, $^4J_{H,H}$ = 1.4 Hz, **H^5**), 7.40 ppm (d, $^4J_{H,H}$ = 0.8 Hz, **H$^{3'}$**).

^{13}C NMR (151 MHz, CD_2Cl_2): δ 163.5 (**C^2**), 161.3 (q, $^2J_{C,F}$ = 38.2 Hz, O**C**OCF$_3$), 160.8 (q, $^2J_{C,F}$ = 39.8 Hz, O**C**OCF$_3$), 148.7 (**C^6**), 145.4 (**C$^{1'}$**), 145.3 (**C^4**), 141.0 (**C$^{2'}$**), 133.1 (q, $^2J_{C,F}$ = 33.1 Hz, **C$^{4'}$**), 127.8 (q, $^3J_{C,F}$ = 3.8 Hz, **C$^{5'}$**), 126.6 (**C^5**), 126.3 (**C$^{6'}$**), 125.4 (q, $^3J_{C,F}$ = 4.0 Hz, **C$^{3'}$**), 123.0 (**C^3**), 122.9 (q, $^1J_{C,F}$ = 271.8 Hz, Ar-**C**F$_3$), 118.0 (q, $^1J_{C,F}$ = 287.3 Hz, OCO**C**F$_3$), 115.8 ppm (q, $^1J_{C,F}$ = 286.3 Hz, OCO**C**F$_3$).

^{19}F NMR (188 MHz, CD_2Cl_2): δ −66.0 (3F, Ar-C**F$_3$**), −76.2 (3F, OCOC**F$_3$**), −77.0 ppm (3F, OCOC**F$_3$**).

MS (ESI): *m/z* (rel. %): 532.004 (40) $[M-OCOCF_3]^+$.

HRMS (ESI): Found 532.0041; calcd for $C_{14}H_7AuF_6NO_2$ $[M-OCOCF_3]^+$: 532.0041.

Elemental Analysis: Anal. calcd. For $C_{16}H_7AuF_9NO_4$: C, 29.79; H, 1.09; N. 2.17. Found: C, 30.31; H, 1.51; N, 2.24.

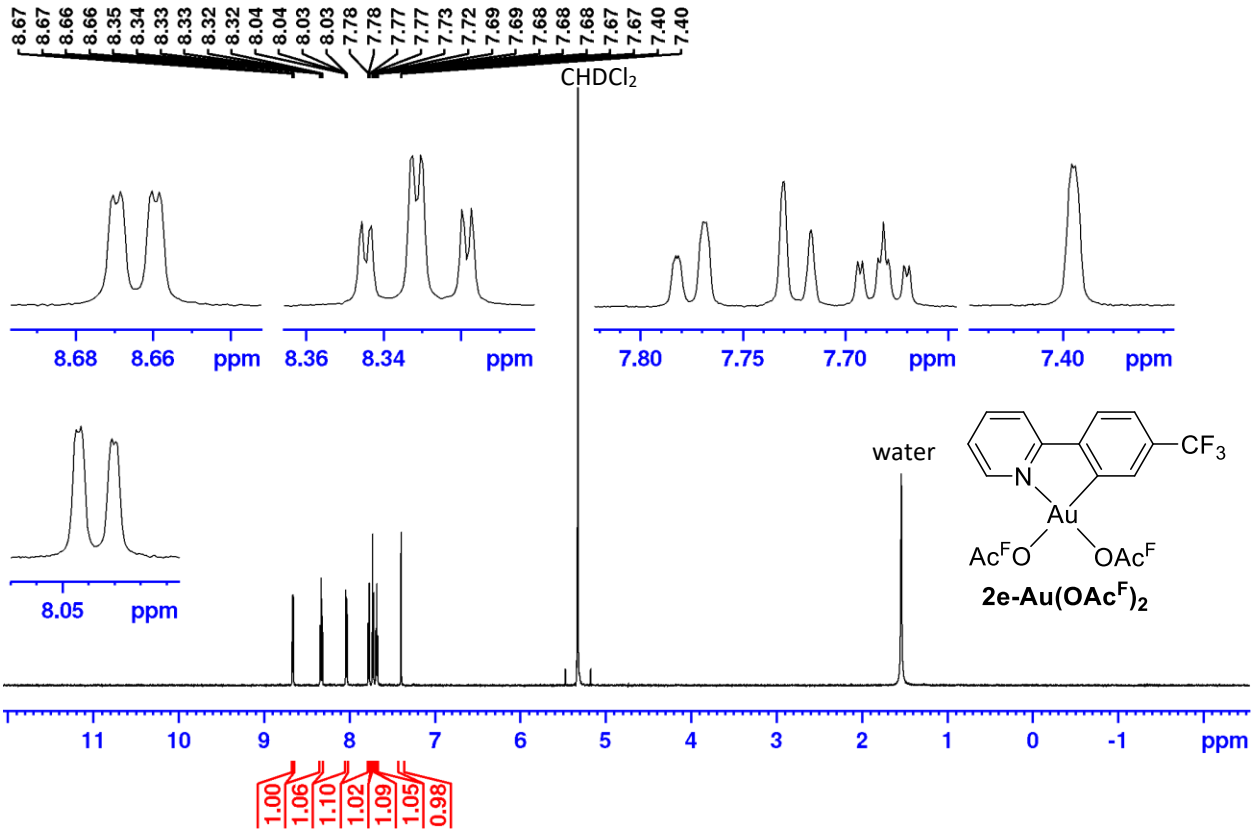


Figure S67. ^{1}H NMR (600 MHz, CD_2Cl_2) of **2e-Au(OAc^{F})$_2$**.

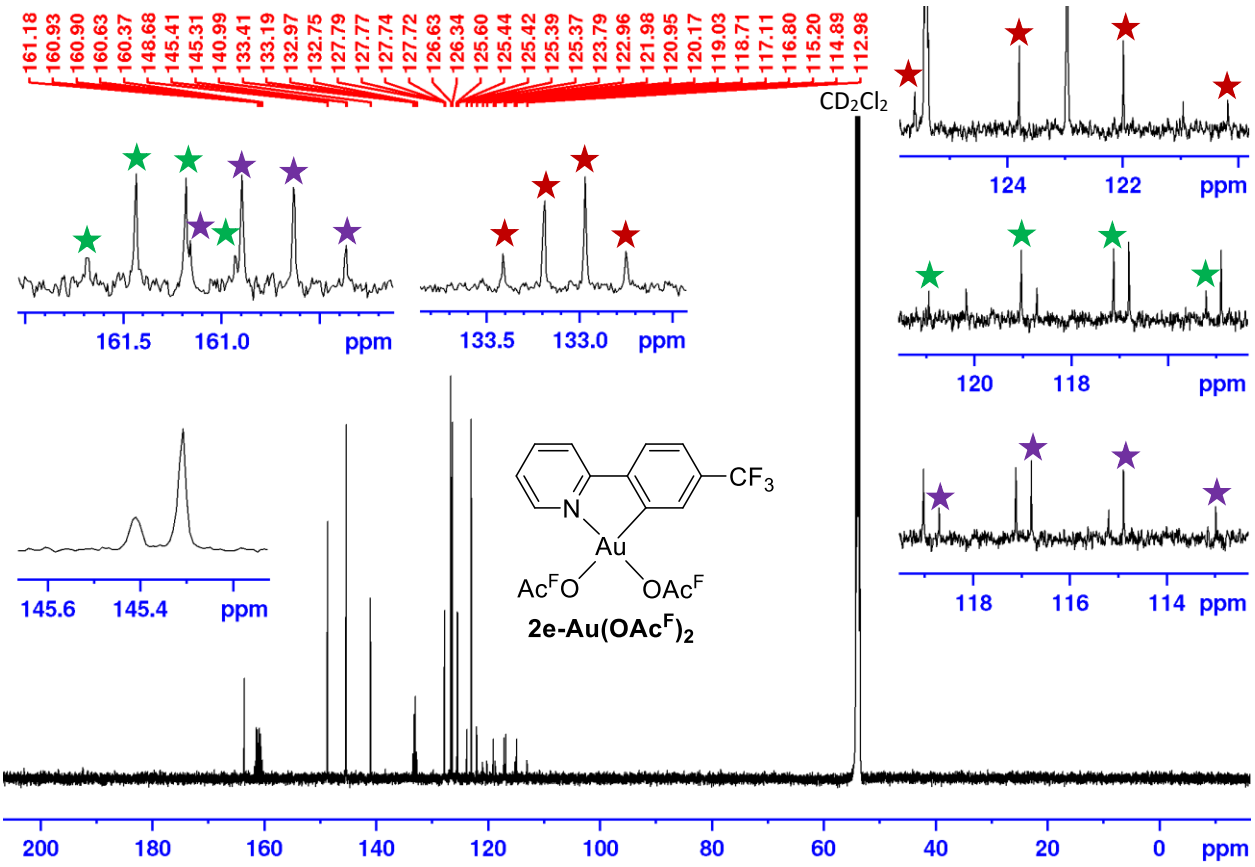


Figure S68. ^{13}C NMR (151 MHz, CD_2Cl_2) of **2e-Au(OAc^F)$_2$**. The quartets corresponding to the three **C**F$_3$ carbons of the trifluoroacetate ligands and the trifluoromethyl group in the phenyl ring are indicated by red, purple and green stars in the inserts. The quartets corresponding to the carbonyl carbons of the trifluoroacetate ligands and the C-**C**F$_3$ carbon of the phenyl ring are indicated by the same colors.

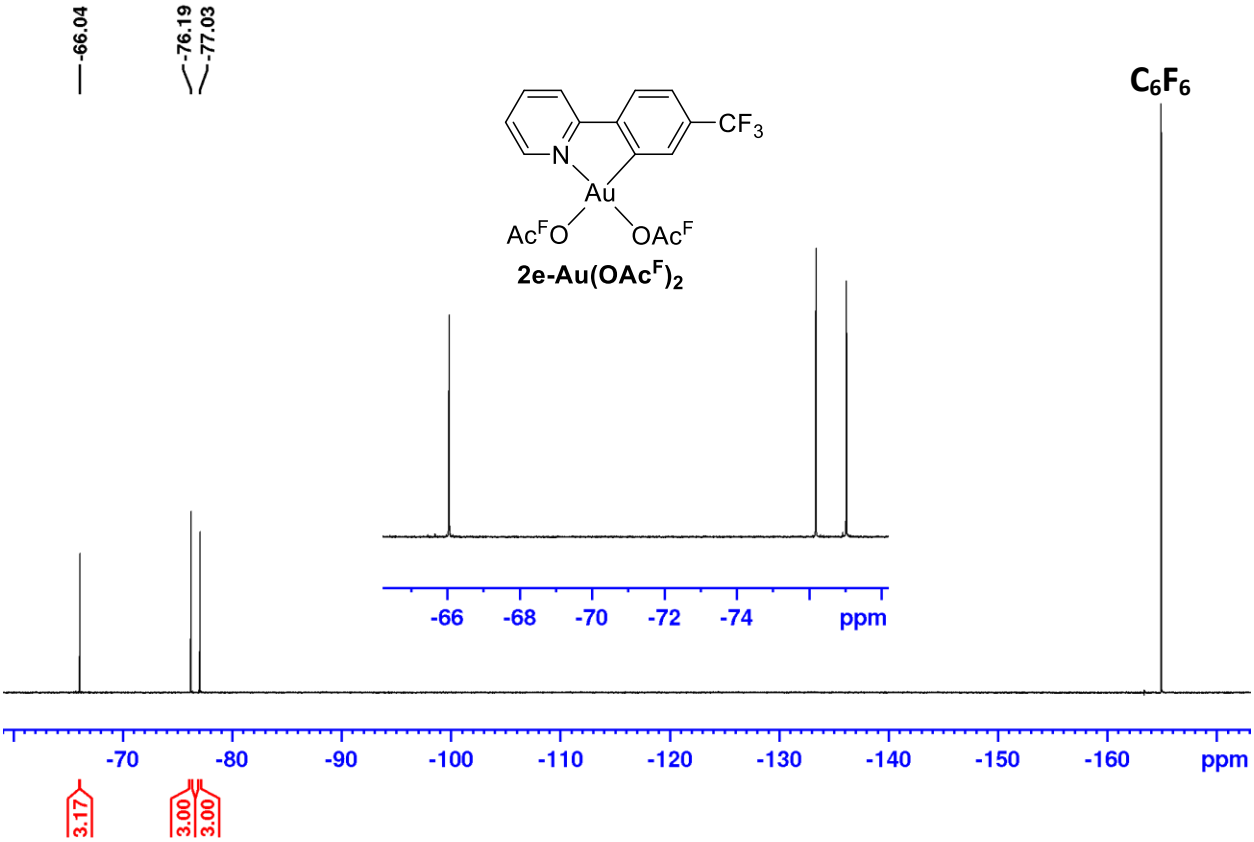
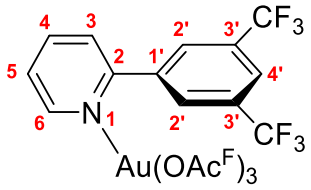


Figure S69. ^{19}F NMR (188 MHz, CD_2Cl_2) of **2e-Au(OAc^F)$_2$**.



1f-Au(OAc^F)$_3$

1f-Au(OAc^F)$_3$. A microwave vessel was charged with $Au(OAc)_3$ (0.383 g, 1.02 mmol, 1.00 equiv.) and **1f** (0.300 g, 1.03 mmol, 1.01 equiv.) in a 1:1 mixture of $HOAc^F$ and water (15 mL). The reaction mixture was heated at 120 °C for 30 min in a microwave. After cooling to room temperature, the yellow solution was filtered to remove insoluble material, and the filtrate was kept at 4-8 °C for several days. During this time, colorless crystals appeared. After one week at 4-8 °C, the crystals were filtered off, washed with water (3x10 mL), and dried under a stream of air for ca. 2 h, furnishing **1f-Au(OAc^F)$_3$** as colorless crystals.

Yield: 0.189 g, 0.228 mmol, 22 %.

^{1}H NMR (800 MHz, CD_2Cl_2): δ 8.98 (dd, 1H, $^3J_{H,H}$ = 6.1, $^4J_{H,H}$ = 1.0 Hz, **H^6**), 8.46 (s, 2H, **H$^{2'}$**), 8.40 (ddd, 1H, $^3J_{H,H}$ = 7.8, $^3J_{H,H}$ = 7.8, $^4J_{H,H}$ = 1.4 Hz, **H^4**), 8.30 (s, 1H, **H$^{4'}$**), 7.91 (ddd, 1H, $^3J_{H,H}$ = 7.7, $^3J_{H,H}$ = 6.2, $^4J_{H,H}$ = 1.6 Hz, **H^5**), 7.88 ppm (dd, 1H, $^3J_{H,H}$ = 7.8, $^4J_{H,H}$ = 1.4 Hz, **H^3**).

^{13}C NMR (201 MHz, CD_2Cl_2): δ 161.1 (q, $^2J_{C,F}$ = 41.0 Hz, O**C**OCF$_3$), 160.5 (q, $^2J_{C,F}$ = 40.7 Hz, O**C**OCF$_3$), 157.9 (**C^2**), 151.6 (**C^6**), 145.5 (**C^4**), 136.8 (**C$^{1'}$**), 134.1 (q, $^2J_{C,F}$ = 34.5 Hz, **C$^{3'}$**), 130.5 (**C^3**), 129.6 (**C$^{2'}$**), 128.5 (**C^5**), 126.5 (**C$^{4'}$**), 123.1 (q, $^1J_{C,F}$ = 273.0 Hz, Ar-**C**F$_3$), 114.0 (q, $^1J_{C,F}$ = 287.8 Hz, OCO**C**F$_3$), 113.7 ppm (q, $^1J_{C,F}$ = 287.8 Hz, OCO**C**F$_3$).

^{19}F NMR (188 MHz, CD_2Cl_2): δ −65.8 (6F, ArC**F**$_3$), −75.3 (6F, OCOC**F$_3$**), −75.5 ppm (3F, OCOC**F$_3$**).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −186.6 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 849.959 (44) $[M+Na]^+$.

HRMS (ESI): Found: 849.9595; calcd for $C_{19}H_7AuF_{15}NNaO_6$ $[M+Na]^+$: 849.9592.

Elemental Analysis: Anal. calcd. For $C_{19}H_7AuF_{15}NO_6$: C, 27.59; H, 0.85; N. 1.69. Found: C, 27.39; H, 0.89; N, 1.73.

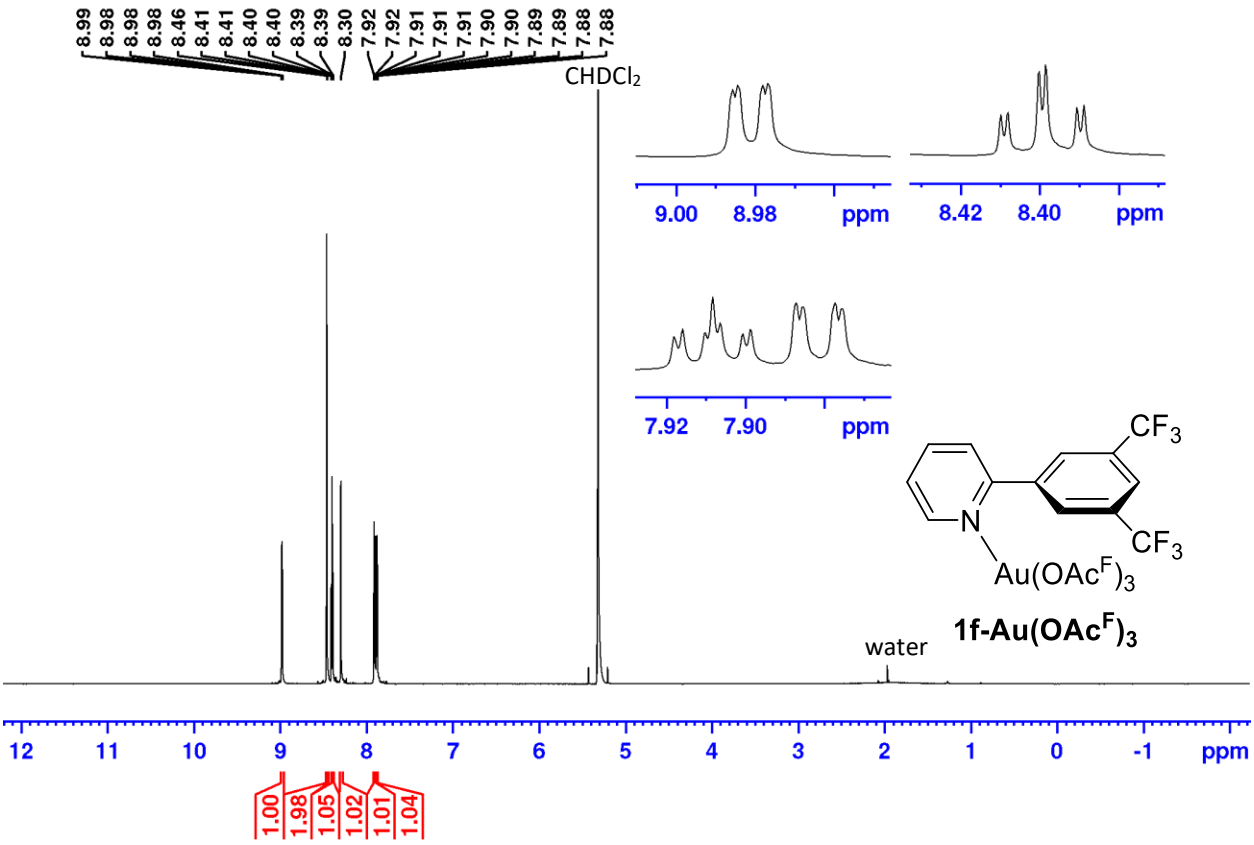


Figure S70. ^{1}H NMR (800 MHz, CD_2Cl_2) of **1f-Au(OAc^{F})$_3$**.

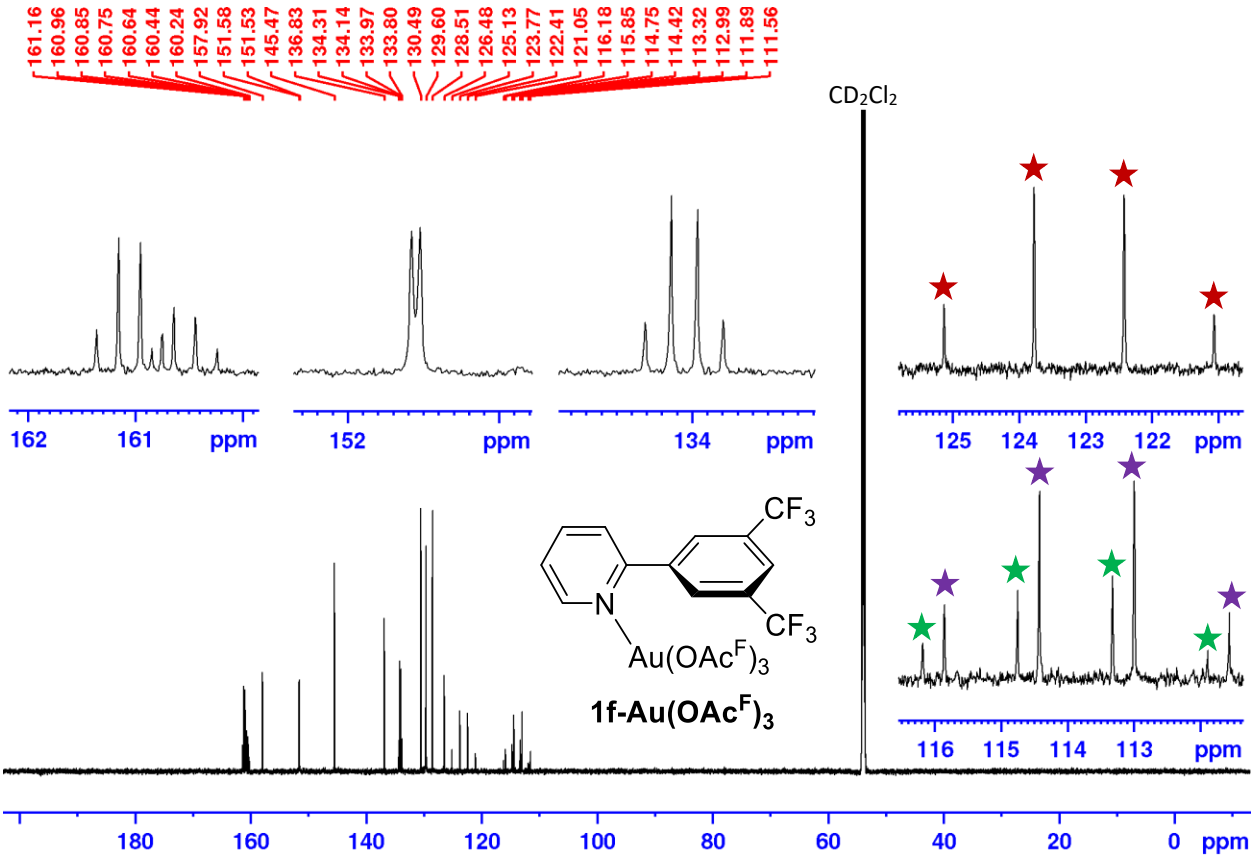


Figure S71. ^{13}C NMR (201 MHz, CD_2Cl_2) of **1f-Au(OAc^F)$_3$**.The three quartets corresponding to the five total **C**F_3 carbons are indicated by red (Ar-**C**F_3), green and purple (OCO**C**F_3) stars in the inserts.

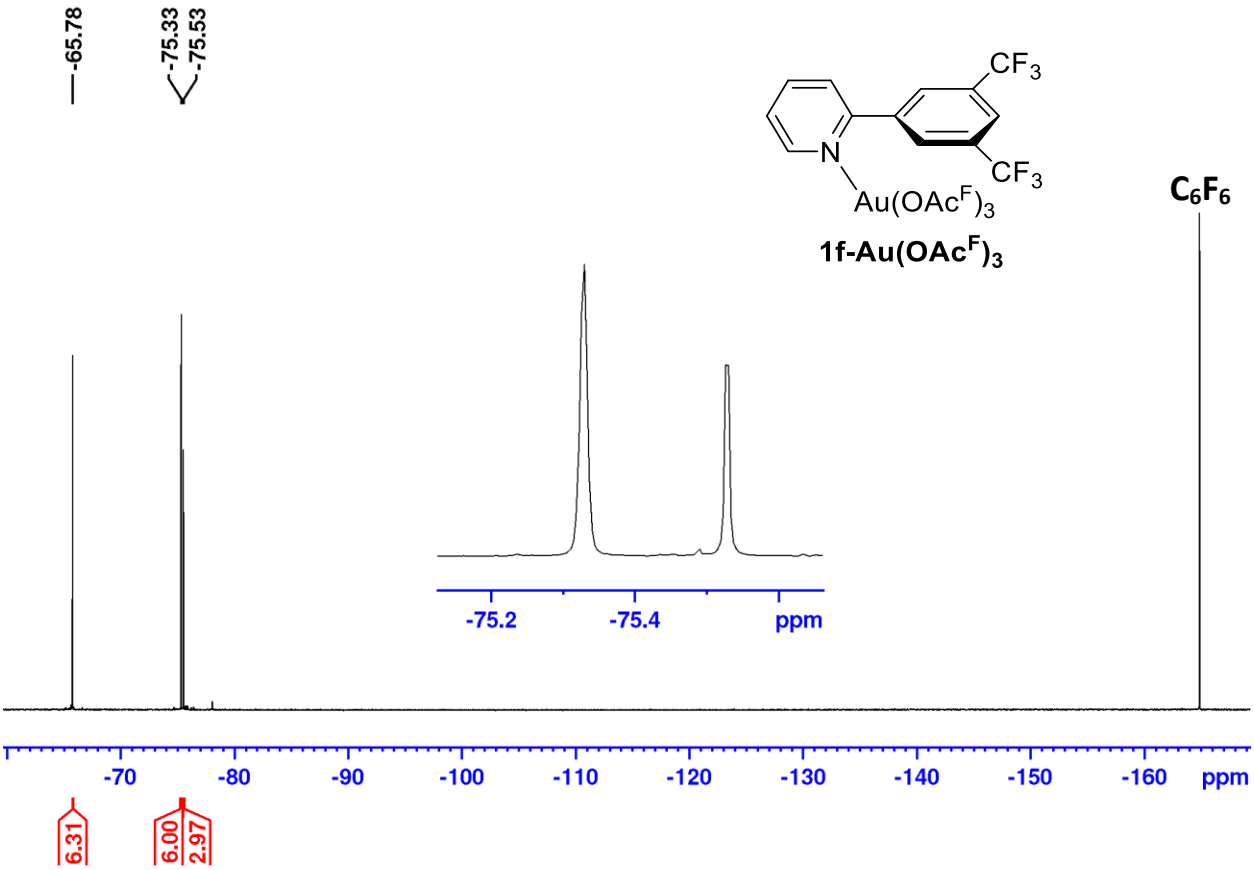


Figure S72. ^{19}F NMR (188 MHz, CD_2Cl_2) of **1f-Au(OAc^F)$_3$**.

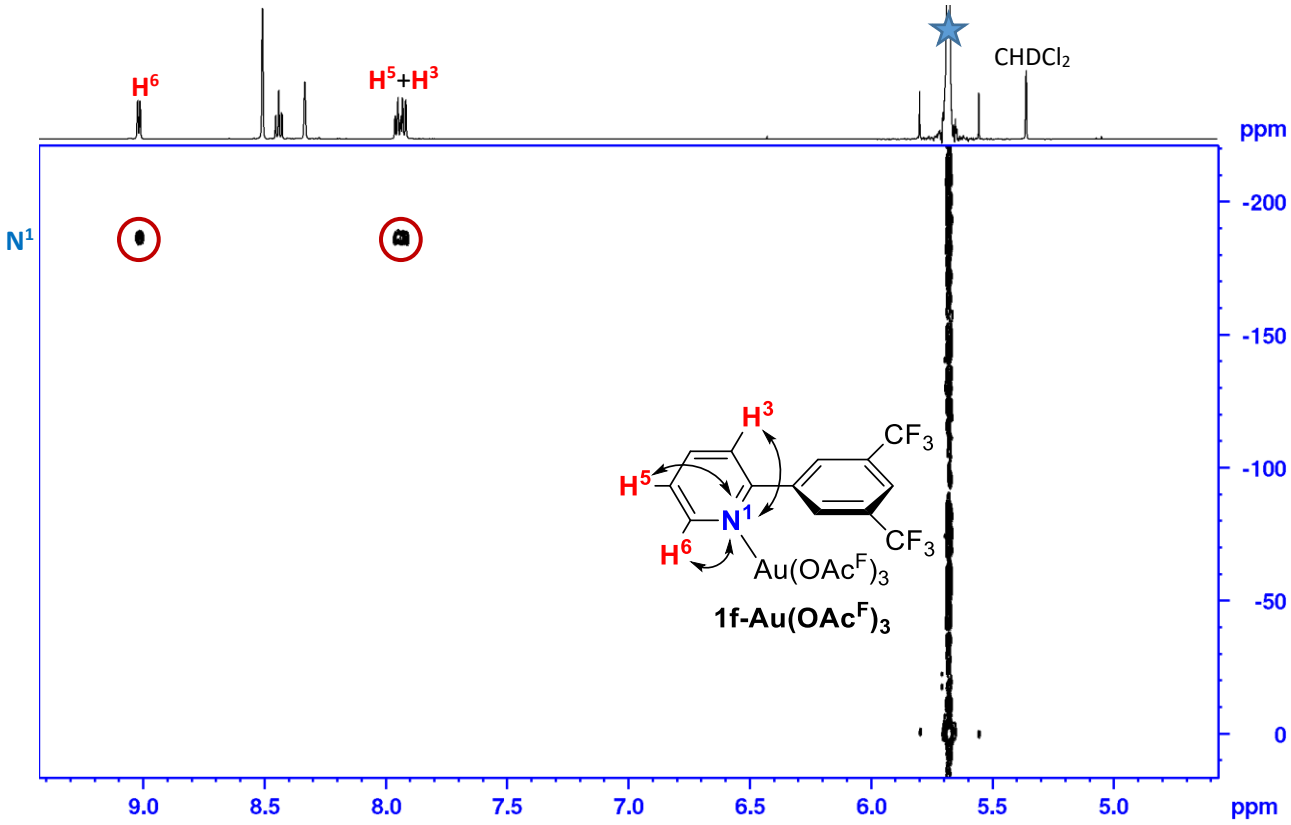
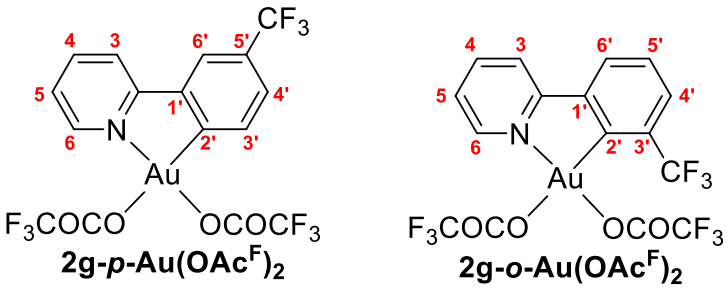


Figure S73. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1f-Au(OAc^F)$_3$**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).

The failure of obtaining cyclometalated **2f-Au(OAc^F)$_2$** is best explained from an electronic perspective. Previously, we reported that the synthesis of pincer complex **3b-AuOAc^F** (derived from the very sterically encumbered ligand **1b**) proceeds via its corresponding (N,C) cyclometalated bis(trifluoroacetate) complex **2b-Au(OAc^F)$_2$**.[2] As the trifluoromethyl group is smaller than the *tert*-butyl group,[24, 25] the formation of **2f-Au(OAc^F)$_2$** should be feasible from a steric point-of-view. It was also observed that the pentafluorophenyl-substituted ligand **1r** gave a cyclometalated complex **2r-Au(OAc^F)$_2$** when reacted with $Au(OAc)_3$, although the effective steric bulk of a pentafluorophenyl substituent is significantly smaller than that of a trifluoromethyl substituent, and more comparable to a methyl group.[25-27] To the best of our knowledge, no examples of cyclometalated Au(III) complexes with a 2-(3,5-bis(trifluoromethyl)phenyl)pyridine ligand backbone have previously been reported. A cyclometalated square planar Pt(II) complex with a 2-(3,5-bis(trifluoromethyl)phenyl)pyridine ligand was described by Ionkin and co-workers.[28] In addition, octahedral Ti(IV),[29, 30] Zr(IV),[30] Ir(III)[8, 31] and Ru(II)[32] complexes with 2-(3,5-bis(trifluoromethyl)phenyl)pyridyl ligands have all been reported in the literature. Bis[2,4,6-tris(trifluoromethyl)phenyl]mercury has also been described, however the arylmercury compound was prepared by transmetalation from the corresponding aryllithium compound,[33, 34] and not by electrophilic

mercuration of the very electron poor aryl ring. If Au-C bond formation takes place by electrophilic C(sp^2)-H bond activation, which is the dominant pathway for formation of cyclometalated Pd(II) and Pt(II) complexes,[35-37] strongly electron-withdrawing substituent(s) in the phenyl ring of the ligand may have a negative effect on the reaction. When the related mono-trifluoromethyl-substituted ligand **1g** was reacted with $Au(OAc)_3$, a mixture of cyclometalated complexes **2g-*p*-Au(OAc^F)$_2$** and **2g-*o*-Au(OAc^F)$_2$** was isolated (see below). This suggests that the steric demands of the trifluoromethyl group is compatible with cyclometalation of Au(III). Furthermore, it hints that the electronic influence is the main factor for the failure of obtaining cyclometalated **2f-Au(OAc^F)$_2$**, as it would be anticipated that ligand **1f** is significantly more electron-deficient at the carbon binding to gold in the hypothetical cyclometalated complex, than the corresponding carbon(s) in ligand **1g**.



2g-*p*-Au(OAc^F)$_2$ and 2g-*o*-Au(OAc^F)$_2$. A microwave vessel was charged with $Au(OAc)_3$ (0.0750 g, 0.200 mmol, 1.00 equiv.) and **1g** (0.0450 g, 0.202 mmol, 1.01 equiv.) in a 1:1 mixture of $HOAc^F$ and water (6 mL). The reaction mixture was heated at 120 °C for 60 min in a microwave. After cooling to room temperature, $HOAc^F$ (6 mL) was added, and the resulting solution was filtered. Water (20 mL) was added to the filtrate, resulting in the precipitation of a solid. After cooling on an ice-water bath for 5 min, the precipitate was filtered off, washed with water (3x5 mL) and Et_2O (5 mL), and dried under a stream of air for ca. 3 h, furnishing a pale gray solid, consisting mainly of **2g-*p*-Au(OAc^F)$_2$** and **2g-*o*-Au(OAc^F)$_2$**, as well as small amounts of other products. The ratio between **2g-*p*-Au(OAc^F)$_2$** and **2g-*o*-Au(OAc^F)$_2$** was found to vary with different batches, from approximately 2:1 (see ^{1}H NMR spectrum in Figure S74) to approximately 4:1 (see ^{1}H NMR spectrum in Figure S75), with **2g-*p*-Au(OAc^F)$_2$** consistently being the major product. This variation may be related to differences in the solubility of the two compounds. No attempts were made of further purifying the mixture.

Yield: 0.0660 g, 0.106 mmol, 53 %.

MS (ESI): *m/z* (rel. %): 426.076 (100) $[M–2OCOCF_3+OMe]^+$.

HRMS (ESI): Found: 426.0761; calcd for $C_{14}H_{15}AuNO_2$ $[M–2OCOCF_3+OMe]^+$: 426.0763.

^{1}H, ^{13}C and ^{19}F NMR data for 2g-*p*-Au(OAc^F)$_2$

^{1}H NMR (800 MHz, CD_2Cl_2): δ 8.66 (dd, $^3J_{H,H}$ = 6.0 Hz, $^4J_{H,H}$ = 1.0 Hz, 1H, **H^6**), 8.32-8.34 (m, 1H, **H^4**), 8.05 (dd, $^3J_{H,H}$ = 8.0 Hz, $^4J_{H,H}$ = 1.0 Hz, 1H, **H^3**), 7.83 (d, $^4J_{H,H}$ = 1.6 Hz, 1H, **H$^{6'}$**), 7.66-7.68 (m, 1H, **H^5**), 7.63 (dd, $^3J_{H,H}$ = 8.4 Hz, $^4J_{H,H}$ = 1.6 Hz, 1H, **H$^{4'}$**), 7.32 ppm (d, $^3J_{H,H}$ = 8.4 Hz, 1H, **H$^{3'}$**).

^{13}C NMR (201 MHz, CD_2Cl_2): δ 163.7 (**C^2**), 161.3 (q, $^2J_{C,F}$ = 37.6 Hz, O**C**OCF$_3$), 160.8 (q, $^2J_{C,F}$ = 39.6 Hz, O**C**OCF$_3$), 148.6 (**C^6**), 145.3 (**C^4**), 144.4 (**C$^{1'}$** or **C$^{2'}$**), 142.7 (**C$^{1'}$** or **C$^{2'}$**), 133.0 (q, $^2J_{C,F}$ = 33.8 Hz, **C$^{5'}$**), 128.8 (**C$^{3'}$**), 129.00-129.04 (m, **C$^{4'}$**), 126.4 (**C^5**), 122.70-122.76 (m, **C$^{6'}$**), 122.6 (**C^3**), 123.6 (q, $^1J_{C,F}$ = 272.2 Hz, Ar-**C**F$_3$), 118.1 (q, $^1J_{C,F}$ = 289.3 Hz, OCO**C**F$_3$), 115.9 ppm (q, $^1J_{C,F}$ = 287.8 Hz, OCO**C**F$_3$).

^{19}F NMR (376 MHz, CD_2Cl_2): δ –65.8 (s, 3F, Ar-C**F**$_3$), –76.0 (s, 3F, OCOC**F**$_3$), –77.05 ppm (s, 3F, OCOC**F**$_3$).

^{1}H, ^{13}C and ^{19}F NMR data for 2g-*o*-Au(OAc^{F})$_2$

^{1}H NMR (800 MHz, CD_2Cl_2): δ 8.58 (dd, $^{3}J_{H,H}$ = 6.1 Hz, $^{4}J_{H,H}$ = 1.1 Hz, 1H, **H^{6}**), 8.29-8.31 (m, 1H, **H^{4}**), 8.00 (dd, $^{3}J_{H,H}$ = 8.2 Hz, $^{4}J_{H,H}$ = 1.3 Hz, 1H, **H^{3}**), 7.82-7.83* (m, 1H, **H$^{6'}$**), 7.70 (dd, $^{3}J_{H,H}$ = 7.8 Hz, $^{4}J_{H,H}$ = 1.4 Hz, 1H, **H$^{4'}$**), 7.63-7.65 (m, 1H, **H$^{5'}$**), 7.59-7.61 ppm (m, 1H, **H^{5}**).

*This resonance partially overlaps with the resonance corresponding to **H$^{6'}$** in **2g-*p*-Au(OAc^{F})$_2$**.

^{13}C NMR (201 MHz, CD_2Cl_2):* δ 164.9 (**C^{2}**), 148.1 (**C^{6}**), 145.2 (**C^{4}**), 131.2 ($^{3}J_{C,F}$ = 6.0 Hz, **C$^{4'}$**), 130.7 (**C$^{5'}$**), 129.4 (**C$^{6'}$**), 125.9 (**C^{5}**), 122.8 ppm (**C^{3}**).

*Most of the quaternary carbons could not be detected and/or identified in an unambiguous manner.

^{19}F NMR (376 MHz, CD_2Cl_2): δ –60.5 (q, $^{8}J_{F,F}$ = 2.6 Hz, Ar-C**F**$_3$), –76.1 (q, $^{8}J_{F,F}$ = 2.6 Hz, 3F, OCOC**F**$_3$), –77.09 ppm (s, 3F, OCOC**F**$_3$).

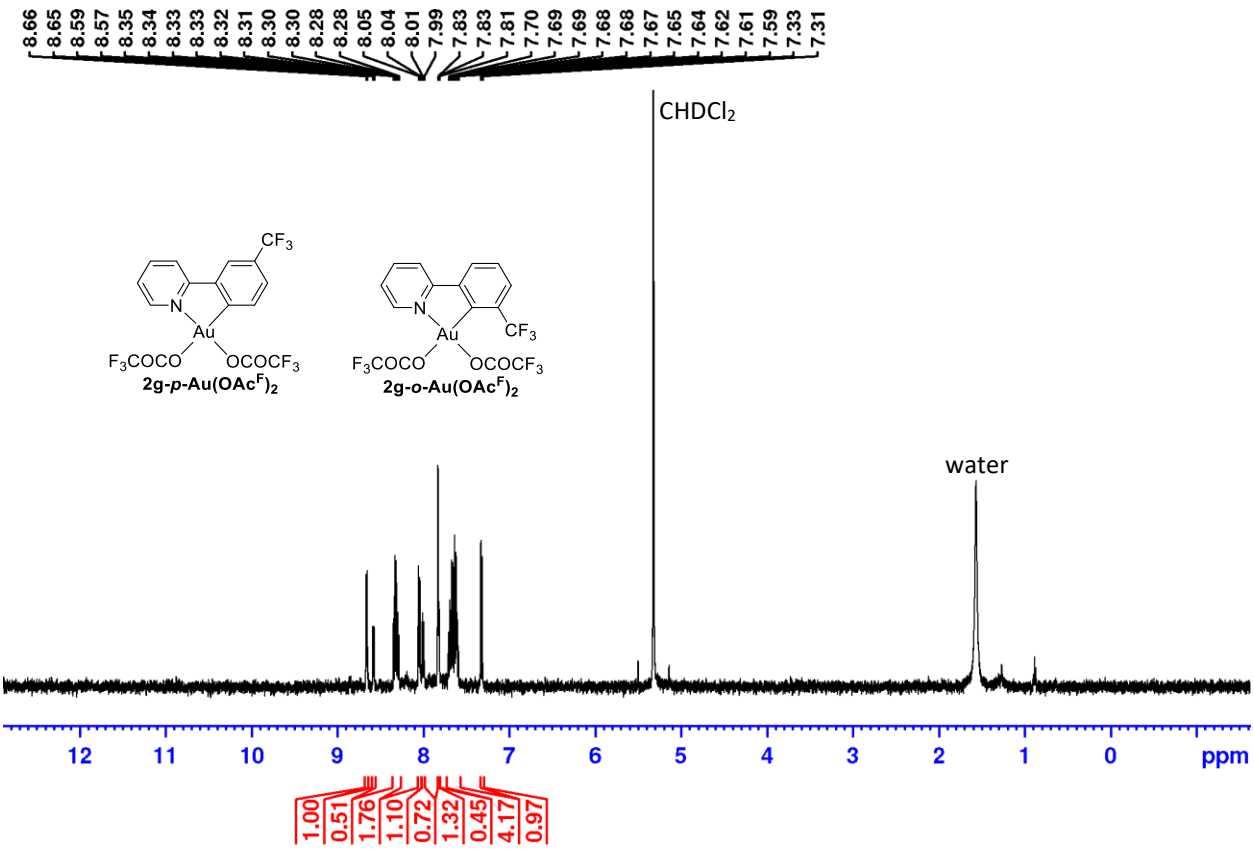


Figure S74. ^{1}H NMR (500 MHz, CD_2Cl_2) of a mixture of **2g-*p*-Au(OAc^{F})$_2$** and **2g-*o*-Au(OAc^{F})$_2$**. The spectrum is integrated with respect to **2g-*p*-Au(OAc^{F})$_2$.**

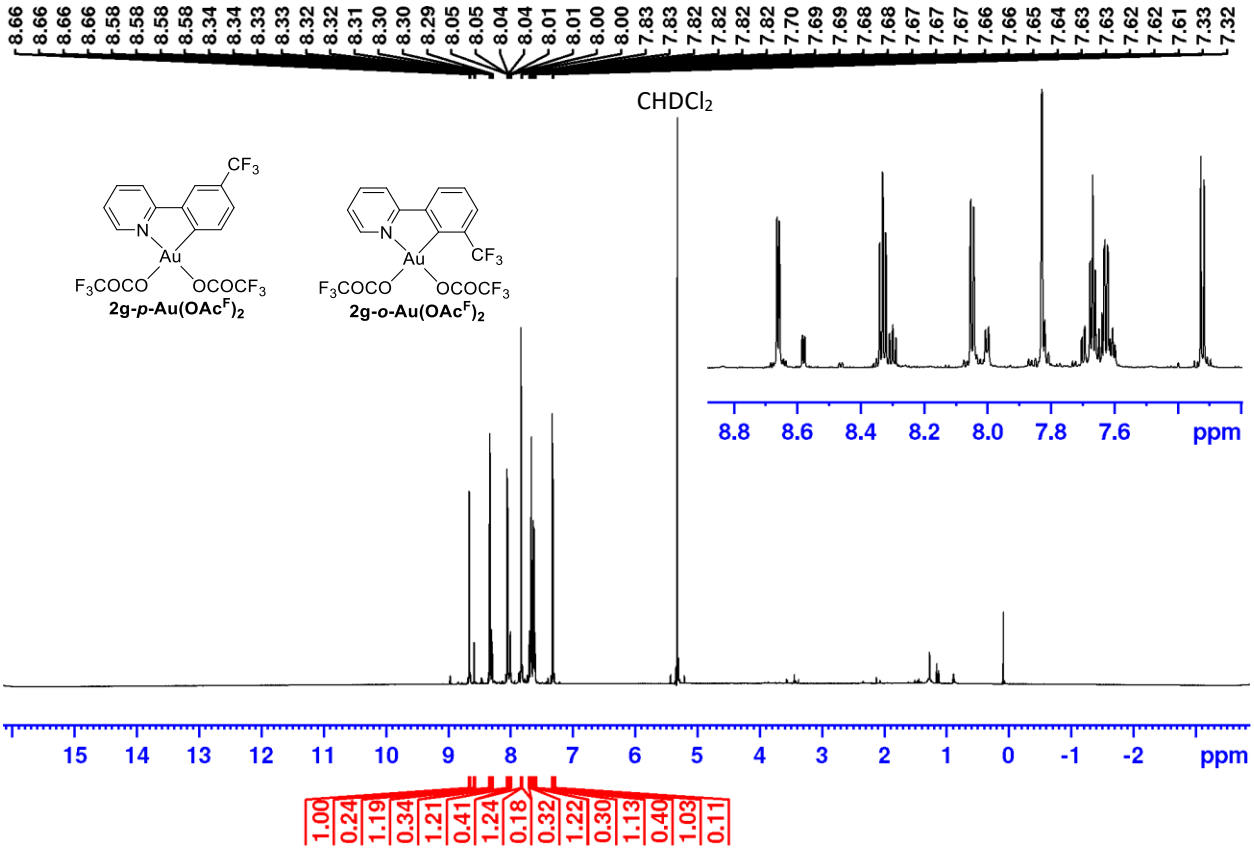


Figure S75. ^{1}H NMR (800 MHz, CD_2Cl_2) of a mixture of **2g-*p*-Au(OAc^{F})$_2$** and **2g-*o*-Au(OAc^{F})$_2$**. The spectrum is integrated with respect to **2g-*p*-Au(OAc^{F})$_2$**. Due to the low purity of the sample, impurities and residual solvents are not indicated.

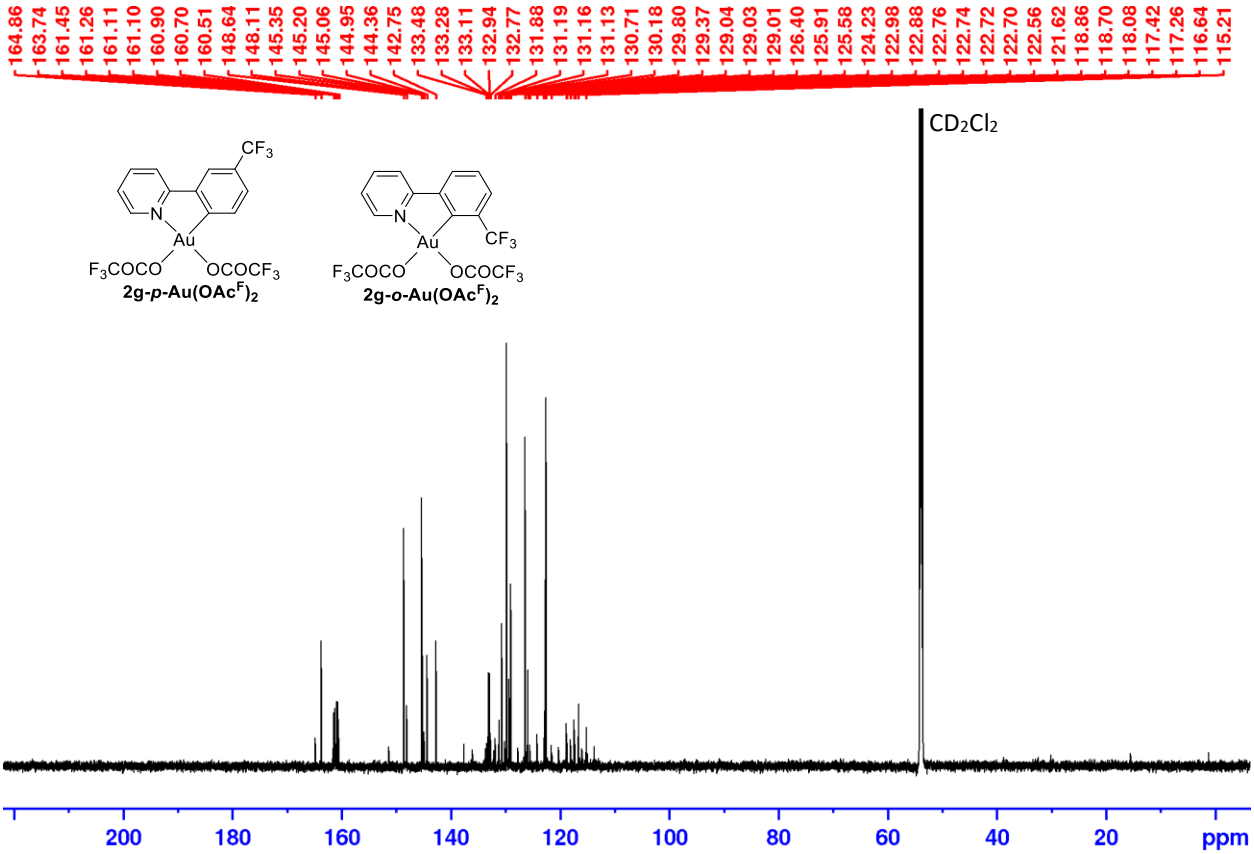


Figure S76. ^{13}C NMR (201 MHz, CD_2Cl_2) of a mixture of **2g-*p*-Au(OAc^F)$_2$** and **2g-*o*-Au(OAc^F)$_2$**.

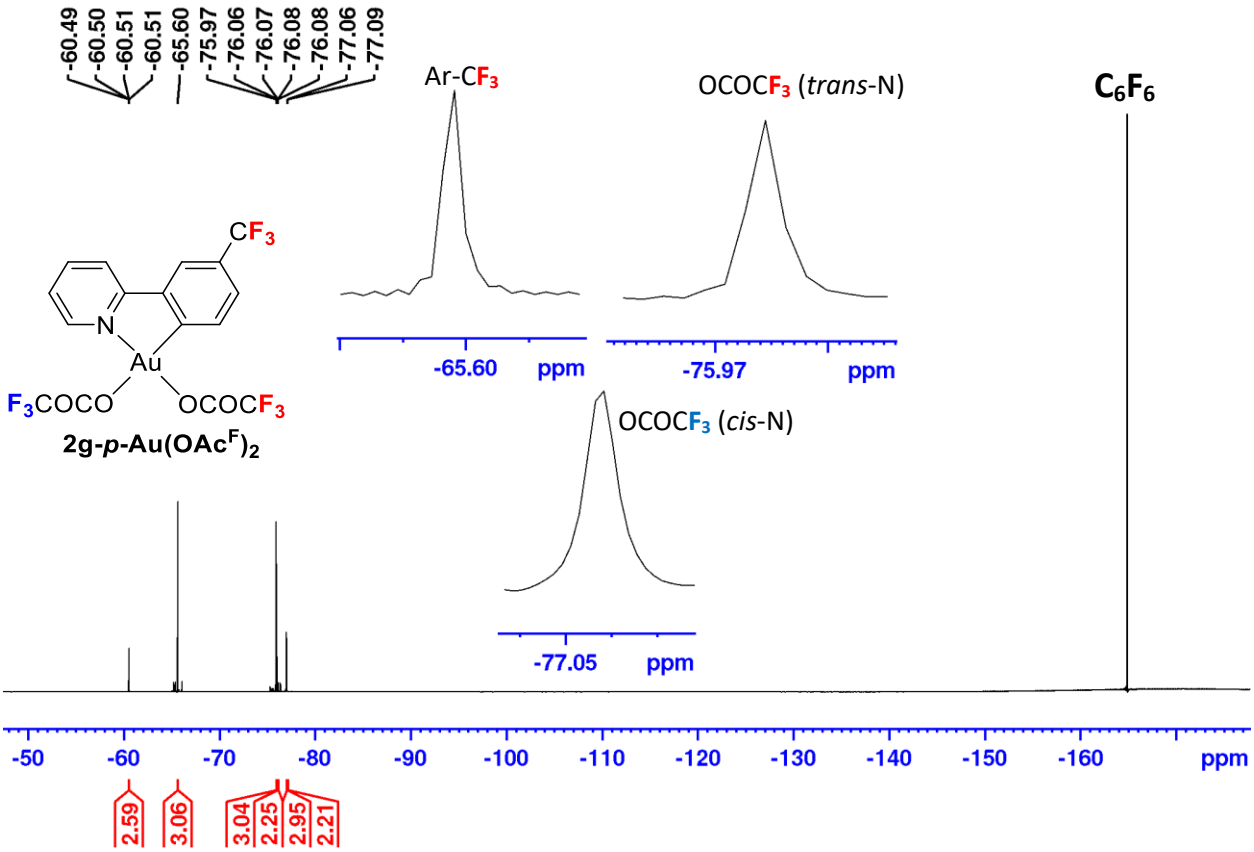


Figure S77. ^{19}F NMR (376 MHz, CD_2Cl_2) of a mixture of **2g-*p*-Au(OAc^F)$_2$** and **2g-*o*-Au(OAc^F)$_2$**. The spectrum is integrated with respect to **2g-*p*-Au(OAc^F)$_2$** and the inserts show the three resonances corresponding to this compound, which are all singlets.

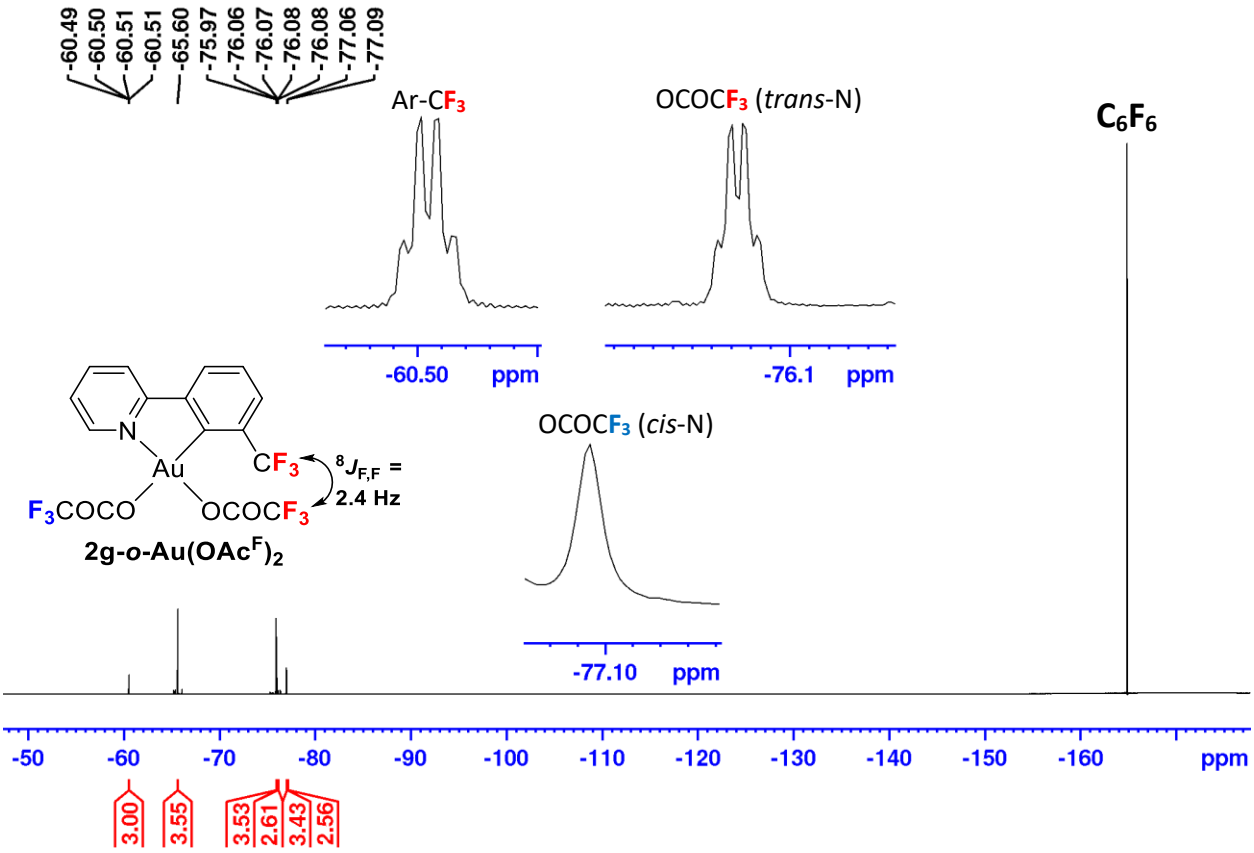
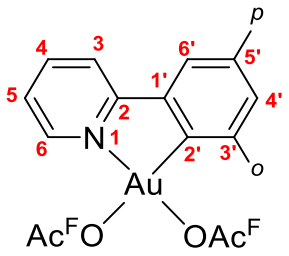


Figure S78. ^{19}F NMR (376 MHz, CD_2Cl_2) of a mixture of **2g-*p*-Au(OAc^F)$_2$** and **2g-*o*-Au(OAc^F)$_2$**. The spectrum is integrated with respect to **2g-*o*-Au(OAc^F)$_2$** and the inserts show the three resonances corresponding to this compound. The resonances corresponding to the aromatic CF_3 group and the trifluoroacetate ligand *trans* to nitrogen appear as quartets, whereas the resonance corresponding to the trifluoroacetate ligand *cis* to nitrogen appears as a singlet.

^{19}F NMR was used to decide the presence of **2g-*o*-Au(OAc^F)$_2$** in an unambiguous manner, and ultimately show that an *ortho*-trifluoromethyl group is compatible with cyclometalation. The resonances corresponding to the aromatic trifluoromethyl group and the trifluoromethyl group of the trifluoroacetate ligand *trans* to nitrogen were both observed as a quartets with $^8J_{F,F}$ = 2.4 Hz (Figure S78). This observation indicates that the two CF_3 groups must be in relatively close spatial proximity to each other,[38] and the corresponding resonances of the major product **2g-*p*-Au(OAc^F)$_2$** were both observed as singlets (Figure S77). Similar long-range ^{19}F-^{19}F couplings were observed between one of the fluorine substituents on the aromatic ring and the trifluoroacetate ligand *trans* to nitrogen in complex **2c-Au(OAc^F)$_2$** (Figure S62). Interestingly, this type of coupling was not observed for complex **2r-Au(OAc^F)$_2$** (Figure S114).



2h-Au(OAc^F)$_2$

2h-Au(OAc^F)$_2$. A microwave vessel was charged with $Au(OAc)_3$ (0.383 g, 1.02 mmol, 1.00 equiv.) and **1h** (0.194 g, 1.06 mmol, 1.04 equiv.) in a mixture of $HOAc^F$ (15 mL) and water (15 mL). The reaction mixture was heated at 120 °C for 30 min in a microwave. After cooling to room temperature, $HOAc^F$ (20 mL) was added to dissolve partially precipitated product, and the resulting solution was filtered to remove insoluble material. Water (50 mL) was added to the filtrate, resulting in the precipitation of a yellow solid. After cooling on an ice-water bath, the precipitate was filtered off, washed with water (3x5 mL) and Et_2O (5 mL), and dried under a stream of air for ca. 1 h. **2h-Au(OAc^F)$_2$** was obtained as a pale yellow solid.

Yield: 0.586 g, 0.968 mmol, 95 %.

^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.52 (dd, $^3J_{H,H}$ = 6.1 Hz, $^4J_{H,H}$ = 0.8 Hz, 1H, **H^6**), 8.19-8.22 (m, 1H, **H^4**), 7.92 (d, $^3J_{H,H}$ = 7.9 Hz, 1H, **H^3**), 7.47-7.50 (m, 1H, **H^5**), 7.24 (s, 1H, **H$^{4'}$**), 6.87 (s, 1H, **H$^{6'}$**), 2.44 (s, 3H, *o*-C**H**$_3$), 2.40 ppm (s, 3H, *p*-C**H**$_3$).

^{13}C NMR (151 MHz, CD_2Cl_2): δ 165.9 (**C^2**), 161.2 (q, $^2J_{C,F}$ = 37.9 Hz, O**C**OCF$_3$), 160.7 (q, $^2J_{C,F}$ = 39.4 Hz, O**C**OCF$_3$), 147.7 (**C^6**), 144.5 (**C^4**), 142.4 (**C$^{1'}$**), 141.9 (**C$^{2'}$**), 140.7 (**C$^{3'}$**), 140.4 (**C$^{5'}$**), 137.4 (**C$^{6'}$**), 124.9 (**C$^{4'}$**), 124.8 (**C^5**), 122.1 (**C^3**), 118.3 (q, $^1J_{C,F}$ = 289.6 Hz, **C**F$_3$), 115.8 (q, $^1J_{C,F}$ = 288.7 Hz, **C**F$_3$), 21.0 (*o*-**C**H$_3$), 20.7 ppm (*p*-**C**H$_3$).

^{19}F NMR (188 MHz, CD_2Cl_2): δ −76.0 (3F, OCOC**F$_3$**), −77.3 ppm (3F, OCOC**F$_3$**).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −167.1 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 437.092 (37) $[M-2OCOCF_3+MeCN+OH]^+$, 492.048 (36) $[M-OCOCF_3]^+$.

HRMS (ESI): Found 492.0480; calcd for $C_{15}H_{12}AuF_3NO_2$ $[M-OCOCF_3]^+$: 492.0480.

Elemental Analysis: Anal. calcd. For $C_{17}H_{12}AuF_6NO_4$: C, 33.74; H, 2.00; N. 2.31. Found: C, 33.71; H, 2.05; N, 2.29.

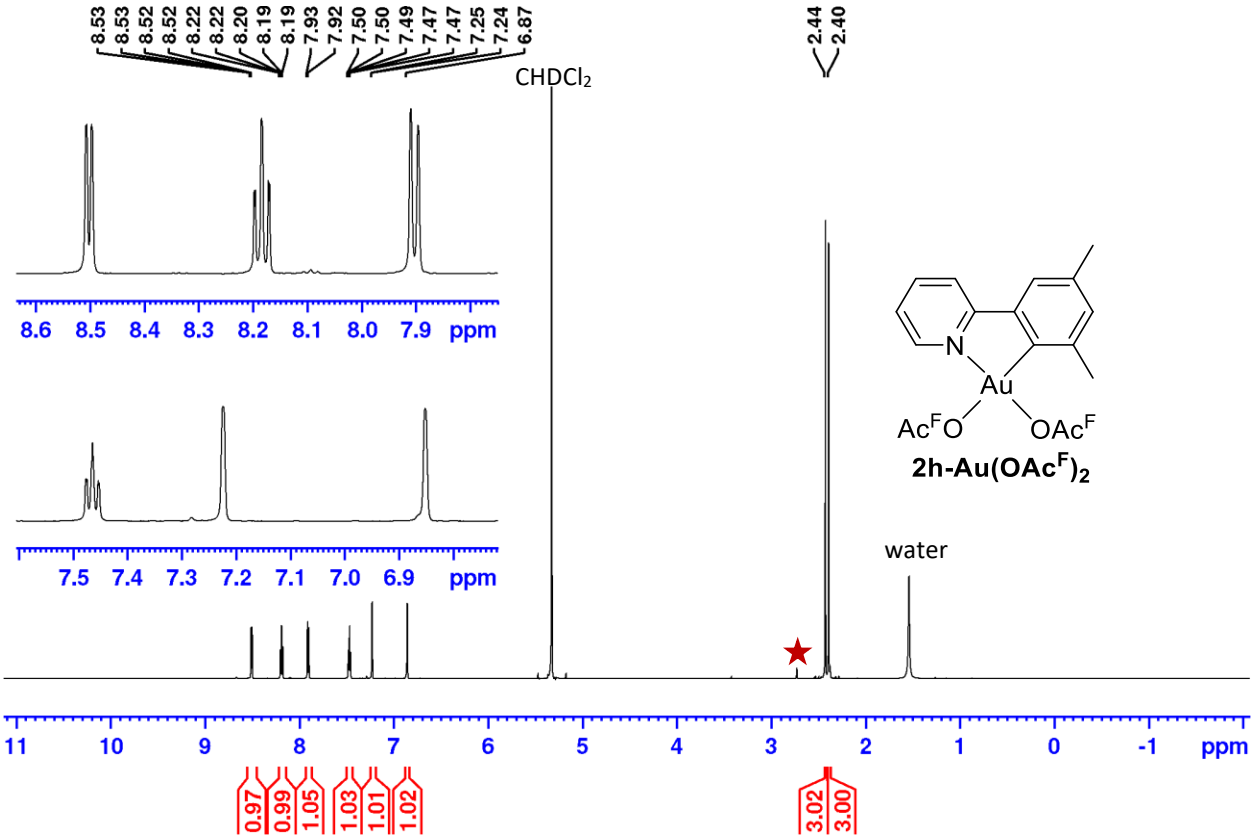


Figure S79. ^{1}H NMR (600 MHz, CD_2Cl_2) of **2h-Au(OAc^{F})$_2$**. The resonance indicated by a red star origins from an unidentified impurity.

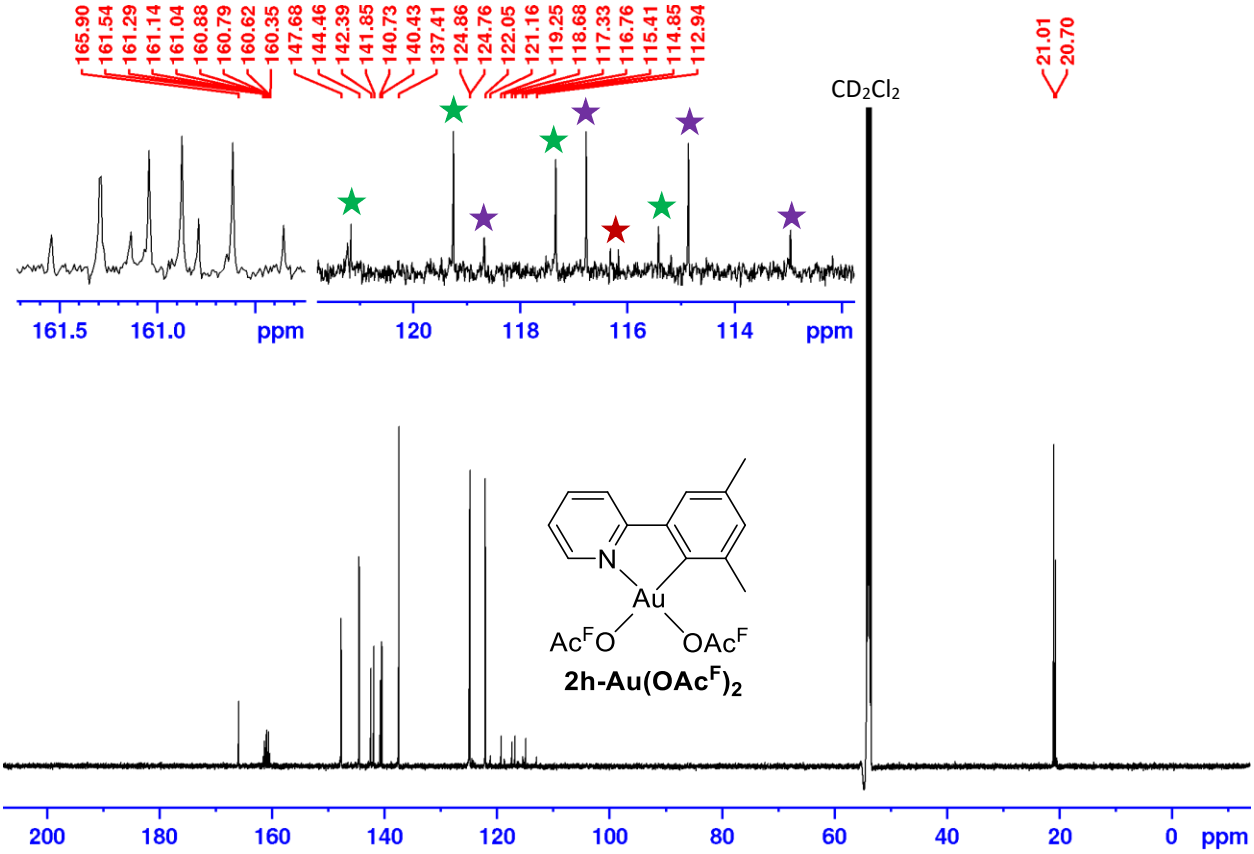


Figure S80. ^{13}C NMR (151 MHz, CD_2Cl_2) of **2h-Au(OAc^F)$_2$**. The quartets corresponding to the two **C**F_3 carbons of the trifluoroacetate ligands are indicated by purple and green stars in the insert to the right. The resonances indicated by a red star origin from an unidentified impurity.

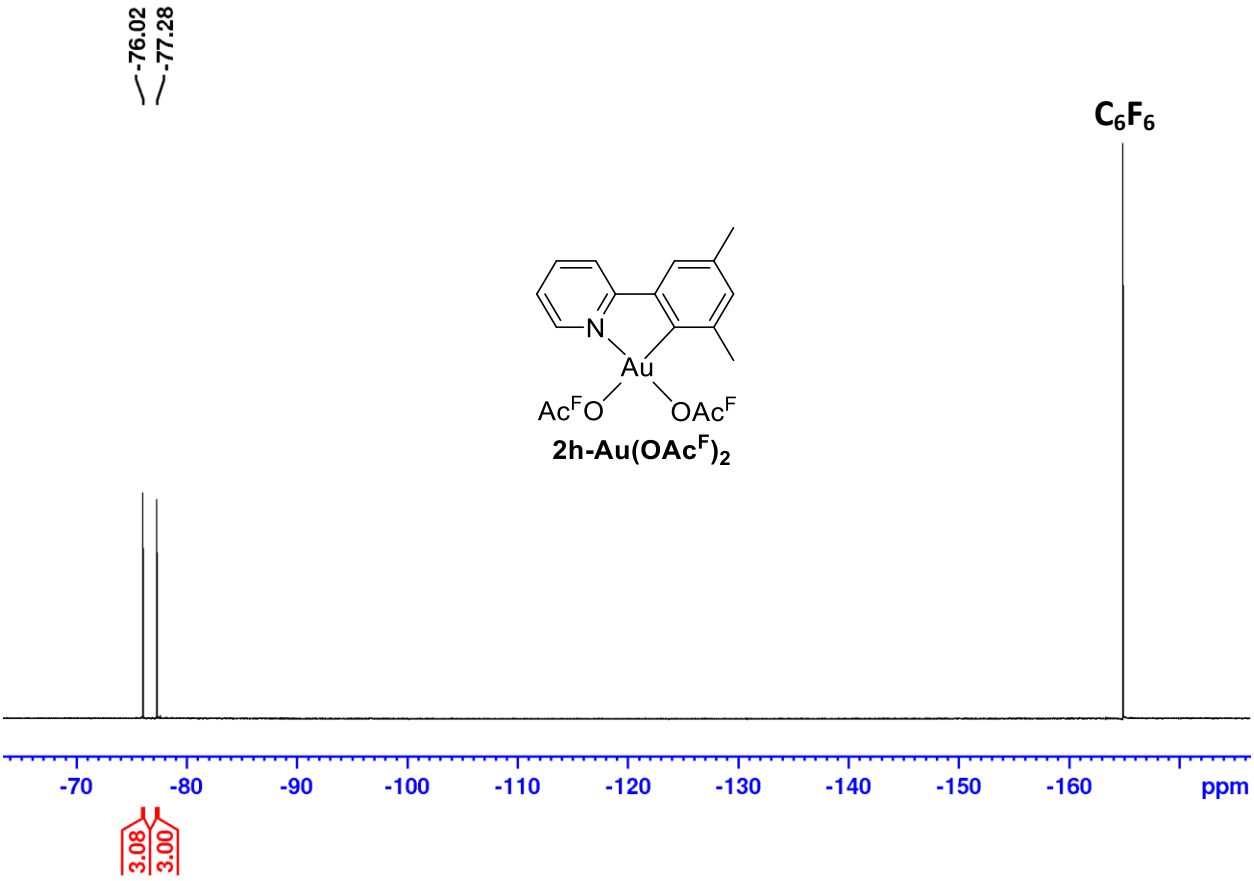


Figure S81. ^{19}F NMR (188 MHz, CD_2Cl_2) of **2h-Au(OAc^F)$_2$**.

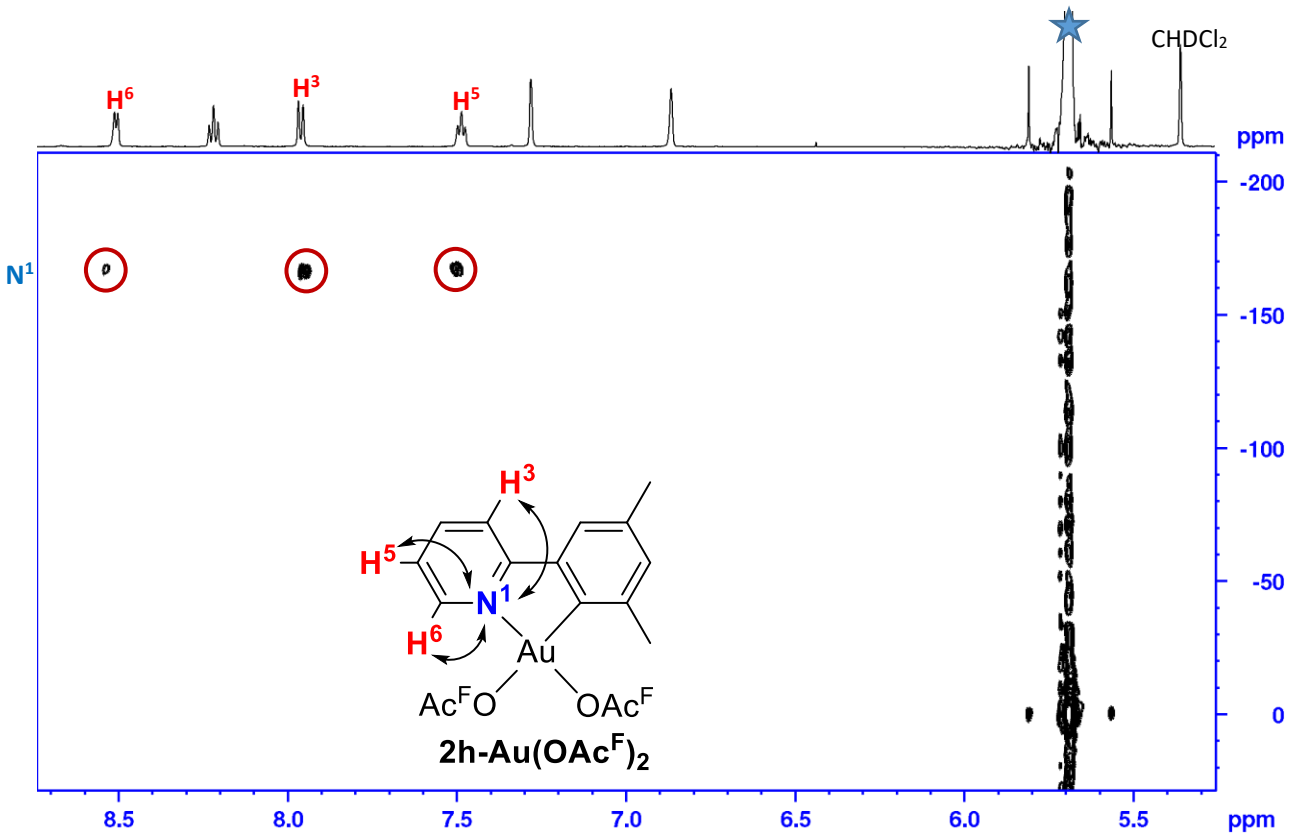


Figure S82. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **2h-Au(OAc^{F})$_2$**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).

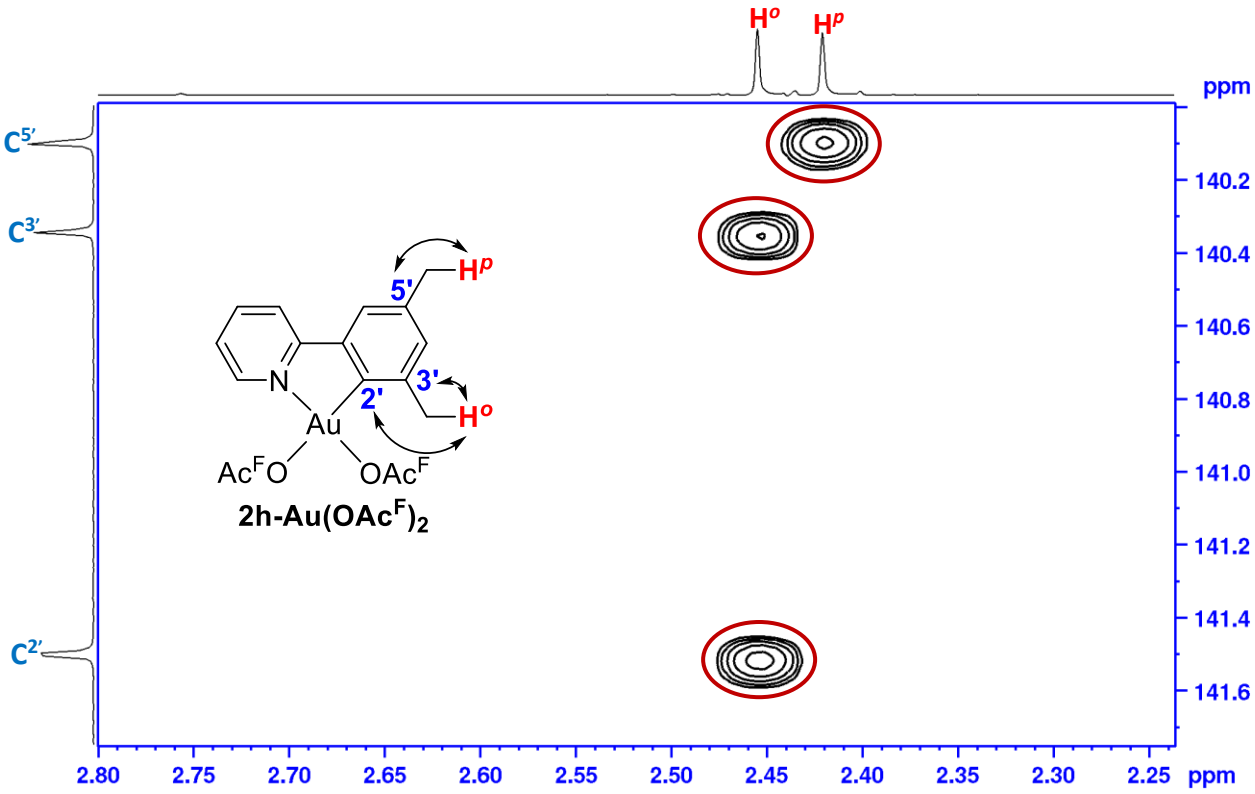
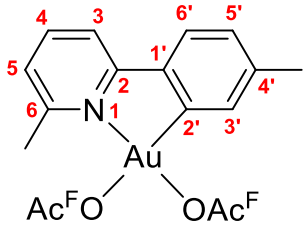


Figure S83. SHMBC (800 MHz, CD_2Cl_2) of **2h-Au(OAc^F)$_2$**.



2i-Au(OAc^F)$_2$

2i-Au(OAc^F)$_2$. A microwave vessel was charged with $Au(OAc)_3$ (0.0750 g, 0.200 mmol, 1.00 equiv.) and **1i** (0.0370 g, 0.202 mmol, 1.01 equiv.) in a 1:1 mixture of $HOAc^F$ and water (6 mL). The reaction mixture was heated at 120 °C for 45 min in a microwave. After cooling to room temperature, $HOAc^F$ (1 mL) was added, and the resulting solution was filtered. Water (8 mL) was added to the filtrate, resulting in the precipitation of a fine solid. After cooling on an ice-water bath for 15 min, and then overnight at 4-8 °C, the precipitate was filtered off, washed with water (3x5 mL) and Et_2O (5 mL), and dried under a stream of air for ca. 3 h, furnishing **2i-Au(OAc^F)$_2$** as a pale yellow solid.

Yield: 0.0630 g, 0.104 mmol, 52 %.

^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.00 (dd, $^3J_{H,H}$ = 7.9 Hz, $^3J_{H,H}$ = 7.9 Hz, 1H), 7.70 (d, $^3J_{H,H}$ = 7.4 Hz, 1H), 7.35 (d, $^3J_{H,H}$ = 7.9 Hz, 1H), 7.26-7.27 (m, 2H), 6.82 (s, 1H), 2.82 (s, 3H), 2.41 ppm (s, 3H).

^{13}C NMR (151 MHz, CD_2Cl_2): δ 165.1, 163.0, 160.4 (q, $^2J_{C,F}$ = 39.5 Hz, O**C**OCF$_3$), 143.8, 143.7, 142.9, 139.5, 131.6, 128.7, 126.9, 125.9, 119.1, 116.1 (q, $^1J_{C,F}$ = 288.0 Hz, OCO**C**F$_3$), 58.0 (O**C**H$_3$), 22.3 ppm (Ar-**C**H$_3$).

Two of the expected resonances, corresponding to the two carbons in one of the trifluoroacetate ligands, could not be observed.

^{19}F NMR (376 MHz, CD_2Cl_2): δ –76.3 (s, 3F, OCOC**F**$_3$), 77.5 ppm (s, 3F, OCOC**F**$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −161.7 ppm (**N^1**).

MS (APPI): *m/z* (rel. %): 492.048 (100) $[M–OCOCF_3]^+$.

HRMS (APPI): Found: 492.0480; calcd for $C_{15}H_{12}AuF_3NO_2$ $[M–OCOCF_3]^+$: 492.0484.

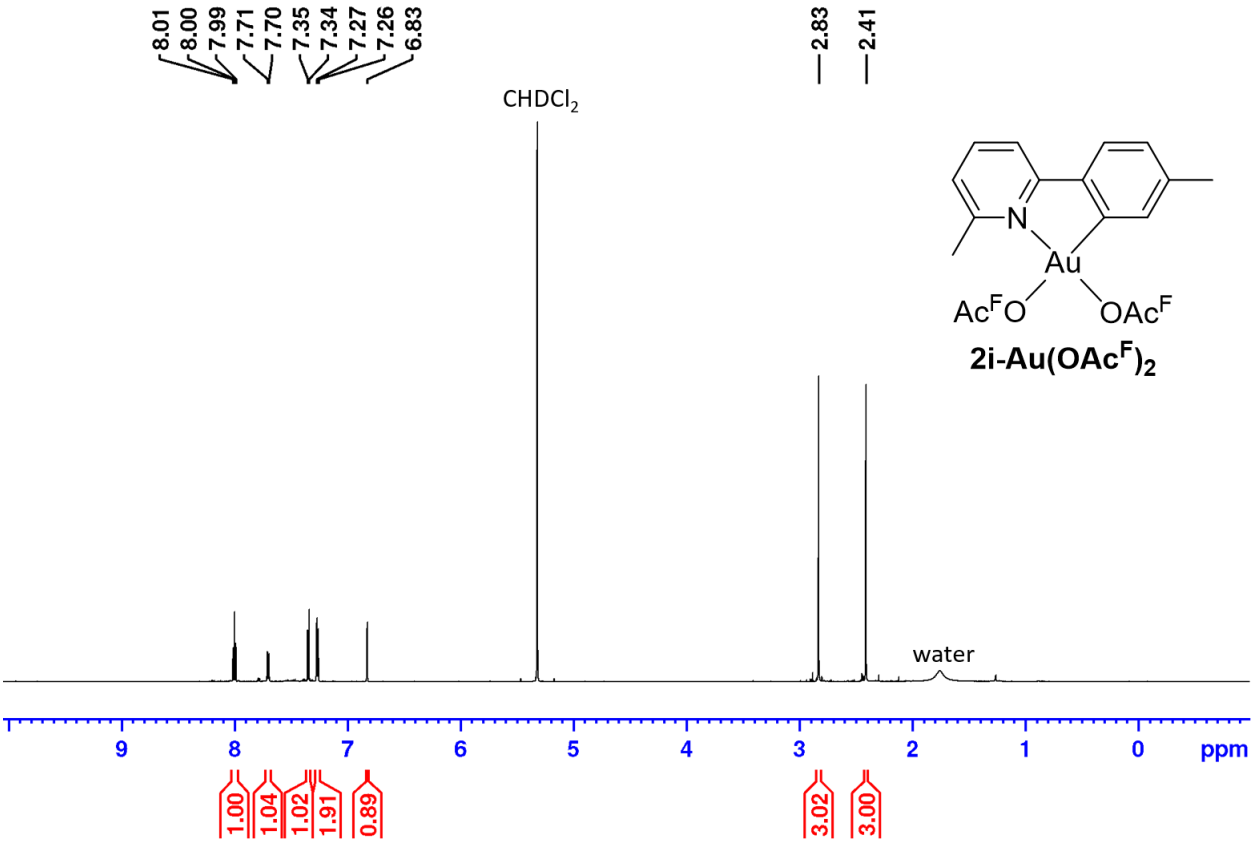


Figure S84. ^{1}H NMR (600 MHz, CD_2Cl_2) of **2i-Au(OAc^{F})$_2$**.

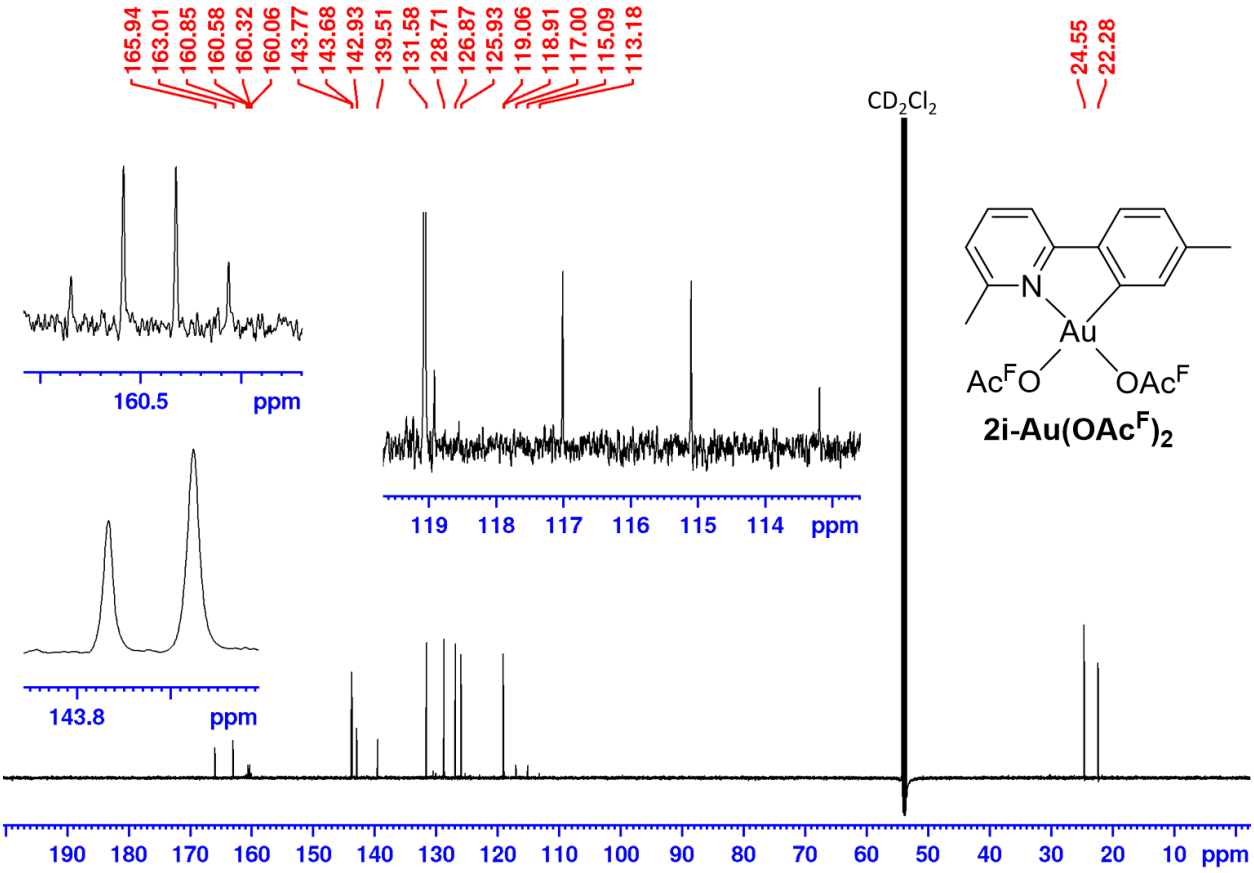


Figure S85. ^{13}C NMR (151 MHz, CD_2Cl_2) of **2i-Au(OAc^F)$_2$**. Two of the expected resonances were not observed.

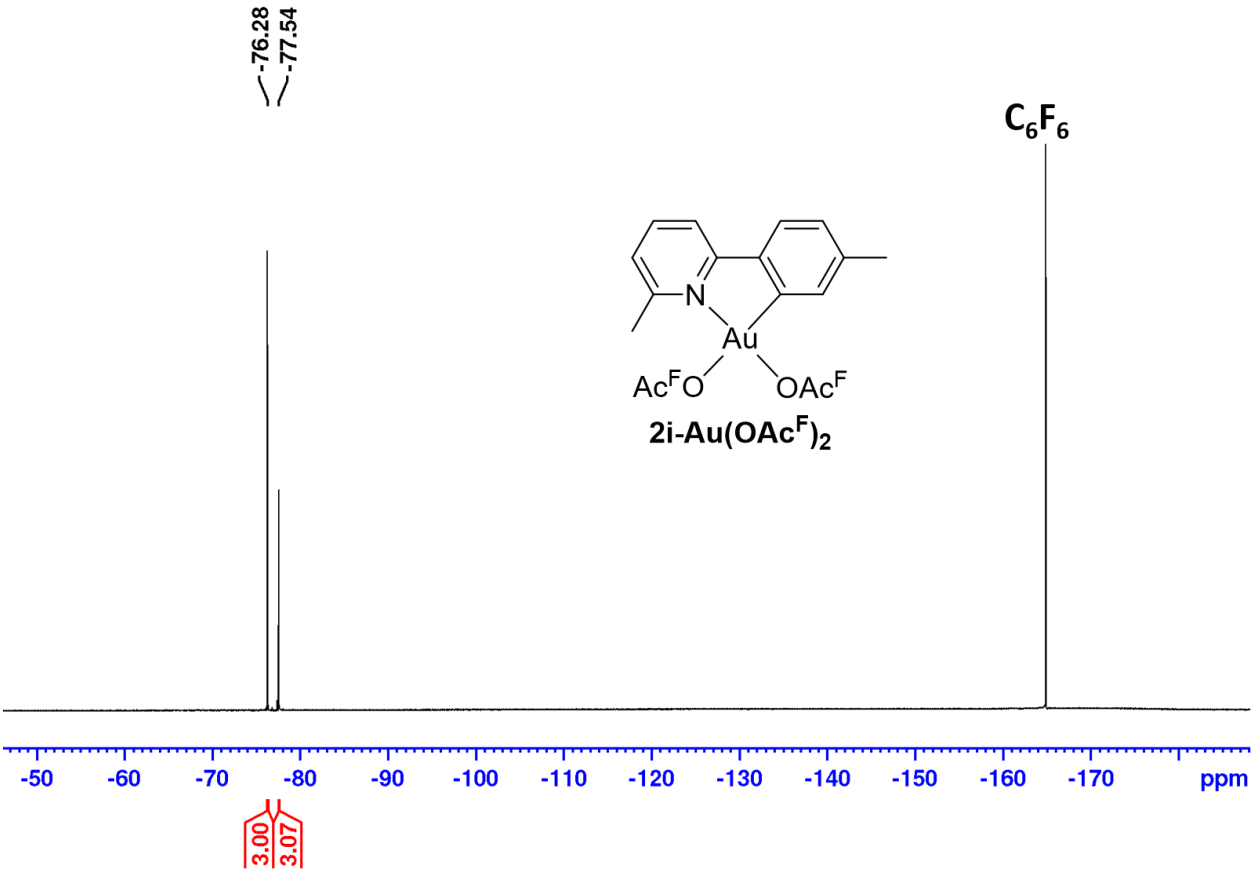


Figure S86. ^{19}F NMR (376 MHz, CD_2Cl_2) of **2i-Au(OAc^F)$_2$**.

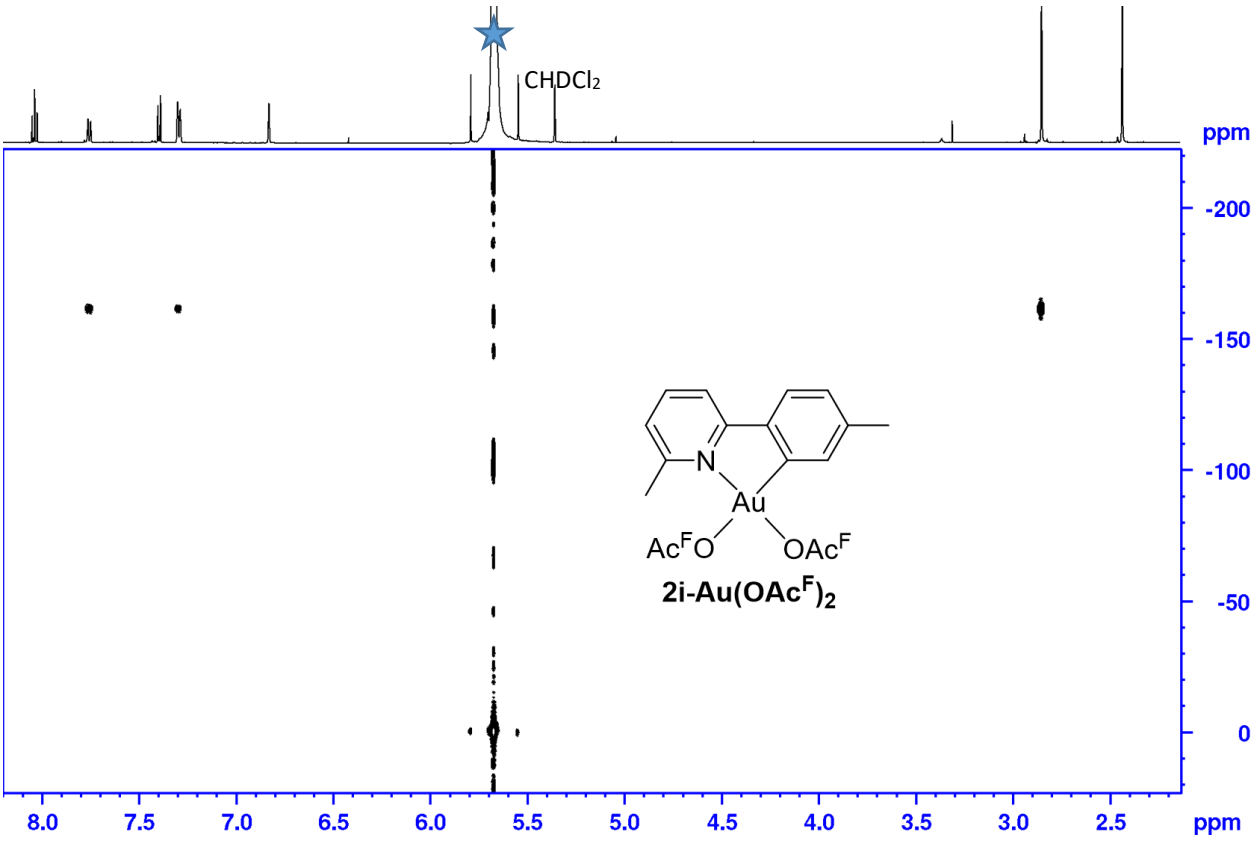
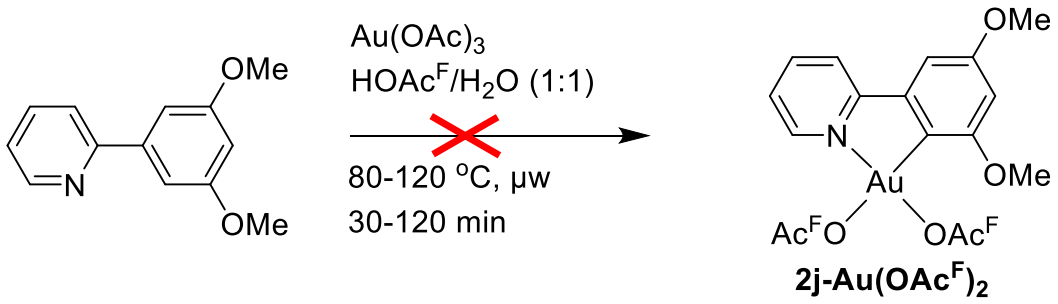
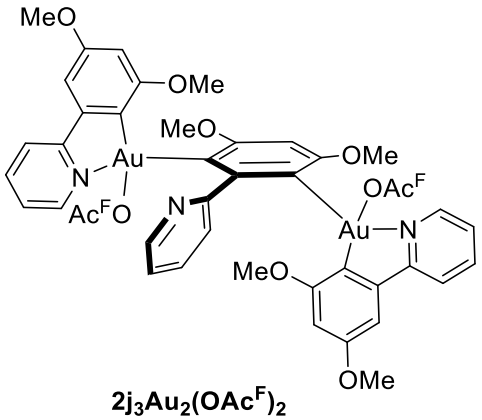


Figure S87. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **2i-Au(OAc^{F})$_2$**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



2j-Au(OAc^F)$_2$

Attempted synthesis of 2j-Au(OAc^F)$_2$. Several attempts of synthesizing **2j-Au(OAc^F)$_2$** were made using different reaction times and temperatures. A cyclometalated complex could not be isolated, and a representative ^{1}H NMR spectrum of a crude product is given below (Figure S89). However, we were able to obtain crystals suitable for single-crystal X-ray diffraction analysis. The analysis showed an unusual dinuclear M_2L_3-type complex (**2j$_3$Au$_2$(OAc^F)$_2$**, Figure S88), but we have no reason to believe that this is the main reaction product, as no other characterization gave any meaningful insights. See Figure S146 and Figure S147 for the ORTEP and Table S7 for crystal and refinement data for **2j$_3$Au$_2$(OAc^F)$_2$**.



2j$_3$Au$_2$(OAc^F)$_2$

Figure S88. M_2L_3-type complex (**2j$_3$Au$_2$(OAc^F)$_2$** characterized by single-crystal X-ray diffraction analysis.

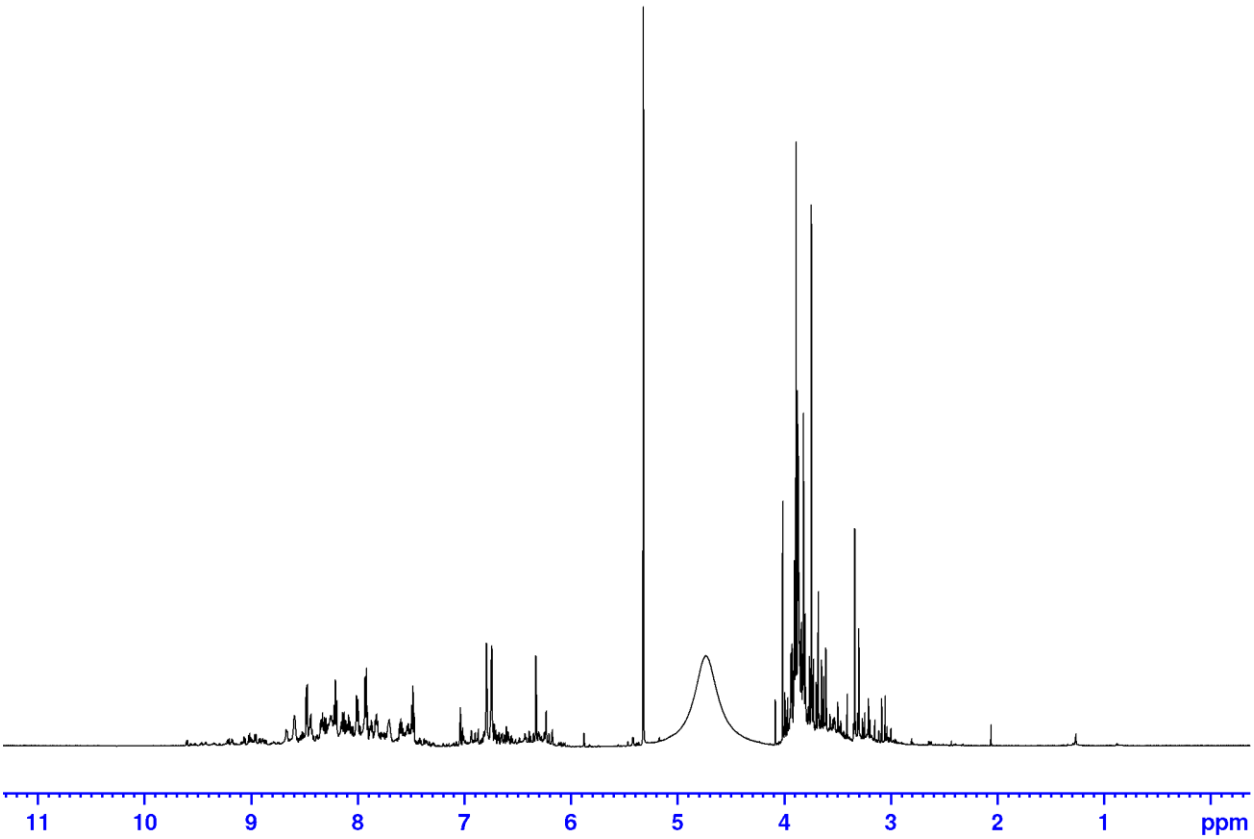
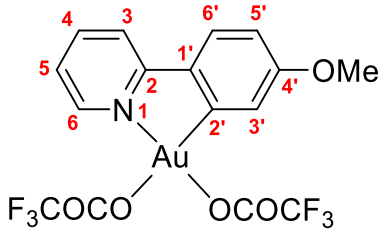


Figure S89. ^{1}H NMR (600 MHz, CD_2Cl_2) of a crude product from the attempted synthesis of **2j-Au(OAc^{F})$_2$**.



2k-Au(OAc^F)$_2$

2k-Au(OAc^F)$_2$. A microwave vessel was charged with $Au(OAc)_3$ (0.0750 g, 0.200 mmol, 1.00 equiv.) and **1k** (0.0370 g, 0.202 mmol, 1.01 equiv.) in a 1:1 mixture of $HOAc^F$ and water (6 mL). The reaction mixture was heated at 100 °C for 30 min in a microwave. After cooling to room temperature, $HOAc^F$ (1 mL) was added, and the resulting solution was filtered. Water (8 mL) was added to the filtrate, resulting in the precipitation of a fine solid. After cooling on an ice-water bath for 15 min, and then overnight at 4-8 °C, the precipitate was filtered off, washed with water (3x5 mL) and Et_2O (5 mL), and dried under a stream of air for ca. 3 h, furnishing **2k-Au(OAc^F)$_2$** as a pale yellow solid.

Yield: 0.0480 g, 0.0790 mmol, 40 %.

^{1}H NMR (800 MHz, CD_2Cl_2): δ 8.46 (dd, $^3J_{H,H}$ = 6.1 Hz, $^4J_{H,H}$ = 1.0 Hz, 1H, **H^6**), 8.15 (ddd, $^3J_{H,H}$ = 8.2 Hz, $^3J_{H,H}$ = 7.5 Hz, $^4J_{H,H}$ = 1.4 Hz, 1H, **H^4**), 7.78 (dd, $^3J_{H,H}$ = 8.2 Hz, $^4J_{H,H}$ = 0.7 Hz, 1H, **H^3**), 7.49 (d, $^3J_{H,H}$ = 8.6 Hz, 1H, **H$^{6'}$**), 7.40-7.42 (m. 1H, **H^5**), 7.00 (dd, $^3J_{H,H}$ = 8.6 Hz, $^4J_{H,H}$ = 2.4 Hz, 1H, **H$^{5'}$**), 6.57 (d, $^4J_{H,H}$ = 2.4 Hz, 1H, **H$^{3'}$**), 3.87 ppm (s, 3H, OC**H**$_3$).

^{13}C NMR (201 MHz, CD_2Cl_2): δ 165.3 (**C^2**), 161.5 (**C$^{4'}$**), 161.3 (q, $^2J_{C,F}$ = 37.7 Hz, O**C**OCF$_3$), 160.7 (q, $^2J_{C,F}$ = 39.4 Hz, O**C**OCF$_3$), 147.6 (**C^6**), 144.5 (**C^4**), 144.0 (**C$^{2'}$**), 133.5 (**C$^{1'}$**), 127.5 (**C$^{6'}$**), 123.8 (**C^5**), 121.4 (**C^3**), 118.7 (q, $^1J_{C,F}$ = 289.9 Hz, OCO**C**F$_3$), 116.5 (**C$^{5'}$**), 116.1 (q, $^1J_{C,F}$ = 288.0 Hz, OCO**C**F$_3$), 113.5 (**C$^{3'}$**), 56.4 ppm (O**C**H$_3$).

^{19}F NMR (188 MHz, CD_2Cl_2): δ –76.2 (s, 3F, OCOC**F**$_3$), –77.1 ppm (s, 3F, OCOC**F**$_3$).

MS (ESI): *m/z* (rel. %): 412.061 (90) $[M–2OCOCF_3+OMe]^+$, 466.069 (100) $[M–2OCOCF_3+2OMe+Na]^+$, 470.019 (33) $[M–2OCOCF_3+^{35}Cl+OMe+Na]^+$, 472.016 (10) $[M–2OCOCF_3+^{37}Cl+OMe+Na]^+$, 548.036 (11) $[M–OCOCF_3+OMe+Na]^+$.

HRMS (ESI): Found: 412.0605; calcd for $C_{13}H_{13}AuNO_2$ $[M–2OCOCF_3+OMe]^+$: 412.0606.

HRMS (ESI): Found: 466.0687; calcd for $C_{14}H_{16}AuNNaO_3$ $[M–2OCOCF_3+2OMe+Na]^+$: 466.0688.

Elemental Analysis: Anal. calcd. For $C_{16}H_{10}AuF_6NO_5$: C, 31.65; H, 1.66; N, 2.31. Found: C, 31.51; H, 1.61; N, 2.24.

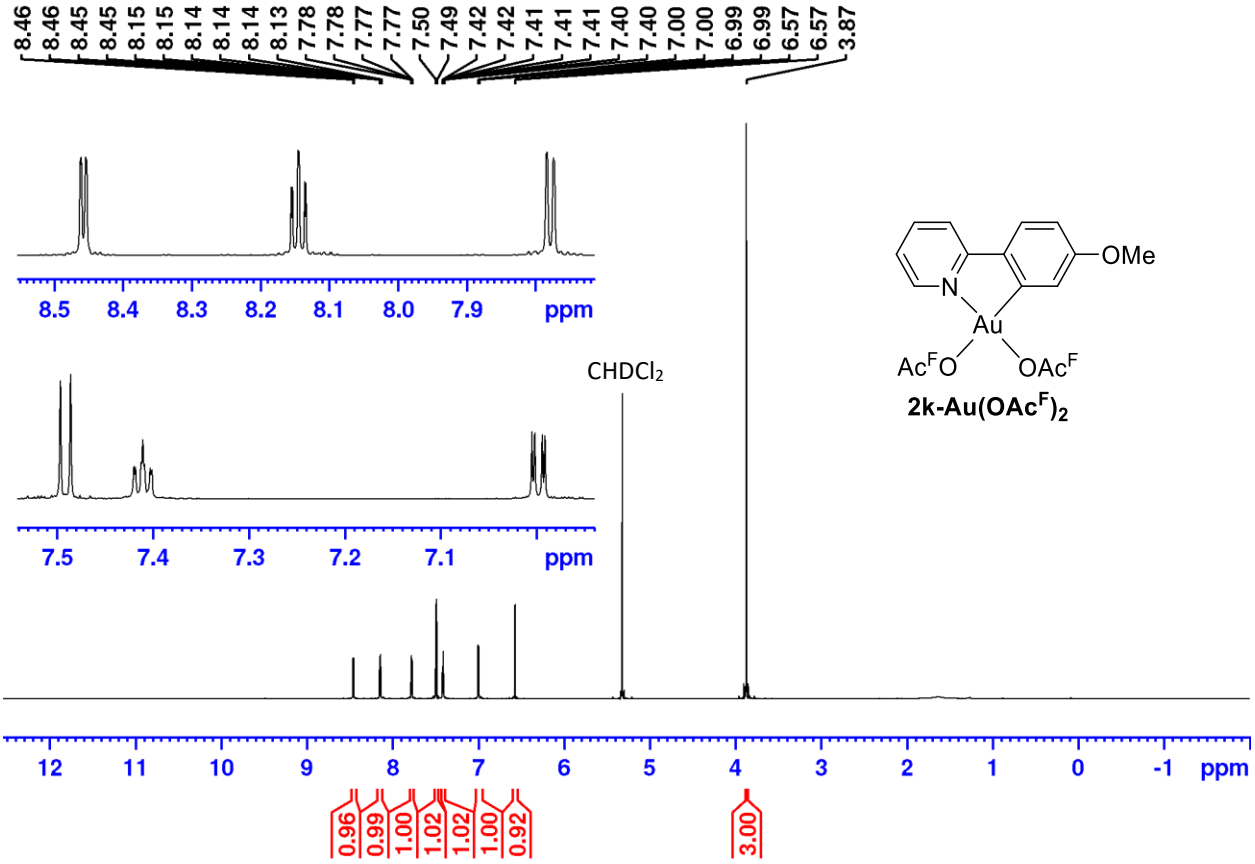


Figure S90. ^{1}H NMR (800 MHz, CD_2Cl_2) of **2k-Au(OAc^{F})$_2$**.

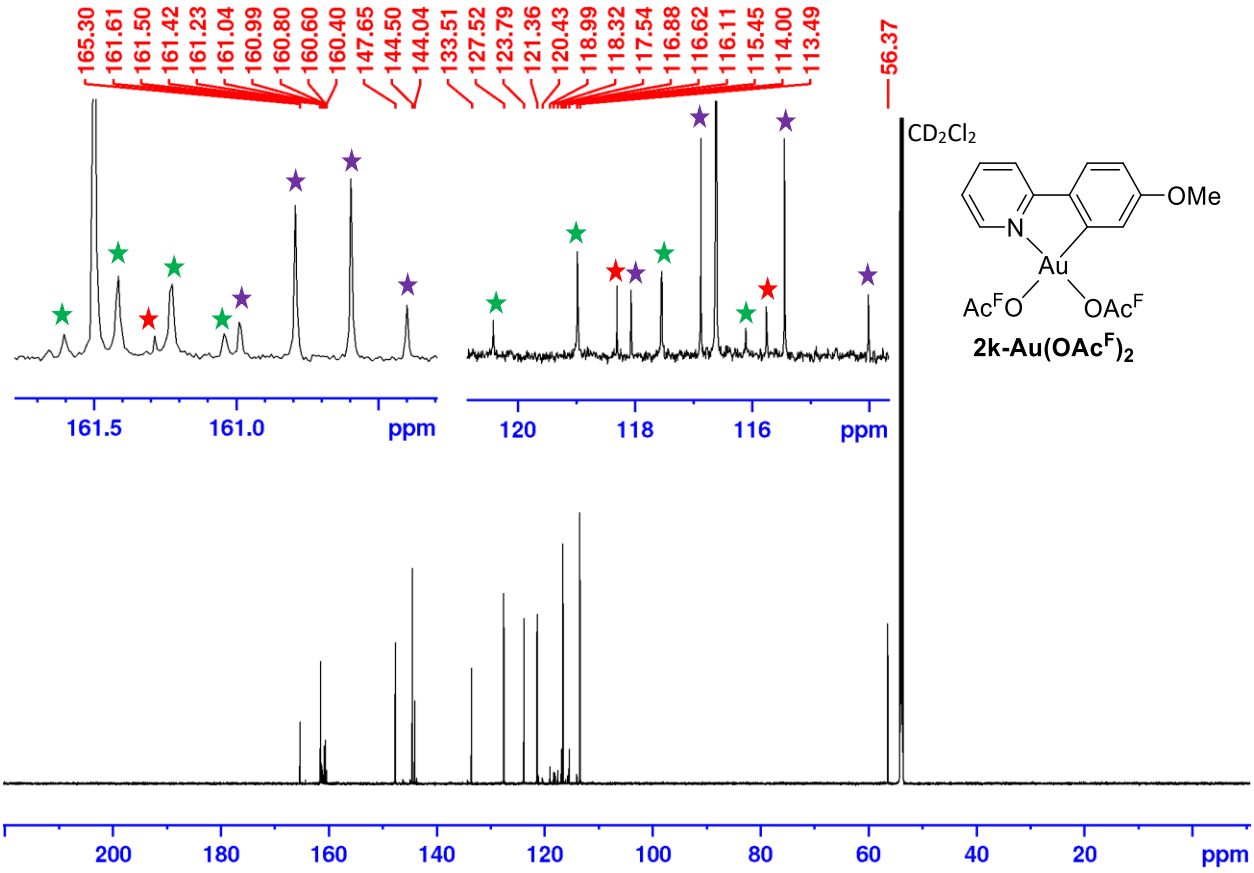


Figure S91. ^{13}C NMR (201 MHz, CD_2Cl_2) of **2k-Au(OAc^F)$_2$**. The quartets corresponding to the two **C**F_3 carbons of the trifluoroacetate ligands are indicated by purple and green stars in the insert to the right. The quartets corresponding to the two carbonyl carbons of the trifluoroacetate ligands are indicated by purple and green stars in the insert to the left. Traces of (an) unidentified impurity/impurities are indicated by red stars.

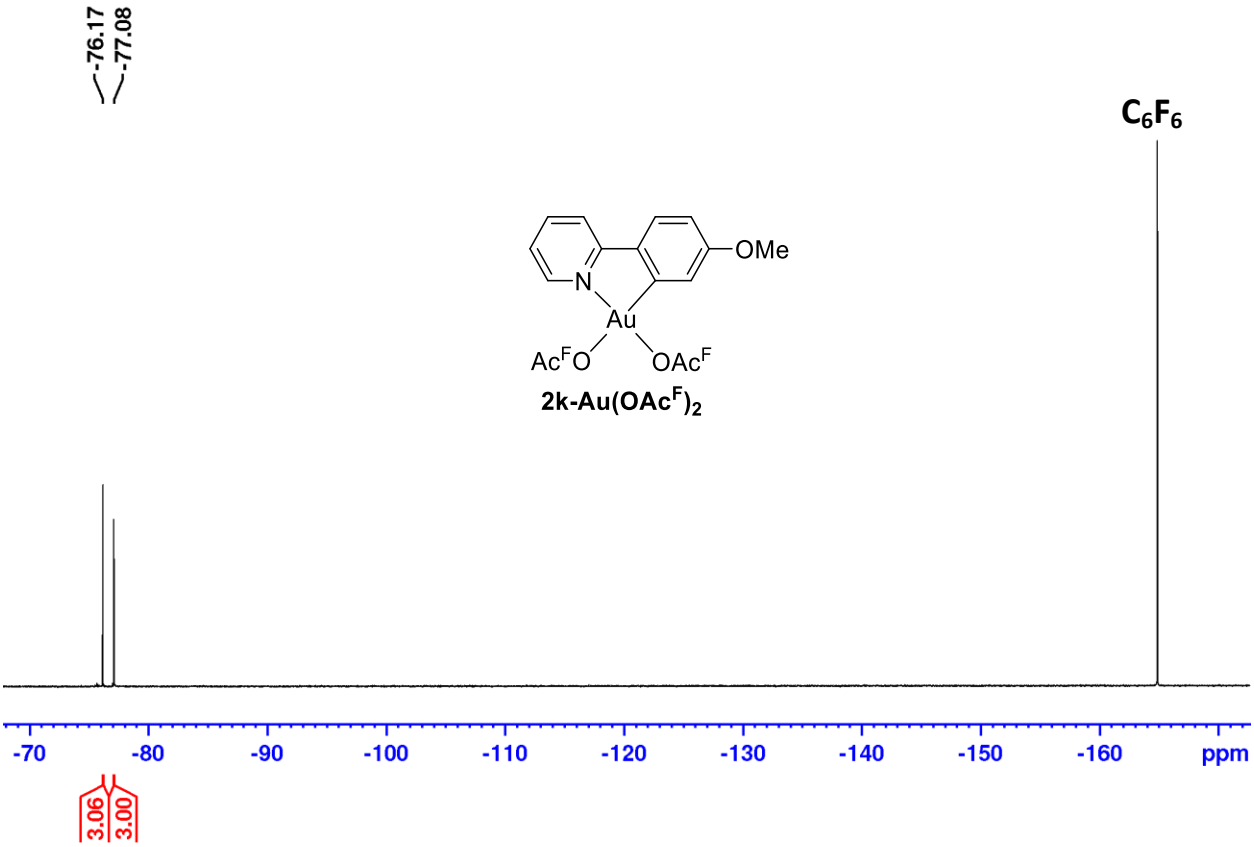
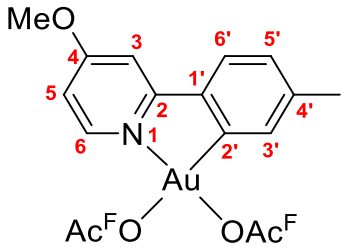


Figure S92. ^{19}F NMR (188 MHz, CD_2Cl_2) of **2k-Au(OAc^F)$_2$**.



2l-Au(OAc^F)$_2$

2l-Au(OAc^F)$_2$. A microwave vessel was charged with $Au(OAc)_3$ (0.385 g, 1.03 mmol, 1.00 equiv.) and **1l** (0.206 g, 1.03 mmol, 1.00 equiv.) in a 1:1 mixture of $HOAc^F$ and water (30 mL). The reaction mixture was heated at 120 °C for 30 min in a microwave. After cooling to room temperature, the resulting solution was filtered. Water (50 mL) was added to the filtrate, resulting in the precipitation of a solid. After cooling on an ice-water bath for 15 min, the precipitate was filtered off, washed with water (3x5 mL) and Et_2O (5 mL), and dried under a stream of air for ca. 3 h, furnishing **2l-Au(OAc^F)$_2$** as a pale yellow solid.

Yield: 0.286 g, 0.461 mmol, 45 %.

^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.20 (d, $^3J_{H,H}$ = 7.0 Hz, 1H, **H^6**), 7.42 (d, $^3J_{H,H}$ = 7.9 Hz, 1H, **H$^{6'}$**), 7.32 (d, $^4J_{H,H}$ = 2.8 Hz, 1H, **H^3**), 7.23 (d, $^3J_{H,H}$ = 7.8 Hz, 1H, **H$^{5'}$**), 6.89 (dd, $^3J_{H,H}$ = 7.1 Hz, $^4J_{H,H}$ = 2.9 Hz, 1H, **H^5**), 6.76 (s, 1H, **H$^{3'}$**), 4.08 (s, 3H, OC**H**$_3$), 2.39 ppm (s, 3H, Ar-C**H**$_3$).

^{13}C NMR (151 MHz, CD_2Cl_2): δ 171.2 (**C^4**), 165.9 (**C^2**), 161.1 (q, $^2J_{C,F}$ = 37.7 Hz, O**C**OCF$_3$), 160.6 (q, $^2J_{C,F}$ = 38.6 Hz, O**C**OCF$_3$), 148.4 (**C^6**), 144.1 (**C$^{4'}$**), 141.7 (**C$^{2'}$**), 138.5 (**C$^{1'}$**), 131.2 (**C$^{5'}$**), 128.7 (**C$^{3'}$**), 125.6 (**C$^{6'}$**), 118.1 (q, $^1J_{C,F}$ = 289.6 Hz, OCO**C**F$_3$), 116.0 (q, $^1J_{C,F}$ = 288.4 Hz, OCO**C**F$_3$), 110.4 (**C^5**), 107.0 (**C^3**), 57.6 (O**C**H$_3$), 22.2 ppm (Ar-**C**H$_3$).

^{19}F NMR (188 MHz, CD_2Cl_2): δ –76.2 (s, 3F, OCOC**F**$_3$), –77.1 ppm (s, 3F, OCOC**F**$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ –187.1 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 508.043 (73) $[M-OCOCF_3]^+$.

HRMS (ESI): Found 508.0429; calcd for $C_{15}H_{12}AuF_3NO_3$ $[M-OCOCF_3]^+$: 508.0429.

Elemental Analysis: Anal. calcd. For $C_{17}H_{12}AuF_6NO_5$: C, 32.87; H, 1.95; N. 2.25. Found: C, 32.73; H, 1.91; N, 2.18.

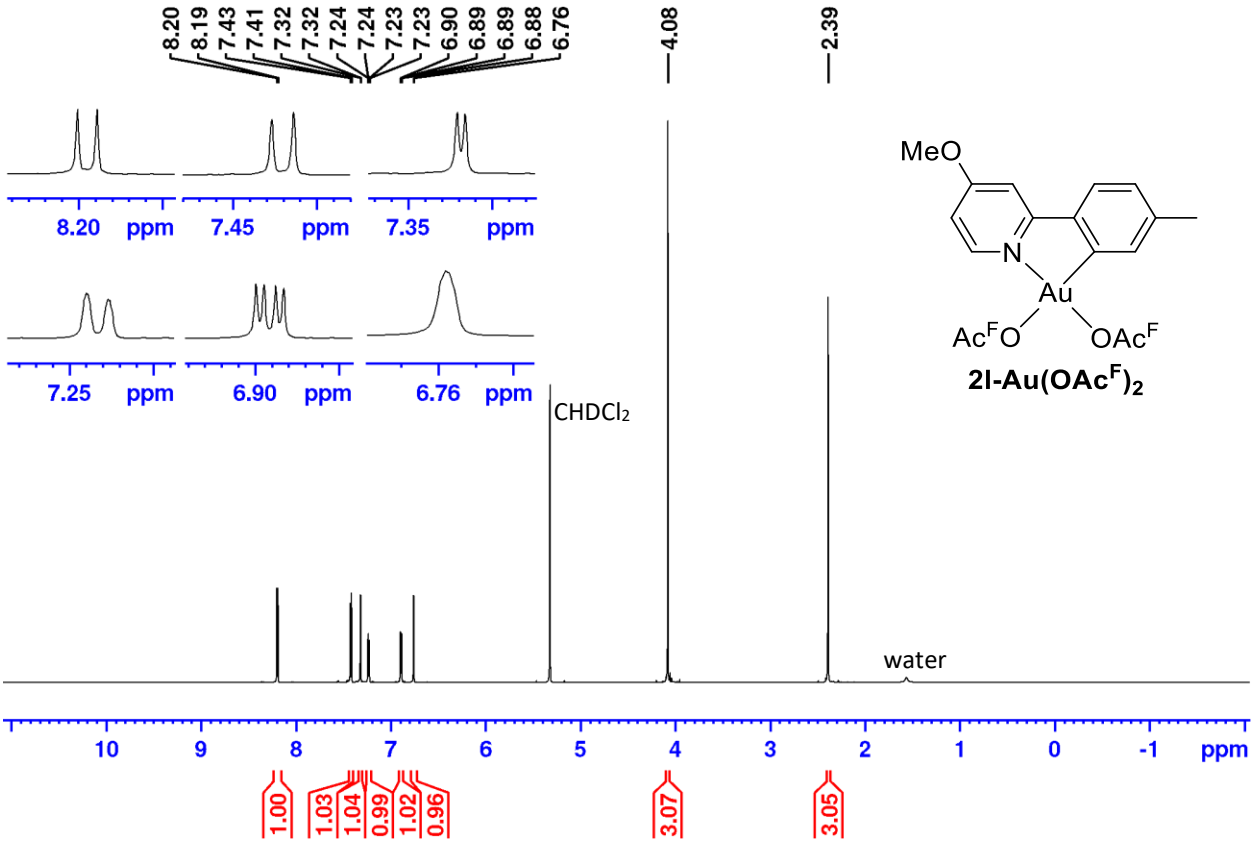


Figure S93. ^{1}H NMR (600 MHz, CD_2Cl_2) of **2l-Au(OAc^{F})$_2$**.

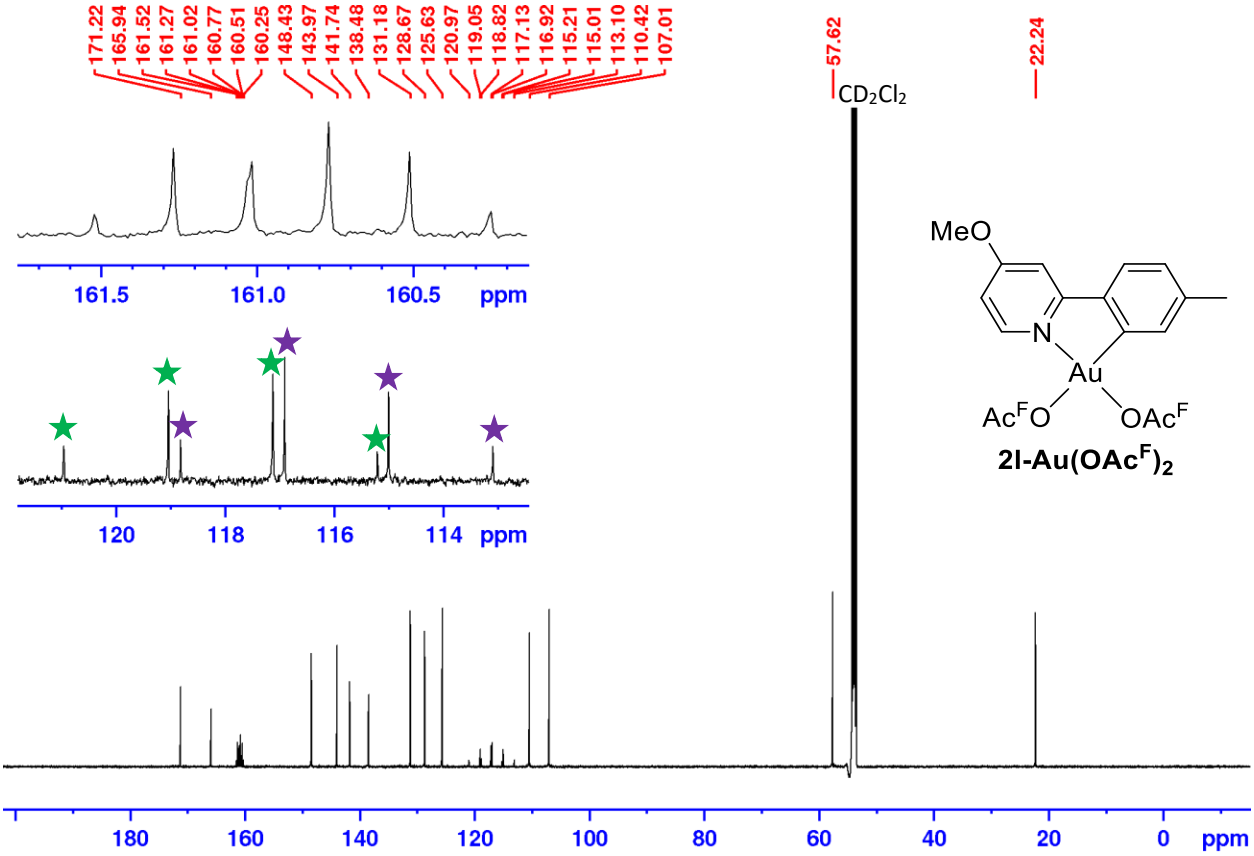


Figure S94. ^{13}C NMR (151 MHz, CD_2Cl_2) of **2l-Au(OAc^F)$_2$**. The quartets corresponding to the two **C**F_3 carbons of the trifluoroacetate ligands are indicated by purple and green stars in the lower insert. The quartets corresponding to the two carbonyl carbons of the trifluoroacetate ligands were found to be partially overlapping (see upper insert).

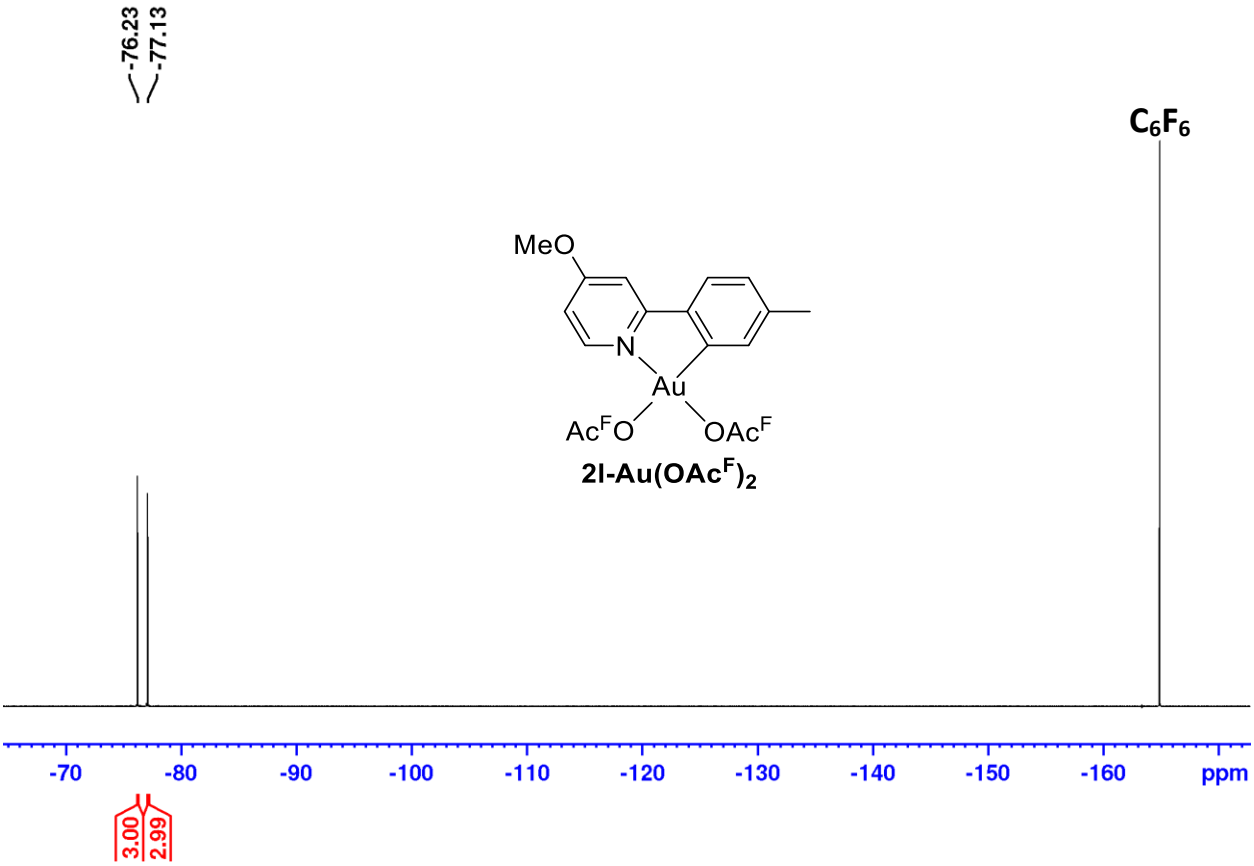


Figure S95. ^{19}F NMR (188 MHz, CD_2Cl_2) of **2l-Au(OAc^F)$_2$**.

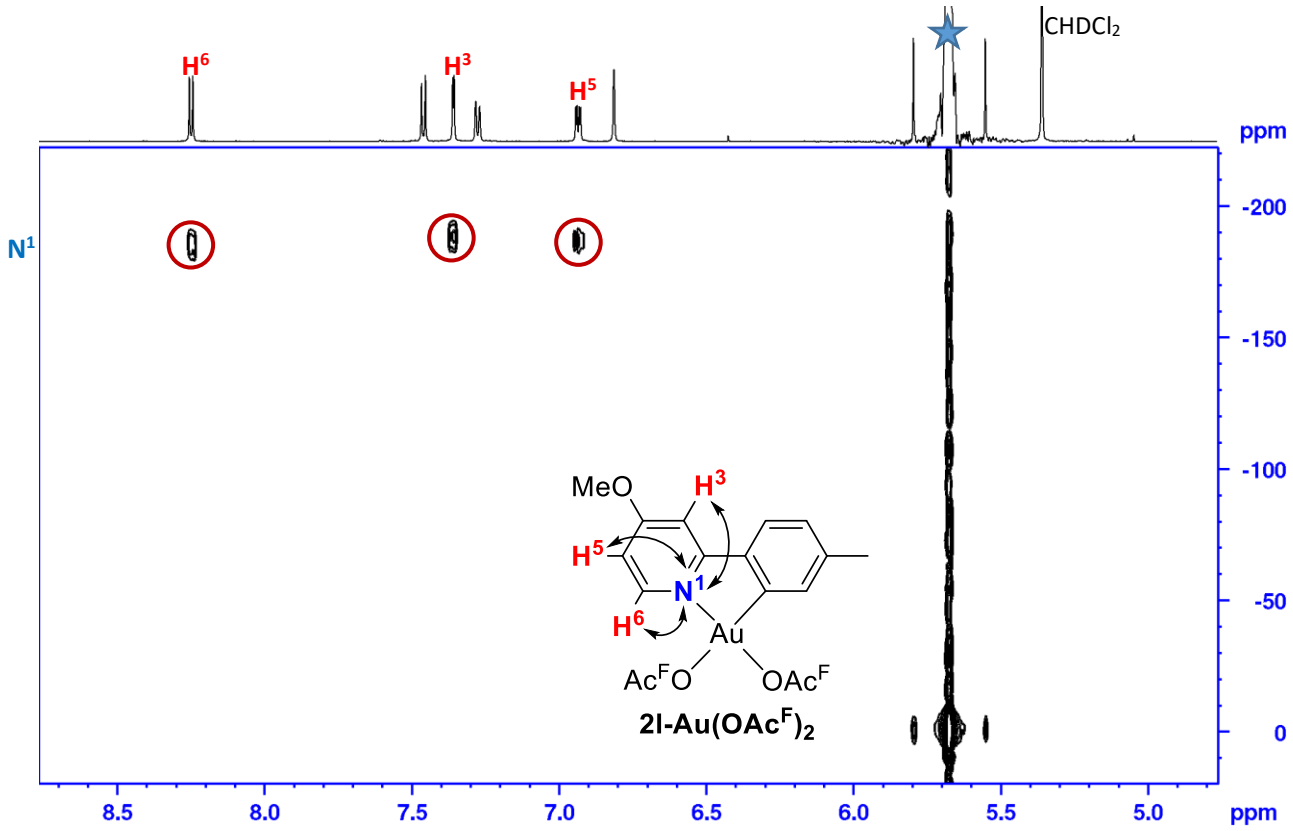
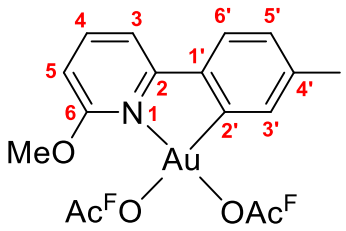


Figure S96. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **2l-Au(OAc^F)$_2$**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



2m-Au(OAc^F)$_2$

2m-Au(OAc^F)$_2$. A microwave vessel was charged with $Au(OAc)_3$ (0.0750 g, 0.200 mmol, 1.00 equiv.) and **1m** (0.0400 g, 0.202 mmol, 1.01 equiv.) in a 1:1 mixture of $HOAc^F$ and water (6 mL). The reaction mixture was heated at 100 °C for 60 min in a microwave. After cooling to room temperature, $HOAc^F$ (1 mL) was added, and the resulting solution was filtered. Water (8 mL) was added to the filtrate, resulting in the precipitation of a solid. After cooling on an ice-water bath for 10 min, the precipitate was filtered off, washed with water (3x5 mL) and Et_2O (5 mL), and dried under a stream of air for ca. 3 h, furnishing **2m-Au(OAc^F)$_2$** as a pale yellow solid.

Yield: 0.0660 g, 0.106 mmol, 53 %.

^{1}H NMR (800 MHz, CD_2Cl_2): δ 8.09 (dd, $^3J_{H,H}$ = 8.2 Hz, $^3J_{H,H}$ = 7.8 Hz, 1H, **H^4**), 7.42 (dd, $^3J_{H,H}$ = 7.7 Hz, $^4J_{H,H}$ = 0.9 Hz, 1H, **H^3**), 7.35 (d, $^3J_{H,H}$ = 7.9 Hz, 1H, **H$^{6'}$**), 7.23-7.25 (m, 1H, **H$^{5'}$**), 6.82 (d, $^4J_{H,H}$ = 0.6 Hz, 1H, **H$^{3'}$**), 6.81 (dd, $^3J_{H,H}$ = 8.5 Hz, $^4J_{H,H}$ = 0.8 Hz, 1H, **H^5**), 4.01 (s, 3H, OC**H**$_3$), 2.40 ppm (s, 3H, Ar-C**H**$_3$).

^{13}C NMR (201 MHz, CD_2Cl_2): δ 165.1 (**C^6**), 163.7 (**C^2**), 161.1 (q, $^2J_{C,F}$ = 36.6 Hz, O**C**OCF$_3$), 160.4 (q, $^2J_{C,F}$ = 39.6 Hz, O**C**OCF$_3$), 146.6 (**C^4**), 143.8 (**C$^{4'}$**), 141.7 (**C$^{2'}$**), 139.5 (**C$^{1'}$**), 131.3 (**C$^{5'}$**), 128.7 (**C$^{3'}$**), 125.9 (**C$^{6'}$**), 118.7 (q, $^1J_{C,F}$ = 289.6 Hz, OCO**C**F$_3$), 116.1 (q, $^1J_{C,F}$ = 288.1 Hz, OCO**C**F$_3$), 113.3 (**C^3**), 106.9 (**C^5**), 58.0 (O**C**H$_3$), 22.3 ppm (Ar-**C**H$_3$).

^{19}F NMR (376 MHz, CD_2Cl_2): δ –76.2 (s, 3F, OCOC**F**$_3$), –76.5 ppm (broadened s, 3F, OCOC**F**$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −187.7 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 426.076 (100) $[M–2OCOCF_3+OMe]^+$.

HRMS (ESI): Found: 426.0761; calcd for $C_{14}H_{15}AuNO_2$ $[M–2OCOCF_3+OMe]^+$: 426.0763.

Elemental Analysis: Anal. calcd. For $C_{17}H_{12}AuF_6NO_5$: C, 32.87; H, 1.95; N. 2.25. Found: C, 32.84; H, 1.97; N, 2.26.

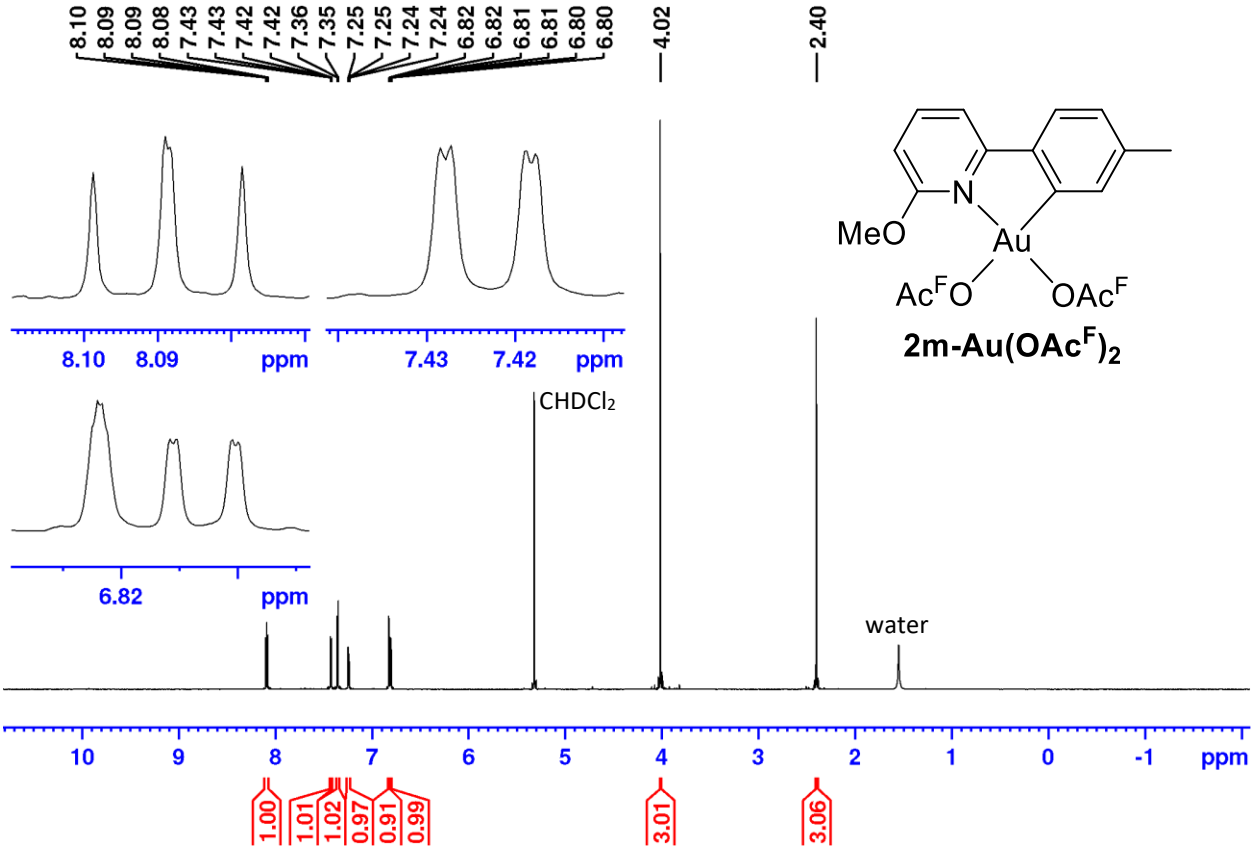


Figure S97. ^{1}H NMR (800 MHz, CD_2Cl_2) of **2m-Au(OAc^{F})$_2$**.

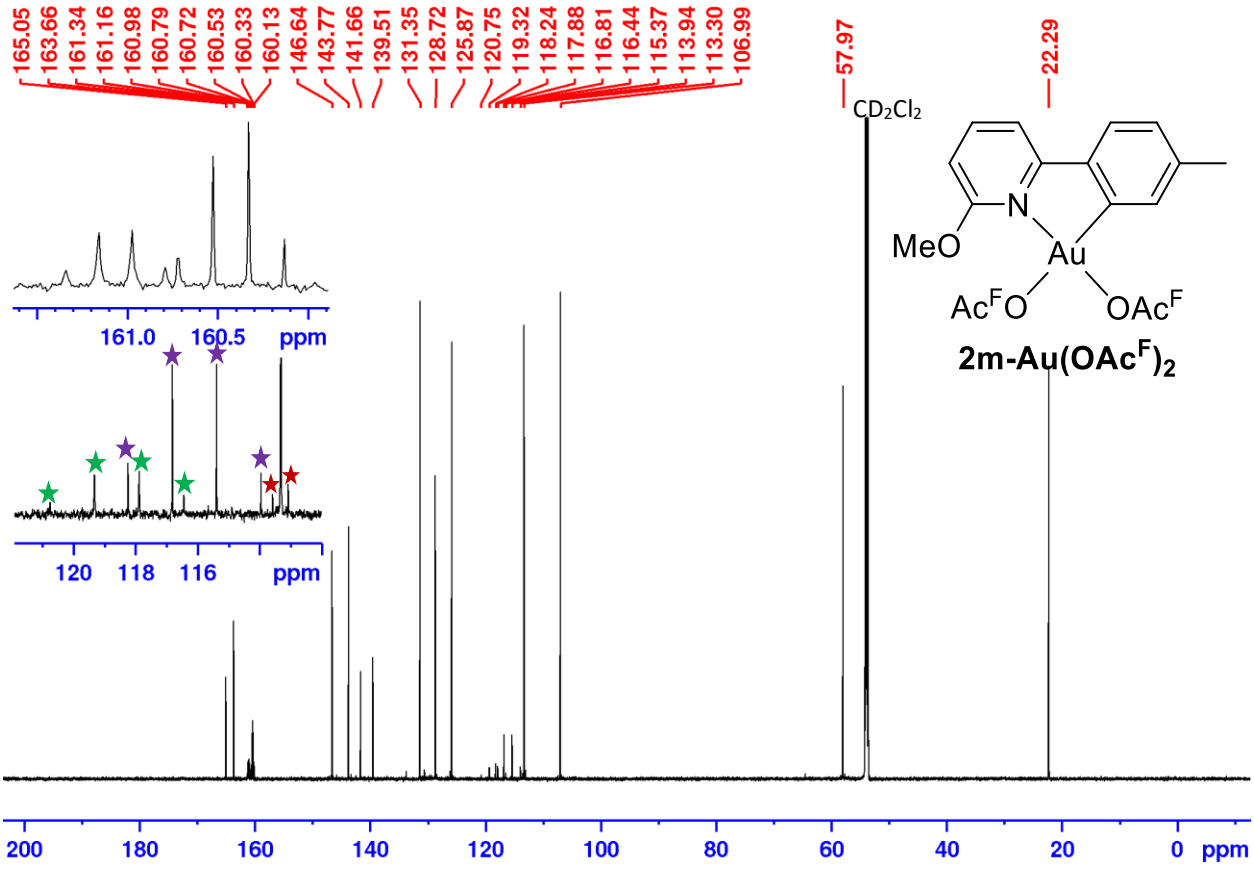


Figure S98. ^{13}C NMR (201 MHz, CD_2Cl_2) of **2m-Au(OAc^F)$_2$**. The quartets corresponding to the two **C**F_3 carbons of the trifluoroacetate ligands are indicated by purple and green stars in the bottom insert. Traces of (an) unidentified impurity/impurities are indicated by red stars.

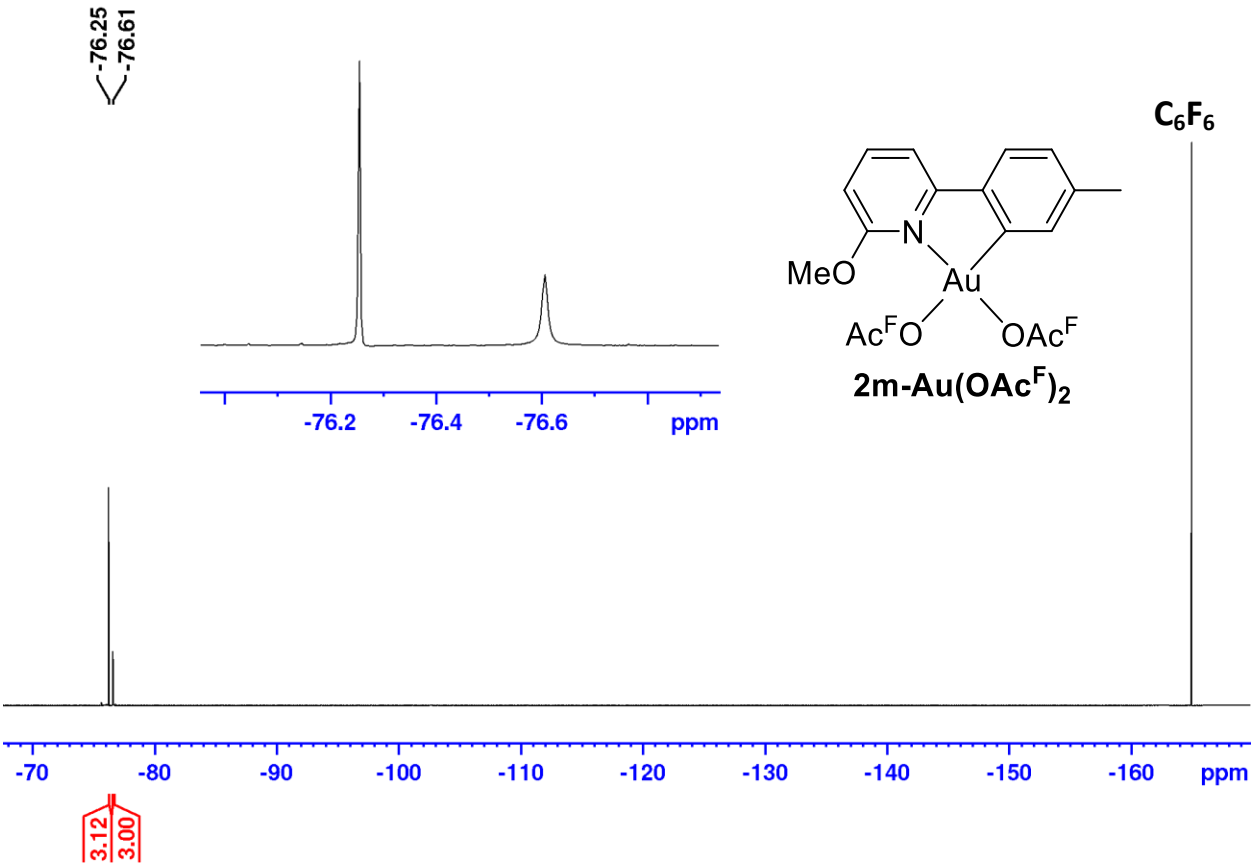


Figure S99. ^{19}F NMR (376 MHz, CD_2Cl_2) of **2m-Au(OAc^F)$_2$**.

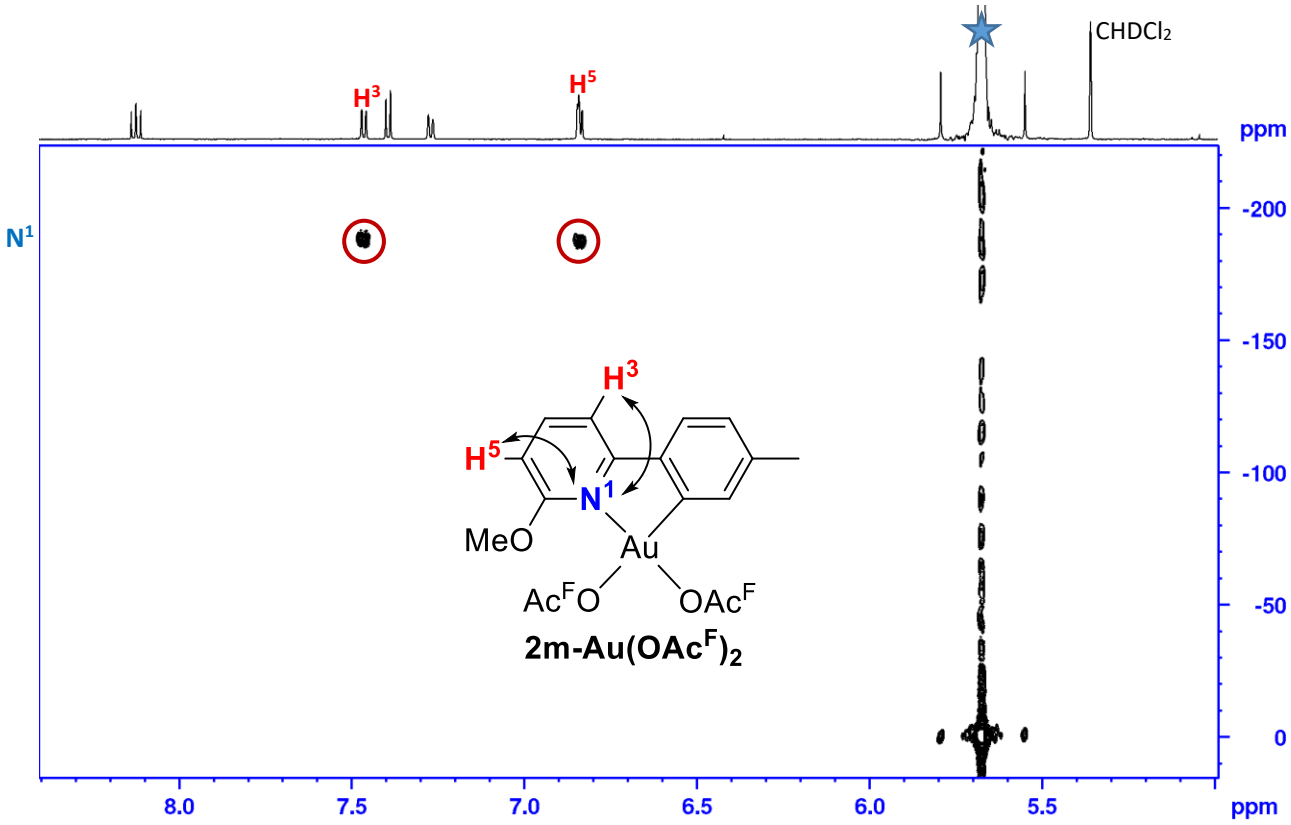
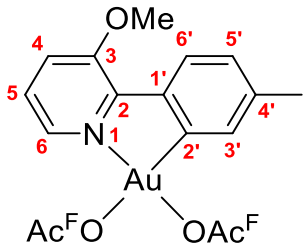


Figure S100. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **2m-Au(OAc^{F})$_2$**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



2n-Au(OAc^F)$_2$

2n-Au(OAc^F)$_2$. A microwave vessel was charged with $Au(OAc)_3$ (0.187 g, 0.500 mmol, 1.00 equiv.) and **1n** (0.100 g, 0.505 mmol, 1.01 equiv.) in a 1:1 mixture of $HOAc^F$ and water (15 mL). The reaction mixture was heated at 100 °C for 30 min in a microwave. After cooling to room temperature, $HOAc^F$ (1.5 mL) was added to dissolve partially precipitated product, and the resulting solution was filtered. Water (15 mL) was added to the filtrate, resulting in the precipitation of a solid. After cooling on an ice-water bath for 5 min, the precipitate was filtered off, washed with water (3x5 mL) and Et_2O (5 mL), and dried under a stream of air for ca. 3 h, furnishing **2n-Au(OAc^F)$_2$** as a yellow solid.

Yield: 0.185 g, 0.299 mmol, 60 %.

^{1}H NMR (800 MHz, CD_2Cl_2): δ 8.22 (dd, $^3J_{H,H}$ = 5.9 Hz, $^4J_{H,H}$ = 1.0 Hz, 1H, **H^6**), 8.07 (d, $^3J_{H,H}$ = 8.0 Hz, 1H, **H$^{6'}$**), 7.74 (dd, $^3J_{H,H}$ = 8.6 Hz, $^4J_{H,H}$ = 0.6 Hz, 1H, **H^4**), 7.46 (dd, $^3J_{H,H}$ = 8.6 Hz, $^3J_{H,H}$ = 5.9 Hz, 1H, **H^5**), 7.23-7.24 (m, 1H, **H$^{5'}$**), 6.82-6.83 (m, 1H, **H$^{3'}$**), 4.12 (s, 3H, OC**H**$_3$), 2.40 ppm (s, 3H, Ar-C**H**$_3$).

^{13}C NMR (201 MHz, CD_2Cl_2): δ 161.2 (q, $^2J_{C,F}$ = 37.7 Hz, O**C**OCF$_3$), 160.6 (q, $^2J_{C,F}$ = 39.2 Hz, O**C**OCF$_3$), 155.2 (**C^3**), 154.2 (**C^2**), 143.2 (**C$^{4'}$**), 142.3 (**C$^{1'}$** or **C$^{2'}$**), 139.7 (**C^6**), 139.3 (**C$^{1'}$** or **C$^{2'}$**), 131.2 (**C$^{5'}$**), 130.8 (**C$^{6'}$**), 128.4 (**C$^{3'}$**), 126.1 (**C^4**), 124.3 (**C^5**), 118.3 (q, $^1J_{C,F}$ = 289.4, OCO**C**F$_3$), 116.2 (q, $^1J_{C,F}$ = 288.1, OCO**C**F$_3$), 57.5 (O**C**H$_3$), 22.2 ppm (Ar-**C**H$_3$).

^{19}F NMR (188 MHz, CD_2Cl_2): δ –76.3 (s, 3F, OCOC**F**$_3$), –77.2 ppm (s, 3F, OCOC**F**$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −164.9 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 508.043 (100) $[M–OCOCF_3]^+$.

HRMS (ESI): Found: 508.0430; calcd for $C_{15}H_{12}AuF_3NO_3$ $[M–OCOCF_3]^+$: 508.0429.

Elemental Analysis: Anal. calcd. For $C_{17}H_{12}AuF_6NO_5$: C, 32.87; H, 1.95; N. 2.25. Found: C, 32.81; H, 1.91; N, 2.23.

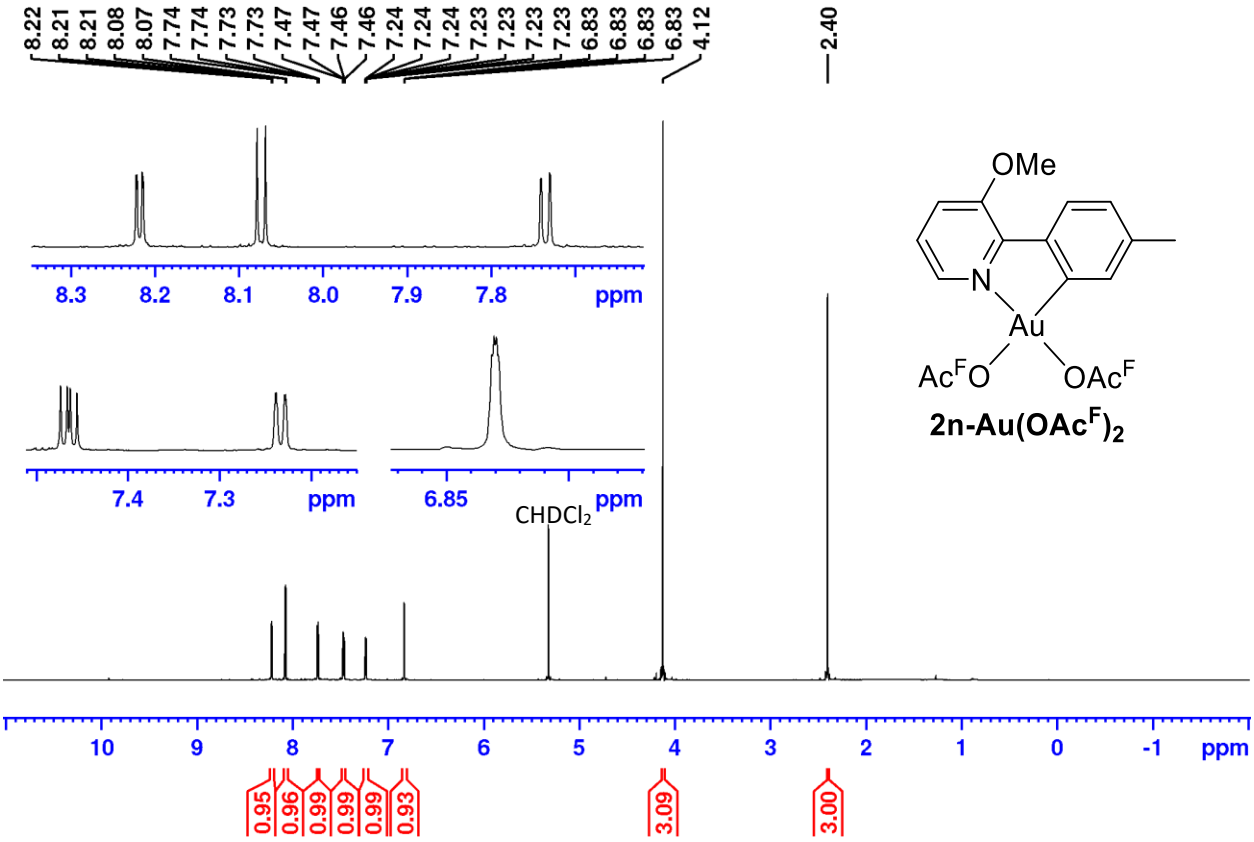


Figure S101. ^{1}H NMR (800 MHz, CD_2Cl_2) of **2n-Au(OAc^{F})$_2$**.

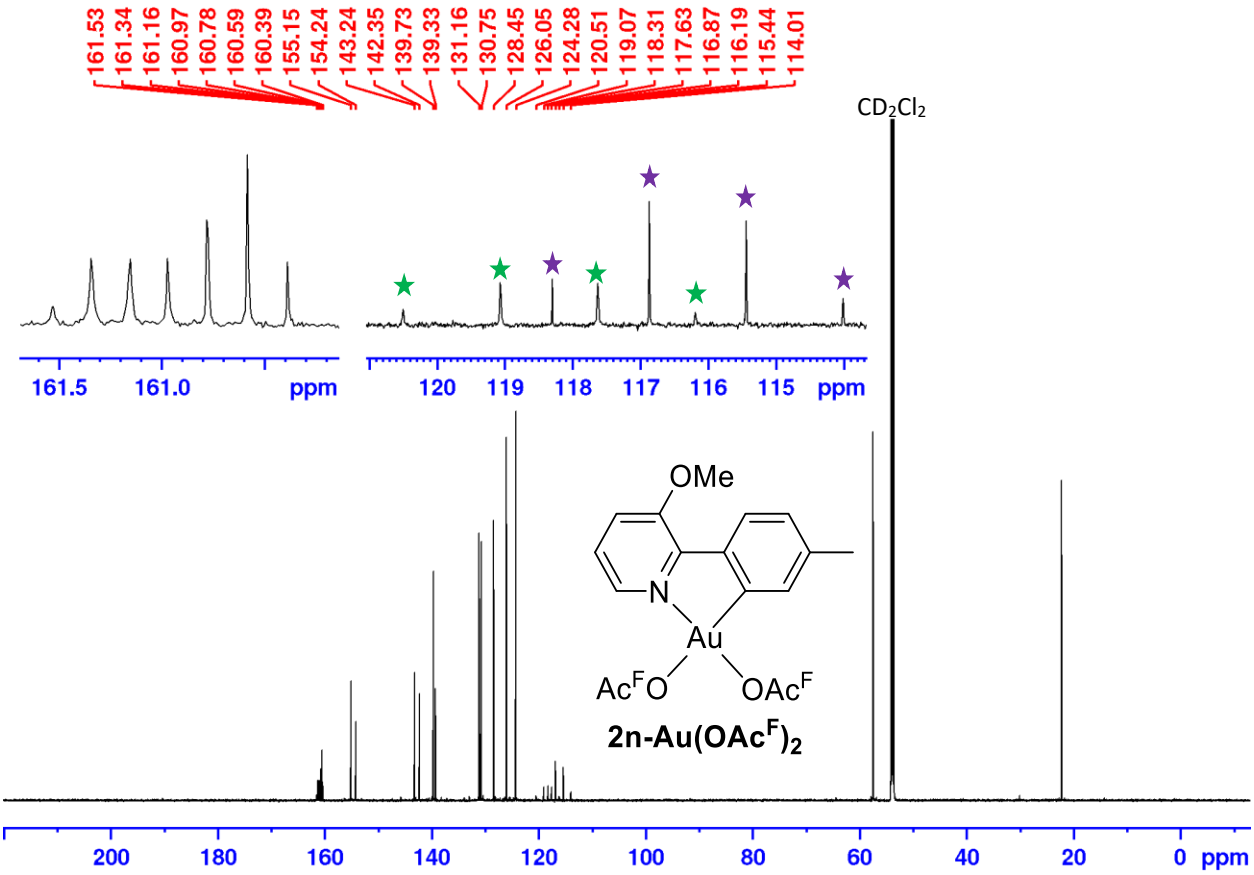


Figure S102. ^{13}C NMR (201 MHz, CD_2Cl_2) of **2n-Au(OAc^F)$_2$**. The quartets corresponding to the two **C**F_3 carbons of the trifluoroacetate ligands are indicated by purple and green stars in the insert to the right. The quartets corresponding to the two carbonyl carbons of the trifluoroacetate ligands were found to partially overlap (see insert to the left).

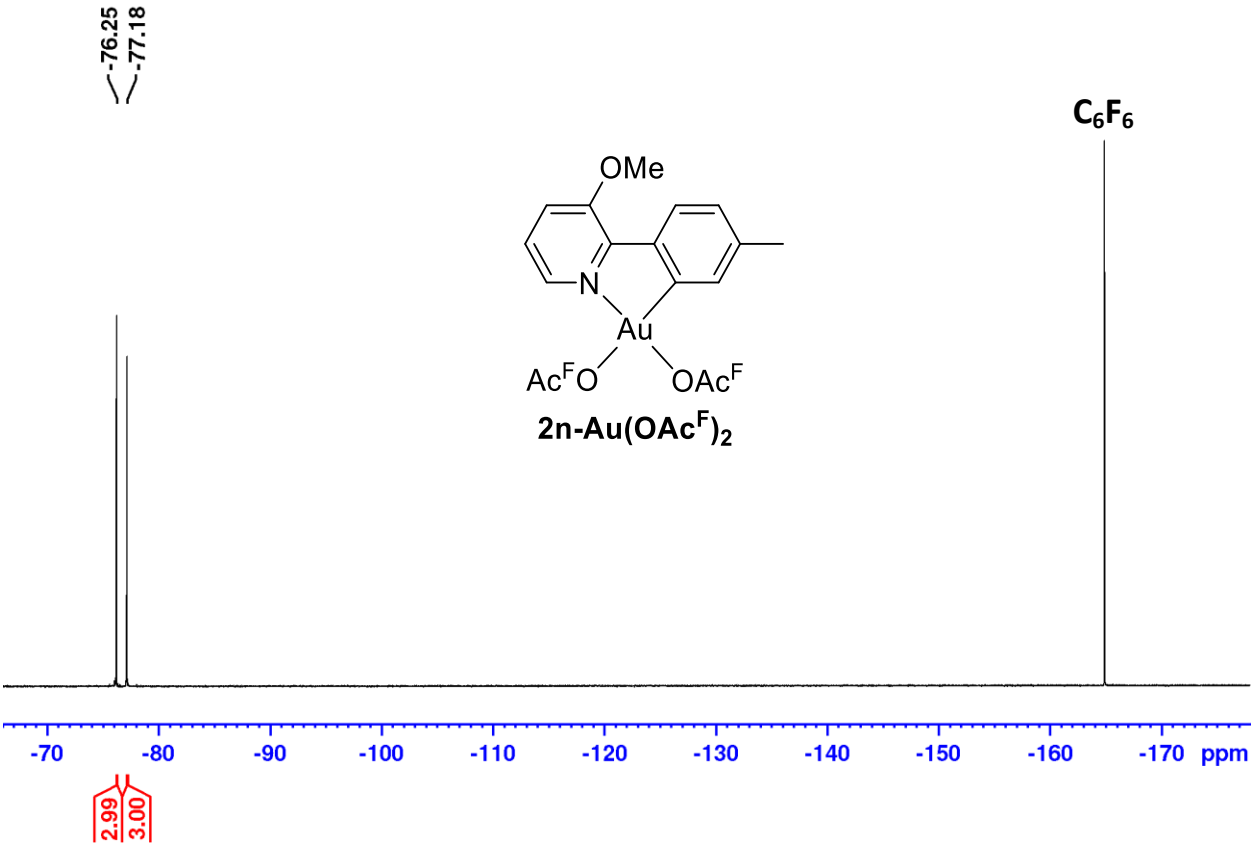


Figure S103. ^{19}F NMR (188 MHz, CD_2Cl_2) of **2n-Au(OAc^F)$_2$**.

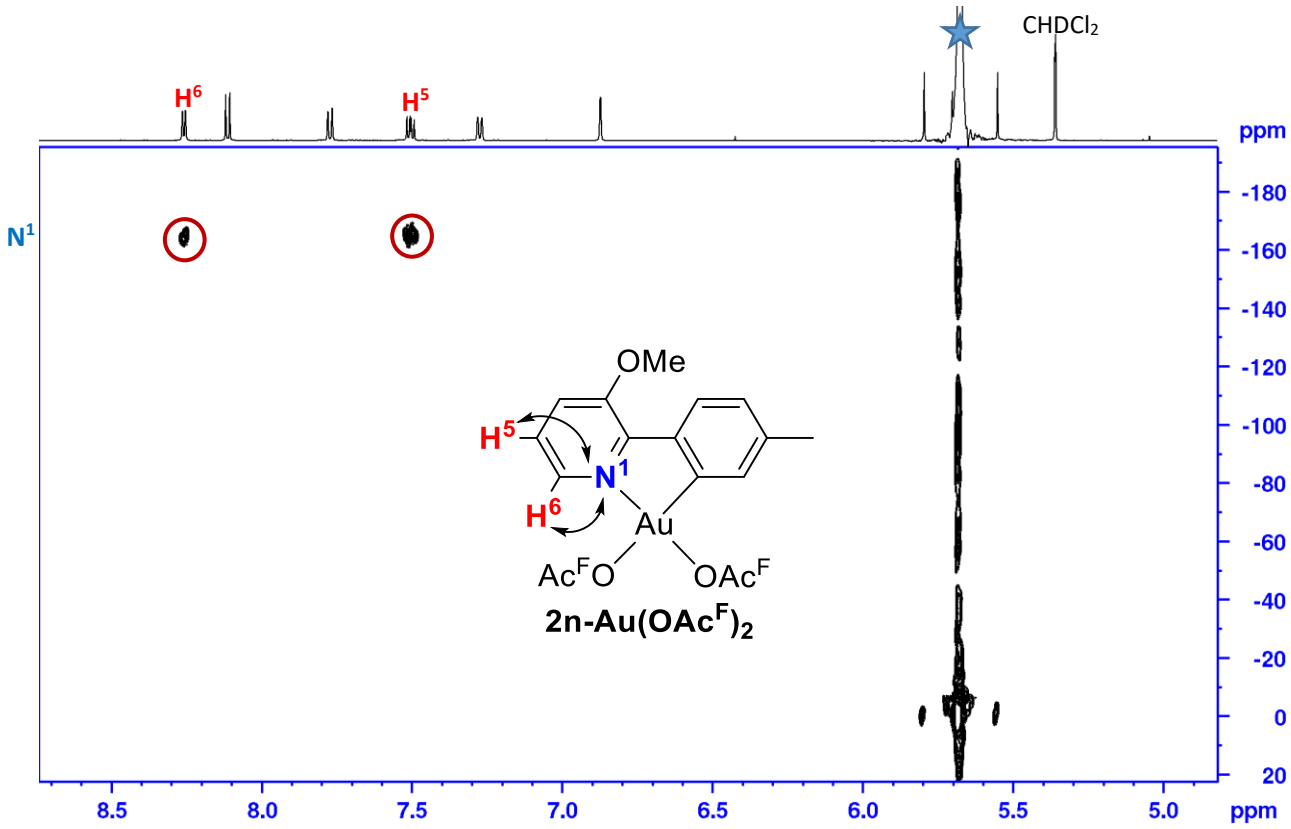
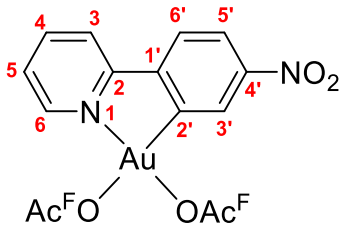


Figure S104. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **2n-Au(OAc^{F})$_2$**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



2o-Au(OAc^F)$_2$

2o-Au(OAc^F)$_2$. A microwave vessel was charged with $Au(OAc)_3$ (0.187 g, 0.500 mmol, 1.00 equiv.) and **1o** (0.101 g, 0.505 mmol, 1.01 equiv.) in a 1:1 mixture of $HOAc^F$ and water (15 mL). The reaction mixture was heated at 120 °C for 30 min in a microwave. After cooling to room temperature, $HOAc^F$ (5 mL) was added to dissolve partially precipitated product, and the resulting solution was filtered. Water (20 mL) was added to the filtrate, resulting in the precipitation of a solid. After cooling on an ice-water bath for 15 min, and then overnight at 4-8 °C, the precipitate was filtered off, washed with water (3x5 mL) and Et_2O (5 mL), and dried under a stream of air for ca. 3 h, furnishing **2o-Au(OAc^F)$_2$** as a pale yellow solid.

Yield: 0.0840 g, 0.135 mmol, 27 %.

^{1}H NMR (800 MHz, CD_2Cl_2): δ 8.70 (ddd, $^3J_{H,H}$ = 6.0, $^4J_{H,H}$ = 1.2, $^4J_{H,H}$ = 0.6 Hz, 1H, **H^6**), 8.35-8.40 (m, 2H, **H^4** + **H$^{5'}$**), 8.07 (dd, $^3J_{H,H}$ = 8.0, $^4J_{H,H}$ = 1.5 Hz, 1H, **H^3**), 7.96 (d, $^4J_{H,H}$ = 2.1 Hz, 1H, **H$^{3'}$**), 7.81 (d, $^3J_{H,H}$ = 8.5 Hz, 1H, **H$^{6'}$**), 7.74 ppm (ddd, 1H, $^3J_{H,H}$ = 7.6 Hz, $^3J_{H,H}$ = 6.1 Hz, $^3J_{H,H}$ = 1.3 Hz, **H^5**).

^{13}C NMR (201 MHz, CD_2Cl_2):* δ 162.7 (**C^2**), 161.5 (q, $^2J_{C,F}$ = 38.2 Hz, O**C**OCF$_3$), 161.0 (q, $^2J_{C,F}$ = 39.7 Hz, O**C**OCF$_3$), 149.1 (**C^6**), 148.1 (Ar-**C**), 147.7 (Ar-**C**), 145.7 (**C^4**), 140.5 (Ar-**C**), 127.5 (**C^5**), 126.8 (**C$^{6'}$**), 125.8 (**C$^{5'}$**), 123.8 (**C^3**), 123.7 (**C$^{3'}$**), 118.2 (q, $^1J_{C,F}$ = 288.6 Hz, OCO**C**F$_3$), 116.0 ppm (q, $^1J_{C,F}$ = 287.9 Hz, OCO**C**F$_3$).

*The quaternary carbons of the aryl ring could not be assigned unambiguously.

^{19}F NMR (376 MHz, CD_2Cl_2): δ –76.0 (s, 3F, C**F**$_3$), –77.0 ppm (s, 3F, C**F**$_3$).

MS (ESI, MeCN): *m/z* (rel. %): 488.946 (17) $[M–2OCOCF_3+2Cl+Na]^+$.

HRMS (ESI, MeCN): Found: 488.9449; calcd for $C_{11}H_7AuCl_2N_2NaO_2$ $[M–2OCOCF_3+2Cl+Na]^+$: 488.9442.

Elemental Analysis: Anal. calcd. For $C_{15}H_7AuF_6N_2O_6$: C, 28.96; H, 1.13; N. 4.50. Found: C, 28.91; H, 1.11; N, 4.45.

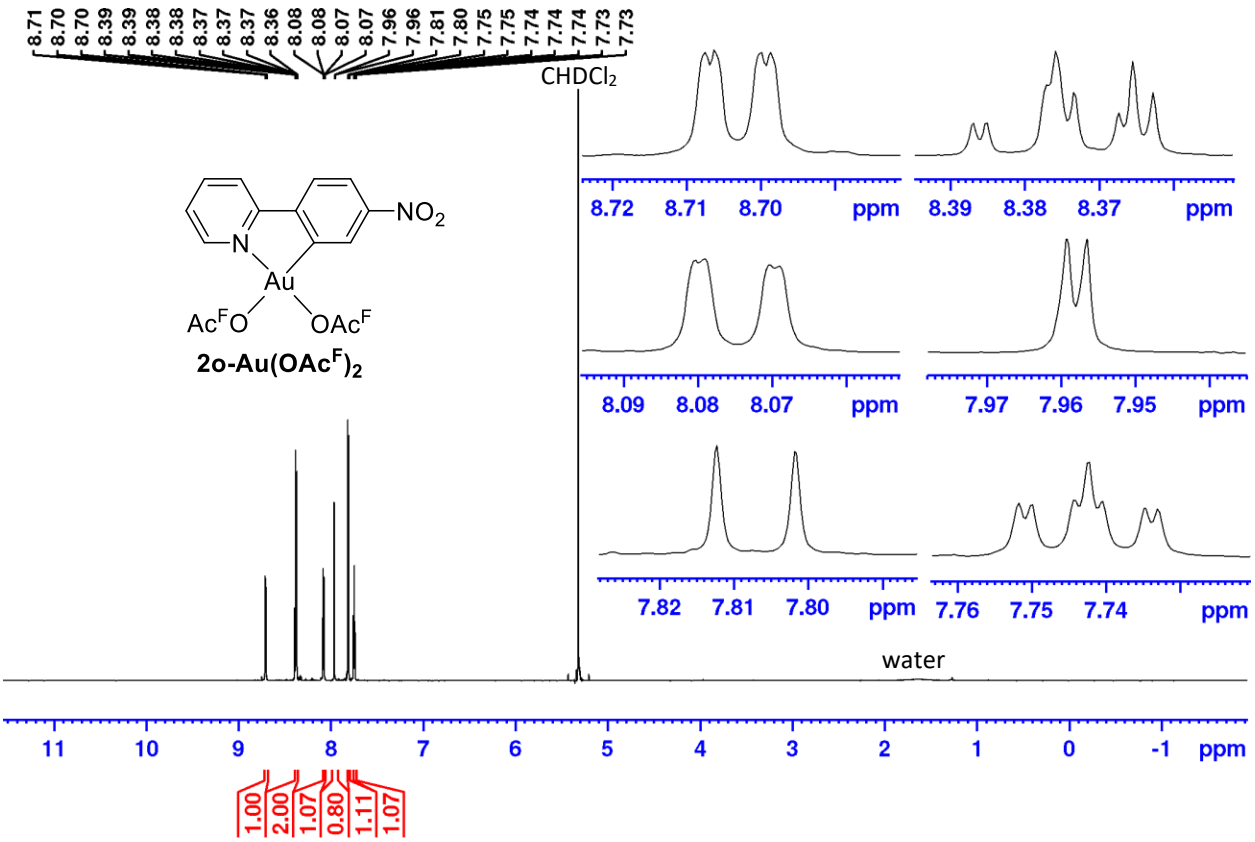


Figure S105. ^{1}H NMR (800 MHz, CD_2Cl_2) of **2o-Au(OAc^{F})$_2$**.

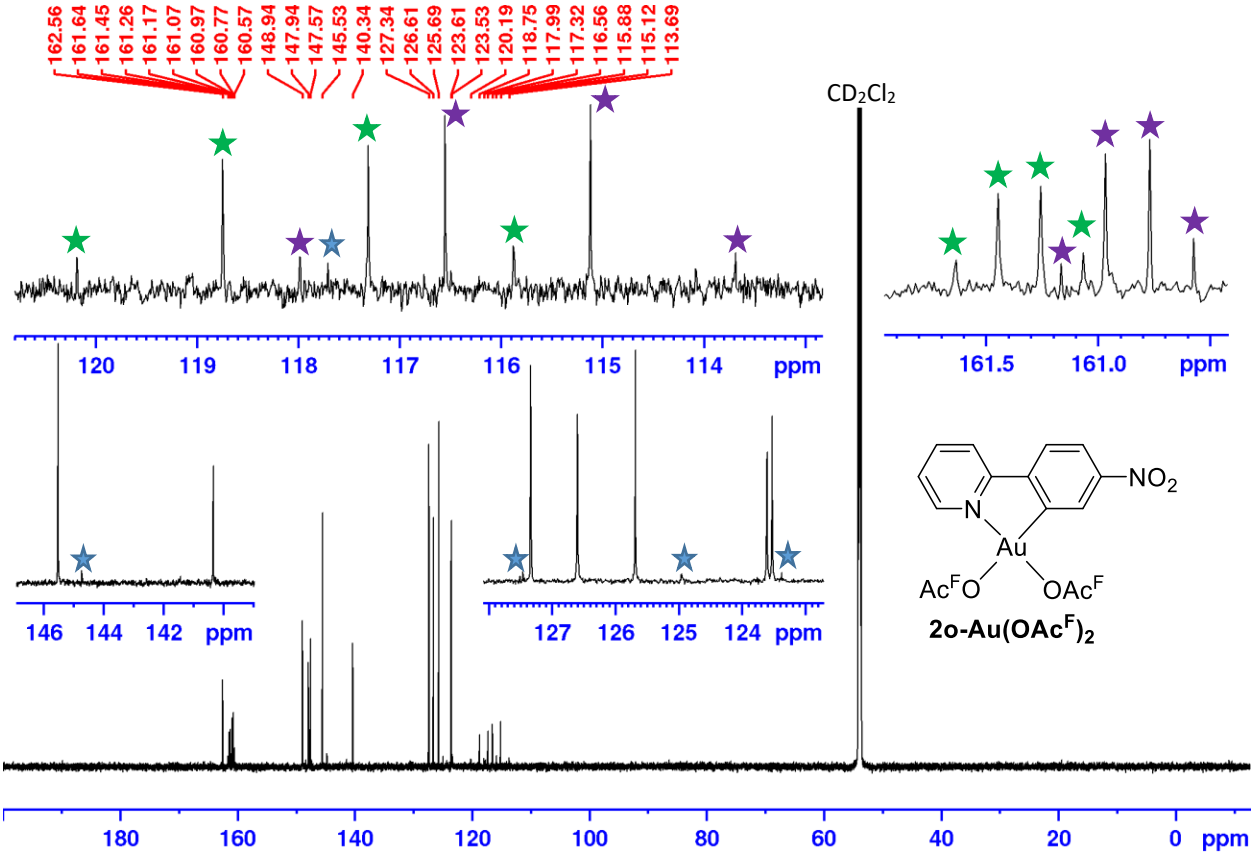


Figure S106. ^{13}C NMR (201 MHz, CD_2Cl_2) of **2o-Au(OAc^F)$_2$**. The quartets corresponding to the two **C**F_3 carbons of the trifluoroacetate ligands are indicated by purple and green stars in the insert to the left. The quartets corresponding to the two carbonyl carbons of the trifluoroacetate ligands are indicated by purple and green stars in the insert to the right. Traces of (an) unidentified impurity/impurities are indicated by blue stars.

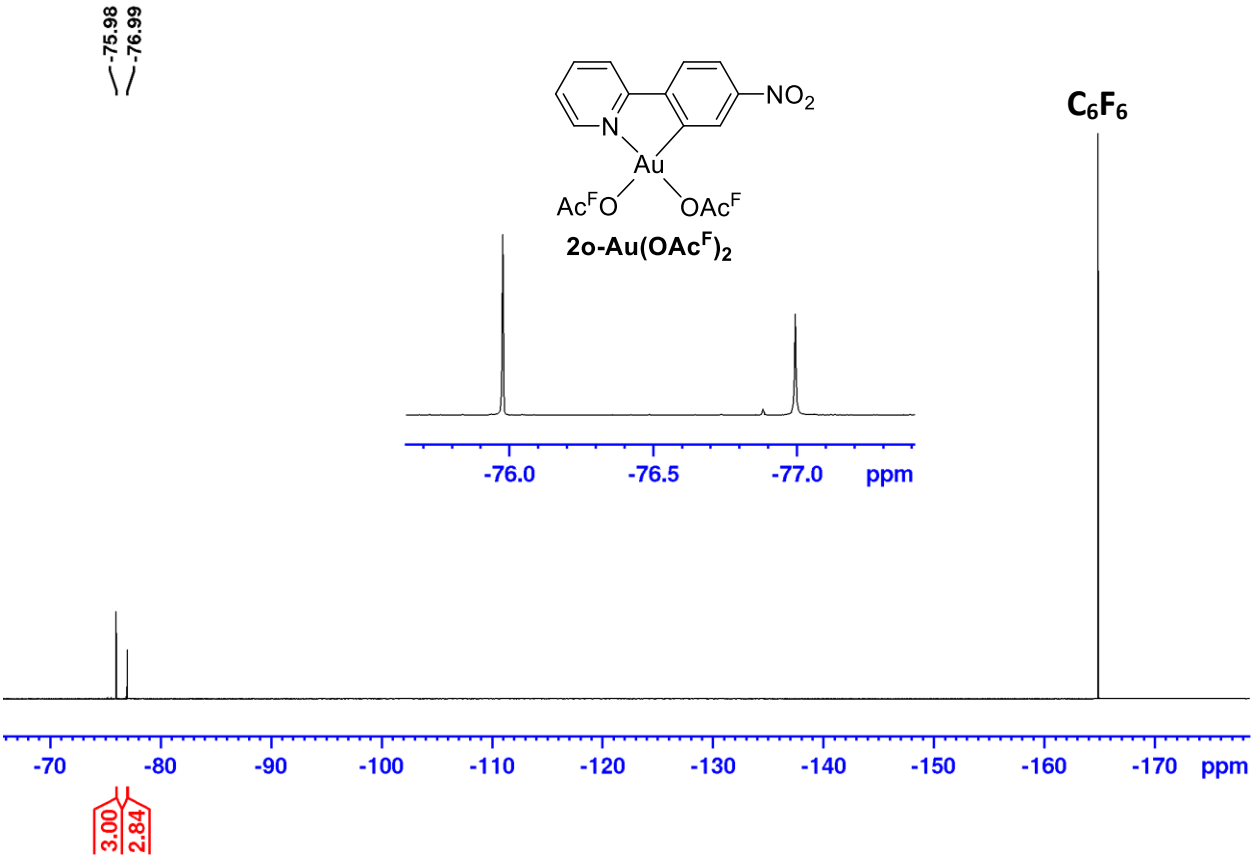
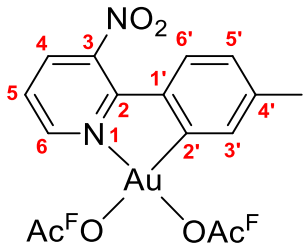


Figure S107. ^{19}F NMR (376 MHz, CD_2Cl_2) of **2o-Au(OAc^F)$_2$**.



2p-Au(OAc^F)$_2$

2p-Au(OAc^F)$_2$. A microwave vessel was charged with $Au(OAc)_3$ (0.187 g, 0.500 mmol, 1.00 equiv.) and **1p** (0.119 g, 0.555 mmol, 1.10 equiv.) in a 1:1 mixture of $HOAc^F$ and water (15 mL). The reaction mixture was heated at 120 °C for 30 min in a microwave. After cooling to room temperature, $HOAc^F$ (20 mL) was added to dissolve partially precipitated product, and the resulting solution was filtered to remove insoluble material. Water (25 mL) was added to the filtrate, resulting in the precipitation of a yellow solid. After cooling on an ice-water bath, the precipitate was filtered off, washed with water (2x5 mL), and dried under a stream of air for ca. 1 h. **2p-Au(OAc^F)$_2$** was obtained as a pale yellow solid.

Yield: 0.207 g, 0.326 mmol, 65 %.

^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.86 (dd, $^3J_{H,H}$ = 6.0 Hz, $^4J_{H,H}$ = 1.3 Hz, 1H, **H^6**), 8.35 (dd, $^3J_{H,H}$ = 8.2 Hz, $^4J_{H,H}$ = 1.3 Hz, 1H, **H^4**), 7.70 (dd, $^3J_{H,H}$ = 8.2 Hz, 6.0 Hz, $^3J_{H,H}$ = 1H, **H^5**), 7.27 (d, $^3J_{H,H}$ = 8.2 Hz, 1H, **H$^{5'}$**), 7.12 (d, 1H, $^3J_{H,H}$ = 8.2 Hz, **H$^{6'}$**), 6.96 (s, 1H, **H$^{3'}$**), 2.46 ppm (s, 3H, Ar-C**H**$_3$).

^{13}C NMR (201 MHz, CD_2Cl_2): δ 161.5 (q, $^2J_{C,F}$ = 38.3 Hz, O**C**OCF$_3$), 160.9 (q, $^2J_{C,F}$ = 39.6 Hz, O**C**OCF$_3$), 157.7 (**C^2**), 151.2 (**C^6**), 147.6 (**C$^{4'}$**), 145.3 (**C^3**), 142.8 (**C$^{2'}$**), 139.0 (**C^4**), 134.6 (**C$^{1'}$**), 132.1 (**C$^{5'}$**), 129.8 (**C$^{3'}$**), 128.4 (**C$^{6'}$**), 124.9 (**C^5**), 118.2 (d (q expected), $^1J_{C,F}$ = 288.8 Hz, OCO**C**F$_3$), 116.1 (q, $^1J_{C,F}$ = 287.9 Hz, OCO**C**F$_3$), 22.7 ppm (Ar-**C**H$_3$).

^{19}F NMR (188 MHz, CD_2Cl_2): δ −76.1 (s, 3F, OCOC**F**$_3$), –77.1 ppm (s, 3F, OCOC**F**$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ −163.9 ppm (**N^1**). The resonance corresponding to the nitrogen in the nitro group was not detected.

MS (ESI): *m/z* (rel. %): 580.976 (23) $[M–OCOCF_3+Na^{35}Cl]^+$, 591.005 (53) $[M–OCOCF_3+NaHCO_2]^+$.

HRMS (ESI): Found: 580.9761/582.9733; calcd for $C_{14}H_9AuClF_3N_2NaO_4$ $[M–OCOCF_3+Na^{35/37}Cl]^+$: 580.9766/582.9737.

HRMS (ESI): Found: 591.0048; calcd for $C_{15}H_{10}AuF_3N_2NaO_6$ $[M–OCOCF_3+NaHCO_2]^+$: 591.0049.

Elemental Analysis: Anal. calcd. For $C_{16}H_9AuF_6N_2O_6$: C, 30.21; H, 1.43; N. 4.40. Found: C, 30.16; H, 1.42; N, 4.40.

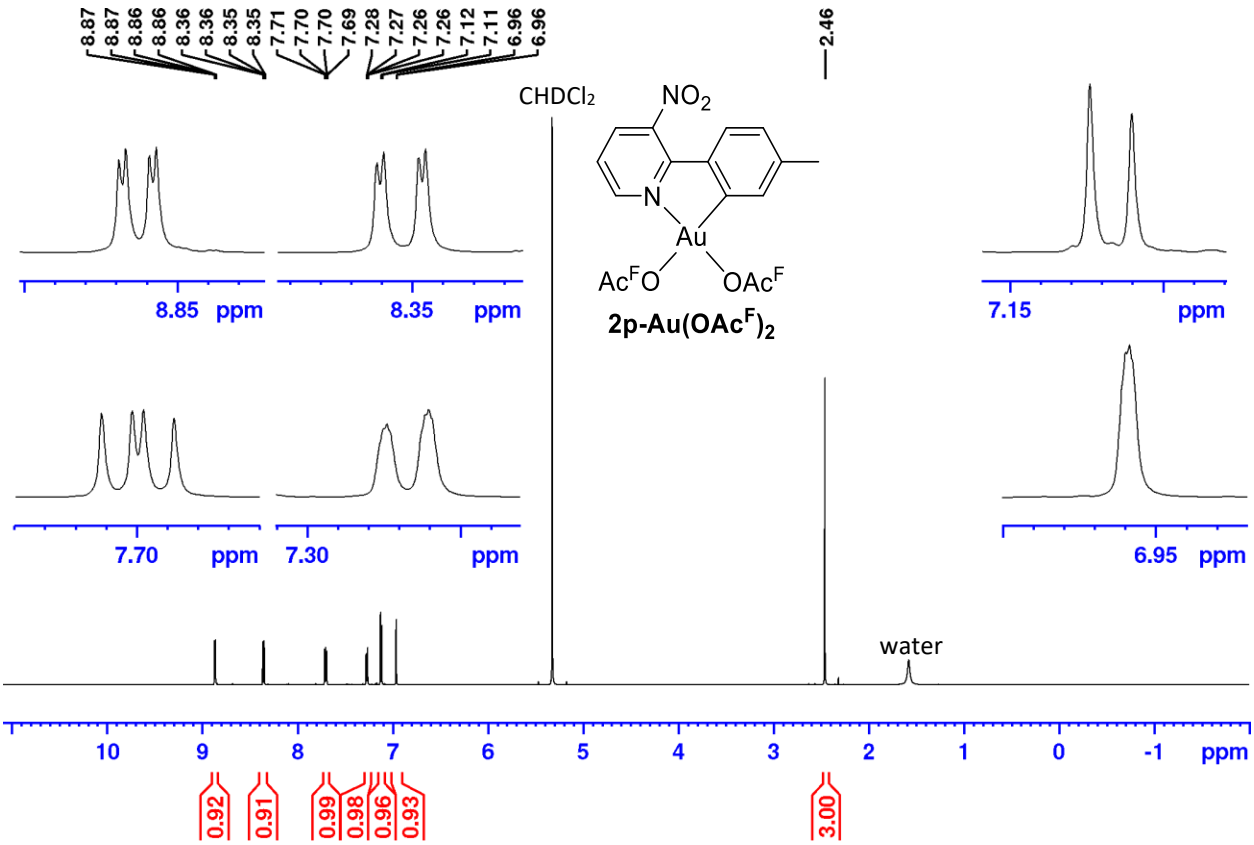


Figure S108. ^{1}H NMR (600 MHz, CD_2Cl_2) of **2p-Au(OAc^F)$_2$**.

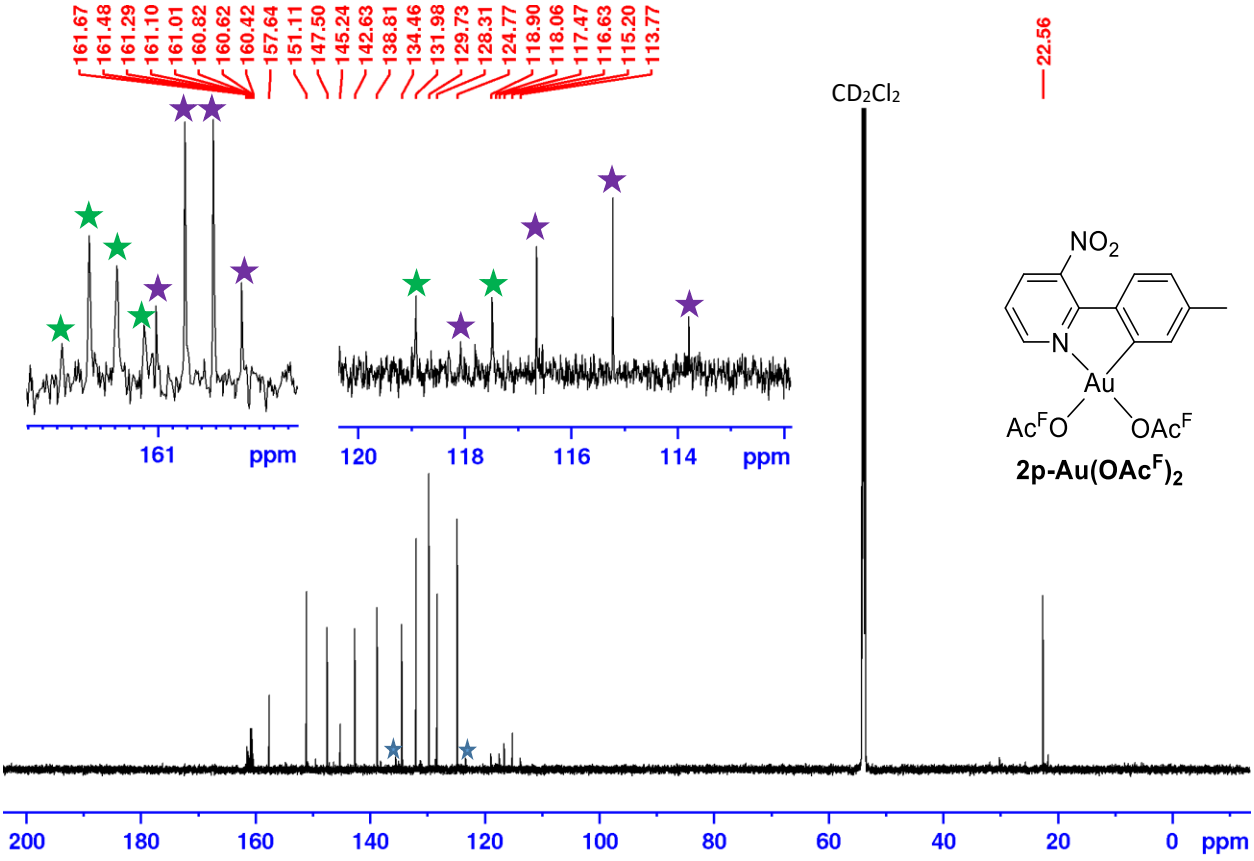


Figure S109. ^{13}C NMR (201 MHz, CD_2Cl_2) of **2p-Au(OAc^F)$_2$**. For one of the expected quartets corresponding to one of the **C**F_3 carbons of the trifluoroacetate ligands, only a doublet could be detected (marked with green stars in the insert to the right). The other quartet (marked with purple stars in the insert to the right) does not show the expected 1:3:3:1 relationship between the individual peaks. Traces of (an) unidentified impurity/impurities are indicated by blue stars.

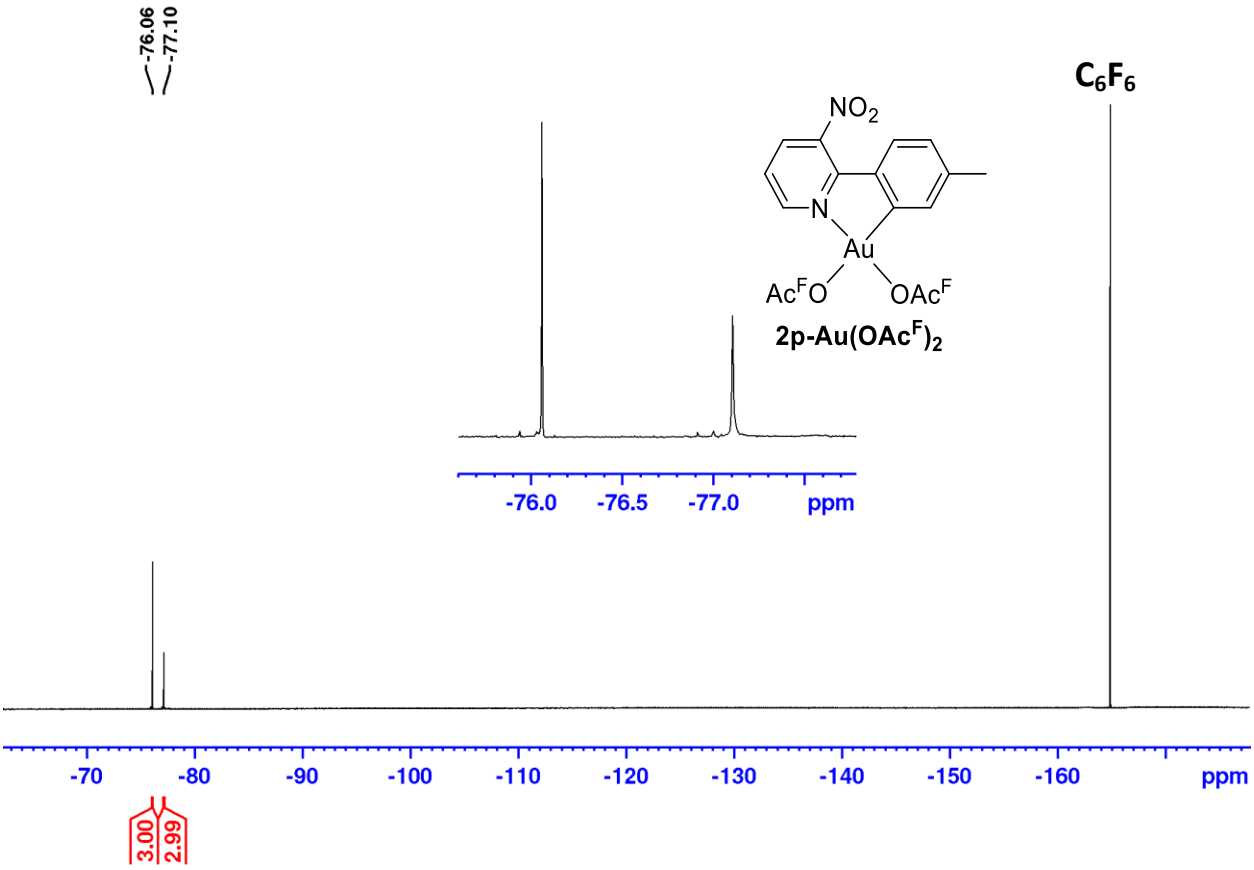


Figure S110. ^{19}F NMR (376 MHz, CD_2Cl_2) of **2p-Au(OAc^F)$_2$**.

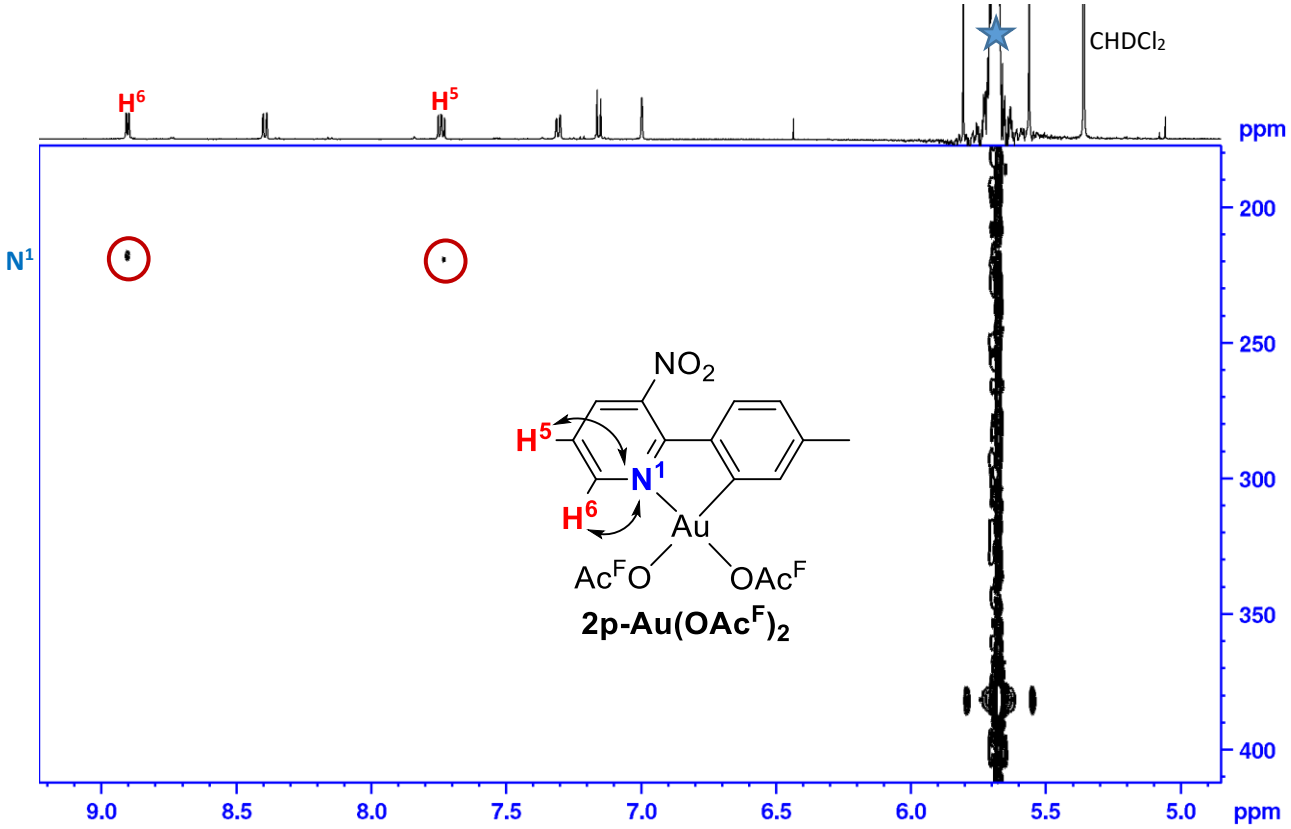
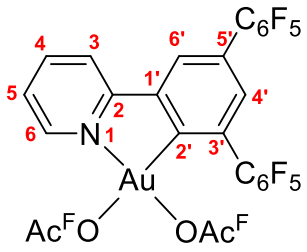


Figure S111. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **2p-Au $(OAc^F)_2$**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection). The resonance corresponding to the nitrogen in the NO_2 group was not detected.



2r-Au(OAc^F)$_2$

2r-Au(OAc^F)$_2$. A microwave vessel was charged with $Au(OAc)_3$ (0.0750 g, 0.200 mmol, 1.00 equiv.) and **1r** (0.0980 g, 0.202 mmol, 1.01 equiv.) in a 1:1 mixture of $HOAc^F$ and water (6 mL). The reaction mixture was heated at 120 °C for 60 min in a microwave. After cooling to room temperature, $HOAc^F$ (2 mL) was added, and the resulting solution was filtered. Water (20 mL) was added to the filtrate, resulting in the precipitation of a solid. After cooling on an ice-water bath for 15 min, and then overnight at 4-8 °C, the precipitate was filtered off, washed with water (3x5 mL) and Et_2O (5 mL), and dried under a stream of air for ca. 3 h, furnishing **2r-Au(OAc^F)$_2$** as a colorless solid.

Yield: 0.0740 g, 0.0810 mmol, 41 %.

^{1}H NMR (800 MHz, CD_2Cl_2): δ 8.61 (dd, $^3J_{H,H}$ = 6.1 Hz, $^4J_{H,H}$ = 1.0 Hz, 1H, **H^6**), 8.34 (ddd, $^3J_{H,H}$ = 8.1 Hz, $^3J_{H,H}$ = 7.7 Hz, $^4J_{H,H}$ = 1.4 Hz, 1H, **H^4**), 8.05 (dd, $^3J_{H,H}$ = 8.2 Hz, $^4J_{H,H}$ = 1.2 Hz, 1H, **H^3**), 7.80 (s, 1H, **H$^{6'}$**), 7.65 (ddd, $^3J_{H,H}$ = 7.6 Hz, $^3J_{H,H}$ = 6.1 Hz, $^4J_{H,H}$ = 1.4 Hz, 1H, **H^5**), 7.27 ppm (s, 1H, **H$^{4'}$**).

^{13}C NMR (201 MHz, CD_2Cl_2): δ 164.3 (**C^2**), 161.2 (q, $^2J_{C,F}$ = 38.4 Hz, O**C**OCF$_3$), 160.4 (q, $^2J_{C,F}$ = 39.6 Hz, O**C**OCF$_3$), 148.4 (**C^6**), 145.4 (**C^4**), 144.6 (m, 2x Ar-**C**-F), 142.2 (d, $^1J_{C,F}$ = 254.8 Hz, Ar-**C**-F), 141.9 (d, $^1J_{C,F}$ = 256.2 Hz, Ar-**C**-F), 141.1 (**C$^{3'}$** + **C$^{5'}$**), 138.6 (d, $^1J_{C,F}$ = 252.5 Hz, Ar-**C**-F), 137.6 (**C$^{4'}$**), 137.2 (d, $^1J_{C,F}$ = 251.1 Hz, Ar-**C**-F), 130.8 (**C$^{1'}$** or **C$^{2'}$**), 129.4 (**C$^{1'}$** or **C$^{2'}$**), 128.3 (**C$^{6'}$**), 126.3 (**C^5**), 122.8 (**C^3**), 117.9 (q, $^1J_{C,F}$ = 288.4 Hz, OCO**C**F$_3$), 115.1 (q, $^1J_{C,F}$ = 288.1 Hz, OCO**C**F$_3$), 113.0 ppm (m, 2x Ar-**C**-C-F).

^{19}F NMR (470 MHz, CD_2Cl_2): δ –75.6 (s, 3F, OCOC**F**$_3$), –77.1 (s, 3F, OCOC**F**$_3$), –143.8 (dd, $^3J_{F,F}$ = 22.1 Hz, $^4J_{F,F}$ = 7.5 Hz, 2F, C$_6$**F**$_5$), –145.2 (dd, $^3J_{F,F}$ = 23.1 Hz, $^4J_{F,F}$ = 7.5 Hz, 2F, C$_6$**F**$_5$), –155.0 (dd, $^3J_{F,F}$ = 21.3 Hz, $^3J_{F,F}$ = 20.3 Hz, 1F, C$_6$**F**$_5$), –156.3 (dd, $^3J_{F,F}$ = 20.8 Hz, $^3J_{F,F}$ = 20.2 Hz, 1F, C$_6$**F**$_5$), –163.6 (m, 2F, C$_6$**F**$_5$), –164.7 ppm (m, 2F, C$_6$**F**$_5$).

^{15}N{^{1}H} NMR (800 MHz, CD_2Cl_2): δ –167.7 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 714.019 (15) [M–2OCOCF$_3$+OMe]$^+$, 768.027 (70) [M–2OCOCF$_3$+2OMe+Na]$^+$, 800.053 (100) [M–2OCOCF$_3$+2OMe+MeOH+Na]$^+$.

HRMS (ESI): Found: 714.0188; calcd for $C_{24}H_9AuF_{10}NO$ $[M–2OCOCF_3+OMe]^+$: 714.0185.

HRMS (ESI): Found: 768.0269; calcd for $C_{25}H_{12}AuF_{10}NNaO_2$ $[M–2OCOCF_3+2OMe+Na]^+$: 768.0266.

HRMS (ESI): Found: 800.0532; calcd for $C_{26}H_{16}AuF_{10}NNaO_3$ $[M–2OCOCF_3+2OMe+MeOH+Na]^+$: 800.0528.

Elemental Analysis: Anal. calcd. For $C_{26}H_6AuF_{16}NO_4$: C, 35.66; H, 0.67; N, 1.54. Found: C, 35.64; H, 0.67; N, 1.54.

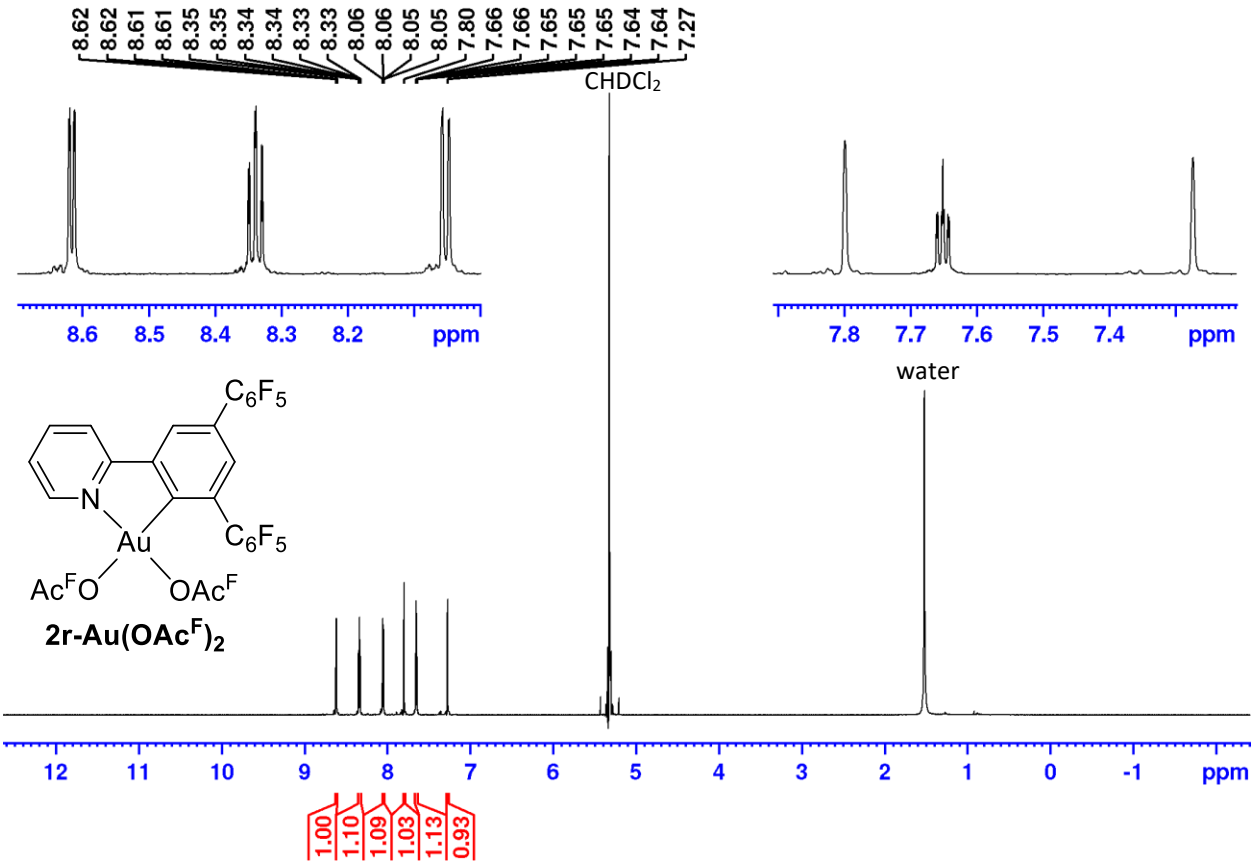


Figure S112. ^{1}H NMR (800 MHz, CD_2Cl_2) of **2r-Au(OAc^F)$_2$**.

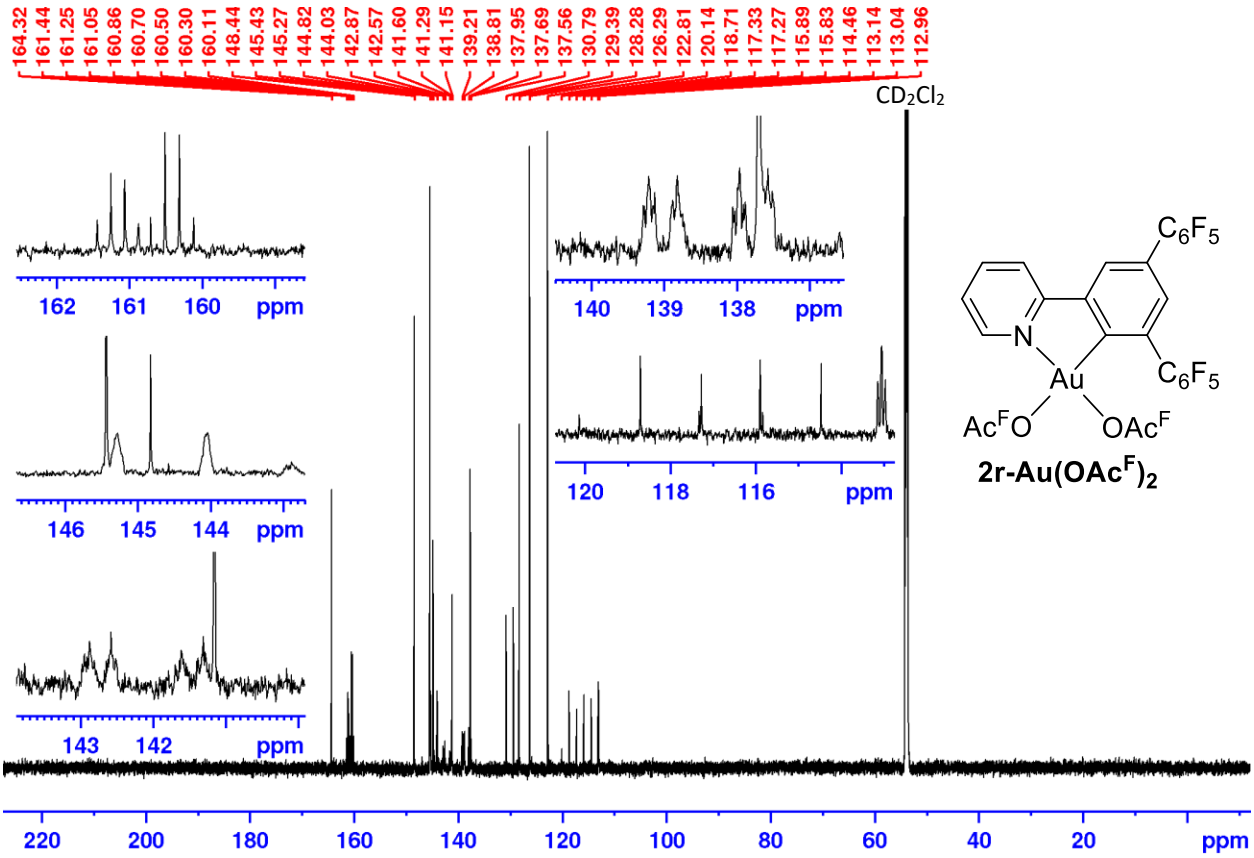


Figure S113. ^{13}C NMR (201 MHz, CD_2Cl_2) of **2r-Au(OAc^F)$_2$**.

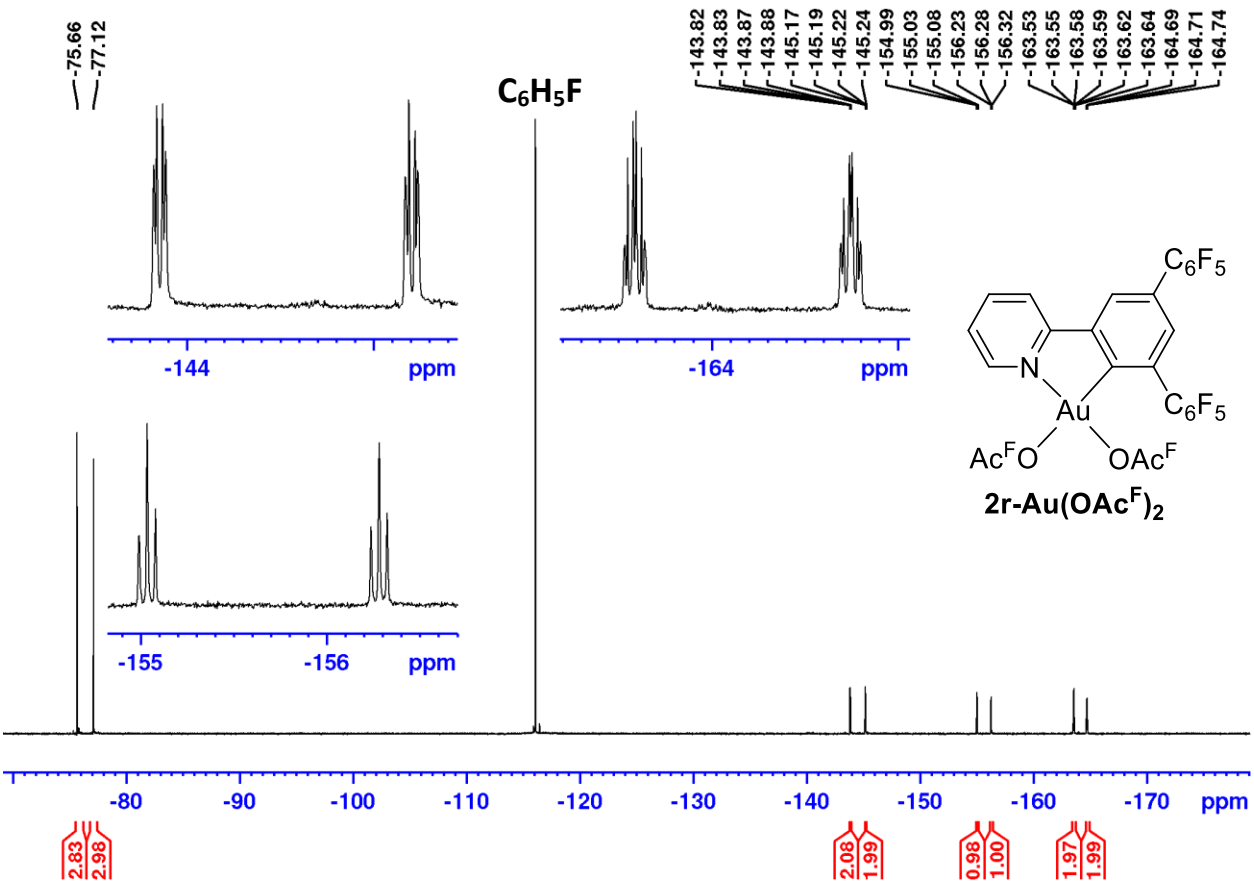


Figure S114. ^{19}F NMR (470 MHz, CD_2Cl_2) of **2r-Au(OAc^F)$_2$**.

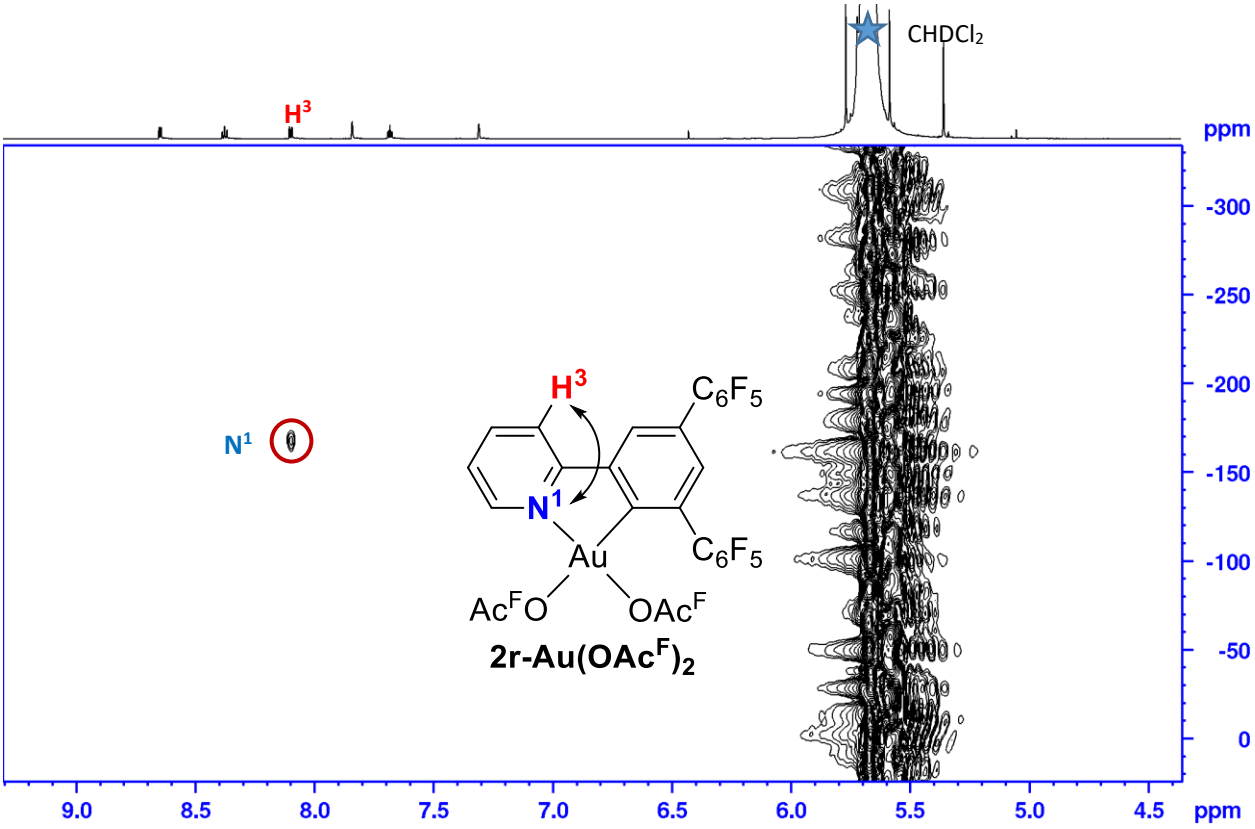
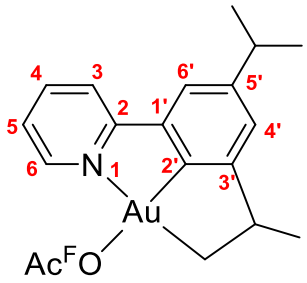


Figure S115. ^{1}H-^{15}N HMBC (800 MHz, CD_2Cl_2) of **2r-Au(OAc^{F})$_2$**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



3s-AuOAc^F

3s-AuOAc^F. A microwave vessel was charged with $Au(OAc)_3$ (0.0750 g, 0.200 mmol, 1.00 equiv.) and **1s** (0.0480 g, 0.202 mmol, 1.01 equiv.) in a 1:1 mixture of $HOAc^F$ and water (6 mL). The reaction mixture was heated at 80 °C for 3.5 h in a microwave. The reaction mixture was kept at 4-8 °C overnight. Addition of $HOAc^F$ (4 mL), followed by water (6 mL), furnishing a white precipitate. The precipitate was collected by filtration, and washed with water (3 x 3 mL). The title compound was obtained as a white solid.

Yield: 0.0410 g, 0.0750 mmol, 38 %.

^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.48 (ddd, $^3J_{H,H}$ = 5.4 Hz, $^4J_{H,H}$ = 1.4 Hz, $^5J_{H,H}$ = 0.8 Hz, 1H, **H^6**), 7.99-8.03 (m, 1H, **H^4**), 7.94 (d, $^3J_{H,H}$ = 8.1 Hz, 1H, **H^3**), 7.50 (ddd, $^3J_{H,H}$ = 7.5 Hz, $^3J_{H,H}$ = 5.4 Hz, $^4J_{H,H}$ = 1.3 Hz, 1H, **H^5**), 7.35 (s, 1H, **H$^{6'}$**), 6.92 (s, 1H, **H$^{4'}$**), 3.50 (sx, $^3J_{H,H}$ = 6.8 Hz, 1H, Ar-C**H**$(CH_2Au)CH_3$), 3.38 (dd, $^2J_{H,H}$ = 10.4 Hz, $^3J_{H,H}$ = 7.3 Hz, 1H, Ar-CH(C**H**$_2$Au)CH_3), 2.97 (dd, $^2J_{H,H}$ = 10.4 Hz, $^3J_{H,H}$ = 5.6 Hz, 1H, Ar-CH(C**H**$_2$Au)CH_3), 2.94 (sp, $^3J_{H,H}$ = 6.9 Hz, 1H, Ar-C**H**$(CH_3)_2$), 1.35 (d, $^3J_{H,H}$ = 7.0 Hz, 3H, Ar-CH(CH_2Au)C**H**$_3$), 1.290 (d, $^3J_{H,H}$ = 6.9 Hz, 3H, Ar-CH(C**H**$_3)_2$), 1.287 ppm (d, $^3J_{H,H}$ = 6.9 Hz, 3H, Ar-CH(C**H**$_3)_2$).

^{13}C NMR (151 MHz, CD_2Cl_2): δ 162.2 (**C^2**), 161.5 (q, $^2J_{C,F}$ = 36.5 Hz, O**C**OCF_3), 161.2 (**C$^{3'}$**), 149.8 (**C$^{5'}$**), 148.1 (**C^6**), 146.3 (**C$^{1'}$**), 141.5 (**C^4**), 139.7 (**C$^{2'}$**), 126.1 (**C$^{4'}$**), 125.1 (**C^5**), 121.1 (**C$^{6'}$**), 120.8 (**C^3**), 118.5 (q, $^1J_{C,F}$ = 290.3 Hz, OCO**C**F_3), 46.7 (Ar-**C**H$(CH_2Au)CH_3$), 41.4 (Ar-CH(**C**H$_2$Au)CH_3), 35.2 (Ar-**C**H$(CH_3)_2$), 24.5 (Ar-CH(**C**H$_3)_2$), 24.3 (Ar-CH(**C**H$_3)_2$), 23.0 ppm (Ar-CH(CH_2Au)**C**H$_3$).

^{19}F NMR (376 MHz, CD_2Cl_2): δ –76.9 ppm (s, 3F, OCOC**F**$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ –111.7 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 434.118 (49) $[M–OCOCF_3]^+$, 452.128 (100) $[M–OCOCF_3+H_2O]^+$, 475.144 (82) $[M–OCOCF_3+MeCN]^+$.

HRMS (ESI): Found: 434.1176; calcd for $C_{17}H_{19}AuN$ $[M–OCOCF_3]^+$: 434.1178.

Elemental Analysis: Anal. calcd. For $C_{17}H_{15}AuF_3NO_2$: C, 41.70; H, 3.50; N, 2.56. Found: C, 41.61; H, 3.48; N, 2.53.

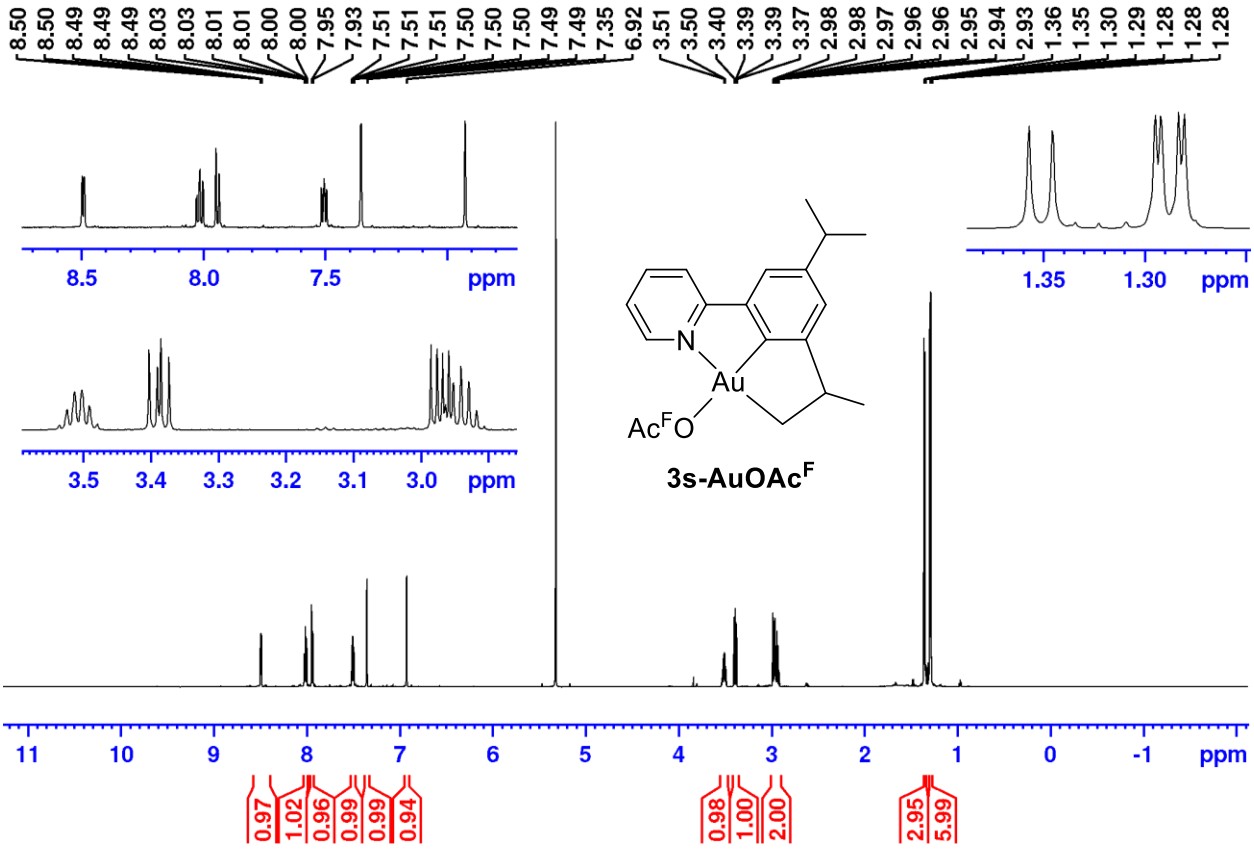


Figure S116. ^{1}H NMR (600 MHz, CD_2Cl_2) of **3s-AuOAc^F**.

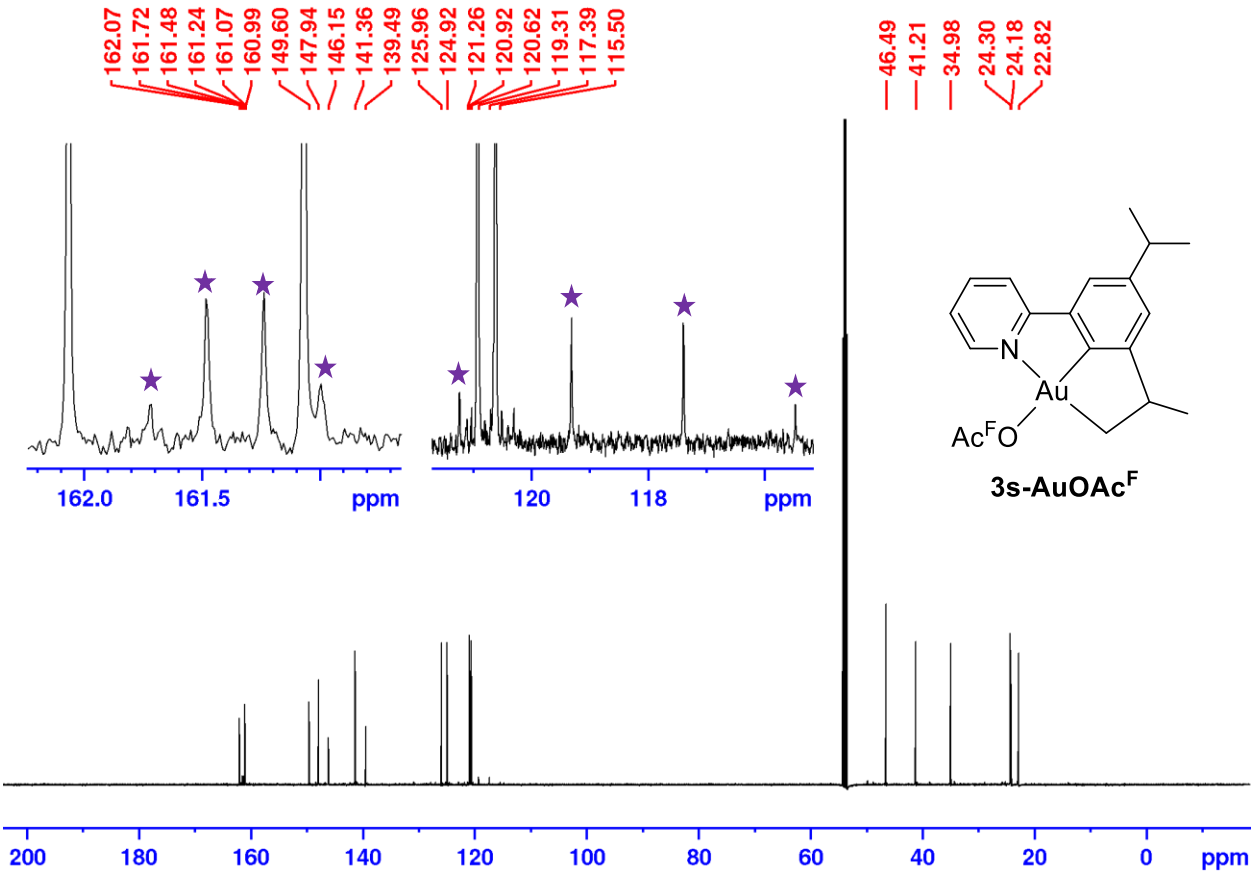


Figure S117. ^{13}C NMR (151 MHz, CD_2Cl_2) of **3s-AuOAc^F**.

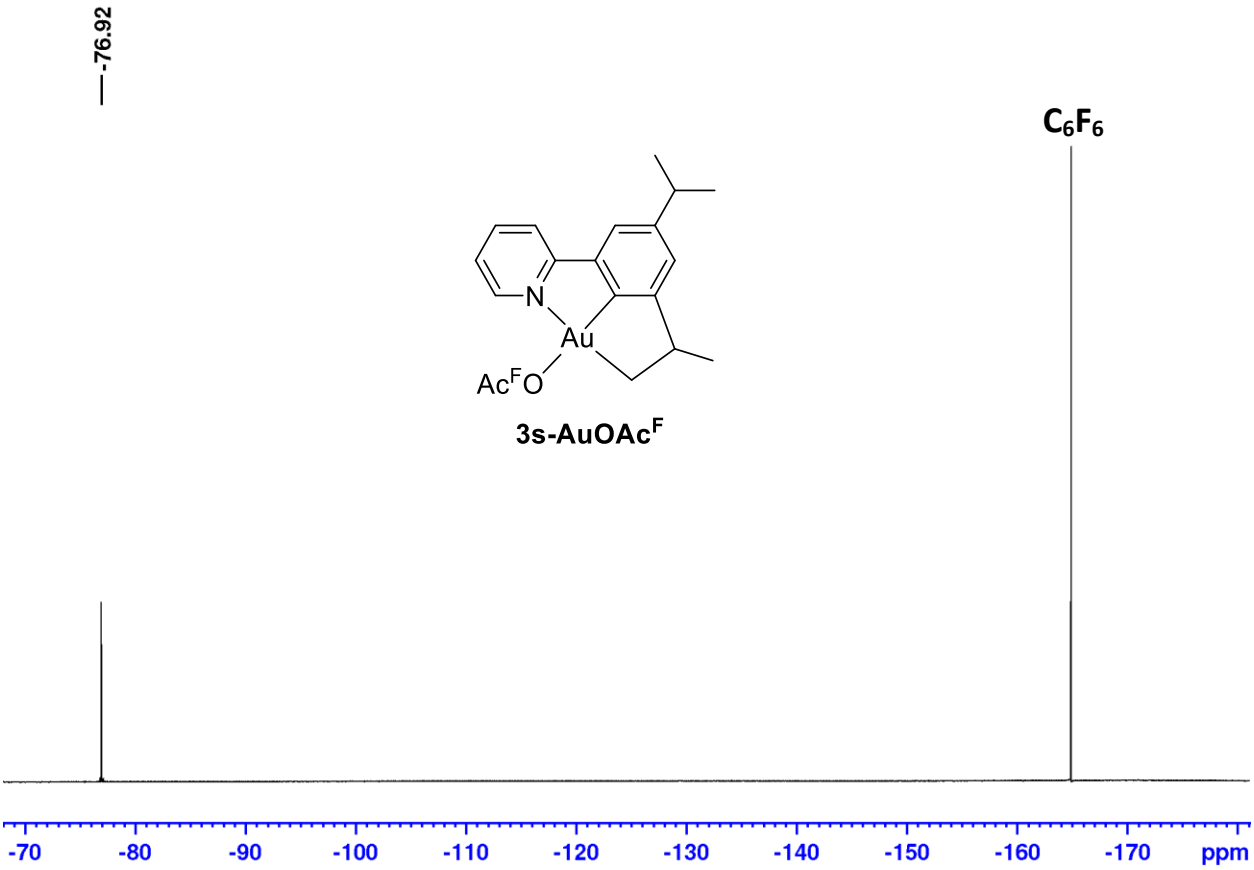


Figure S118. ^{19}F NMR (376 MHz, CD_2Cl_2) of **3s-AuOAc^F**.

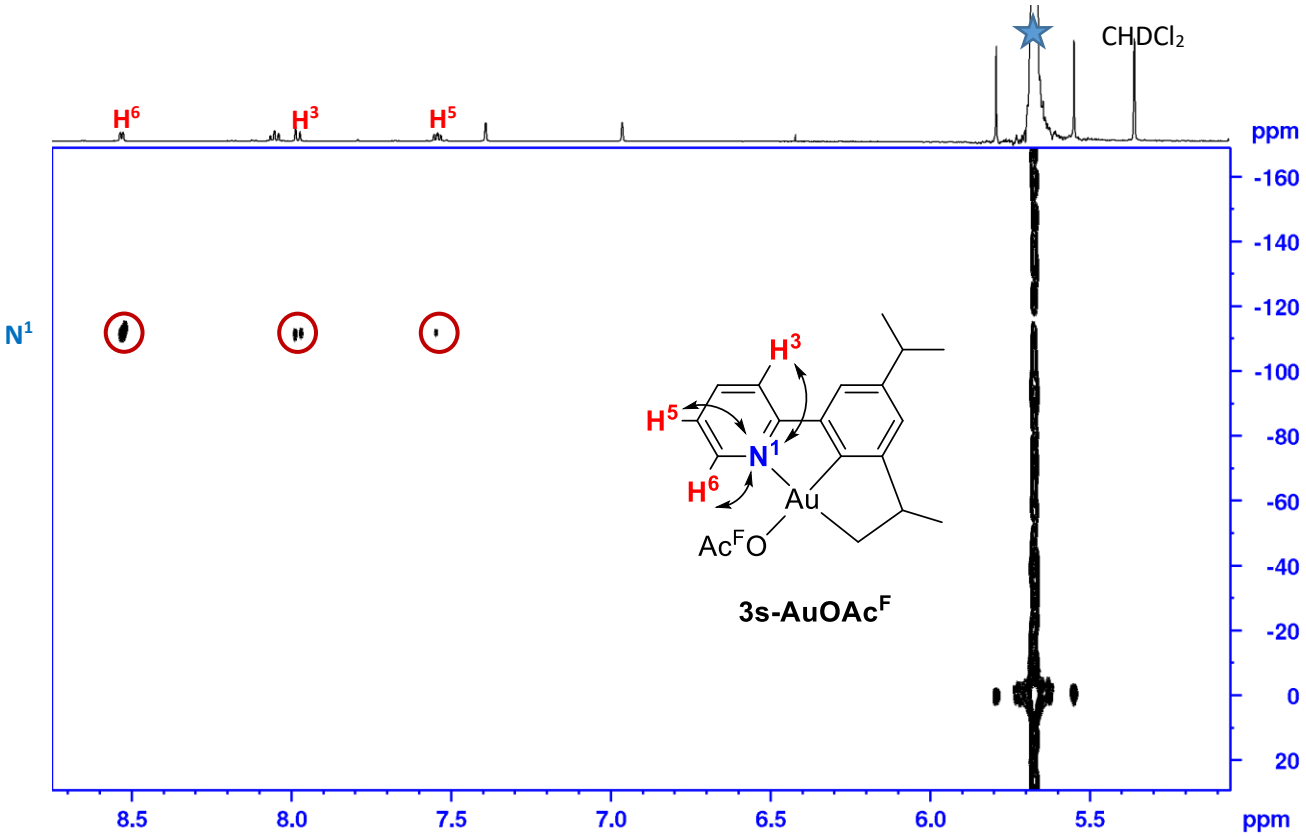
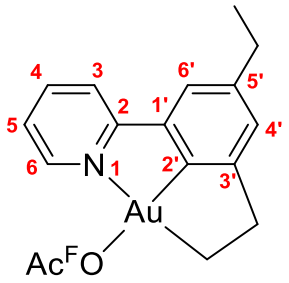


Figure S119. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **3s-AuOAc^{F}**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



3t-AuOAc^F

3t-AuOAc^F. A microwave vessel was charged with $Au(OAc)_3$ (0.0750 g, 0.200 mmol, 1.00 equiv.) and **1t** (0.0440 g, 0.202 mmol, 1.04 equiv.) in a 1:1 mixture of $HOAc^F$ and water (6 mL). The reaction mixture was heated at 80 °C for 3 h in a microwave. The reaction mixture was kept at 4-8 °C overnight. Addition of $HOAc^F$ (2 mL), followed by water (3 mL), furnishing a white precipitate. The precipitate was collected by filtration, and washed with water (3 x 3 mL) and pentane (5 mL). The title compound was obtained as a white solid.

Yield: 0.0680 g, 0.131 mmol, 65 %.

^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.45-8.47 (m, 1H, **H^6**), 7.99-8.01 (m, 1H, **H^4**), 7.90 (d, $^3J_{H,H}$ = 8.0 Hz, 1H, **H^3**), 7.47 (ddd, $^3J_{H,H}$ = 7.6, $^3J_{H,H}$ = 5.4, $^4J_{H,H}$ = 1.3 Hz, 1H, **H^5**), 7.31 (s, 1H, **H$^{6'}$**), 6.99 (s, 1H, **H$^{4'}$**), 3.27–3.30 (m, 2H, Ar-CH_2C**H**$_2$Au), 3.18–3.20 (m, 2H, Ar-C**H**$_2$$CH_2$Au), 2.65 (q, $^3J_{H,H}$ = 7.6 Hz, 2H, Ar-C**H**$_2$$CH_3$), 1.25 ppm (t, $^3J_{H,H}$ = 7.6 Hz, 3H, Ar-CH_2C**H**$_3$).

^{13}C NMR (151 MHz, CD_2Cl_2): δ 162.5 (**C^2**), 161.5 (d (q expected), $^2J_{C,F}$ = 36.3 Hz, O**C**OCF_3), 158.3 (**C$^{3'}$**), 148.2 (**C$^{5'}$**), 148.0 (**C^6**), 145.0 (**C$^{1'}$**), 141.5 (**C^4**), 139.4 (**C$^{2'}$**), 126.9 (**C$^{4'}$**), 125.0 (**C^5**), 122.0 (**C$^{6'}$**), 120.9 (**C^3**), 118.5 (d (q expected), $^1J_{C,F}$ = 290.5 Hz, OCO**C**F_3), 40.3 (Ar-**C**H_2CH_2Au), 32.2 (Ar-CH_2**C**H_2Au), 29.7 (Ar-**C**H_2CH_3), 16.2 ppm (Ar-CH_2**C**H_3).

^{19}F NMR (376 MHz, CD_2Cl_2): δ –76.9 ppm (s, 3F, OCOC**F**$_3$).

^{15}N{^{1}H} NMR (600 MHz, CD_2Cl_2): δ –110.7 ppm (**N^1**).

MS (ESI): *m/z* (rel. %): 406.087 (63) $[M–OCOCF_3]^+$, 424.097 (100) $[M–OCOCF_3+H_2O]^+$, 447.113 (54) $[M–OCOCF_3+MeCN]^+$.

HRMS (ESI): Found: 406.0867; calcd for $C_{15}H_{15}AuN$ $[M–OCOCF_3]^+$: 406.0865.

Elemental Analysis: Anal. calcd. For $C_{17}H_{15}AuF_3NO_2$: C, 39.32; H, 2.91; N, 2.70. Found: C, 39.27; H, 2.87; N, 2.69.

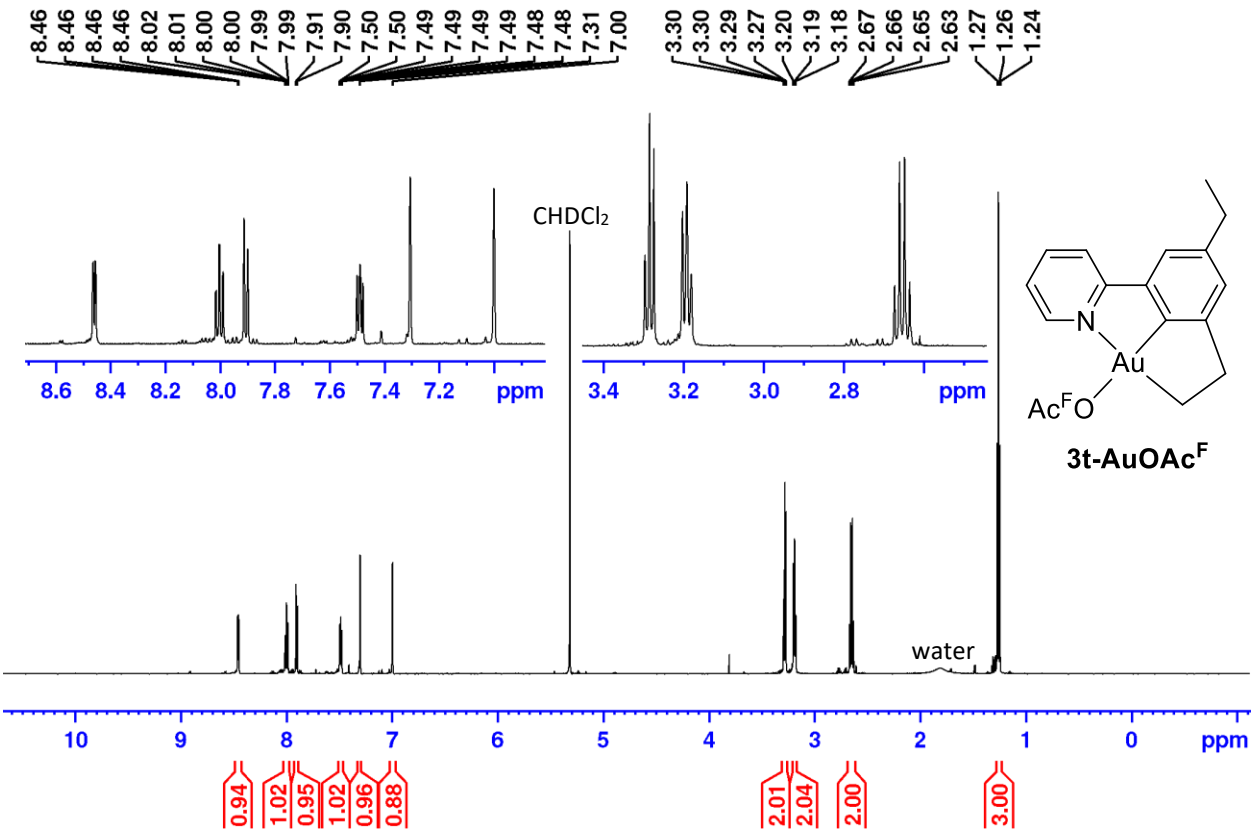


Figure S120. ^{1}H NMR (600 MHz, CD_2Cl_2) of **3t-AuOAc^{F}**.

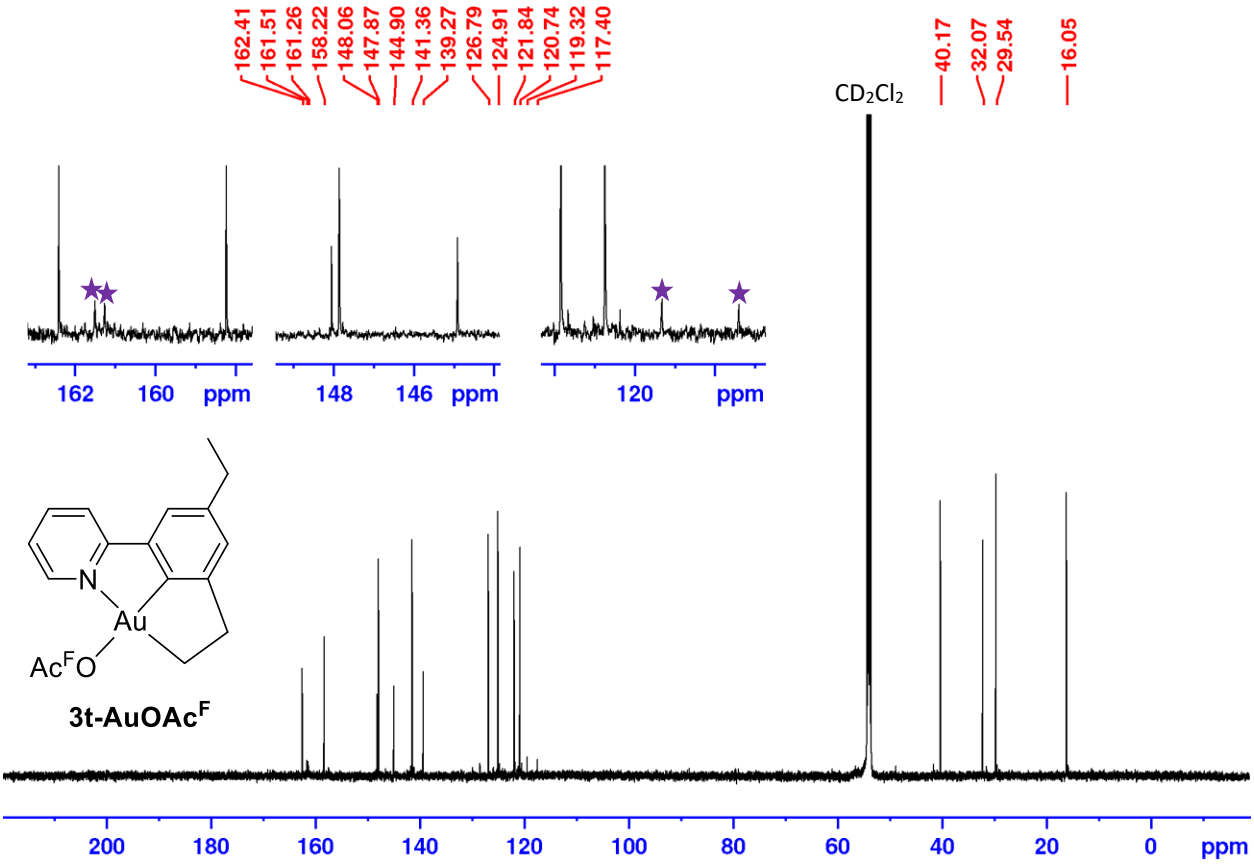


Figure S121. ^{13}C NMR (151 MHz, CD_2Cl_2) of **3t-AuOAc^F**. The doublet (quartet expected) corresponding to the **C**F_3 carbon of the trifluoroacetate ligand is indicated by purple stars in the insert to the right. The doublet (quartet expected) corresponding to the carbonyl carbon of the trifluoroacetate ligand is indicated by purple stars in the insert to the left.

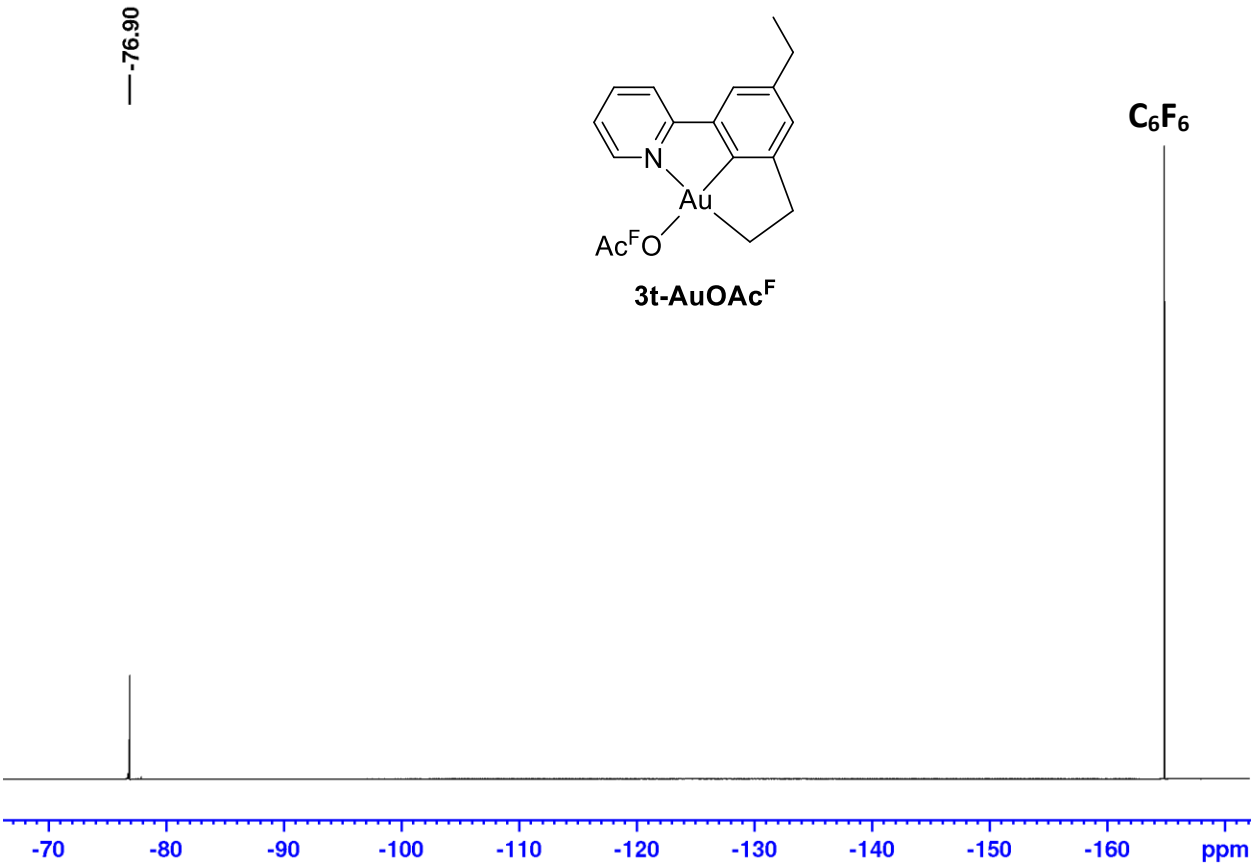


Figure S122. ^{19}F NMR (376 MHz, CD_2Cl_2) of **3t-AuOAc^F**.

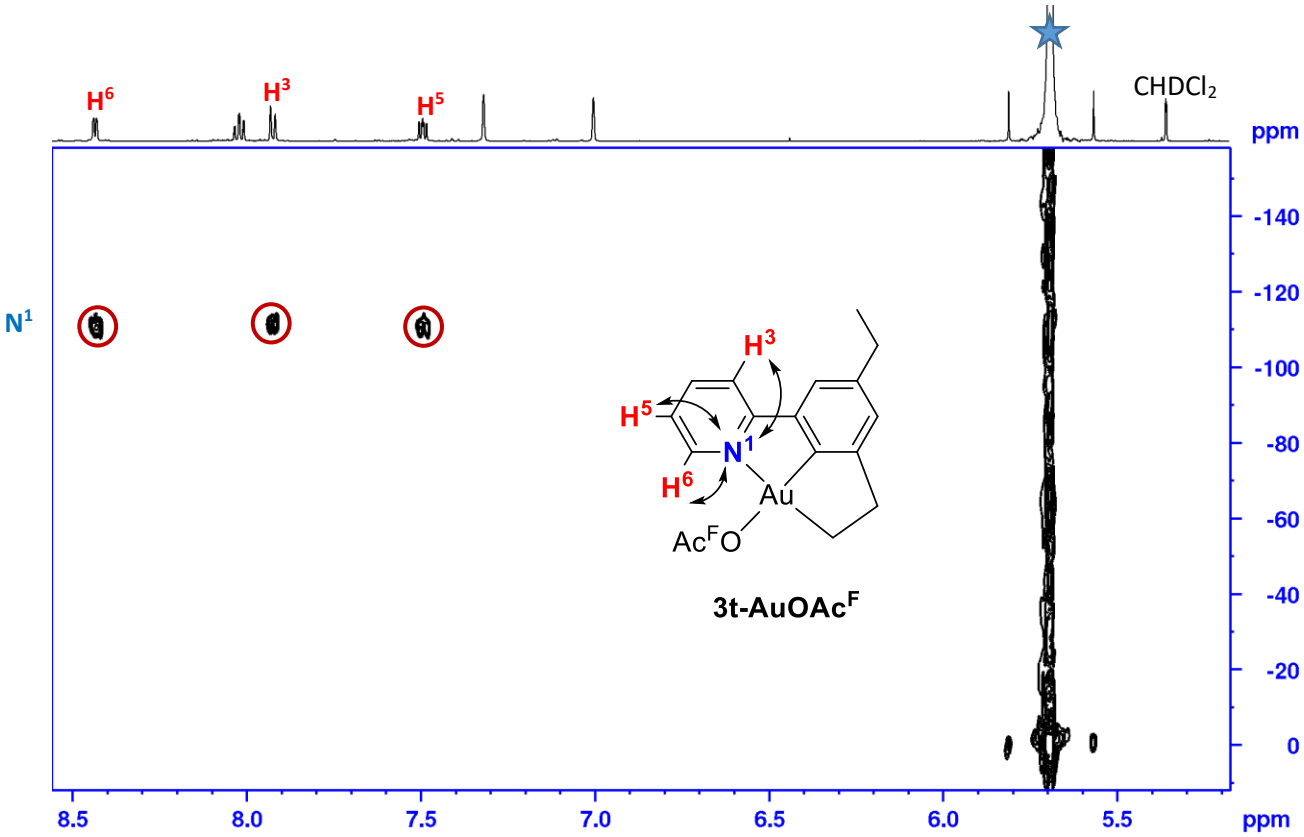


Figure S123. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **3t-AuOAc^{F}**, showing the region between 5.0 ppm and 8.5 ppm. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).

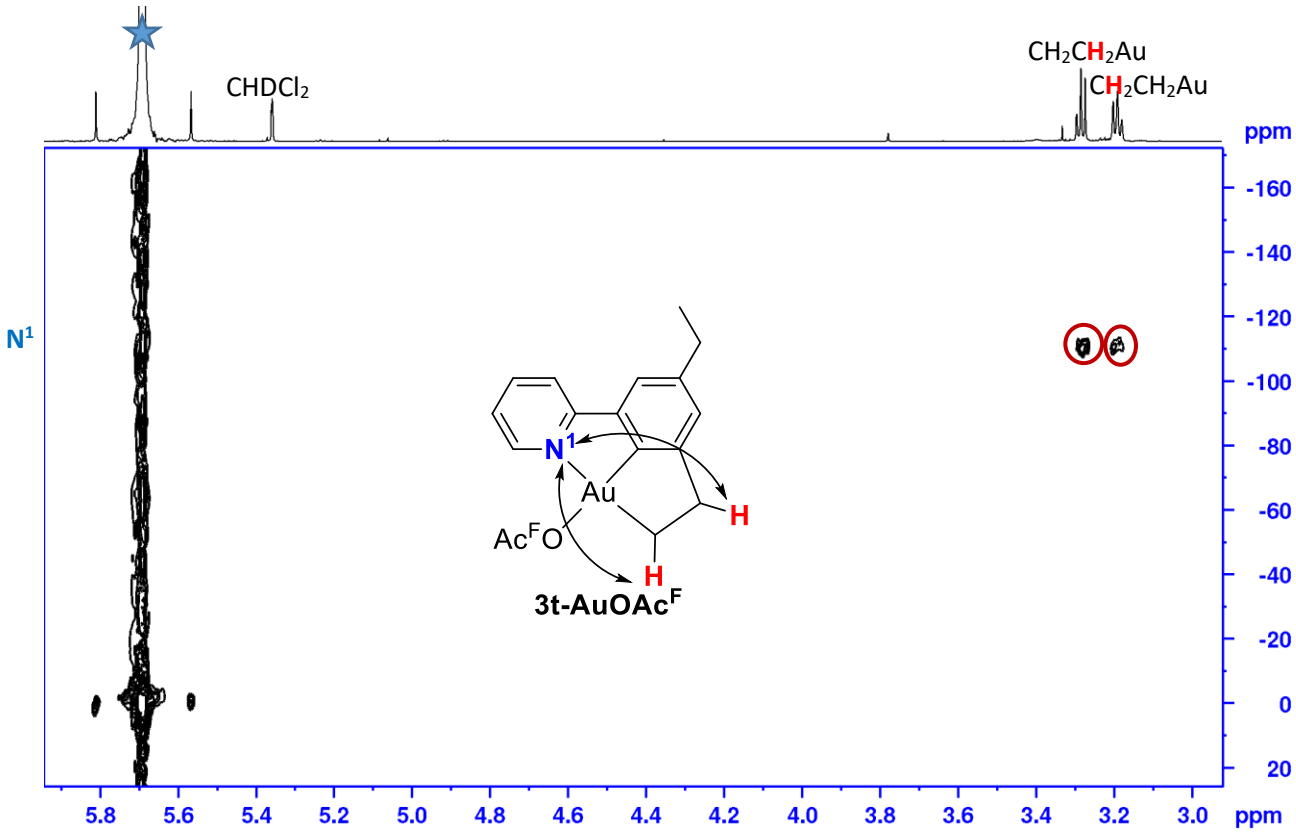
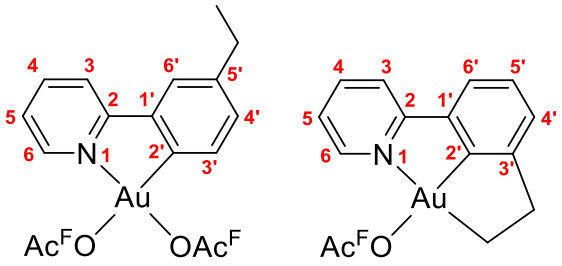


Figure S124. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **3t-AuOAc^{F}**, showing the region between 3.0 ppm and 6.0 ppm. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).



2u-*p*-Au(OAc^F)$_2$ **3u-AuOAc^F**

2u-*p*-Au(OAc^F)$_2$ and 3u-AuOAc^F. A microwave vessel was charged with $Au(OAc)_3$ (0.0750 g, 0.200 mmol, 1.00 equiv.) and **1u** (0.0370 g, 0.202 mmol, 1.01 equiv.) in a 1:1 mixture of $HOAc^F$ and water (6 mL). The reaction mixture was heated at 80 °C for 3 h in a microwave. After cooling to room temperature, water (2 mL) was added to the strongly yellow solution, furnishing a white precipitate The precipitate was collected by filtration and washed with water (3 x 3 mL). The title compounds were obtained as a white solid (0.0630 g). No attempts were made to separate the two complexes. The ratio between **2u-*p*-Au(OAc^F)$_2$** and **3u-AuOAc^F** was determined to be approximately 9:5 in favor of **2u-*p*-Au(OAc^F)$_2$**, based on integration of the ^{1}H NMR spectrum, resulting in an overall yield of 56 % (0.0403 mmol **3u-AuOAc^F**, 20 %; 0.0717 mmol **2u-*p*-Au(OAc^F)$_2$**, 36 %).

Analytical data for 3u-AuOAc^F

^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.48 (d, $^3J_{H,H}$ = 5.0 Hz, 1H, **H^6**), 8.02 (m, 1H, **H^4**), 7.92 (d, $^3J_{H,H}$ = 8.0 Hz, 1H, **H^3**), 7.52–7.50 (m, 1H, **H^5**), 7.47 (d, $^3J_{H,H}$ = 7.7 Hz, 1H, **H$^{6'}$**), 7.25 (m, 1H, **H$^{5'}$**), 7.14 (d, $^3J_{H,H}$ = 8.2 Hz, 1H, **H$^{4'}$**), 3.32 (dd, $^3J_{H,H}$ = 6.4 Hz, $^3J_{H,H}$ = 6.4 Hz, 2H, Ar-CH_2C**H**$_2$Au), 3.24 ppm (dd, 2H, $^3J_{H,H}$ = 6.6 Hz, $^3J_{H,H}$ = 6.6 Hz, Ar-C**H**$_2$$CH_2$Au).

^{13}C NMR (201 MHz, CD_2Cl_2): δ 162.4 (**C^2**), 161.6 (q, $^2J_{C,F}$ = 36.4 Hz, O**C**OCF_3), 158.7 (**C$^{3'}$**), 151.1 (**C$^{2'}$**), 148.0 (**C^6**), 141.7 (**C^4**), 139.6 (**C$^{1'}$**), 128.5 (**C$^{5'}$**), 127.2 (**C$^{4'}$**), 125.2 (**C^5**), 122.3 (**C$^{6'}$**), 121.0 (**C^3**), 118.5 (q, $^1J_{C,F}$ = 290.1 Hz, OCO**C**F_3), 40.5 (Ar-**C**H_2CH_2Au), 32.5 ppm (Ar-CH_2**C**H_2Au).

^{19}F NMR (376 MHz, CD_2Cl_2): δ –76.9 ppm (s, 3F, OCOC**F**$_3$).

MS (ESI): *m/z* (rel. %): 436/438 (48/16) [M–$OCOCF_3$+ $Na^{35/37}Cl]^+$.

HRMS (ESI): Found: 436.0138/438.0109; calcd for $C_{13}H_{11}AuClNNa$ [M–$OCOCF_3$+$Na^{35/37}Cl]^+$: 436.0143/438.0114.

Analytical data for 2u-*p*-Au(OAc^{F})$_2$

^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.56 (d, $^{3}J_{H,H}$ = 5.9 Hz, 1H, **H^{6}**), 8.22 (m, 1H, **H^{4}**), 7.95 (d, $^{3}J_{H,H}$ = 8.1 Hz, 1H, **H^{3}**), 7.53–7.51 (m, 1H, **H^{5}**), 7.38 (d, $^{3}J_{H,H}$ = 1.9 Hz, 1H, **H$^{6'}$**), 7.16 (dd, $^{3}J_{H,H}$ = 8.4 Hz, $^{4}J_{H,H}$ = 2.0 Hz, 1H, **H$^{4'}$**), 6.98 (d, $^{3}J_{H,H}$ = 8.3 Hz, 1H, **H$^{3'}$**), 2.74 (q, $^{3}J_{H,H}$ = 7.6 Hz, 2H, C**H**$_2$), 1.29 ppm (t, $^{3}J_{H,H}$ = 7.6 Hz, 3H, C**H**$_3$).

^{13}C NMR (201 MHz, CD_2Cl_2): δ 165.4 (**C^{2}**), 161.5 (q, $^{2}J_{C,F}$ = 37.8 Hz, O**C**OCF$_3$), 160.9 (q, $^{2}J_{C,F}$ = 39.2 Hz, O**C**OCF$_3$), 148.3 (**C^{6}**), 147.7 (**C$^{5'}$**), 144.9 (**C^{4}**), 141.6 (**C$^{1'}$**), 140.6 (**C$^{2'}$**), 132.4 (**C$^{4'}$**), 128.8 (**C$^{3'}$**), 125.9 (**C$^{6'}$**), 125.3 (**C^{5}**), 122.1 (**C^{3}**), 118.5 (q, $^{1}J_{C,F}$ = 289.0 Hz, OCO**C**F$_3$), 116.2 (q, $^{1}J_{C,F}$ = 287.9 Hz, OCO**C**F$_3$), 29.0 (**C**H$_2$), 15.7 ppm (**C**H$_3$).

^{19}F NMR (376 MHz, CD_2Cl_2): δ –76.1 (s, 3F, OCOC**F**$_3$), –77.1 ppm (s, 3F, OCOC**F**$_3$).

MS (ESI): *m/z* (rel. %): 482 (20) [M–2(OCOCF$_3$)+^{35}Cl+CO$_2$H]$^{+}$.

HRMS (ESI): Found: 482.0192/484.0163; calcd for $C_{13}H_{11}AuClNNa$ [M–2(OCOCF$_3$)+$^{35/37}$Cl+CO$_2$H]$^{+}$: 482.0198/484.0169.

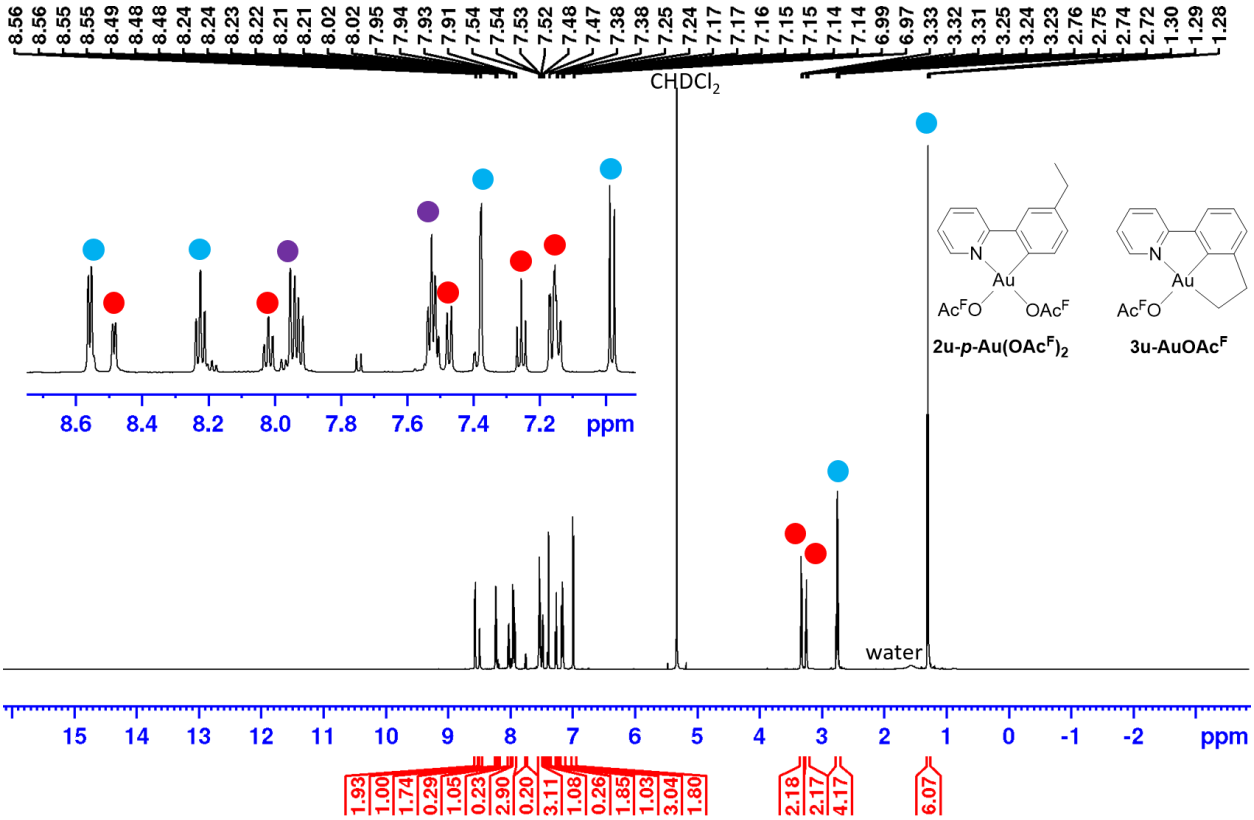


Figure S125. ^{1}H NMR (600 MHz, CD_2Cl_2) of a mixture of **3u-AuOAc^F** and **2u-*p*-Au(OAc^F)$_2$**. Resonances arising from **3u-AuOAc^F** are marked with red circles, resonances arising from **2u-*p*-Au(OAc^F)$_2$** are marked with blue circles and overlapping resonances are marked with purple circles.

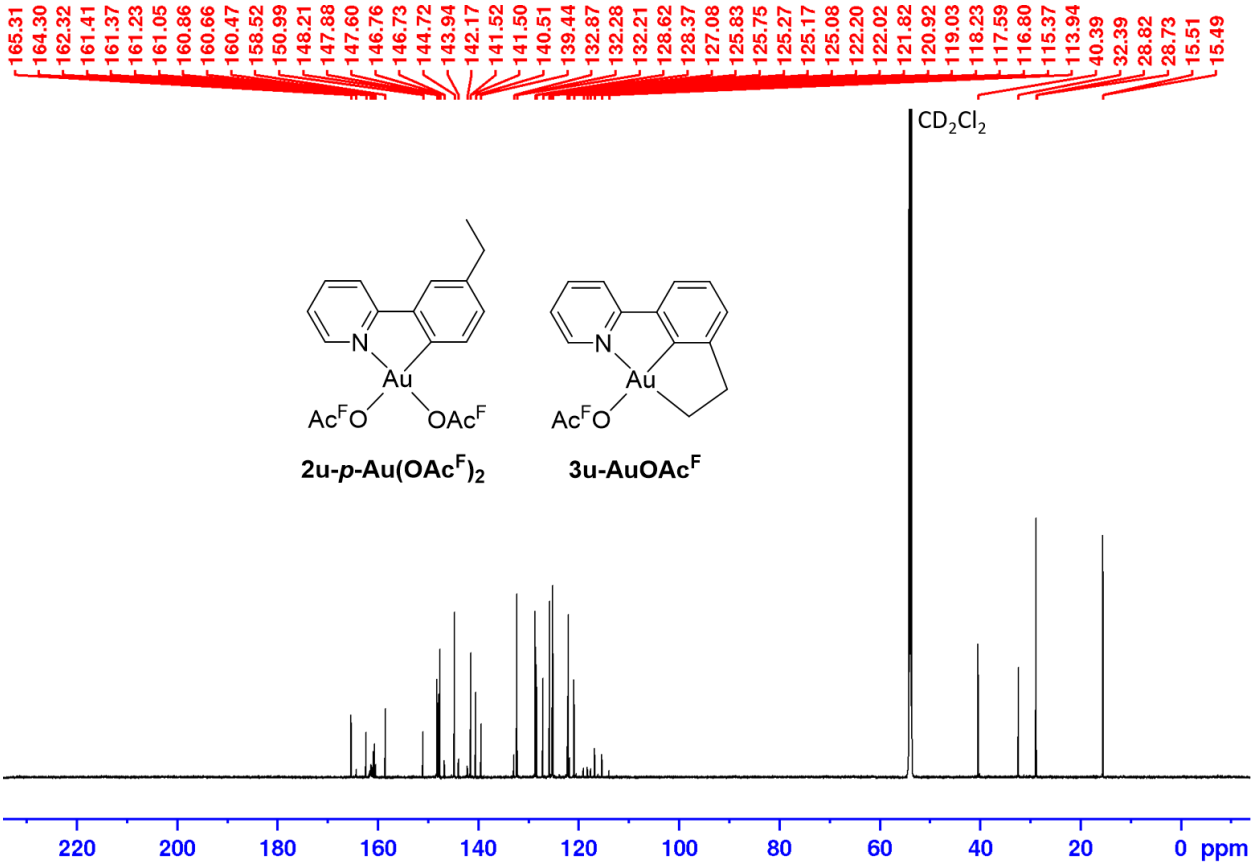


Figure S126. ^{13}C NMR (201 MHz, CD_2Cl_2) of a mixture of **3u-AuOAc^F** and **2u-*p*-Au(OAc^F)$_2$**.

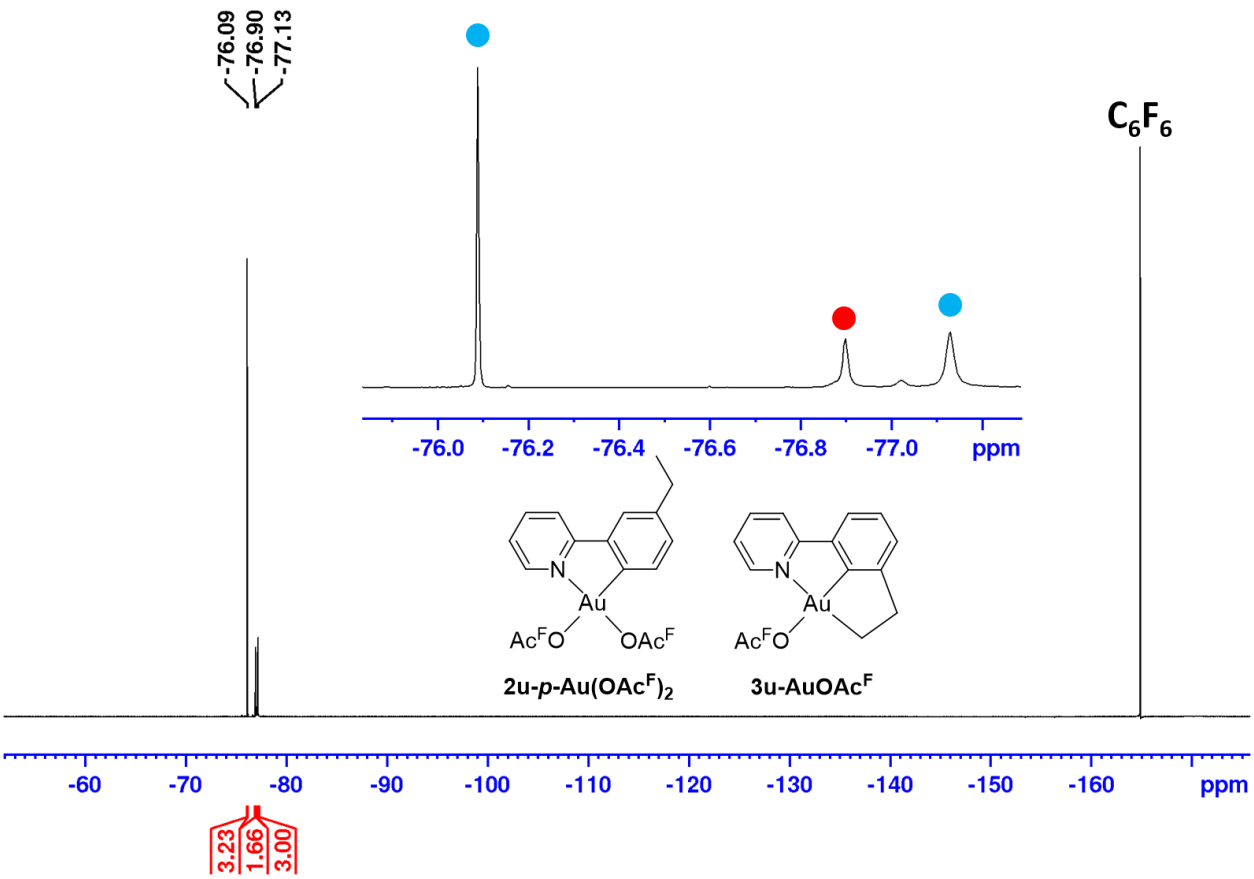


Figure S127. ^{19}F NMR (376 MHz, CD_2Cl_2) of a mixture of **3u-AuOAc^F** and **2u-*p*-Au(OAc^F)$_2$**. The resonance arising from **3u-AuOAc^F** is marked with a red circle and the resonances arising from **2u-*p*-Au(OAc^F)$_2$** are marked with blue circles.

^{1}H-^{15}N HMBC spectra of previously reported Au(III) complexes

For δ^{15}N of each compound, see Table S1. The spectra are presented in Figure S128—Figure S136.

Table S1. Overview of δ^{15}N for a selection of the complexes studied herein, as well as relevant previosuly reported Au(III) complexes.[1-5, 39] $\delta^{15}N_{ligand}$ are given as well, together with the coordination shifts ($\Delta\delta^{15}$N) and Au-N bond lengths from the corresponding crystal structure, if available. The data were collected through ^{1}H-^{15}N HMBC experiments (600 or 800 MHz). All measurements were done in CD_2Cl_2. Unless otherwise noted, the data (NMR and X-ray diffraction) were collected in this work.

Complex	δ^{15}N	$\delta^{15}N_{ligand}$	$\Delta\delta^{15}$N	Au-N [Å]	Ligand *trans* to pyridine-N	Ligand *cis* to pyridine-N
1f-Au(OAc^F)$_3$	−186.5	−72.2	−114.0	n/a	[OAc^F]$^-$	
2d-Au(OAc^F)$_2$	−160.4	−64.9	−95.5	2.013(4)		
2h-Au(OAc^F)$_2$	−167.1	−72.6	−94.5	1.9996(19)		
2i-Au(OAc^F)$_2$	−161.7	−73.5	−88.2	2.034(3)		
2l-Au(OAc^F)$_2$	−187.1	−94.2	−92.9	1.999(4)		
2m-Au(OAc^F)$_2$	−187.7	−121.5	−66.1	2.0426(17)		
2n-Au(OAc^F)$_2$	−164.9	−63.9	−101.0	1.9974(19)		
2p-Au(OAc^F)$_2$	−163.9	−59.4	−104.5	2.008(3)		
2r-Au(OAc^F)$_2$	−167.7	−73.0	−94.0	1.999(12)		
2a-Au(OAc^F)$_2$	−165.6	−74.9	−90.7	1.991(6)[1]	[OAc^F]$^-$	[OAc^F]$^-$
2a-Au(OAc)$_2$	−164.4	−74.9	−89.5	n/a	[OAc]$^-$	[OAc]$^-$
2a-Au(CH_2=$CHCH_2$)Br	−122.6	−74.9	−47.7	2.11(3)[5]	CH_2=$CHCH_2^-$	Br^-
2a-Au(C_6H_5)Br	−127.9	−74.9	−53.0	2.121(3)[40]	$C_6H_5^-$	Br^-
2a-Au(CH_3)Br	−121.6	−74.9	−46.7	2.1280(17)[40]	CH_3^-	Br^-
2a-Au(CH_3)$_2$	−131.0	−74.9	−56.1	2.130(3)[1]	CH_3^-	CH_3^-
[2a-Au(C,N)]$^+$[OAc^F]$^-$	−129.0[39]	−74.9	−54.1	2.126(2)[39]	-$OCH_2CH_2^-$	-OC(CH_3)=NH
3b-AuOAc^F	−111.6	−72.4	−39.2	2.135(3)[2]	Ar$C(CH_3)_2CH_2^-$	[OAc^F]$^-$
3s-AuOAc^F	−111.7	−73.6	−38.1	2.144(3)	Ar$CH(CH_3)CH_2^-$	[OAc^F]$^-$
3t-AuOAc^F	−110.7	−73.6	−37.1	2.15(2)	Ar$CH_2CH_2^-$	[OAc^F]$^-$

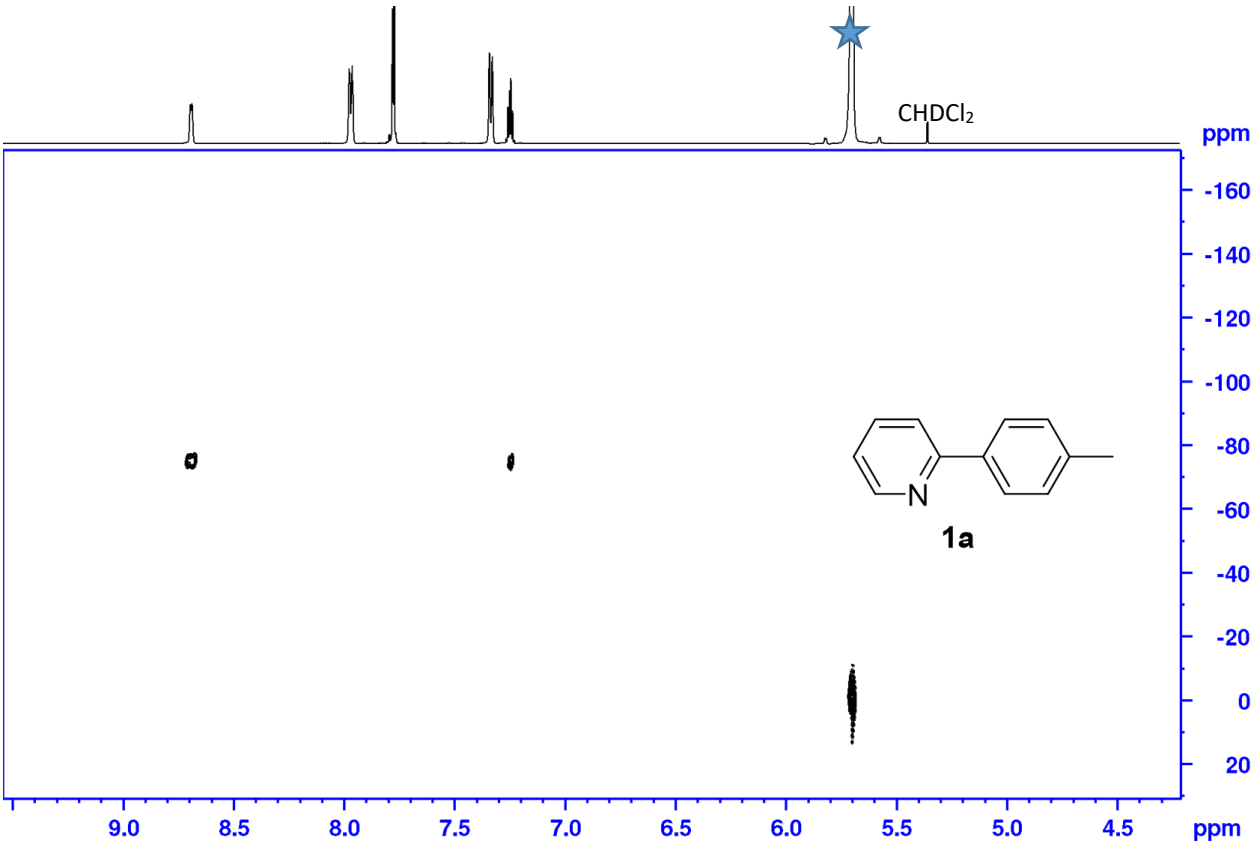


Figure S128. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1a**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).

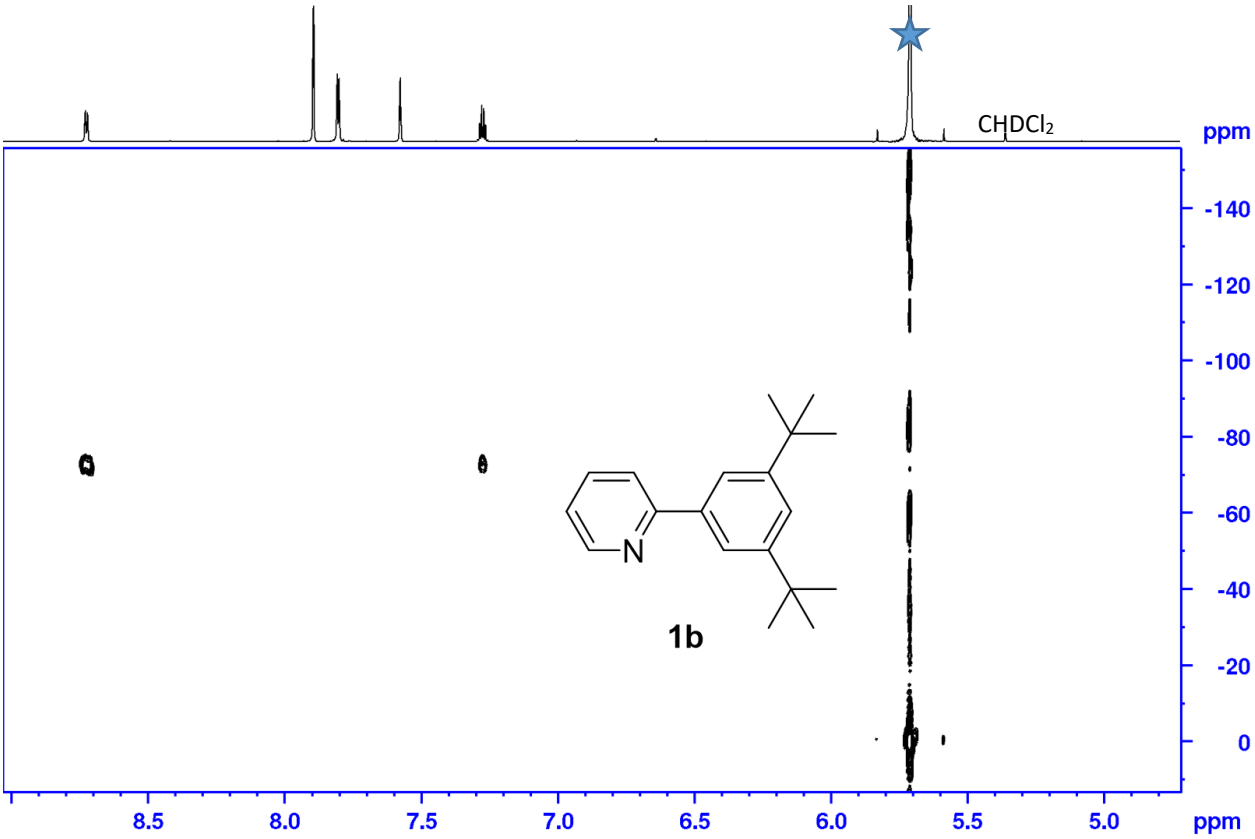


Figure S129. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **1b**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).

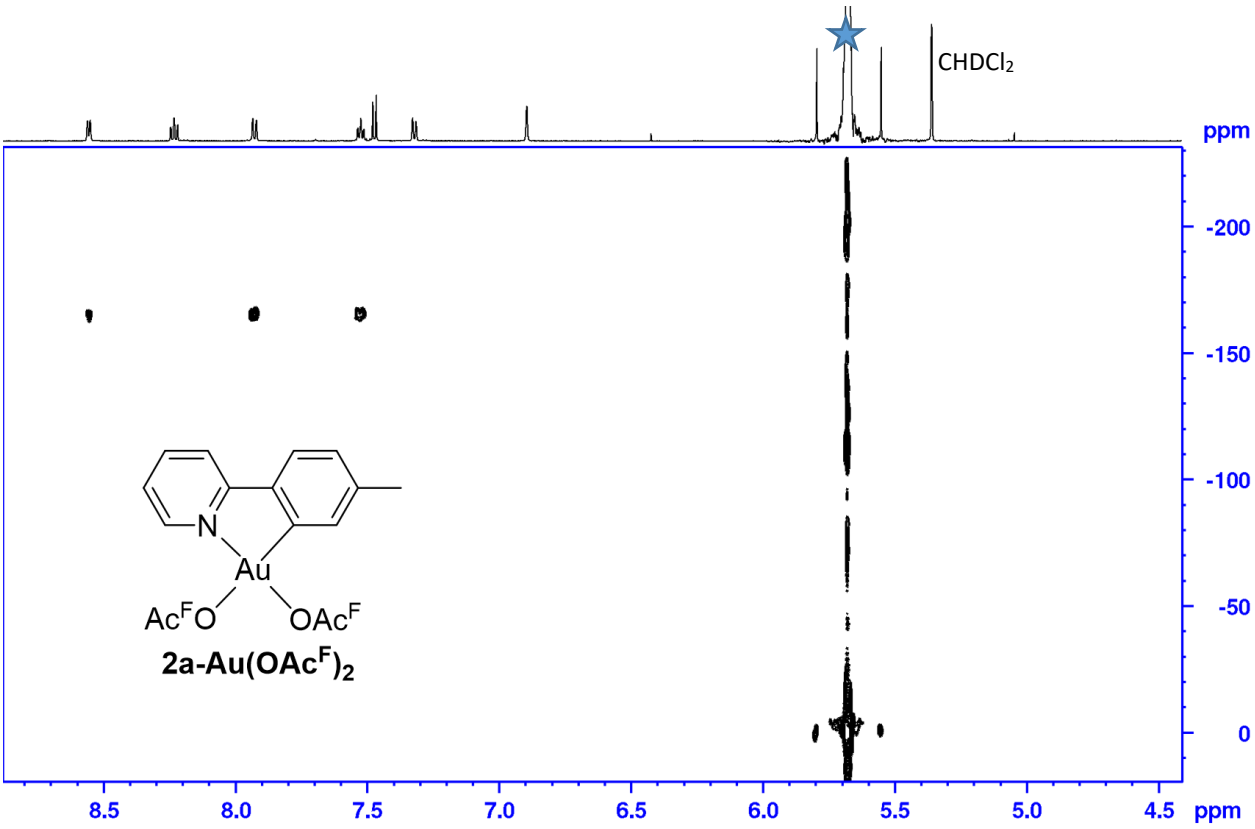


Figure S130. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **2a-Au(OAc^{F})$_2$**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).

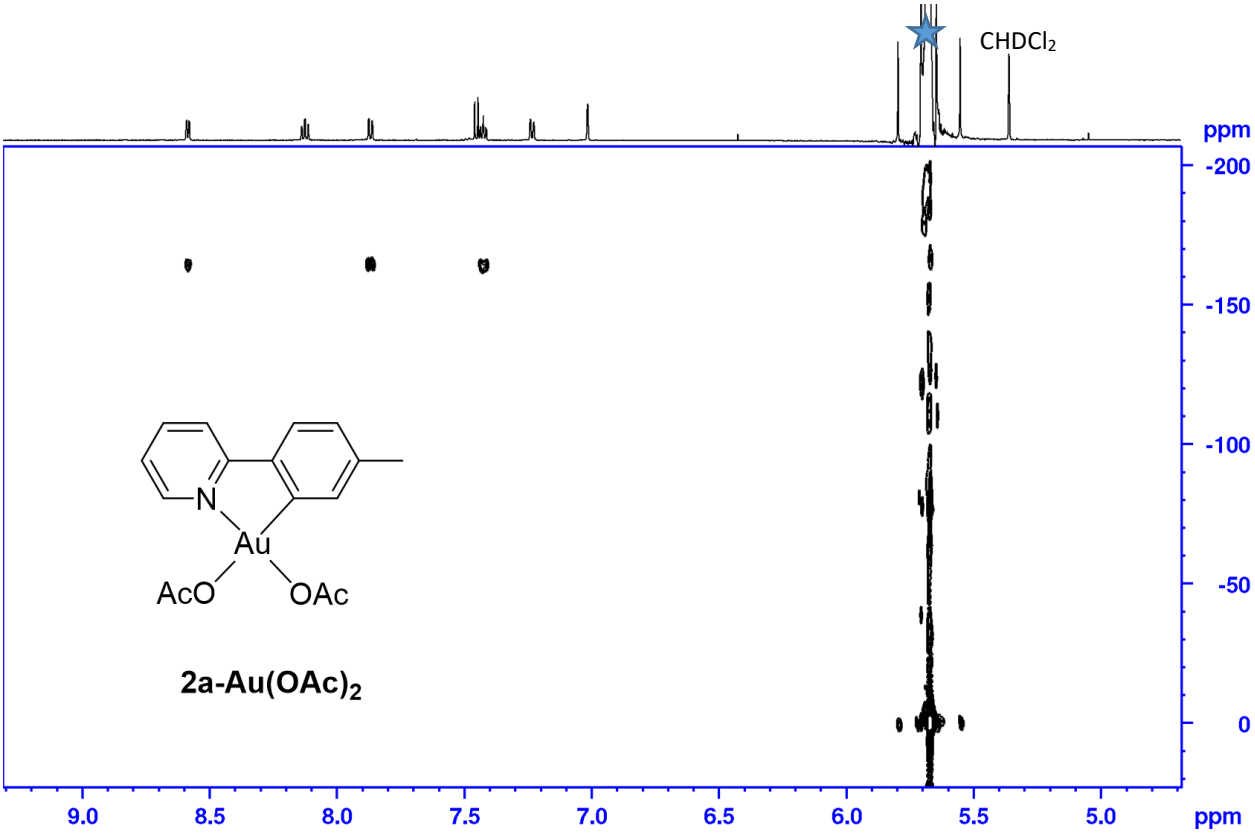


Figure S131. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **2a-Au(OAc)$_2$**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).

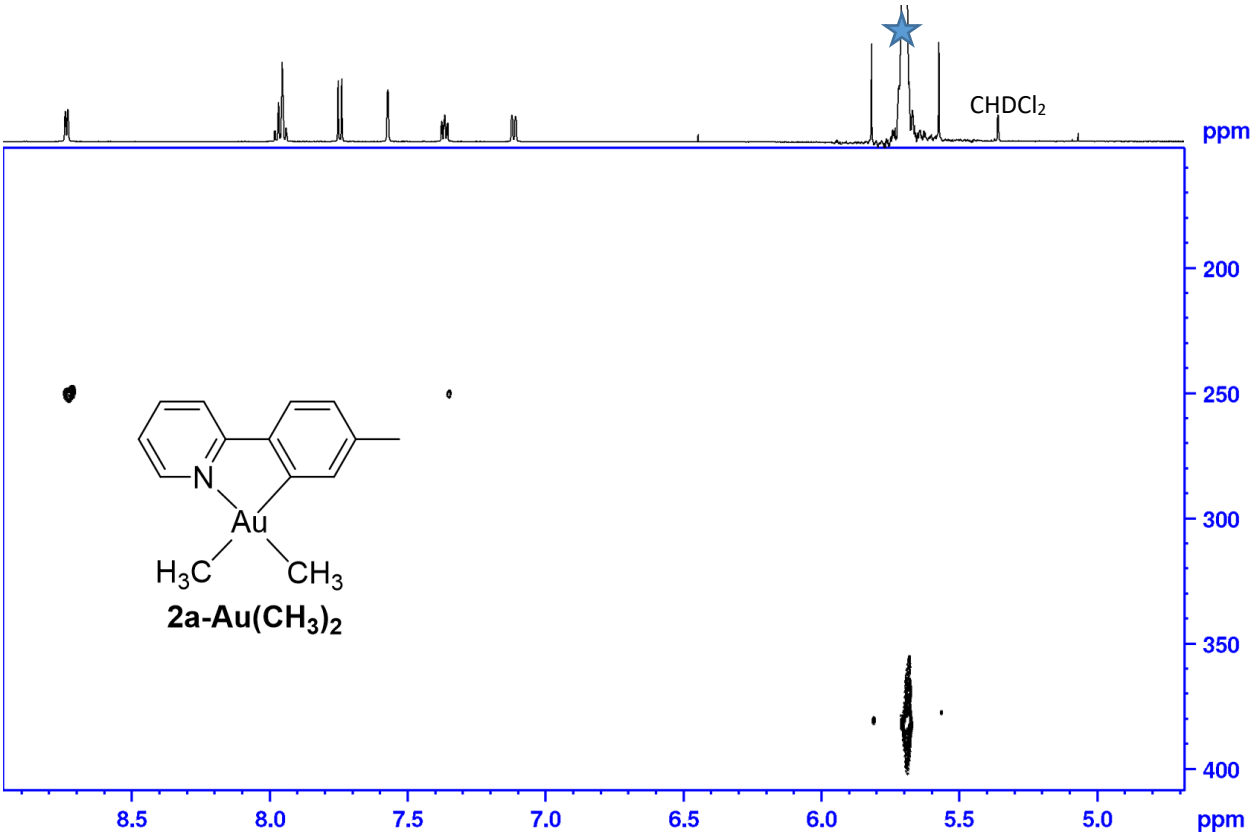


Figure S132. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **2a-Au(CH_3)$_2$**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).

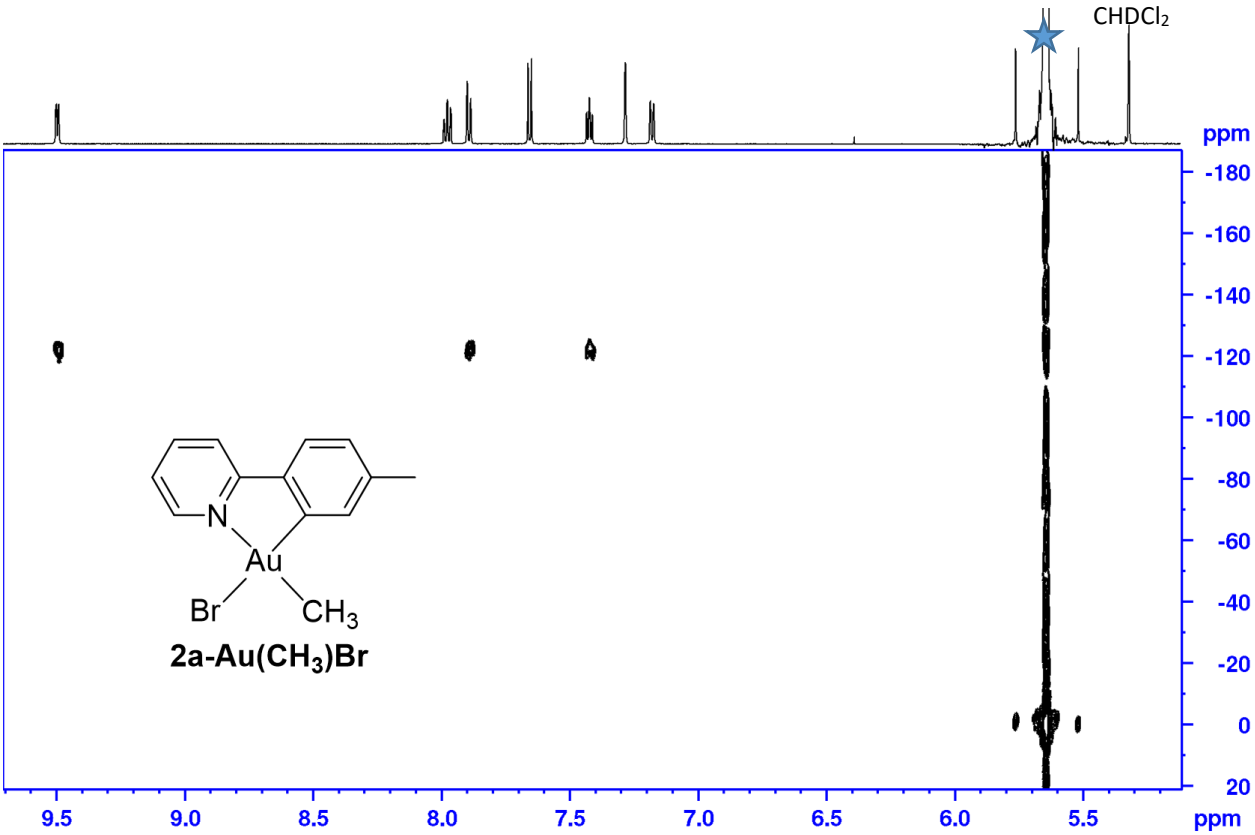


Figure S133. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **2a-Au(CH_3)Br**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).

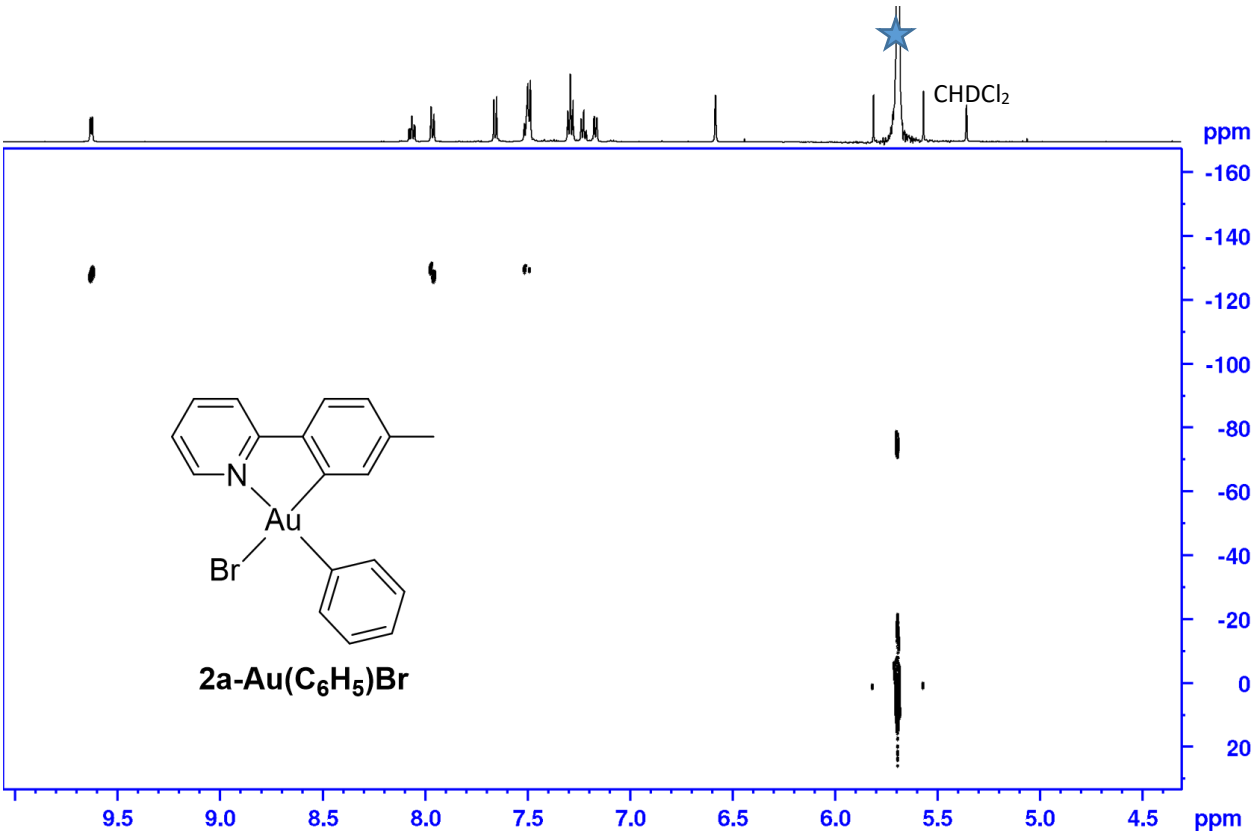


Figure S134. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **2a-Au(C_6H_5)Br**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).

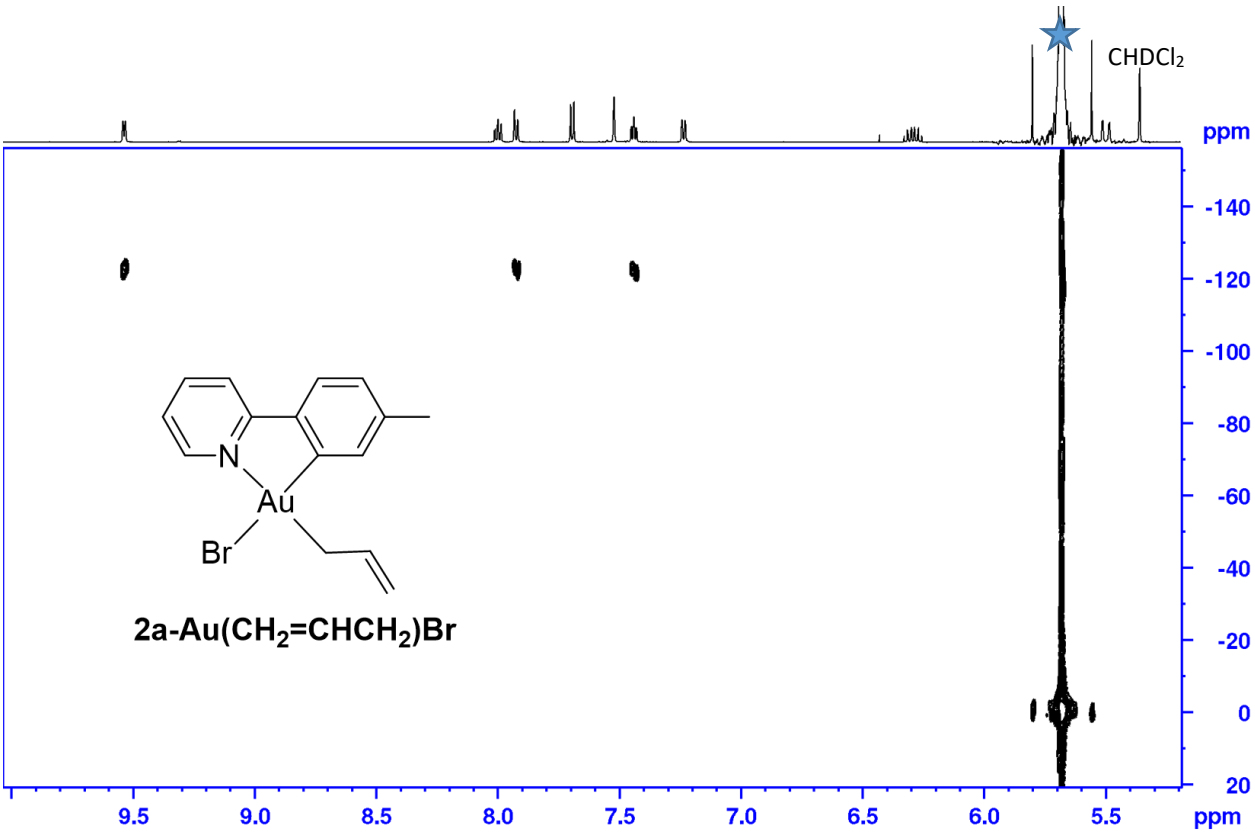


Figure S135. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **2a-Au(CH_2=$CHCH_2$)Br**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).

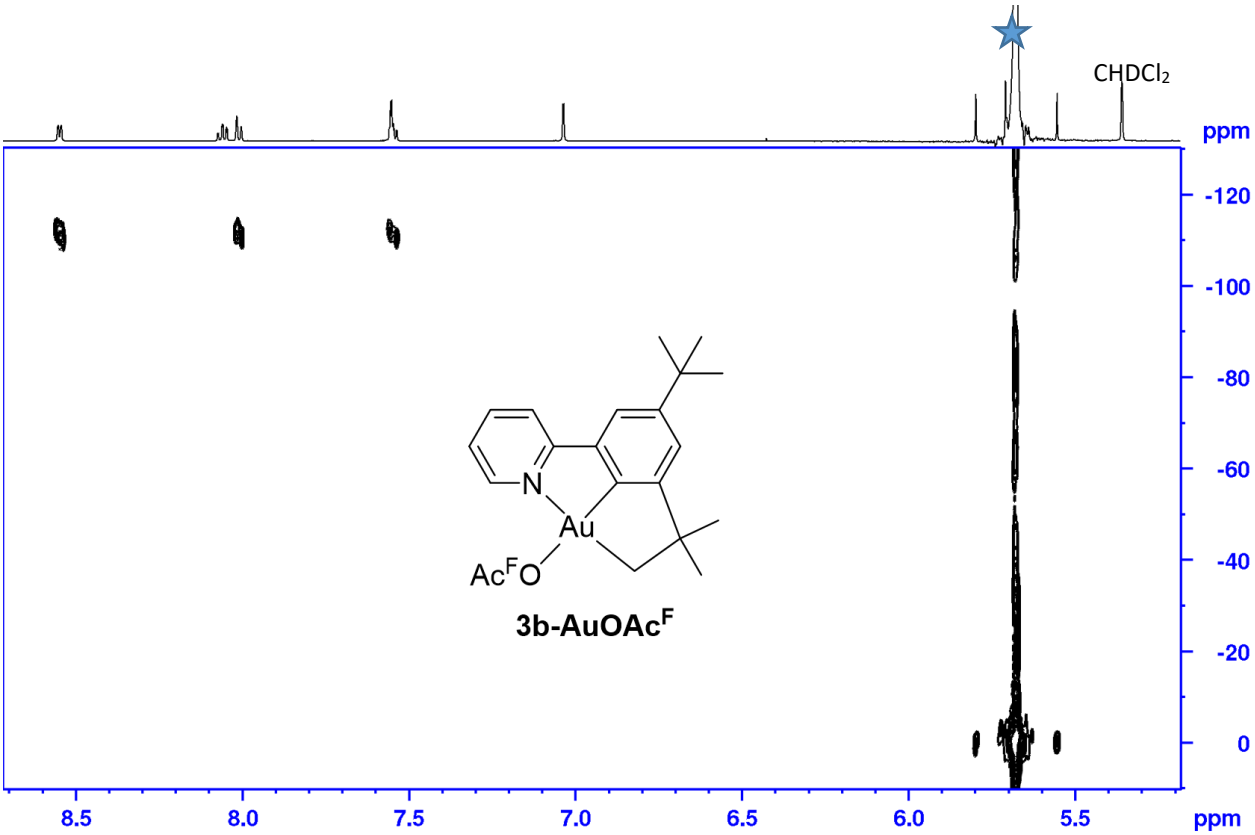


Figure S136. ^{1}H-^{15}N HMBC (600 MHz, CD_2Cl_2) of **3b-AuOAc^{F}**. The chemical shifts have been calibrated using CH_3NO_2 as an external standard (blue star in the projection).

Crystallographic methods

Single-crystal diffraction data were acquired on a Bruker D8 Venture equipped with a Photon 100 CMOS area detector, and using Mo Kα radiation (λ = 0.71073 Å) or Cu Kα radiation (λ = 1.5406 Å) from an Incoatec iμS microsource. Data reduction was performed with the Bruker Apex3 Suite, the structures were solved with ShelXT[41] and refined with ShelXL.[42] Olex2 was used as user interface.[43] The cif files were edited with enCIFer v. 1.4.[44] Full details of the data collection, structure solution and refinement for each compound are contained in the cif files, available from https://www.ccdc.cam.ac.uk/ (CCDC numbers: 2115512 (**2c-Au(OAc^F)$_2$**), 2122527 (**2d-Au(OAc^F)$_2$**), 2085151 (**2e-Au(OAc^F)$_2$**), 2086346 (**2h-Au(OAc^F)$_2$**), 2126159 (**2i-Au(OAc^F)$_2$**), 2126283 (**2j$_3$Au$_2$(OAc^F)$_2$**), 2122284 (**2l-Au(OAc^F)$_2$**), 2111917 (**2m-Au(OAc^F)$_2$**), 2105655 (**2n-Au(OAc^F)$_2$**), 2086931 (**2o-Au(OAc^F)$_2$**), 2126114 (**2p-Au(OAc^F)$_2$**), 2130186 (**2r-Au(OAc^F)$_2$**), 2126097 (**3s-AuOAc^F**) and 2114274 (**3t-AuOAc^F**)). The data are summarized in Table S2–Table S15. For comments on level A and/or level B alerts in the cifs of **2j$_3$Au$_2$(OAc^F)$_2$** and **3t-AuOAc^F**, see the text below Figure S147 and Figure S162, respectively.

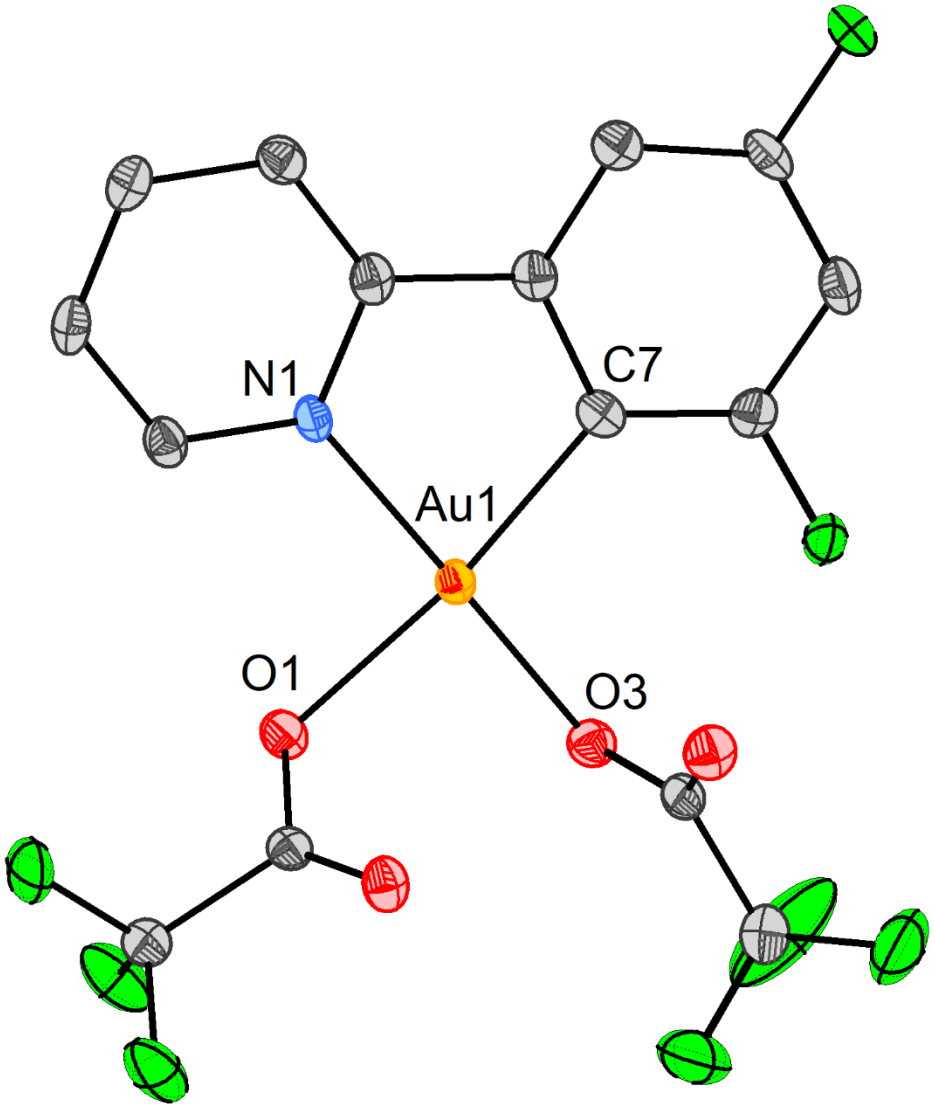


Figure S137. ORTEP plot of **2c-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms have been omitted for clarity.

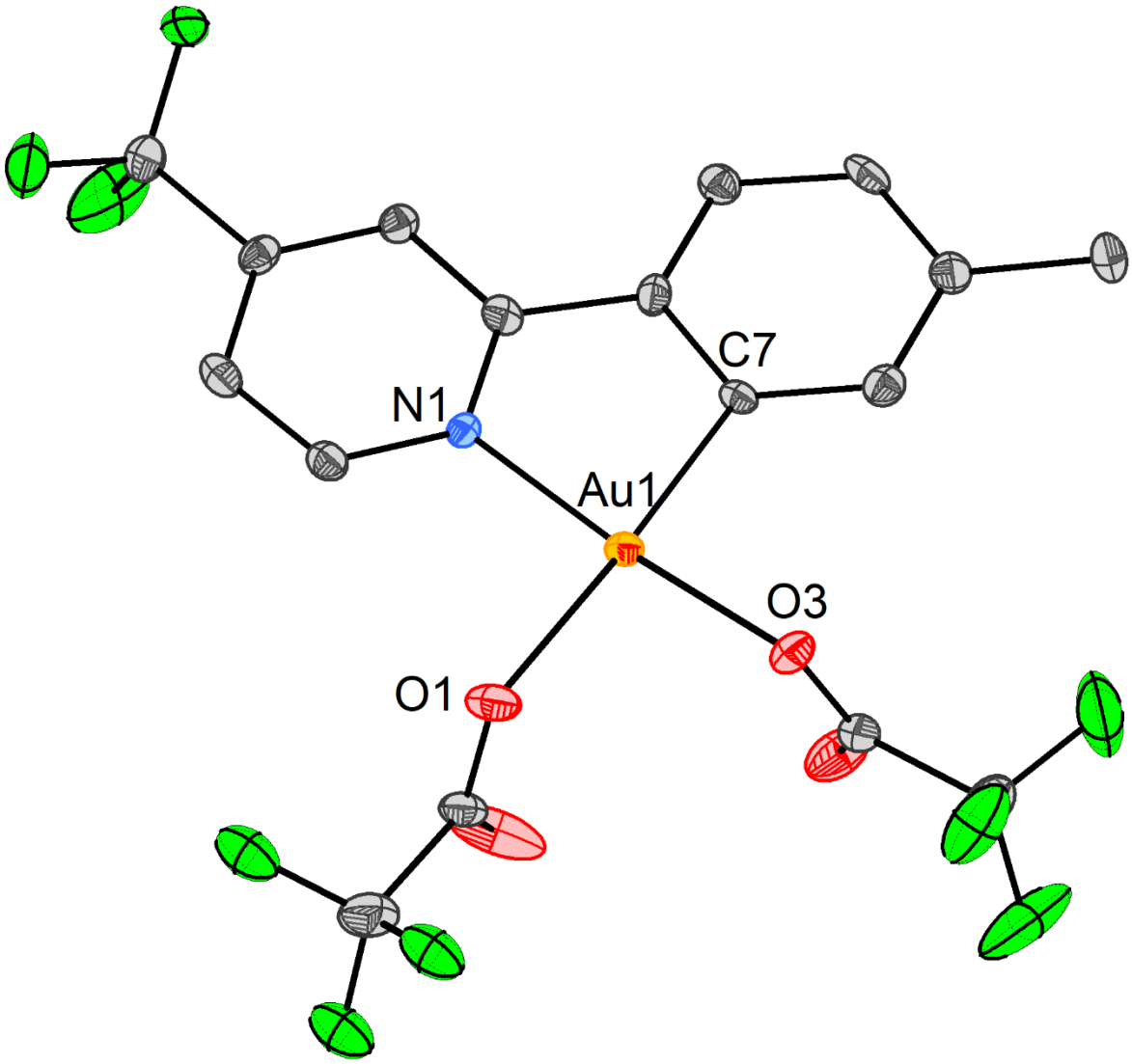


Figure S138. ORTEP plot of **2d-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Only one of the two molecules in the asymmetric unit is shown. Hydrogen atoms, disorder in the trifluoroacetate ligand *trans* to C7, and an associated CH_2Cl_2 molecule (solvent of crystallization) have been omitted for clarity.

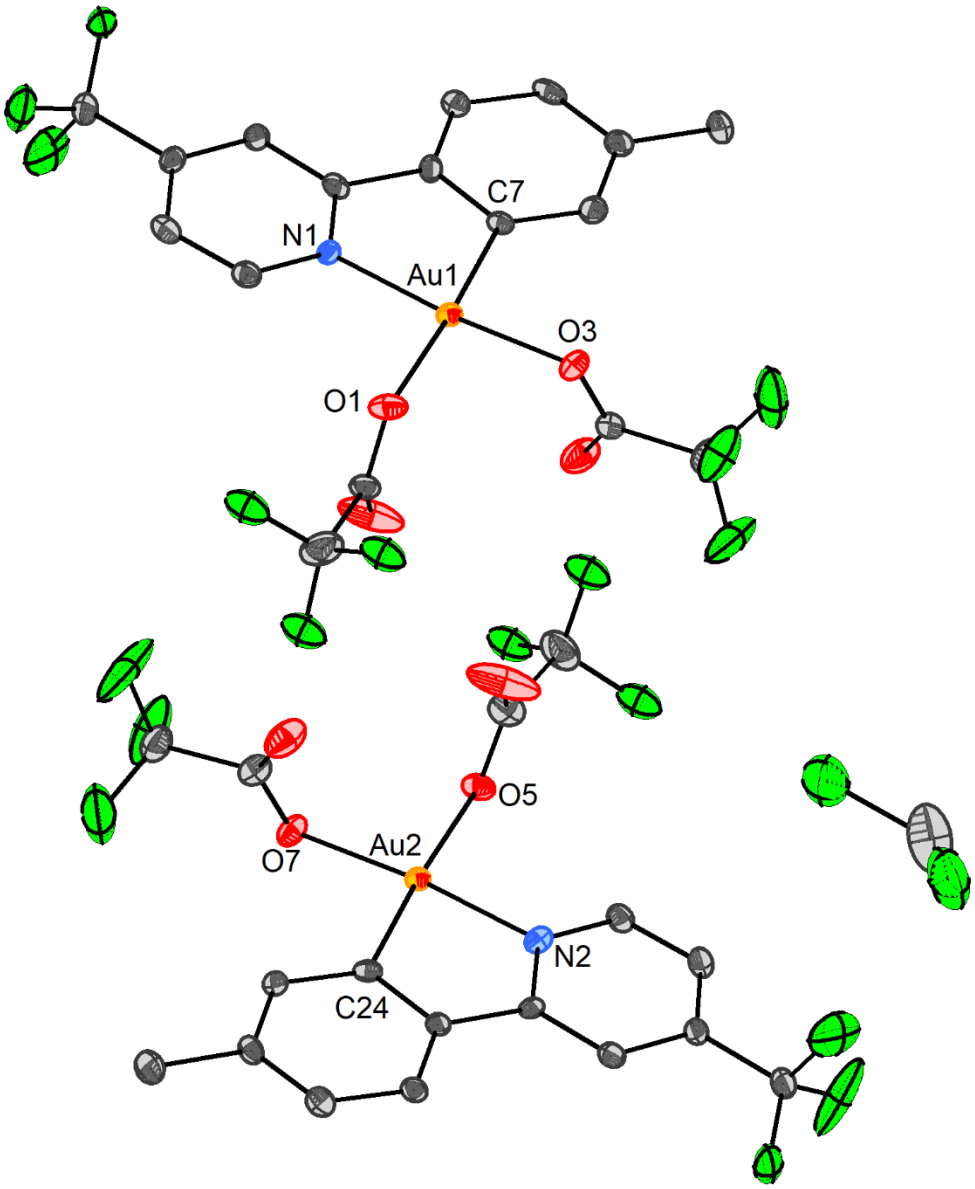


Figure S139. ORTEP plot of **2d-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Both molecules in the asymmetric unit are shown. Hydrogen atoms and disorder in the trifluoroacetate ligand *trans* to C7 have been omitted for clarity.

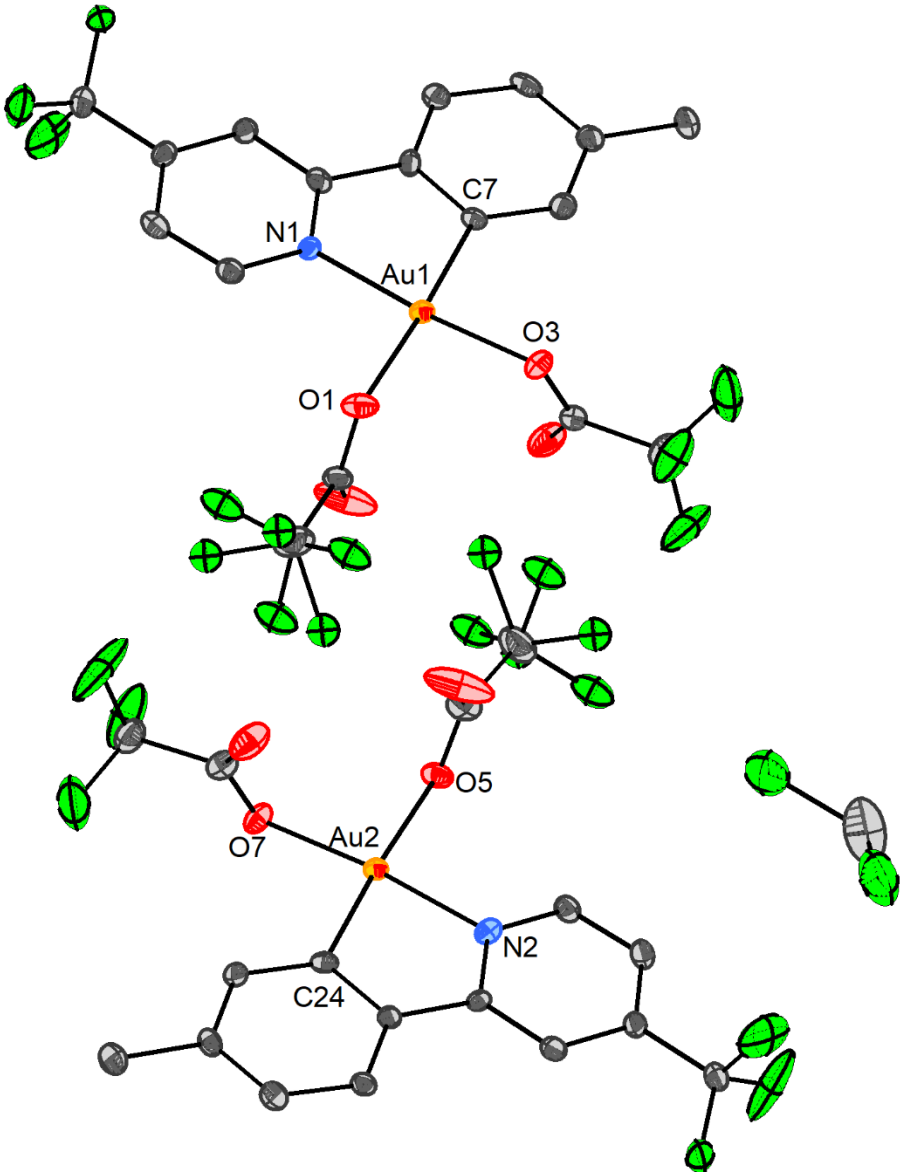


Figure S140. ORTEP plot of **2d-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Both molecules in the asymmetric unit are shown. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): Au1—O3, 2.008(4); Au1—O1, 2.114(4); Au1—N1, 2.013(4); Au1—C7, 1.995(5); Au2—O7, 2.009(4); Au2—O5, 2.113(4); Au2—N2, 2.008(4); Au2—C24, 2.001(5); O3—Au1—O1, 88.41(17); O3—Au1—N1, 174.92(17); N1—Au1—O1, 94.74(17); C7—Au1—O3, 94.73(18); C7—Au1—O1, 176.60(19); C7—Au1—N1, 82.03(19); O7—Au2—O5; 88.84(16); N2—Au2—O7; 174.47(18); N2—Au2—O5; 94.42(17); C24—Au2—O7; 94.57(19); C24—Au2—O5, 176.39(19); C24—Au2—N2, 82.1(2).

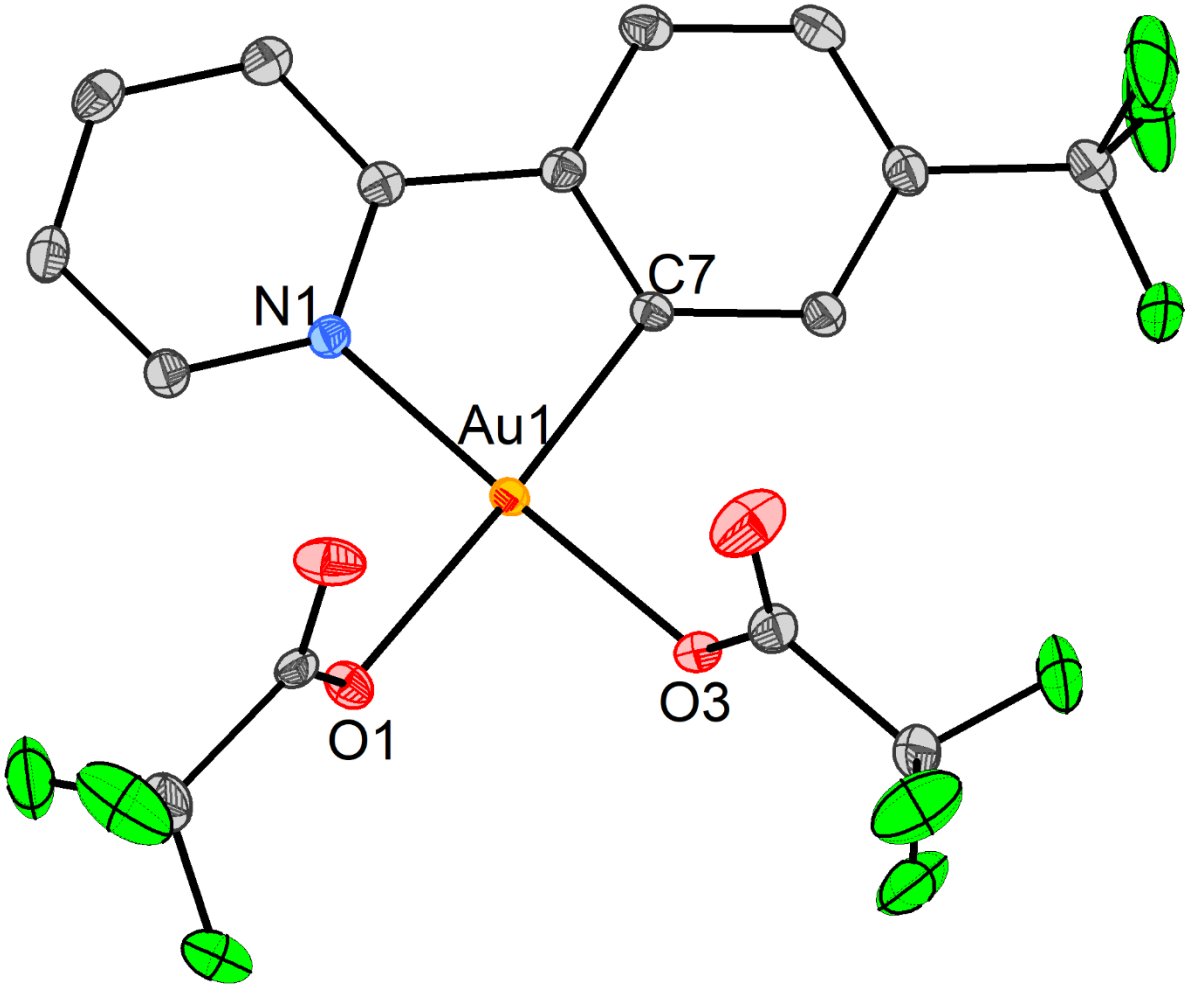


Figure S141. ORTEP plot of **2e-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms have been omitted for clarity.

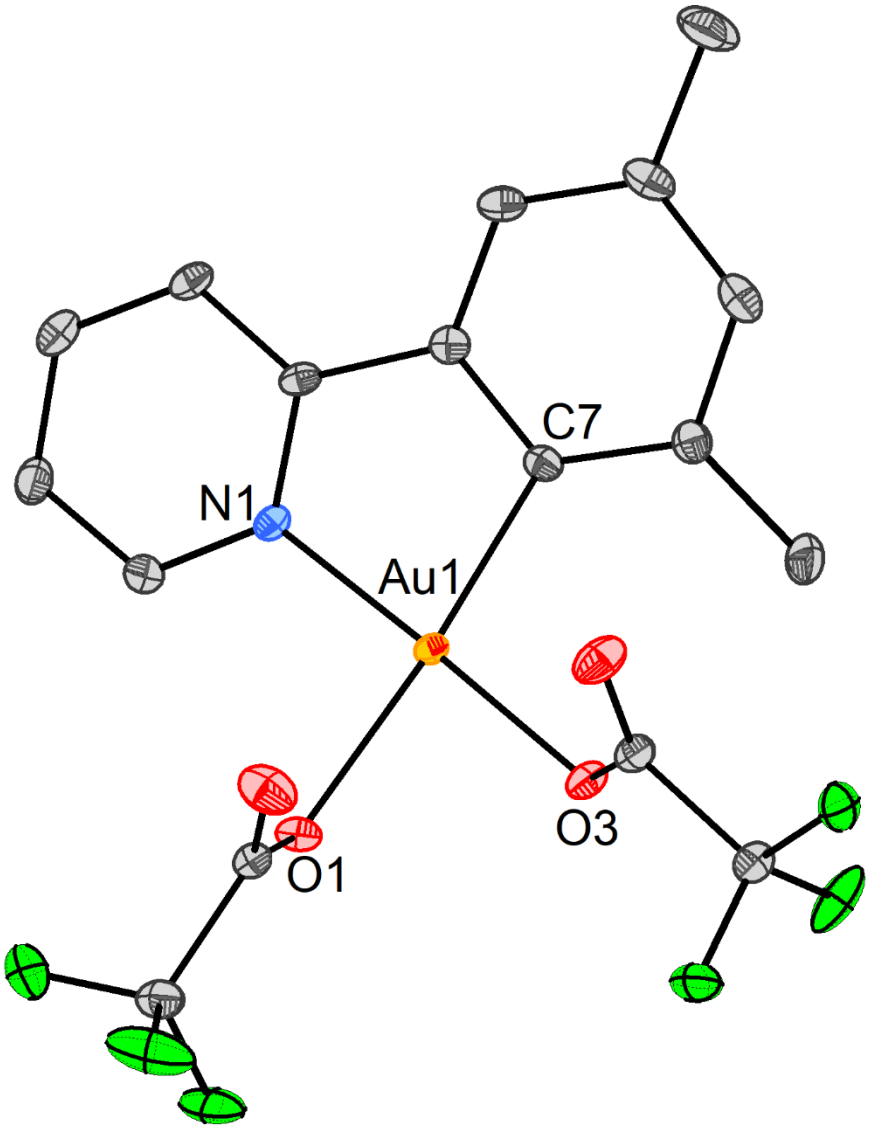


Figure S142. ORTEP plot of **2h-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms have been omitted for clarity.

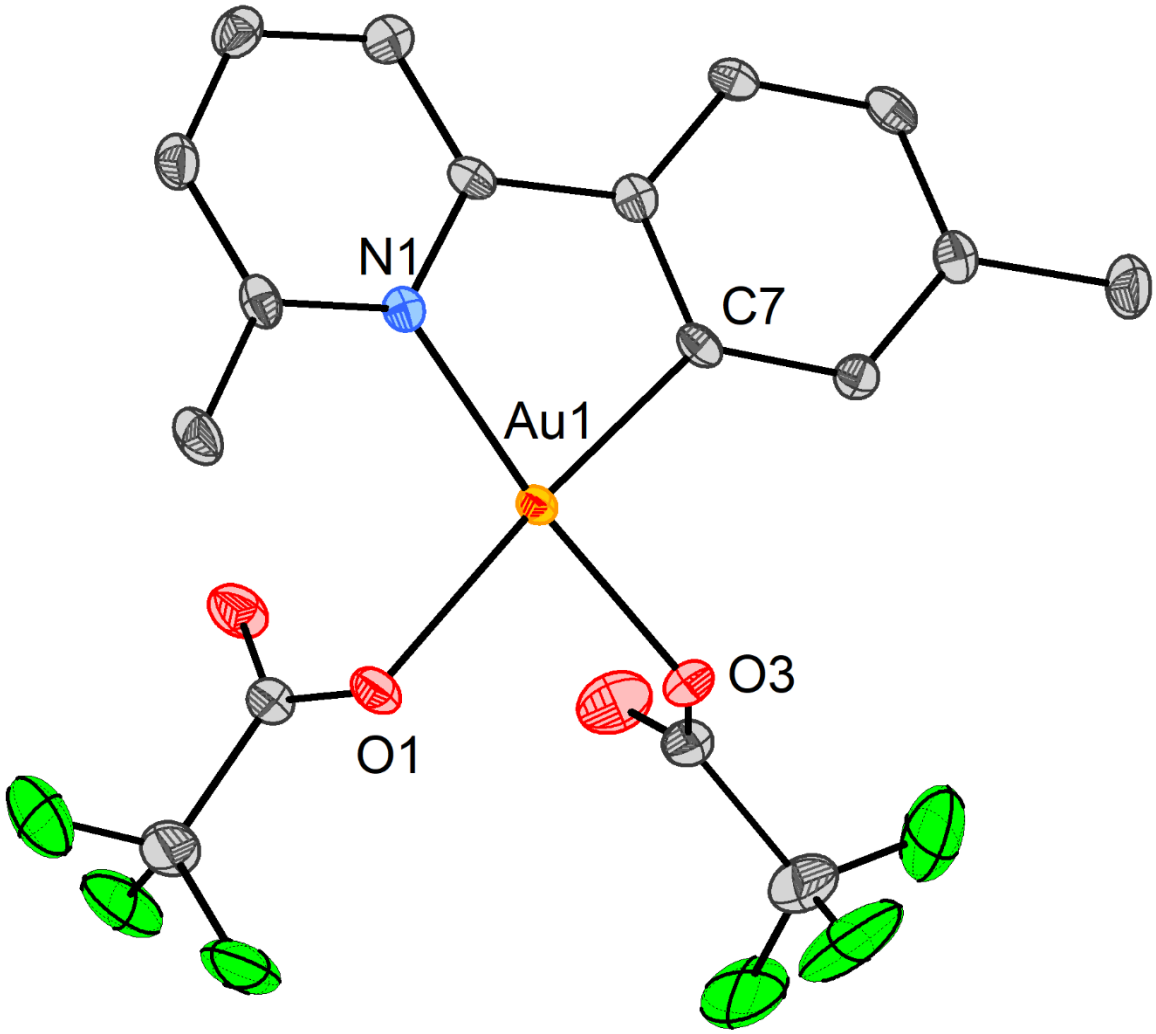


Figure S143. ORTEP plot of **2i-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Only one of the two molecules in the asymmetric unit is shown. Hydrogen atoms and an associated CH_2Cl_2 molecule (solvent of crystallization) have been omitted for clarity.

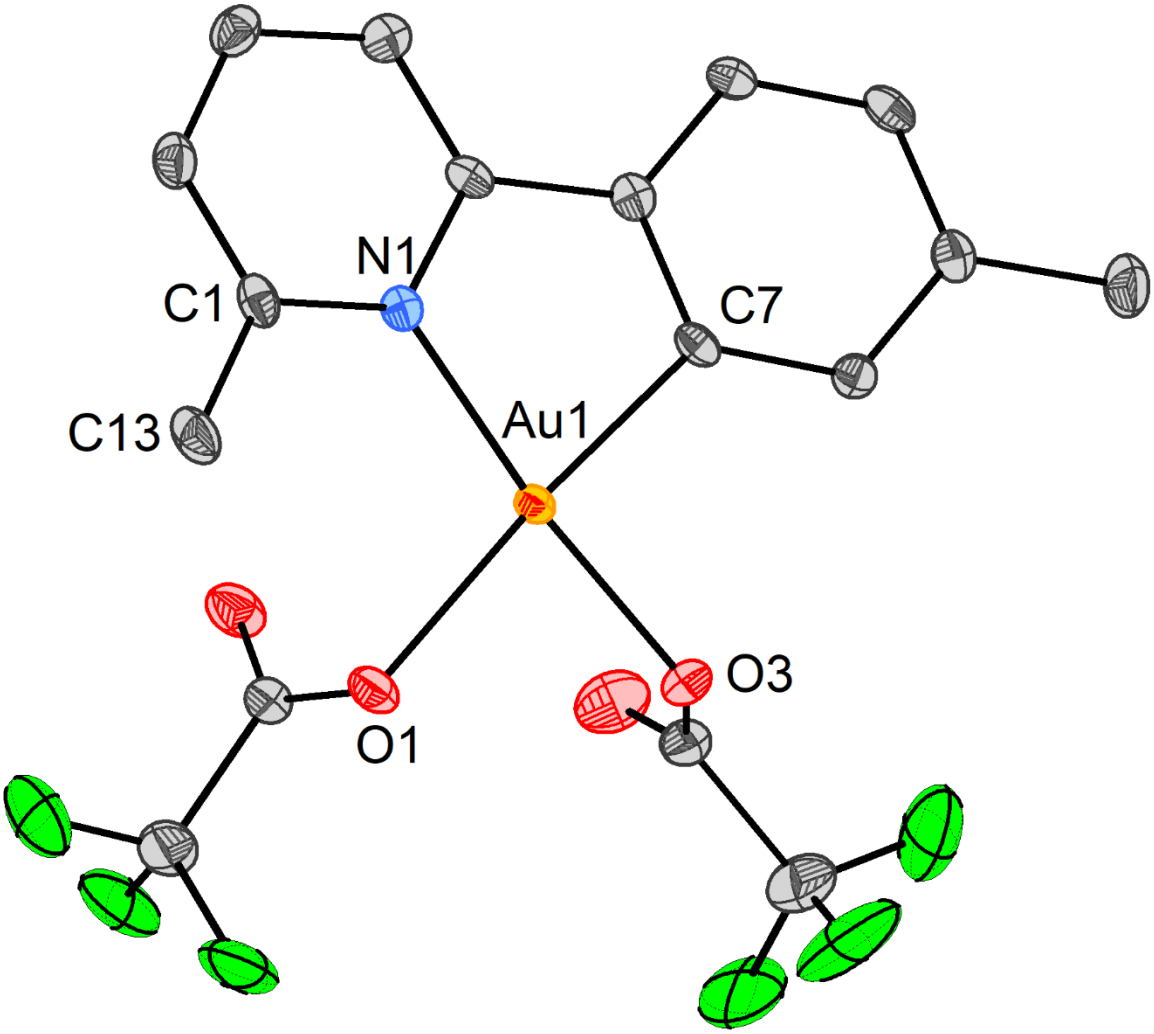


Figure S144. ORTEP plot of **2i-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Only one of the two molecules in the asymmetric unit is shown. Hydrogen atoms and an associated CH_2Cl_2 molecule (solvent of crystallization) have been omitted for clarity.

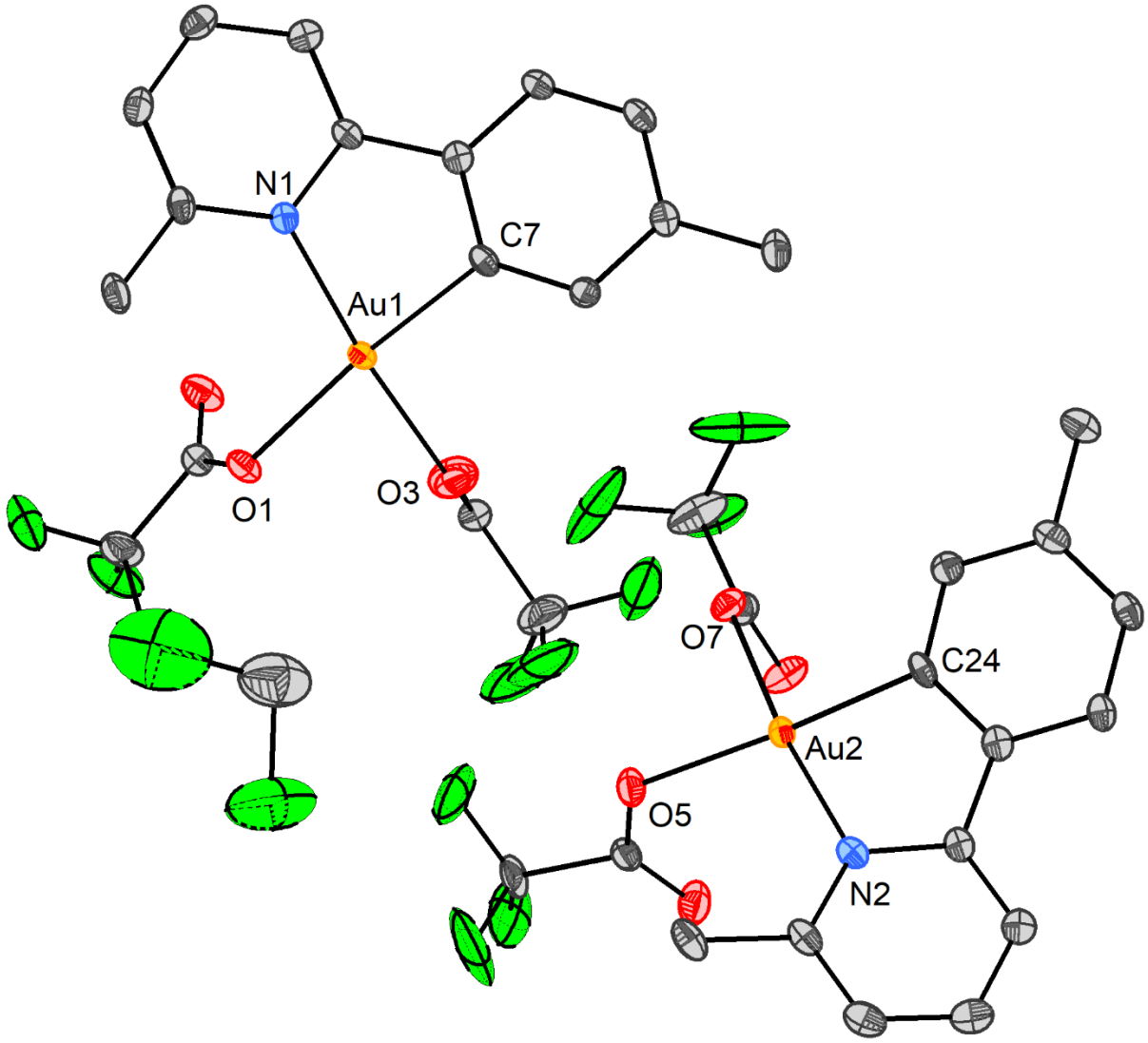


Figure S145. ORTEP plot of **2i-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Both molecules in the asymmetric unit are shown. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): Au1—O1, 2.113(2); Au1—O3, 2.011(2); Au1—N1, 2.034(3); Au1—C7, 1.994(3); Au2—O5, 2.112(3); Au2—O7, 2.010(3); Au2—N2, 2.033(3); Au2—C24, 1.992(3); O3—Au1—O1, 82.24(10); O3—Au1—N1, 173.84(11); N1—Au1—O1, 103.80(11); C7—Au1—O1, 172.37(12); C7—Au1—O3, 92.46(12); C7—Au1—N1, 81.65(13); O7—Au2—O5, 82.01(11); O7—Au2—N2, 173.39(11); N2—Au2—O5, 104.53(11); C24—Au2—O5, 172.55(12); C24—Au2—O7, 91.75(13); C24—Au2—N2, 81.65(13).

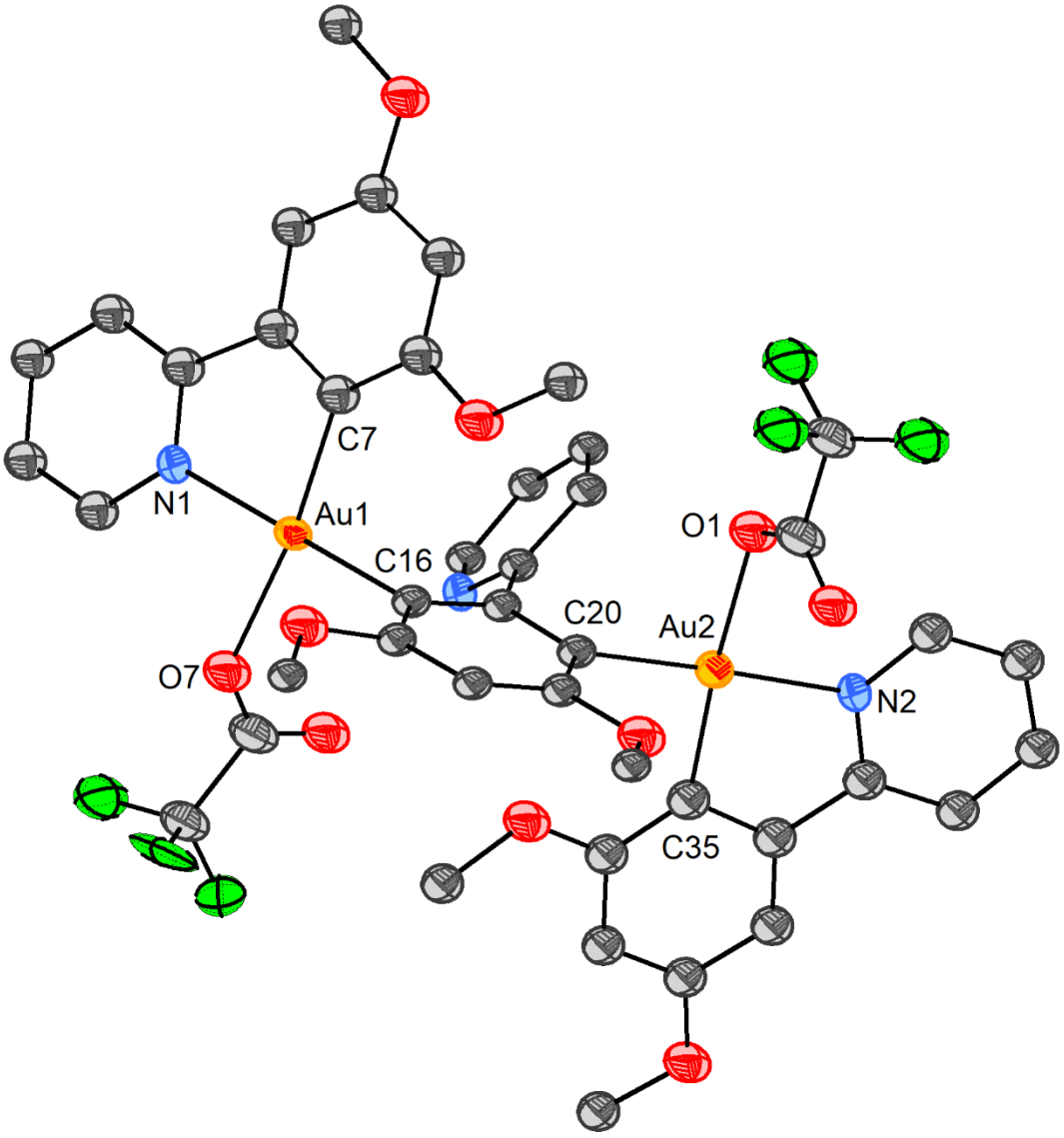


Figure S146. ORTEP plot of **2j$_3$Au$_2$(OAc^F)$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): Au1—O7, 2.116(17); Au1—N1, 2.112(19); Au1—C7, 2.01(2); Au1—C16, 2.07(2); Au2—O1, 2.145(17); Au2—N2, 2.104(18); Au2—C20, 2.05(2); Au2—C35, 2.03(3); N1—Au1—O7, 90.9(7); C7—Au1—O7, 172.6(9); C7—Au1—N1 82.2(8); C7—Au1—C16, 98.0(10); C16—Au1—O7, 89.0(8); C16—Au1—N1, 178.4(9); N2—Au2—O1, 93.3(7); C20—Au2—O1, 88.3(8); C20—Au2—N2, 178.2(8); C35—Au2—O1, 174.6(9); C35—Au2—N2, 81.5(9); C35—Au2—C20, 96.9(10).

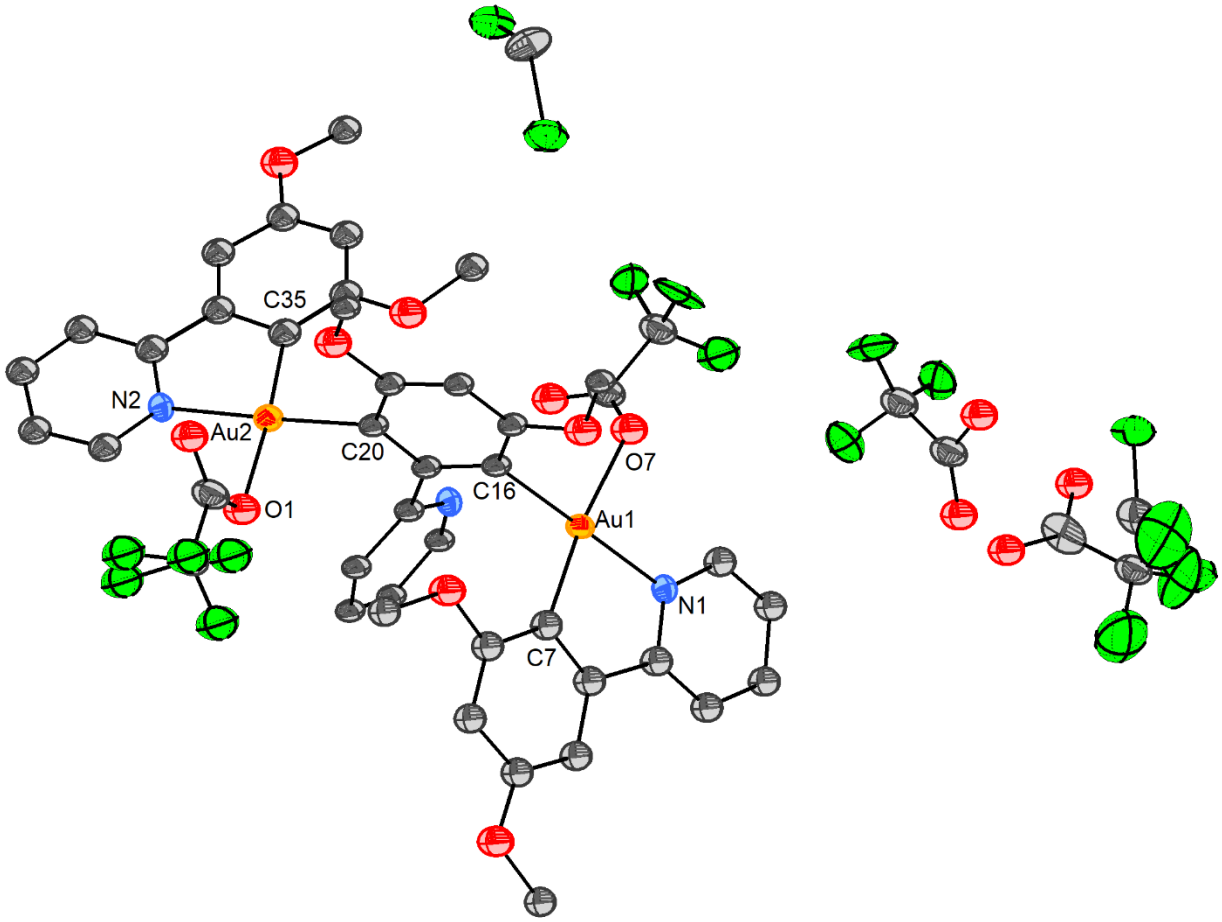


Figure S147. ORTEP plot of **2j$_3$Au$_2$(OAc^F)$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms have been omitted for clarity. Disordered fluorine atoms in the trifluoroacetate ligand bonded to Au2 and solvent molecules (CH_2Cl_2 and (H)OAc^F) are shown.

A low $(\sin\theta/\lambda)_{max}$ value (0.530) was found for the chosen crystal of **2j$_3$Au$_2$(OAc^F)$_2$**. The crystal was a weak scatterer with a relatively complex structure, these data were the best possible. Compared to other structures with better resolution, the geometry of the main moiety seems to be reasonable.

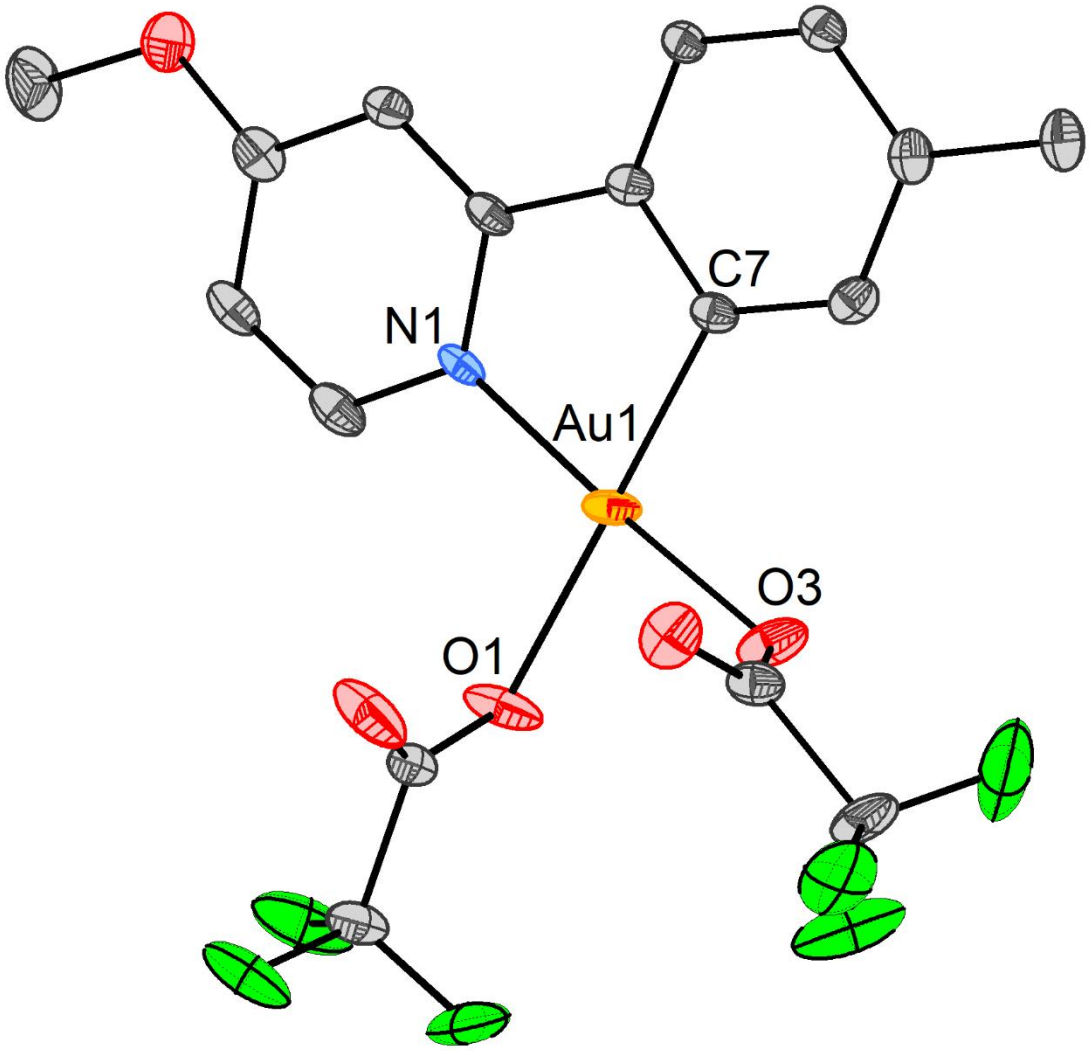


Figure S148. ORTEP plot of **2l-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms and disorder in the trifluoroacetate ligand *trans* to N1 have been omitted for clarity.

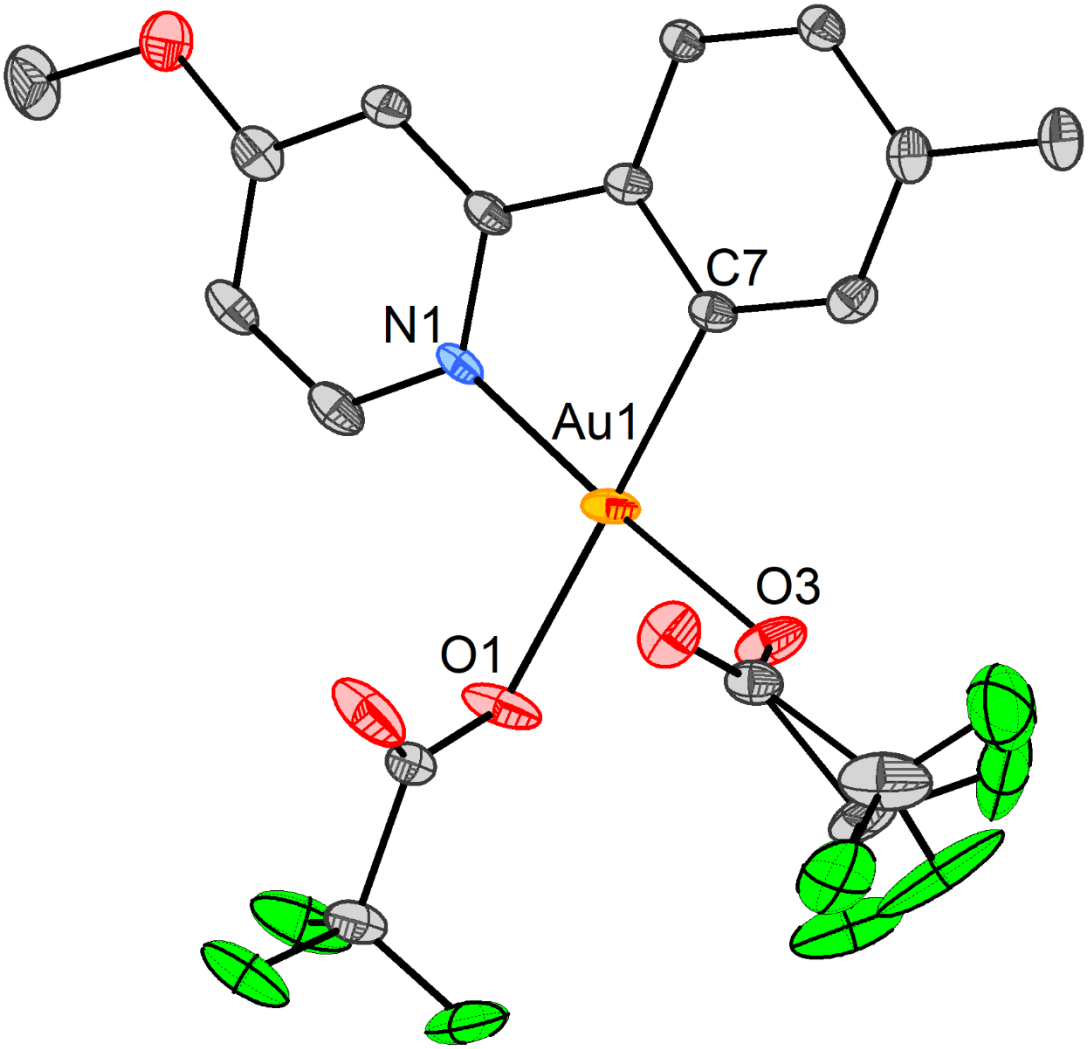


Figure S149. ORTEP plot of **2I-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms have been omitted for clarity. The disorder in the trifluoroacetate ligand *trans* to N is shown.

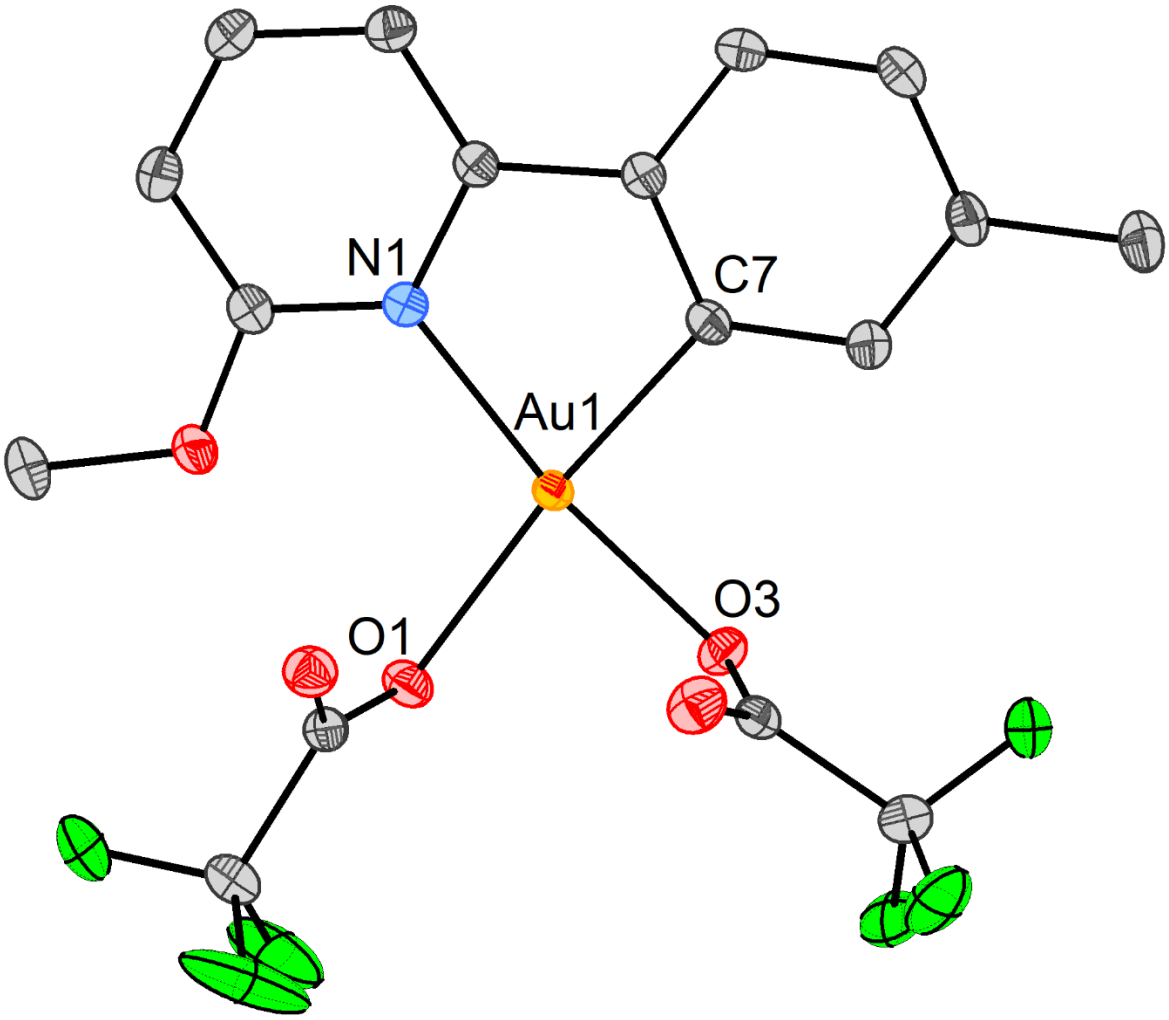


Figure S150. ORTEP plot of **2m-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms and an associated CH_2Cl_2 molecule (solvent of crystallization) have been omitted for clarity.

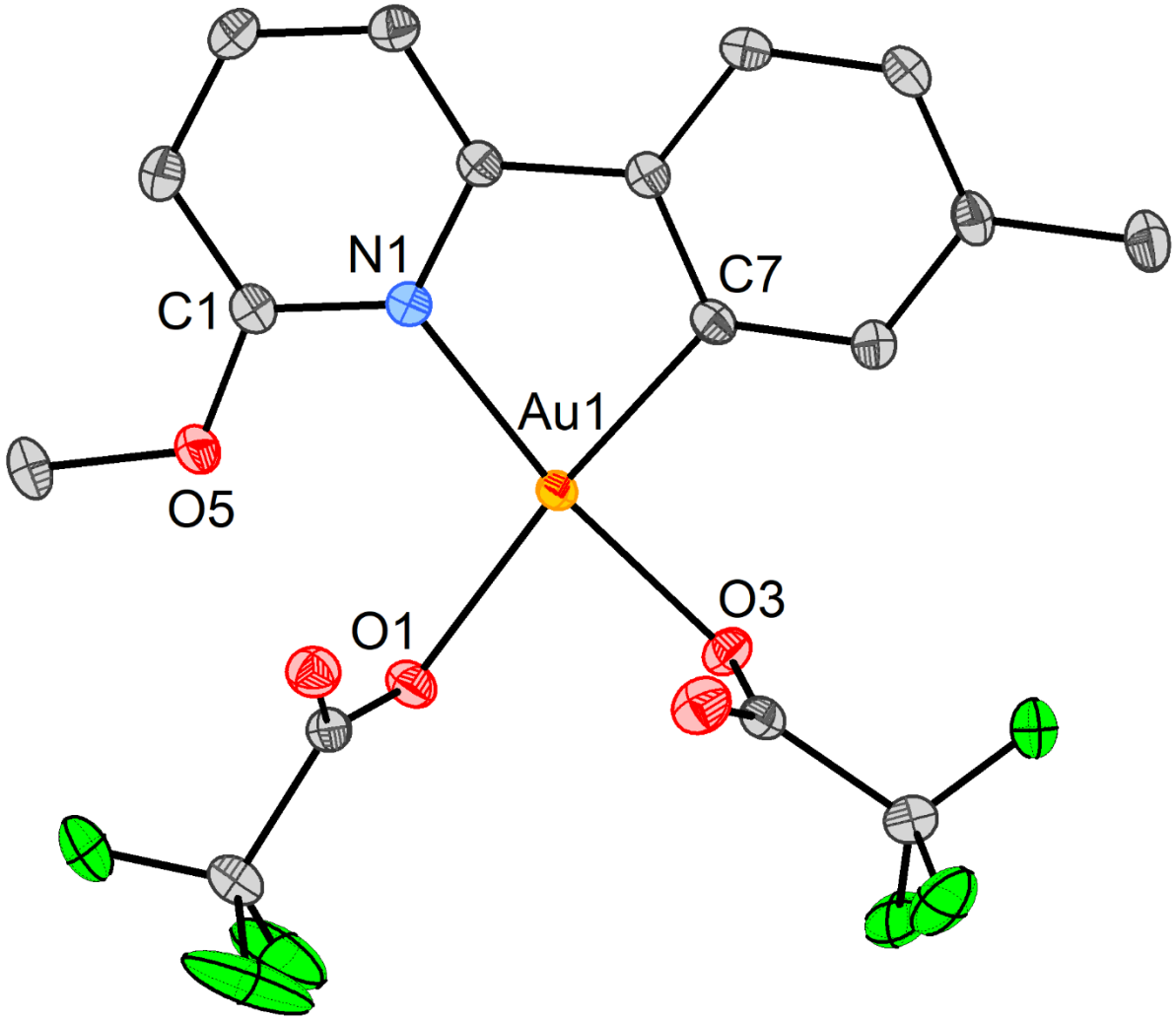


Figure S151. ORTEP plot of **2m-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms and an associated CH_2Cl_2 molecule (solvent of crystallization) have been omitted for clarity.

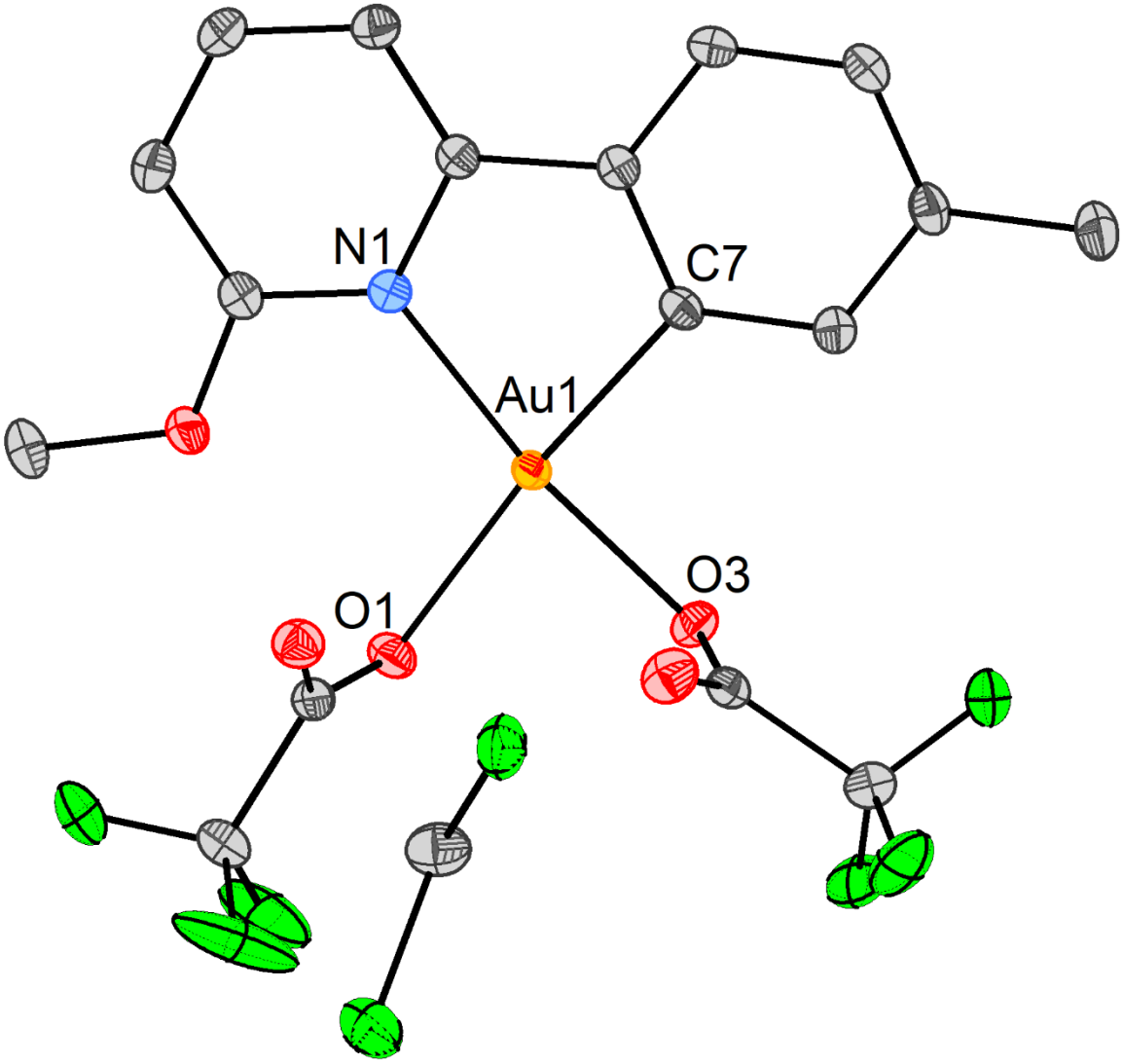


Figure S152. ORTEP plot of **2m-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms have been omitted for clarity.

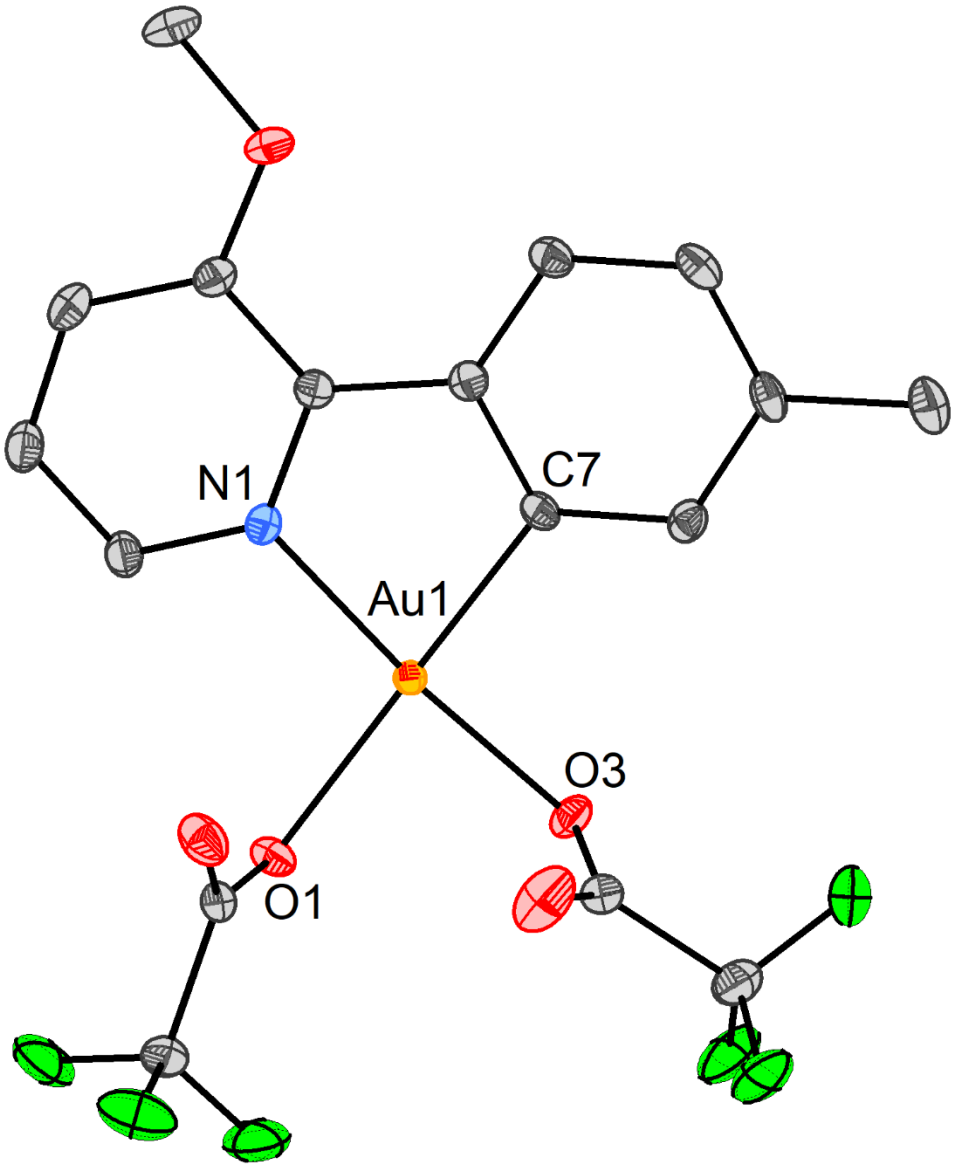


Figure S153. ORTEP plot of **2n-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms have been omitted for clarity.

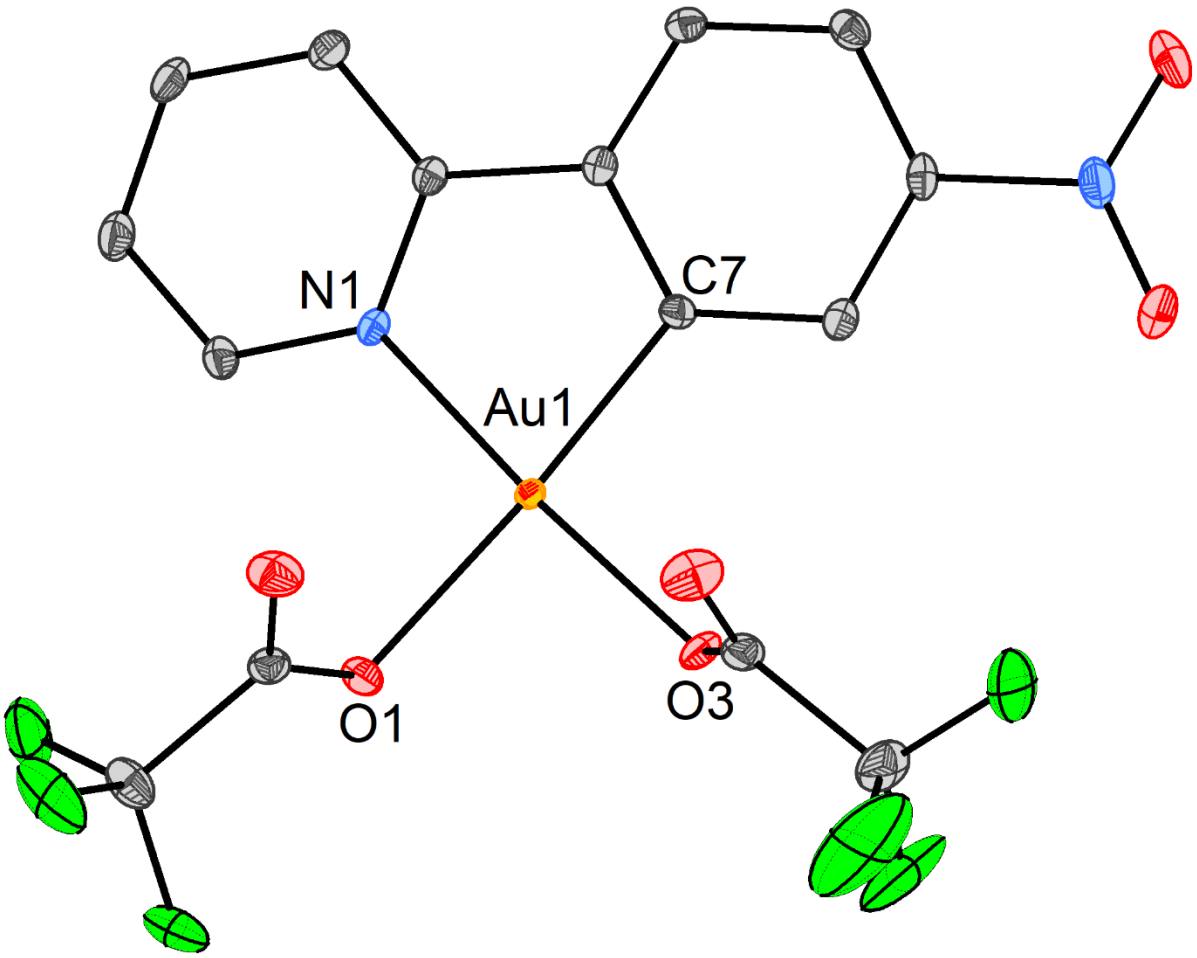


Figure S154. ORTEP plot of **2o-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms have been omitted for clarity.

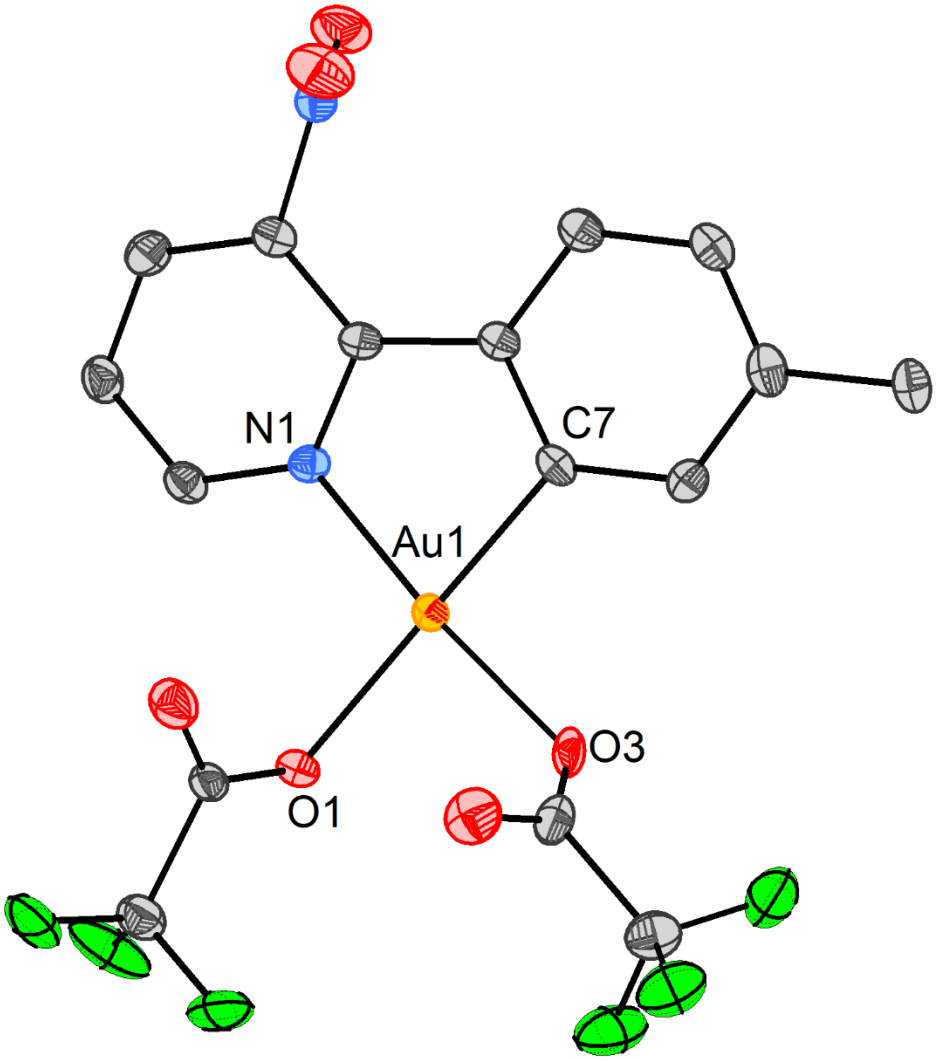


Figure S155. ORTEP plot of **2p-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms and a disordered CH_2Cl_2 molecule (solvent of crystallization) have been omitted for clarity.

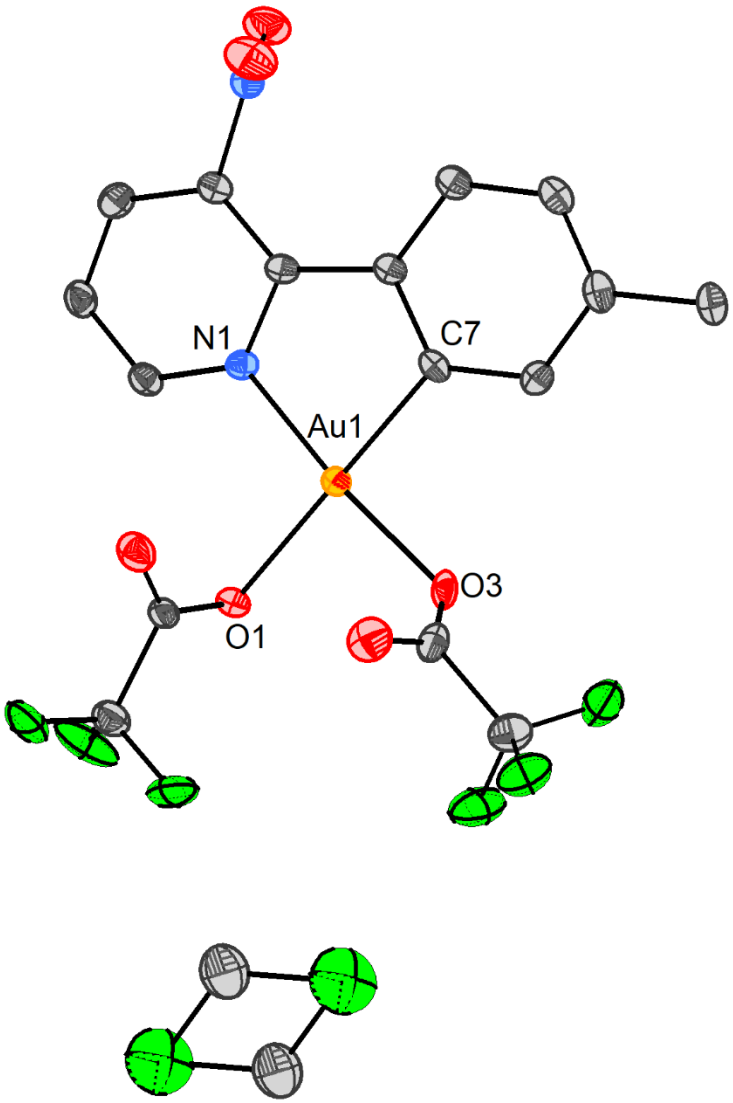


Figure S156. ORTEP plot of **2p-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms have been omitted for clarity.

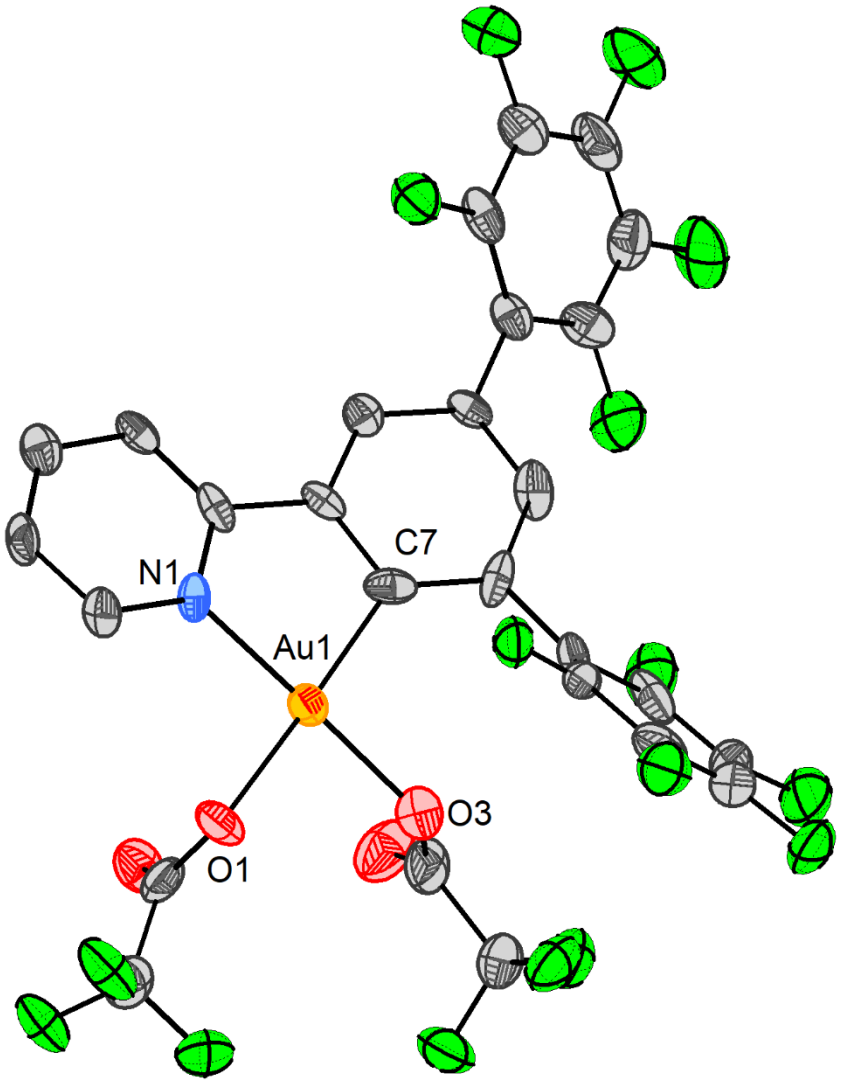


Figure S157. ORTEP plot of **2r-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms have been omitted for clarity.

A low $(\sin\theta/\lambda)_{max}$ value (0.500) was found for the chosen crystal of **2r-Au(OAc^{F})$_2$**. The crystal was a twinned weak scatterer with a relatively complex structure, these data were the best possible. Compared to other structures with better resolution, the geometry of the main moiety seems to be reasonable.

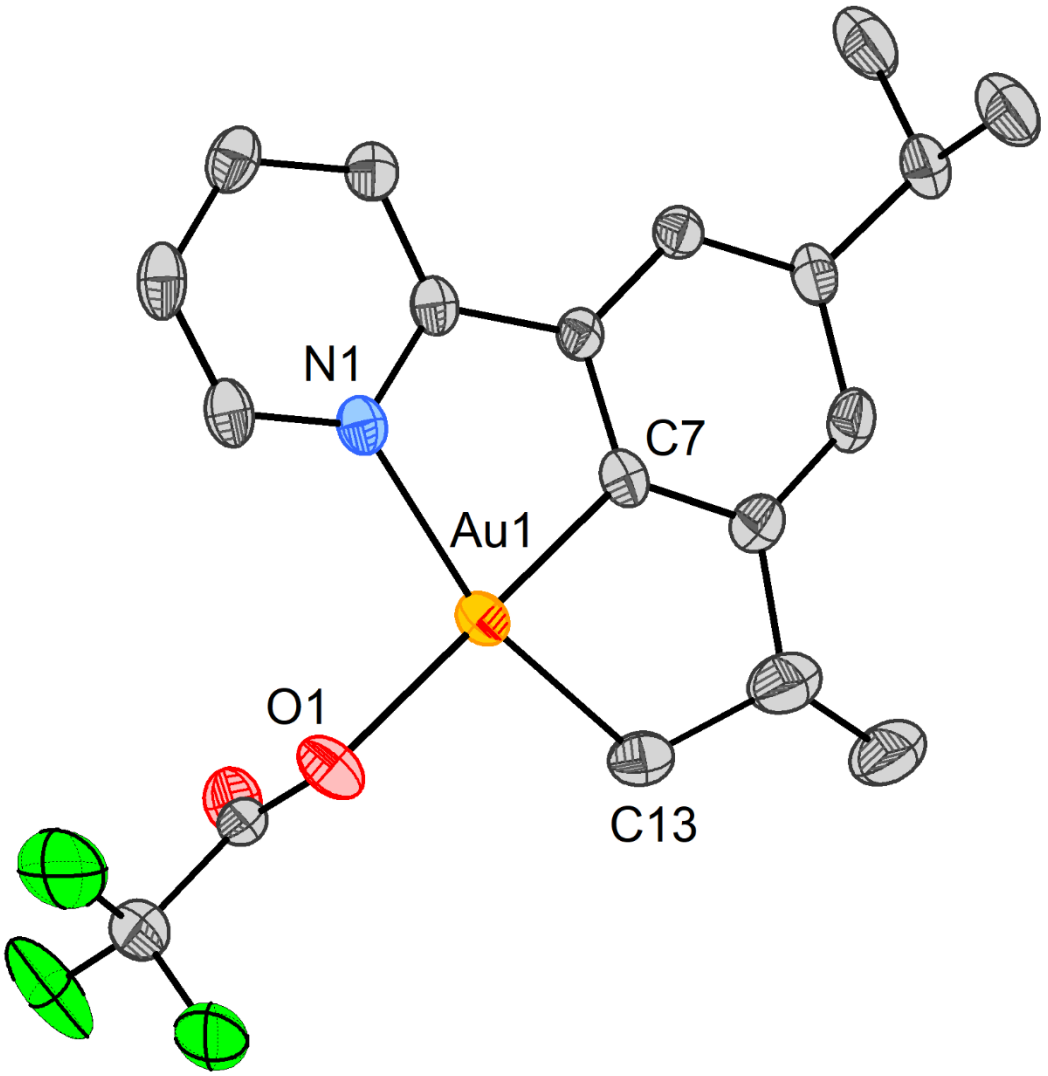


Figure S158. ORTEP plot of **3s-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Only one of the two molecules in the asymmetric unit is shown. Hydrogen atoms and disorder in one of the isopropyl groups have been omitted for clarity.

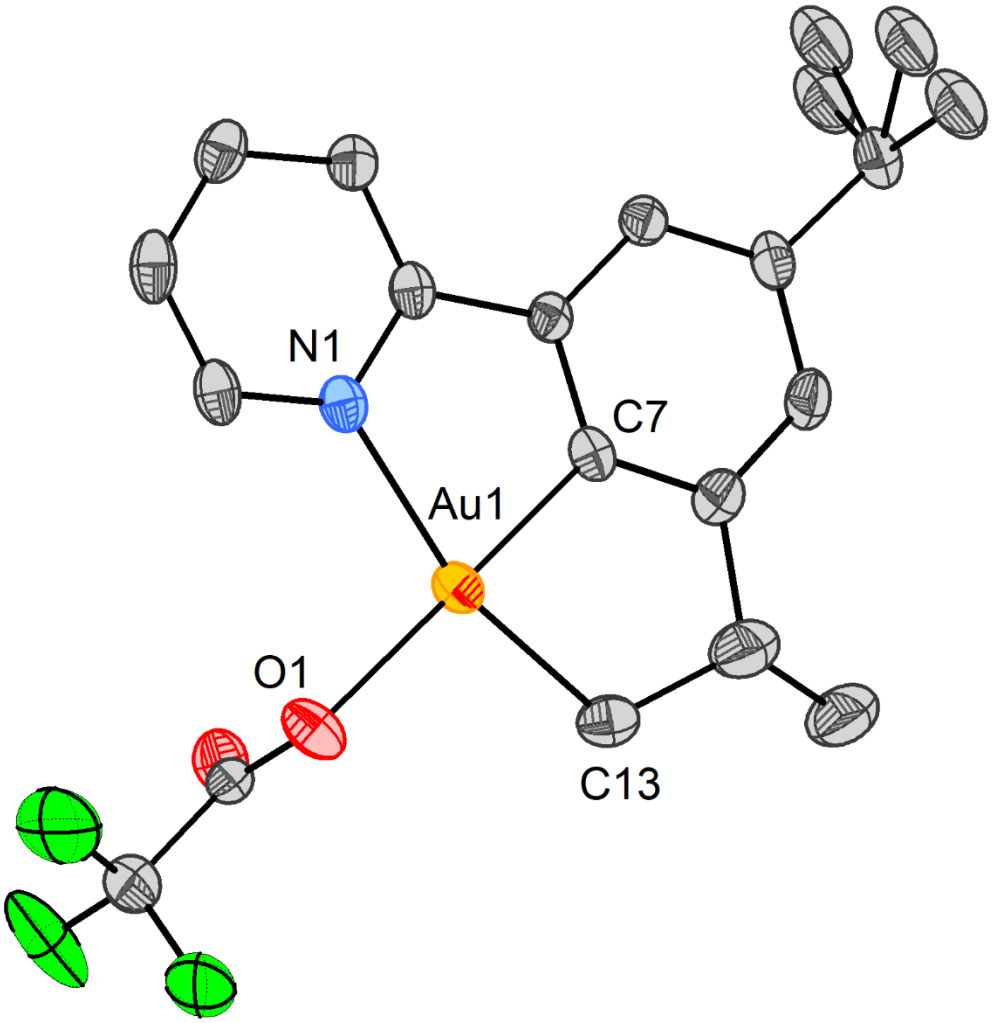


Figure S159. ORTEP plot of **3s-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Only one of the two molecules in the asymmetric unit is shown. Hydrogen atoms have been omitted for clarity.

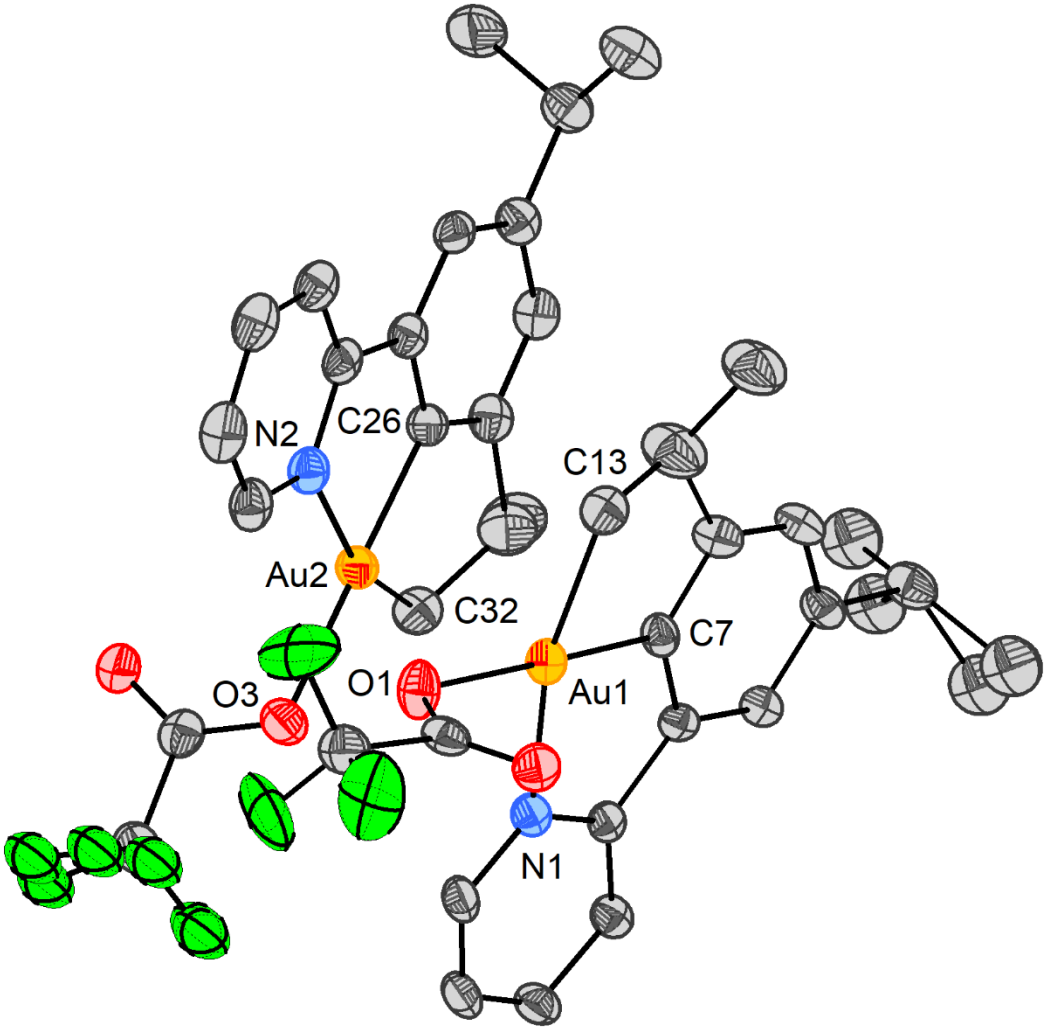


Figure S160. ORTEP plot of **3s-Au(OAc^{F})$_2$**. Ellipsoids are shown at 50 % probability level. Both molecules in the asymmetric unit are shown. The gold atoms in the two molecules are separated by 3.2322(3) Å. Hydrogen atoms have been omitted for clarity. Selected bond lengths (Å) and angles (°): Au1—O1, 2.108(3); Au1—N1, 2.144(3); Au1—C7, 1.954(3); Au1—C13, 2.055(4); Au1—Au2, 3.2322(3); Au2—O3, 2.114(3); Au2—N2, 2.144(3); Au2—C26, 1.953(4); Au2—C32, 2.050(4); O1—Au1—N1, 98.52(11); O1—Au1—Au2, 87.75(7); N1—Au1—Au2, 85.46(8); C7—Au1—O1, 177.53(13); C7—Au1—N1, 80.59(13); C7—Au1—C13, 81.33(15); C7—Au1—Au2, 89.88(10); C13—Au1—O1, 99.67(14); C13—Au1—N1, 161.67(14); C13—Au1—Au2, 97.48(11); O3—Au2—Au1, 79.99(7); O3—Au2—N2, 99.16(12); N2—Au2—Au1, 83.29(8); C26—Au2—Au1, 98.65(11); C26—Au2—O3, 178.64(13); C26—Au2—N2, 80.54(14); C26—Au2—C32, 81.70(16); C32—Au2—Au1, 102.77(12); C32—Au2—O3, 98.67(14); C32—Au2—N2, 161.92(14).

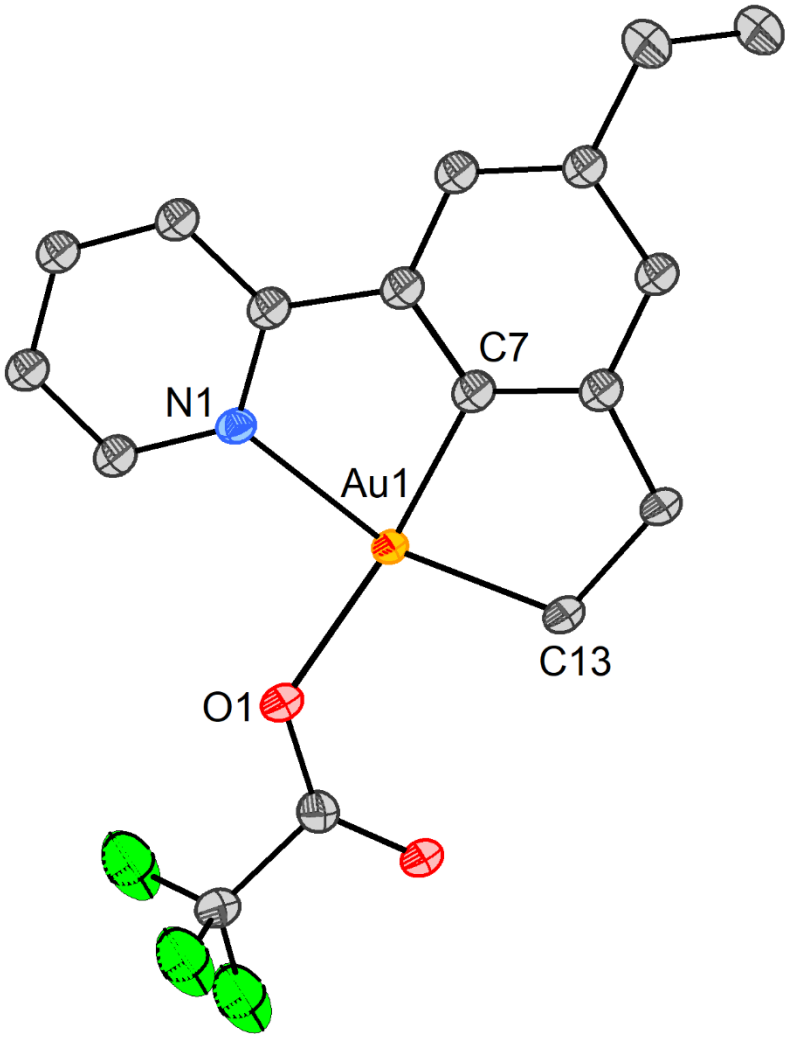


Figure S161. ORTEP plot of **3t-AuOAc^{F}**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms have been omitted for clarity. Only one of the four molecules in the asymmetric unit is shown.

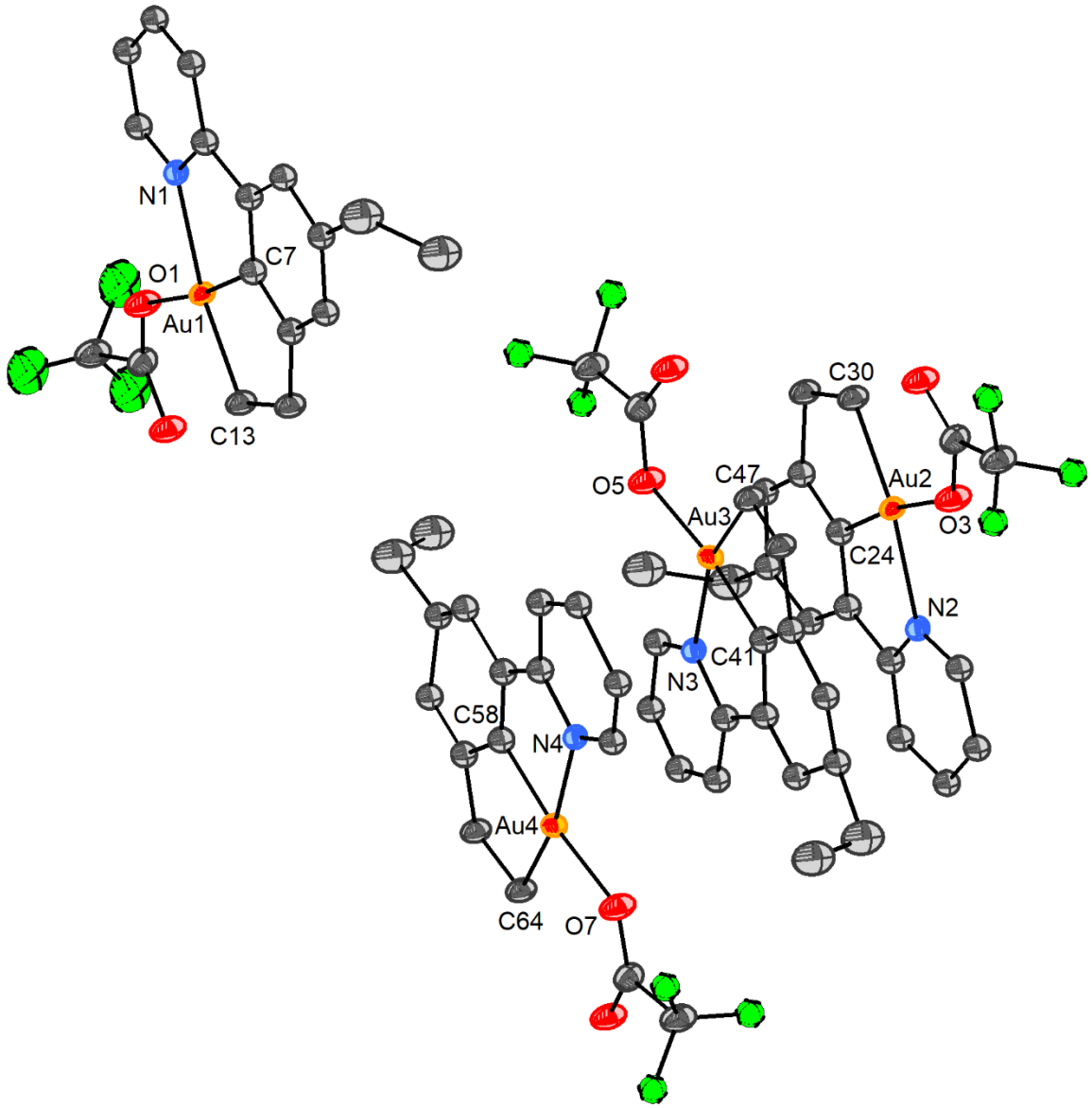
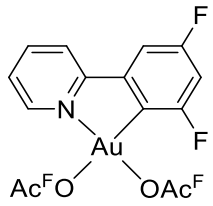


Figure S162. ORTEP plot of **3t-AuOAc^{F}**. Ellipsoids are shown at 50 % probability level. Hydrogen atoms have been omitted for clarity. All four molecules in the asymmetric unit are shown. Selected bond lengths (Å) and angles (°): Au1—O1, 2.076(18); Au1—N1, 2.15(2); Au1—C7, 1.94(2); Au1—C13, 2.04(3); Au2—O3, 2.129(18); Au2—N2, 2.14(2); Au2—C24, 1.96(2); Au2—C30, 2.06(3); Au3—O5, 2.078(17); Au3—N3, 2.128(18); Au3—C41, 1.95(2); Au3—C47, 2.079(19); Au4—O7, 2.115(17); Au4—N4, 2.159(18); Au4—C58, 1.94(2); Au4—C64, 2.029(19); O1—Au1—N1, 93.2(8); C7—Au1—O1, 173.2(10); C7—Au1—N1, 80.0(10); C7—Au1—C13, 83.0(11); C13—Au1—O1, 103.7(9); C13—Au1—N1, 163.0(9); O3—Au2—N2, 91.7(8); C24—Au2—O3, 172.5(10); C24—Au2—N2, 80.8(10); C24—Au2—C30, 82.9(11); C30—Au2—O3, 104.6(9); C30—Au2—N2, 163.7(9); O5—Au3—N3, 93.3(6); O5—Au3—C47, 107.9(6); C41—Au3—O5, 172.5(7); C41—Au3—N3, 79.6(7); C41—Au3—C47, 79.2(7); C47—Au3—N3, 158.8(6); O7—Au4—N4, 91.1(6); C58—Au4—O7, 172.0(7); C58—Au4—N4, 81.2(6); C58—Au4—C64, 86.4(7); C64—Au4—O7, 101.3(6); C64—Au4—N4, 167.6(6).

Several issues in the structure of **3t-AuOAc^{F}** were encountered (see cif for full details). The structure is complex and contains significant disorder, which could not be well modelled despite several different strategies being tested. Significant restraint of the thermal parameters was required to get the refinement

to this stage, which unfortunately led to some positional oscillation in atoms, which would have had highly anisotropic thermal parameters if allowed to refine freely. The overall geometry of the structure seems reasonable compared to other similar complexes. The disorder in the structure may be due to weak intermolecular interactions, which allow each molecule to have a slightly different position/orientation; and molecular flexibility, which allows every molecule to have a slightly different shape/configuration. The reported crystal structure therefore represents an average of the possible orientations and configurations of the molecules in this system, represented by the four independent molecules in the asymmetric unit. We were also able to solve the crystal structure with a smaller unit cell containing one molecule in the asymmetric unit, but the signs of disorder in the resulting model were so excessive that it could not be refined.

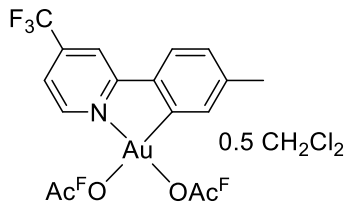
Table S2. Crystal and refinement data for **2c-Au(OAc^F)$_2$**.



2c-Au(OAc^F)$_2$

Crystal data	
Identification code, CCDC number	IL_MA_48, 2115512
Chemical formula	$C_{15}H_6AuF_8NO_4$
M_r	613.17
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, *b*, *c* (Å)	9.0823 (9), 9.6035 (9), 9.6741 (9)
α, β, γ (°)	99.749 (2), 103.932 (2), 94.850 (2)
V (Å^3)	800.19 (13)
Z	2
Radiation type	Mo *K*α
μ (mm^{-1})	9.31
Crystal size (mm)	0.4 × 0.14 × 0.05
Data collection	
Diffractometer	Bruker D8 Venture, Bruker *SMART APEX2* area detector
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1222 before and 0.0611 after correction. The Ratio of minimum to maximum transmission is 0.6453. The λ/2 correction factor is Not present.
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	23774, 4025, 3665
R_{int}	0.055
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.670
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.025, 0.052, 1.04
No. of reflections	4025
No. of parameters	262
No. of restraints	0
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0171P)^2 + 1.8796P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.86, -0.93

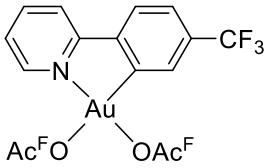
Table S3. Crystal and refinement data for **2d-Au(OAc^F)$_2$**.



2d-Au(OAc^F)$_2$

Crystal data	
Identification code, CCDC number	IL_4cf3, 2122527
Chemical formula	$C_{17}H_9AuF_9NO_4 \cdot 0.5CH_2Cl_2$
M_r	701.68
Crystal system, space group	Monoclinic, $P2_1$
Temperature (K)	100
a, b, c (Å)	8.3096 (4), 24.4047 (13), 10.1744 (5)
β (°)	101.993 (1)
V (Å^3)	2018.26 (18)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	7.53
Crystal size (mm)	0.45 × 0.12 × 0.08
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1009 before and 0.0594 after correction. The Ratio of minimum to maximum transmission is 0.5983. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.446, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	43389, 12387, 11761
R_{int}	0.031
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.717
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.022, 0.046, 1.02
No. of reflections	12387
No. of parameters	601
No. of restraints	1
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0103P)^2 + 0.7666P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.03, -1.05

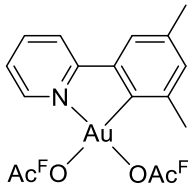
Table S4. Crystal and refinement data for **2e-Au(OAc^F)$_2$**.



2e-Au(OAc^F)$_2$

Crystal data	
Identification code, CCDC number	ILMA64, 2085151
Chemical formula	$C_{16}H_7AuF_9NO_4$
M_r	645.19
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	7.9194 (7), 22.7352 (19), 9.8659 (8)
β (°)	100.171 (2)
V (Å^3)	1748.4 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	8.53
Crystal size (mm)	1.3 × 0.1 × 0.1
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1160 before and 0.0465 after correction. The Ratio of minimum to maximum transmission is 0.4099. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.330, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	39659, 6415, 5833
R_{int}	0.031
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.774
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.023, 0.050, 1.12
No. of reflections	6415
No. of parameters	280
No. of restraints	0
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0154P)^2 + 4.6906P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.62, -1.46

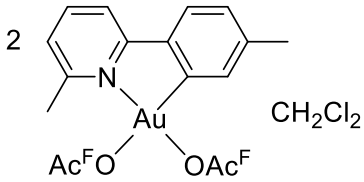
Table S5. Crystal and refinement data for **2h-Au(OAc^F)$_2$**.



2h-Au(OAc^F)$_2$

Crystal data	
Identification code, CCDC number	IL_dimethyl, 2086346
Chemical formula	$C_{17}H_{12}AuF_6NO_4$
M_r	605.24
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	10.349 (3), 19.446 (5), 9.020 (3)
β (°)	104.225 (8)
V (Å^3)	1759.6 (9)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	8.45
Crystal size (mm)	0.52 × 0.4 × 0.28
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1203 before and 0.0499 after correction. The Ratio of minimum to maximum transmission is 0.5557. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.415, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	46689, 5371, 5078
R_{int}	0.037
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.715
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.018, 0.039, 1.19
No. of reflections	5371
No. of parameters	264
No. of restraints	0
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0097P)^2 + 2.6789P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.98, -1.41

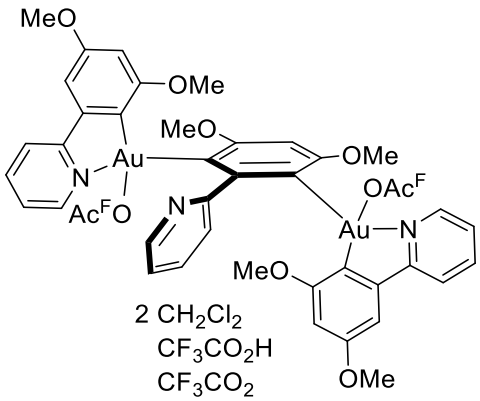
Table S6. Crystal and refinement data for **2i-Au(OAc^F)$_2$**.



2i-Au(OAc^F)$_2$

Crystal data	
Identification code, CCDC number	IL183_freezer, 2126159
Chemical formula	$2(C_{17}H_{12}AuF_6NO_4)\cdot CH_2Cl_2$
M_r	1295.41
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	12.9432 (7), 24.5659 (13), 12.8760 (7)
β (°)	93.769 (1)
V (Å^3)	4085.2 (4)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	7.41
Crystal size (mm)	0.46 × 0.1 × 0.07
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1138 before and 0.0561 after correction. The Ratio of minimum to maximum transmission is 0.6481. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.484, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	183078, 12987, 10781
R_{int}	0.054
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.735
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.032, 0.063, 1.07
No. of reflections	12987
No. of parameters	554
No. of restraints	0
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0204P)^2 + 15.8963P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.30, -1.98

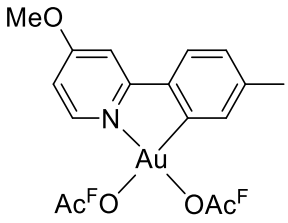
Table S7. Crystal and refinement data for **2j$_3$Au$_2$(OAc^F)$_2$**.



2j$_3$Au$_2$(OAc^F)$_2$

Crystal data	
Identification code, CCDC number	test_1ang, 2126283
Chemical formula	$C_{43}H_{35}Au_2F_6N_3O_{10}\cdot 2(CH_2Cl_2)\cdot CF_3CO_2H\cdot CF_3CO_2$
M_r	1658.57
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, b, c (Å)	11.978 (2), 14.129 (3), 16.804 (4)
α, β, γ (°)	86.730 (5), 82.867 (5), 76.625 (4)
V (Å^3)	2744.0 (10)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	5.64
Crystal size (mm)	0.4 × 0.34 × 0.09
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1365 before and 0.0949 after correction. The Ratio of minimum to maximum transmission is 0.5506. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.410, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	47330, 6777, 5268
R_{int}	0.080
θ_{max} (°)	22.1
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.530
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.091, 0.233, 1.29
No. of reflections	6777
No. of parameters	413
No. of restraints	29
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + 232.7055P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	3.28, -4.04

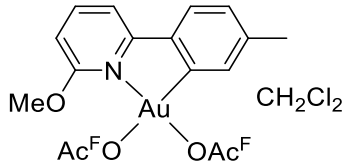
Table S8. Crystal and refinement data for **2I-Au(OAc^F)$_2$**.



2I-Au(OAc^F)$_2$

Crystal data	
Identification code, CCDC number	IL_dime, 2122284
Chemical formula	$C_{17}H_{12}AuF_6NO_5$
M_r	621.24
Crystal system, space group	Monoclinic, $P2_1/n$
Temperature (K)	100
a, b, c (Å)	8.8236 (8), 9.7870 (9), 21.7712 (19)
β (°)	101.618 (2)
V (Å^3)	1841.6 (3)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	8.08
Crystal size (mm)	0.44 × 0.29 × 0.12
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1055 before and 0.0545 after correction. The Ratio of minimum to maximum transmission is 0.4769. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.356, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	47169, 5624, 5229
R_{int}	0.044
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.715
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.038, 0.077, 1.43
No. of reflections	5624
No. of parameters	301
No. of restraints	31
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + 11.9551P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.72, -2.79

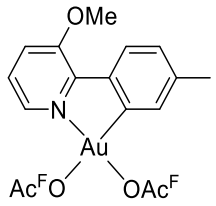
Table S9. Crystal and refinement data for **2m-Au(OAc^F)$_2$**.



2m-Au(OAc^F)$_2$

Crystal data	
Identification code, CCDC number	IL_161_freezer, 2111917
Chemical formula	$C_{17}H_{12}AuF_6NO_5 \cdot CH_2Cl_2$
M_r	706.17
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, b, c (Å)	9.3498 (6), 10.7363 (7), 10.9287 (7)
α, β, γ (°)	91.934 (1), 93.962 (1), 98.824 (1)
V (Å^3)	1080.38 (12)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	7.14
Crystal size (mm)	0.23 × 0.13 × 0.05
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.0868 before and 0.0465 after correction. The Ratio of minimum to maximum transmission is 0.7323. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.546, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	55997, 6630, 6201
R_{int}	0.035
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.716
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.018, 0.039, 1.06
No. of reflections	6630
No. of parameters	300
No. of restraints	0
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0164P)^2 + 1.1797P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.97, -0.78

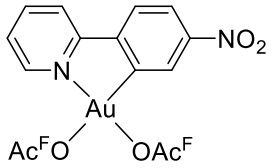
Table S10. Crystal and refinement data for **2n-Au(OAc^F)$_2$**.



2n-Au(OAc^F)$_2$

Crystal data	
Identification code, CCDC number	IL_155_shorter, 2105655
Chemical formula	$C_{17}H_{12}AuF_6NO_5$
M_r	621.24
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, b, c (Å)	9.207 (1), 9.8687 (10), 11.0143 (12)
α, β, γ (°)	81.490 (2), 67.125 (2), 83.432 (2)
V (Å^3)	910.14 (17)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	8.17
Crystal size (mm)	0.71 × 0.35 × 0.16
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1210 before and 0.0621 after correction. The Ratio of minimum to maximum transmission is 0.3667. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.274, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	41502, 5610, 5215
R_{int}	0.049
$(\sin \theta/\lambda)_{max}$ (Å^{-1})	0.717
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.019, 0.042, 1.04
No. of reflections	5610
No. of parameters	273
No. of restraints	0
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0172P)^2 + 0.6464P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.40, -1.28

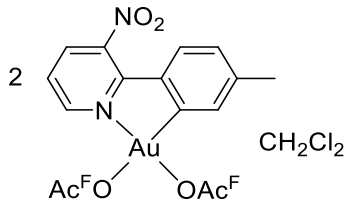
Table S11. Crystal and refinement data for **2o-Au(OAc^F)$_2$**.



2o-Au(OAc^F)$_2$

Crystal data	
Identification code, CCDC number	IL_MA_98, 2086931
Chemical formula	$C_{15}H_7AuF_6N_2O_6$
M_r	622.19
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, b, c (Å)	7.3280 (5), 10.7406 (7), 11.6341 (7)
α, β, γ (°)	89.684 (1), 77.095 (1), 81.102 (1)
V (Å^3)	881.42 (10)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	8.45
Crystal size (mm)	0.43 × 0.37 × 0.1
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1213 before and 0.0471 after correction. The Ratio of minimum to maximum transmission is 0.4931. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.368, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	38944, 5421, 5278
R_{int}	0.034
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.716
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.016, 0.041, 1.17
No. of reflections	5421
No. of parameters	271
No. of restraints	0
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0168P)^2 + 1.1321P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.26, -1.62

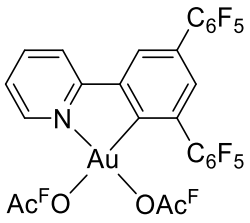
Table S12. Crystal and refinement data for **2p-Au(OAc^F)$_2$**.



2p-Au(OAc^F)$_2$

Crystal data	
Identification code, CCDC number	IL_MA_75, 2126114
Chemical formula	$2(C_{16}H_9AuF_6N_2O_6)\cdot CH_2Cl_2$
M_r	1357.36
Crystal system, space group	Monoclinic, $P2_1/c$
Temperature (K)	100
a, b, c (Å)	7.8990 (4), 13.1289 (6), 18.9100 (9)
β (°)	101.648 (1)
V (Å^3)	1920.68 (16)
Z	2
Radiation type	Mo $K\alpha$
μ (mm^{-1})	7.90
Crystal size (mm)	0.22 × 0.12 × 0.05
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.0932 before and 0.0448 after correction. The Ratio of minimum to maximum transmission is 0.6732. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.502, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	36782, 4839, 4326
R_{int}	0.033
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.670
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.022, 0.049, 1.09
No. of reflections	4839
No. of parameters	307
No. of restraints	2
H-atom treatment	H atoms treated by a mixture of independent and constrained refinement
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0161P)^2 + 6.3832P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	0.76, -1.13

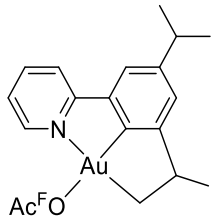
Table S13. Crystal and refinement data for **2r-Au(OAc^F)$_2$**.



2r-Au(OAc^F)$_2$

Crystal data	
Identification code, CCDC number	IL_134, 2130186
Chemical formula	$C_{27}H_6AuF_{16}NO_4$
M_r	909.29
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, *b*, *c* (Å)	8.0544 (3), 12.1925 (6), 15.7587 (7)
α, β, γ (°)	86.998 (4), 82.480 (3), 73.200 (3)
V (Å^3)	1468.59 (11)
Z	2
Radiation type	Cu *K*α
μ (mm^{-1})	10.72
Crystal size (mm)	0.14 × 0.03 × 0.03
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan TWINABS-2012/1 (Bruker,2012) was used for absorption correction. For component 1: wR2(int) was 0.1038 before and 0.0560 after correction. For component 2: wR2(int) was 0.1055 before and 0.0544 after correction. The Ratio of minimum to maximum transmission is 0.71. Final HKLF 4 output contains 12412 reflections, R_{int} = 0.0767 (9567 with I > 3sig(I), R_{int} = 0.0683)
T_{min}, T_{max}	0.714, 0.725
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	7414, 7414, 6056
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.500
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.062, 0.143, 1.07
No. of reflections	7414
No. of parameters	443
No. of restraints	36
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0563P)^2 + 13.002P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.70, -0.97

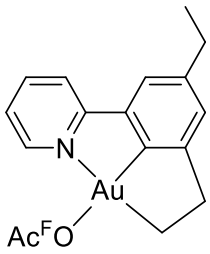
Table S14. Crystal and refinement data for **3s-AuOAc^F**.



3s-AuOAc^F

Crystal data	
Identification code, CCDC number	IL_60_tol, 2126097
Chemical formula	$C_{19}H_{18.5}AuF_3NO_2$
M_r	546.81
Crystal system, space group	Triclinic, $P\bar{1}$
Temperature (K)	100
a, b, c (Å)	9.0910 (5), 14.2888 (8), 16.1720 (9)
α, β, γ (°)	65.308 (1), 78.665 (1), 82.526 (1)
V (Å^3)	1868.71 (18)
Z	4
Radiation type	Mo $K\alpha$
μ (mm^{-1})	7.91
Crystal size (mm)	0.19 × 0.13 × 0.04
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.1158 before and 0.0491 after correction. The Ratio of minimum to maximum transmission is 0.7113. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.530, 0.745
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	57959, 7703, 6644
R_{int}	0.038
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.627
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.022, 0.049, 1.03
No. of reflections	7703
No. of parameters	476
No. of restraints	20
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0142P)^2 + 5.004P]$ where $P = (F_o^2 + 2F_c^2)/3$
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	1.31, -0.84

Table S15. Crystal and refinement data for **3t-AuOAc^F**.



3t-AuOAc^F

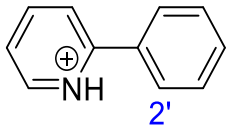
Crystal data	
Identification code, CCDC number	IL_63_tol, 2114274
Chemical formula	$0.25(C_{17}H_{15}AuF_{2.706}NO_2)\cdot 0.75(C_{17}H_{15}AuF_3NO_2)$
M_r	517.91
Crystal system, space group	Monoclinic, *Cc*
Temperature (K)	100
a, *b*, *c* (Å)	26.1042 (19), 13.5893 (10), 19.3988 (14)
β (°)	112.368 (2)
V (Å^3)	6363.7 (8)
Z	16
Radiation type	Mo *K*α
μ (mm^{-1})	9.29
Crystal size (mm)	0.22 × 0.18 × 0.15
Data collection	
Diffractometer	Bruker D8 Venture
Absorption correction	Multi-scan *SADABS2016*/2 (Bruker,2016/2) was used for absorption correction. wR2(int) was 0.0992 before and 0.0444 after correction. The Ratio of minimum to maximum transmission is 0.8177. The λ/2 correction factor is Not present.
T_{min}, T_{max}	0.610, 0.746
No. of measured, independent and observed [$I > 2\sigma(I)$] reflections	84078, 19420, 13543
R_{int}	0.037
$(\sin\theta/\lambda)_{max}$ (Å^{-1})	0.716
Refinement	
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, *S*	0.033, 0.079, 1.02
No. of reflections	19420
No. of parameters	367
No. of restraints	5
H-atom treatment	H-atom parameters constrained
Weighting scheme	$w = 1/[\sigma^2(F_o^2) + (0.0286P)^2 + 73.1986P]$ where $P = (F_o^2 + 2F_c^2)/3$
$(\Delta/\sigma)_{max}$	1.312
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e Å^{-3})	2.68, -1.56
Absolute structure	Refined as an inversion twin.
Absolute structure parameter	0.482 (19)

Computational details

Calculations were carried out at the DFT level as implemented in the Gaussian16 software package.[45] The hybrid PBE0+GD3 functional[46, 47] including Grimme's model for dispersion forces was used to optimize all geometries. This methodology was selected based on previous studies which have proven its solid performance in the modelling of Au(III) complexes.[39, 48-51] C, H, F, N and O were described with the all-electron triple-ζ 6-311+G** basis set,[52, 53] whereas Au was described with the Stuttgart-Köln basis set including a small-core quasi-relativistic pseudopotential.[54, 55] NBO7 calculations were performed in order to analyze the natural charges.[56] Geometries were fully optimized without any constraint. Vibrational frequencies were computed at the same level of theory to classify all stationary points as either saddle points (transition states, with a single imaginary frequency) or energy minima (reactants, intermediates and products, with only real frequencies). The Gibbs free energy used in the discussion includes both the thermochemistry and the refined energy. All optimizations were carried out in solvent (CH_2Cl_2 or $HOAc^F$) using the SMD solvation model.[57] $HOAc^F$ was defined as eps = 8.55, epsinf = 2.26 and rsolv = 13.7. In the bimolecular steps, the energies were corrected for the 1 M standard state.

Formal Charge Analysis calculations

In order to assess the electronic properties of the (N,C) ligands depicted in Scheme 1, main text, in a systematic manner, and possibly explain some of the experimental observations, natural charge analysis of the protonated bidentate (N,C) ligands was performed (Table S16). Protonated ligands were used to model the *N*-coordinated Au(III) adducts that initially form during cyclometalation. The natural charge of the carbon (C2') within each ligand that would bind Au(III) under experimental conditions was calculated and compared to those of the 2-phenylpyridinium cation (**ppy-H$^+$**, Figure S163).



ppy-H$^+$

Figure S163. The phenylpyridinium cation.

From the analysis, the natural charge of C2' varies only to a minor extent for the 4'-substituted ligands compared to **ppy-H$^+$** ($\Delta \leq 0.020$). A broader range was found for the ligands containing electron-donating or electron-withdrawing groups in the 3' and/or 5' positions. For ligand **1h-H$^+$**, bearing methyl groups in *ortho* and *para* positions relative to C2', a small negative change in the natural charge was found ($\Delta = -0.008$), consistent with the mild electron-donating ability of alkyl groups. For ligand **1c-H$^+$**, having fluorine groups in the same positions, a much larger change was observed ($\Delta = -0.084$), in line with fluorine being an activating, *ortho*/*para* directing group in electrophilic aromatic substitutions. An even more negative natural charge was found for C2' in 3',5'-dimethoxy-substituted ligand **1j-H$^+$** ($\Delta = -0.120$). While **1c** and **1h** furnished cyclometalated Au(III) complexes in high yields, ligand **1j** yielded a mixture of a unidentifiable species. The larger negative Δ found for **1j** compared to **1c** and **1h** may suggest that **1j** is too electron rich to give a clean reaction under the experimental conditions for cyclometalation. This once again illustrates the resemblance of cyclometalation reactions of electron poor late transition metals and electrophilic aromatic substitution reactions.[58, 59]

For the ligands containing electron-withdrawing groups in the *ortho*/*para* positions relative to C2', the lowest natural charges of C2' were found for ligands **1r-H$^+$** (R = 3',5'-di(pentafluorophenyl), $\Delta = 0.041$) and **1f-H$^+$** (R = 3',5'-di(trifluoromethyl), $\Delta = 0.061$). These findings are in accordance with literature reports on the less powerful electron-withdrawing properties of the pentafluorophenyl group relative to the trifluoromethyl group,[60] and also agrees with the experimental findings. As discussed above, ligand **1r**

furnished the (N,C) complex **2r-Au(OAc^F)$_2$** upon reaction with Au(OAc)$_3$, whereas ligand **1f** failed to yield any cyclometalated complex. For ligand **1g-H$^+$**, two static isomers were modelled: the *ortho* isomer **1g-*o*-H$^+$** (R = 3'-trifluoromethyl) and the *para* isomer **1g-*p*-H$^+$** (R = 5'-trifluoromethyl). We found that the *ortho* isomer had a significantly lower natural charge at C2' than the *para* isomer, which is consistent with the *para* isomer **1g-*p*-Au(OAc^F)$_2$** always being the main isomer obtained experimentally.

Table S16. Absolute and relative formal charges at C2' in protonated ligands.

Protonated ligand	Charge of C2'	ΔC2'
ppy-H$^+$	-0.19526	0
1a-H$^+$	-0.18608	0.009
1c-H$^+$	-0.27967	-0.084
1d-H$^+$	-0.18099	0.014
1e-H$^+$	-0.17479	0.020
1f-H$^+$	-0.13399	0.061
1g-*p*-H$^+$	-0.17066	0.025
1g-*o*-H$^+$	-0.15729	0.038
1h-H$^+$	-0.20283	-0.008
1i-H$^+$	-0.19340	0.002
1j-H$^+$	-0.31507	-0.120
1k-H$^+$	-0.17786	0.017
1l-H$^+$	-0.18894	0.006
1m-H$^+$	-0.18651	0.000
1n-H$^+$	-0.18888	0.006
1o-H$^+$	-0.18412	0.011
1p-H$^+$	-0.17743	0.018
1r-H$^+$	-0.15380	0.041

Color code: green shade: *para*-substituted on phenyl; red shade: di-substituted on phenyl; blue shade: pyridine-substituted; yellow shade: mono-substituted on phenyl. Red name: electron-donating substituent on phenyl; blue name: electron-withdrawing substituent on phenyl; black name: methyl in *para* position on phenyl.

DFT calculations on the formation of 2s-Au(OAc^F)$_2$

Table S17. Gibbs energies in CH_2Cl_2 (SMD), calculated for the C(sp^2)-H activation step furnishing **2s-Au(OAc^F)$_2$** from **1s-H$^+$** (and [Au(OAc^F)$_4$]$^-$). The latter is set as the reference energy.

Structure	Gibbs energy [kcal mol^{-1}]
1s-H$^+$ and [Au(OAc^F)$_4$]$^-$	0.0
1s-Au(OAc^F)$_3$	-6.5
TSA	[15.0]
2s-Au(OAc^F)$_2$	-22.9

DFT calculations on the formation of 3u-AuOAc^F

DFT calculations on the formation of **3u-AuOAc^F** were performed for both cyclometalation steps. Due to the unsymmetrically substituted phenyl ring in ligand **1u**, two possible bis(trifluoroacetate) complexes can be obtained in the initial C(sp^2)-H activation reaction, as already discussed for ligand **1g** (see the discussion related to the characterization of **2g-*p*-Au(OAc^F)$_2$** and **2g-*o*-Au(OAc^F)$_2$**). Since a potential preference is of interest, this step was investigated thoroughly. The protonated ligand **1u-H$^+$** and the [Au(OAc^F)$_4$]$^-$ anion were used as the energy reference (Figure S164). The energy difference for the two stable conformations of the free ligand is only 0.6 kcal mol^{-1}, hence both reaction pathways are considered possible. Formation of the *N*-coordinated complexes **1u-*o*-Au(OAc^F)$_3$** and **1u-*p*-Au(OAc^F)$_3$** are both exergonic processes. For the following C(sp^2)-H activation step, the energy barrier is 19.7 kcal mol^{-1} when ethyl is *ortho* to the newly formed Au-C bond, and 22.5 kcal mol^{-1} when ethyl is *para* to the Au-C bond. This energy barrier found for the complex bearing the ethyl group *ortho* to the carbon that undergoes C-H activation is 2 kcal mol^{-1} lower than seen in the same step for the more sterically crowded isopropyl analog **3s-AuOAc^F** ($\Delta G^{\ddagger}$ = 21.6 kcal mol^{-1}). The bis(trifluoroacetate) complex (**2u-*o*-Au(OAc^F)$_2$**) that may undergo C(sp^3)–H activation has a similar thermodynamic energy difference compared to its energy reference as that seen for **3s-Au(OAc^F)$_2$**, meaning the *ortho*-substituted **2u-*o*-Au(OAc^F)$_2$** is a relatively stable species. The energy barrier (Table S18) for the dissociation step (25.9 kcal mol^{-1}) furnishing the agostic intermediate [**2u-*o*-Au-OAc^F**]$^+$[**OAc^F**]$^-$ is similar to that observed in the formation of both **3s-Au-OAc^F** and **3t-Au-OAc^F** (22.1 and 25.0 kcal mol^{-1}, respectively). The proton abstraction by [OAc^F]$^-$ is barrier-free. Overall, the **3u-AuOAc^F** pincer complex is more thermodynamically stable than **2u-*p*-Au(OAc^F)$_2$**, albeit only with a relatively small

margin (ΔG = −2.7 kcal mol^{-1}). This correlates well with the experimental observations, where a mixture of **3u-AuOAc^F** and **2u-*p*-Au(OAc^F)$_2$** was obtained.

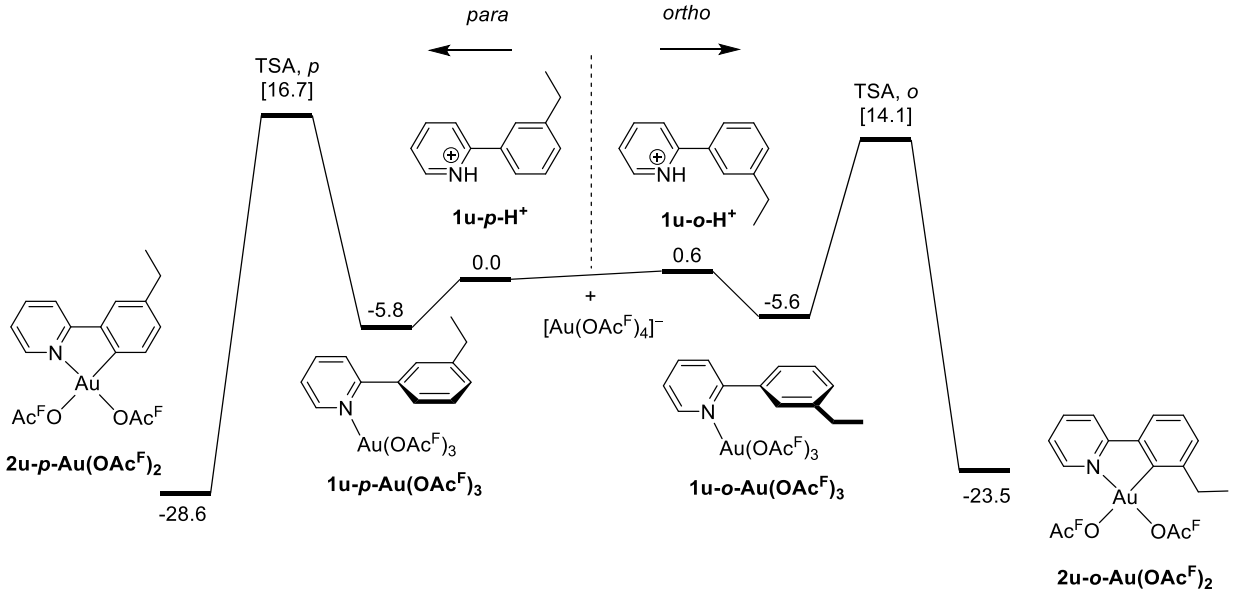


Figure S164. Free energy profile in kcal mol^{-1} for the C(sp^2)-H activation reaction furnishing **2u-o-Au(OAc^F)$_2$** and **2u-p-Au(OAc^F)$_2$**. The energies of all minima and transition states in brackets are computed in CH_2Cl_2 (SMD).

Table S18. Gibbs energies in CH_2Cl_2 (SMD), calculated for the C(sp^3)-H activation step furnishing **3u- AuOAc^F** from its bis(trifluoroacetate) precursor **2u-o-Au(OAc^F)$_2$**. The latter is set as the reference energy.

Structure	Gibbs energy [kcal mol^{-1}]
2u-*o*-Au(OAc^F)$_2$	0.0
TS1	[25.9]
[2u-*o*-Au-OAc^F]$^+$[OAc^F]$^-$	22.9
TS2	[23.9]
3u-AuOAc^F	-7.8

Optimized Cartesian coordinates (in Å) and energies (G, in Hartrees)

ppy-H^+

C	2.73802100	-1.13178700	-0.37697200
C	0.71871300	0.06866500	0.01087700
C	1.46448100	1.18148400	0.38487700
C	2.84899200	1.12245400	0.37319100
C	3.50069500	-0.04939100	-0.00775200
H	3.14701300	-2.08027500	-0.70023000
H	0.86701300	-1.84709800	-0.67066000
H	0.94665000	2.07623700	0.70626900
H	3.42539000	1.99103400	0.67323200
H	4.58033900	-0.12308200	-0.02189300
C	-0.74758000	0.02652100	0.00746100
C	-1.46925300	1.16576500	-0.36544200
C	-1.43310600	-1.13430900	0.38380900
C	-2.85658200	1.13713600	-0.37279500
H	-0.94347200	2.06456300	-0.67081300
C	-2.82112400	-1.15378900	0.37792000
H	-0.89108600	-2.01375200	0.71989800
C	-3.53436900	-0.02112400	-0.00276600
H	-3.41023900	2.02056200	-0.67308200
H	-3.34656900	-2.05290400	0.68225500
N	1.39873200	-1.03792700	-0.35897400
H	-4.61947700	-0.03955600	-0.00660500

1a-H^+

C	3.20180600	-1.13951000	-0.36720200
C	1.18262400	0.06758800	0.00988400
C	1.93258200	1.18342300	0.37108800

C	3.31614900	1.12214100	0.35836600
C	3.96651000	-0.05517200	-0.01047800
H	3.60878200	-2.09227600	-0.68034700
H	1.32989900	-1.85459600	-0.65447000
H	1.41708000	2.08221300	0.68465200
H	3.89420900	1.99288200	0.64891400
H	5.04601500	-0.13063900	-0.02426100
C	-0.28079700	0.02872300	0.00998200
C	-1.00671400	1.17109800	-0.34934400
C	-0.97550600	-1.12801900	0.37770100
C	-2.39076500	1.14503500	-0.35345500
H	-0.48374400	2.07393000	-0.64796200
C	-2.36293500	-1.13995300	0.37546700
H	-0.44181300	-2.01430100	0.70955000
C	-3.09503900	-0.00972000	0.00582300
H	-2.93936300	2.03593000	-0.64504400
H	-2.88799900	-2.04065900	0.67885200
N	1.86214400	-1.04324400	-0.35003700
C	-4.59212600	-0.02557100	-0.01600900
H	-5.00180900	0.83957300	0.51410600
H	-4.96117000	0.02395000	-1.04655800
H	-4.98983000	-0.93366900	0.44189100

1c-H$^+$

C	3.30170500	-1.05808100	-0.54448300
C	1.28603700	0.06771300	0.02537700
C	2.02807900	1.11402800	0.55672800
C	3.41400200	1.05978900	0.53230700
C	4.06455600	-0.04025900	-0.02021800
H	3.71068900	-1.94696400	-1.00717600

H	1.43444700	-1.72913300	-0.93275000
H	1.51242300	1.95345500	1.00540800
H	5.14422700	-0.10972800	-0.04884100
C	-0.18334400	0.02607600	0.01864700
C	-0.89338200	1.21500500	-0.16231700
C	-0.85979000	-1.18400000	0.19550400
C	-2.27313300	1.15791900	-0.17312600
H	-0.39236900	2.16358400	-0.31498500
C	-2.24119100	-1.16925300	0.17638200
H	-0.34457300	-2.12060000	0.38091100
C	-2.98348400	-0.01738300	-0.00780300
N	1.96333800	-0.97091300	-0.50786400
H	3.98969600	1.87588700	0.95521400
H	-4.06695300	-0.03445500	-0.01887800
F	-2.95939000	2.29414100	-0.36012800
F	-2.89519600	-2.32580600	0.35503500

1d-H$^+$

C	-1.43962900	2.39645100	-0.32185300
C	0.14526400	0.62760700	-0.11161900
C	-0.90787900	-0.28132300	0.00981200
C	-2.21035500	0.17426500	-0.03848900
C	-2.49654800	1.53064800	-0.20103500
H	-1.54918200	3.46359900	-0.46492600
H	0.56787200	2.59899300	-0.41070700
H	-0.68967300	-1.32935400	0.16650600
H	-3.51174800	1.90456200	-0.23824800
C	1.55679200	0.25652300	-0.05224000
C	1.97293000	-0.99324500	-0.52657100
C	2.51151900	1.13007900	0.48581800

C	3.31030300	-1.34925000	-0.47434600
H	1.25494000	-1.67965700	-0.96293400
C	3.84428000	0.75846200	0.54033100
H	2.21713500	2.08935600	0.90292300
C	4.27027400	-0.48314900	0.05734400
N	-0.18280800	1.92525400	-0.27915000
H	4.56844500	1.43882400	0.97810100
H	3.61799100	-2.31767400	-0.85695800
C	-3.36150700	-0.79010800	0.12900700
F	-2.97145300	-2.06376500	0.05516500
F	-4.29300500	-0.59361400	-0.81224300
F	-3.95411500	-0.61628400	1.31958800
C	5.71732200	-0.86303100	0.08978000
H	6.22128000	-0.43575200	0.96041700
H	5.84535300	-1.94785600	0.10463900
H	6.22779100	-0.48242400	-0.80299400

1e-H$^+$

C	-4.24230800	1.14486900	-0.39415900
C	-2.23950400	-0.07111400	0.01233200
C	-2.99304500	-1.17449000	0.39103800
C	-4.37822600	-1.10299300	0.37357400
C	-5.01625000	0.07087000	-0.01964400
H	-4.64213100	2.09381200	-0.72728300
H	-2.36418100	1.84346500	-0.68031900
H	-2.48418000	-2.07169800	0.72007000
H	-6.09507400	0.15440700	-0.04015200
C	-0.77063100	-0.04193000	0.01647900
C	-0.05895900	-1.18445400	-0.35911700
C	-0.07972600	1.10944800	0.40647900

C	1.32683700	-1.17370300	-0.35503300
H	-0.58837800	-2.07721800	-0.67364500
C	1.30605900	1.11971700	0.41371800
H	-0.61396700	1.99299900	0.74214900
C	2.00389900	-0.02231700	0.03381300
H	1.87627000	-2.05929400	-0.65332100
H	1.83948200	2.00956500	0.72867500
N	-2.90491600	1.04025300	-0.36768200
C	3.50349400	0.00960700	-0.00225900
H	-4.96357000	-1.96419600	0.67729700
F	4.04441600	-1.20739900	0.15634800
F	4.01719900	0.79948500	0.95400600
F	3.96064100	0.48517100	-1.17958000

1f-H$^+$

C	-4.39158700	-0.88703500	0.69862900
C	-2.36577500	0.11870700	-0.03241200
C	-3.09463700	1.08246400	-0.71406500
C	-4.48167900	1.04969000	-0.67984900
C	-5.14333200	0.05217500	0.03008700
H	-4.81074700	-1.69337900	1.28651600
H	-2.53192700	-1.51525500	1.18201800
H	-2.57043900	1.83738600	-1.28595400
H	-6.22371600	0.00118400	0.06990400
C	-0.89656800	0.05620500	-0.02149700
C	-0.15507300	1.23911400	0.01195700
C	-0.23543300	-1.17085700	-0.05718700
C	1.22958600	1.18156200	0.01933500
H	-0.65734100	2.19963800	0.04827400
C	1.15334900	-1.20703400	-0.04237300

H	-0.79519200	-2.09859100	-0.12865900
C	1.89771000	-0.03769200	-0.00198500
N	-3.05275400	-0.82284200	0.64825100
H	-5.04845600	1.80136800	-1.21847900
H	2.98056200	-0.07282700	0.00708200
C	1.83366700	-2.54483600	-0.11041300
C	2.01790300	2.45770100	0.10804400
F	1.35152400	-3.39050000	0.81799500
F	1.64017200	-3.13686300	-1.30385100
F	3.15426100	-2.45936400	0.07763200
F	3.22632200	2.34346600	-0.45833400
F	1.38839700	3.47850700	-0.49340300
F	2.21907500	2.82690700	1.38795200

1g-*p*-H$^+$

C	-4.19408700	0.40324500	0.59576600
C	-1.93062900	0.05456400	-0.05074500
C	-2.28061500	-1.18500200	-0.57209500
C	-3.59534800	-1.62072800	-0.49892800
C	-4.57055000	-0.81789900	0.08754000
H	-4.87247200	1.09402100	1.07958900
H	-2.66962700	1.68422100	0.93447500
H	-1.52263300	-1.78982400	-1.05365900
H	-3.86341300	-2.58682900	-0.91261300
H	-5.60440600	-1.13136100	0.15342300
C	-0.56946900	0.60745100	-0.09453100
C	0.52149200	-0.24871900	0.06430000
C	-0.35025700	1.97225200	-0.31072000
C	1.80980800	0.26491600	0.00912700
H	0.36644100	-1.30518900	0.25312000

C	0.94267800	2.47185800	-0.36673000
H	-1.18627200	2.64688300	-0.46852300
C	2.02970900	1.62147300	-0.20922300
H	1.10525200	3.52890300	-0.54522900
N	-2.91147700	0.79050500	0.51430800
H	3.04006800	2.01189300	-0.25588900
C	2.97506000	-0.67264900	0.13407600
F	2.71397600	-1.70079000	0.95840500
F	4.07519700	-0.06267400	0.59772200
F	3.30645500	-1.21329500	-1.05744500

1g-*o*-H$^+$

C	3.47200900	-1.57757900	-0.53665500
C	1.95771000	0.17921500	-0.00924100
C	2.99179800	0.88000900	0.59819500
C	4.26747300	0.33638800	0.63082400
C	4.51545200	-0.91025000	0.06148800
H	3.56471800	-2.54257200	-1.01801600
H	1.51094400	-1.52440700	-1.03677600
H	2.78071000	1.83620300	1.06033400
H	5.07133800	0.88257200	1.11226000
H	5.50074500	-1.35796100	0.07543500
C	0.57267800	0.66335900	-0.08460900
C	-0.49906000	-0.21690700	0.07397400
C	0.32639000	2.02251200	-0.30257600
H	-0.33276400	-1.26744000	0.28916800
C	-0.97640900	2.49288000	-0.37133600
H	1.15607800	2.70816800	-0.43799900
C	-2.04601100	1.61881800	-0.21930600
H	-1.16142200	3.54649300	-0.54846600

N	2.25130200	-1.02032800	-0.55420800
H	-3.06444800	1.98713100	-0.27029100
C	-1.79845600	0.26897700	0.00799700
C	-2.94372800	-0.69129600	0.14041700
F	-3.27097200	-1.23976100	-1.04921400
F	-4.05312500	-0.10442000	0.61021600
F	-2.65635800	-1.71389100	0.96330700

1h-H$^+$

C	3.33433600	-1.04704700	-0.56121200
C	1.31426700	0.07113800	0.02736700
C	2.06414600	1.10825500	0.57472800
C	3.44794800	1.05304500	0.54730300
C	4.09894900	-0.03996100	-0.02343100
H	3.74079500	-1.92976300	-1.03786600
H	1.46331500	-1.70730500	-0.95781500
H	1.55044500	1.93936600	1.04040700
H	5.17853500	-0.10950700	-0.05396600
C	-0.15153800	0.02796700	0.02071100
C	-0.87055500	1.21874400	-0.12438000
C	-0.83188900	-1.18550000	0.15732500
C	-2.26155700	1.20539400	-0.14965300
H	-0.34338400	2.15951300	-0.24839700
C	-2.22512500	-1.21986500	0.14602600
H	-0.28639300	-2.11312700	0.31185300
C	-2.91841500	-0.02000100	-0.01358500
N	1.99482400	-0.95780700	-0.52231800
H	4.02541600	1.86099300	0.98354300
H	-4.00582200	-0.03875200	-0.03050700
C	-2.96300000	-2.51141200	0.33955000

H	-2.34871000	-3.37004000	0.05754400
H	-3.24653200	-2.63734800	1.39071100
H	-3.88263700	-2.53335300	-0.25098400
C	-3.04438200	2.47093300	-0.33761400
H	-2.39211800	3.34707200	-0.34279500
H	-3.59332700	2.45052600	-1.28504300
H	-3.78245300	2.59623900	0.46073700

1i-H$^+$

C	-0.83459900	0.40748700	-0.06785900
C	-2.83473100	1.70069800	-0.33324900
C	-3.60793800	0.56651100	-0.10800700
H	-1.18601500	-1.54351700	0.38549400
H	-3.31905600	2.65008700	-0.53632000
H	-4.68974500	0.60850100	-0.12416400
C	0.61570800	0.20107500	-0.04620700
C	1.45831200	1.19813000	0.45643900
C	1.18263800	-0.98375700	-0.53086400
C	2.83033300	1.00352200	0.48617300
H	1.03746000	2.11848200	0.84813900
C	2.55659800	-1.16416000	-0.50245800
H	0.55699000	-1.75582500	-0.97078900
C	3.40491000	-0.17961700	0.01263600
H	3.46964900	1.78300800	0.89001400
H	2.98113100	-2.08187200	-0.89851800
N	-1.63471200	-0.65939200	0.15843300
C	4.88511000	-0.39766700	0.07636500
H	5.43018500	0.54901800	0.05111900
H	5.15354000	-0.90759300	1.00927900
H	5.23138800	-1.02468600	-0.74916800

C	-1.45011300	1.62660700	-0.31761300
H	-0.84058700	2.49694100	-0.52423200
C	-2.98453900	-0.64133300	0.14489800
C	-3.68746000	-1.92305400	0.40972300
H	-3.43027700	-2.66180000	-0.35616100
H	-3.39070100	-2.32966300	1.38170300
H	-4.76635100	-1.77198700	0.40471300

1j-H$^+$

C	-3.62400300	0.94812400	-0.66348900
C	-1.60530600	-0.10008000	0.04145000
C	-2.35128000	-1.08771400	0.67505900
C	-3.73573900	-1.04382500	0.63081700
C	-4.38729200	-0.01164500	-0.04228300
H	-4.03173600	1.78101400	-1.22174900
H	-1.74952100	1.57769000	-1.10424000
H	-1.83551800	-1.86903200	1.21810300
H	-4.31267200	-1.81285600	1.13312200
H	-5.46697700	0.04767700	-0.08805700
C	-0.13835600	-0.04082300	0.03860600
C	0.58198800	-1.23362100	-0.03508300
C	0.50028800	1.20033300	0.10247200
C	1.97742700	-1.17246300	-0.06585600
H	0.06078000	-2.17963400	-0.10170200
C	1.89671400	1.23850100	0.08290000
H	-0.07719800	2.10918500	0.21568900
C	2.62761700	0.05717600	-0.00569000
N	-2.28491900	0.87151000	-0.60452000
H	3.71115300	0.09561700	-0.02683000
O	2.77517100	-2.25232300	-0.16209200

O	2.62064700	2.37147700	0.15197300
C	2.17067200	-3.53465000	-0.24387900
H	1.58301300	-3.75631600	0.65364000
H	1.53762900	-3.62092100	-1.13382900
H	2.99273000	-4.24622200	-0.31816400
C	1.93376100	3.61222900	0.21634700
H	1.30391900	3.76556500	-0.66719700
H	1.32590800	3.68592400	1.12480000
H	2.70744500	4.37925700	0.24078300

1k-H$^+$

C	3.67527200	-1.02229100	-0.36678300
C	1.58626400	0.06723300	0.01152800
C	2.27710400	1.23123400	0.34892300
C	3.66008700	1.25246400	0.31948500
C	4.37794400	0.10944100	-0.03636600
H	4.13401400	-1.95591200	-0.66623000
H	1.84832200	-1.84996400	-0.62892300
H	1.71713100	2.10466600	0.65750200
H	5.46001600	0.09764400	-0.05851800
C	0.13198800	-0.06076500	0.02686200
C	-0.66917700	1.04880300	-0.25990800
C	-0.49762600	-1.27991600	0.33256900
C	-2.05195800	0.95979300	-0.25361300
H	-0.21189300	1.99744300	-0.52095800
C	-1.87256600	-1.37674000	0.35072500
H	0.08363500	-2.15918600	0.59858800
C	-2.66494300	-0.25856000	0.05608300
H	-2.63989300	1.83580700	-0.49748700
H	-2.36080400	-2.31087100	0.60645700

N	2.33163400	-1.00457300	-0.33950900
H	4.18799600	2.16075800	0.58986300
O	-3.99007200	-0.45048400	0.09893200
C	-4.84699500	0.65423700	-0.16460800
H	-4.70197800	1.03396600	-1.18135900
H	-5.86226200	0.27233600	-0.06326700
H	-4.68751000	1.45959400	0.56006200

1l-H$^+$

C	-2.16520500	1.92568400	-0.36677500
C	-0.40746400	0.35431700	-0.08265300
C	-1.33944000	-0.64175500	0.11117900
C	-2.70909400	-0.35084200	0.06549600
C	-3.12695400	0.97018300	-0.17658000
H	-2.40074400	2.96276200	-0.56955200
H	-0.18640000	2.34813100	-0.50662000
H	-1.01831000	-1.65254700	0.32790900
H	-4.16925100	1.25298100	-0.22126200
C	1.04184900	0.13436800	-0.03502000
C	1.58452800	-1.07004100	-0.49539200
C	1.90133300	1.10867600	0.48232800
C	2.95264000	-1.28343700	-0.44826600
H	0.93584700	-1.83421000	-0.91062200
C	3.26917000	0.88288900	0.52834600
H	1.50598100	2.03472500	0.88912800
C	3.82089900	-0.31170600	0.05944300
H	3.35785300	-2.22095400	-0.81765800
H	3.92010000	1.64432000	0.94767100
N	-0.86082500	1.61216800	-0.31969100
C	5.30094000	-0.53985600	0.07723200

H	5.53919400	-1.58663000	0.28362100
H	5.73560700	-0.29306000	-0.89862600
H	5.79318800	0.08571700	0.82553900
O	-3.52587400	-1.36634800	0.27313000
C	-4.94004300	-1.14044800	0.26444700
H	-5.26751600	-0.78049300	-0.71465100
H	-5.38930600	-2.11092600	0.46722700
H	-5.22243500	-0.43238700	1.04797600

1m-H$^+$

C	-2.64211800	-0.30125300	0.06013100
C	-0.41233500	0.56522400	-0.08113000
C	-2.30236200	2.02064500	-0.30872800
C	-3.18154700	0.96206800	-0.14172100
H	-0.95111400	-1.38201200	0.27816500
H	-2.70280000	3.01541600	-0.47335300
H	-4.25230600	1.10843700	-0.16493800
C	1.01456600	0.23889600	-0.04523500
C	1.93445300	1.18278300	0.42884500
C	1.48818000	-1.00205700	-0.48487600
C	3.28601300	0.88537700	0.46463000
H	1.58831700	2.14398300	0.79431200
C	2.84510000	-1.28730900	-0.44830800
H	0.80778400	-1.74399900	-0.89396700
C	3.76784500	-0.35400200	0.02890500
H	3.98395900	1.62590800	0.84447200
H	3.19577500	-2.24979500	-0.80823200
N	-1.30097300	-0.44625700	0.08714700
C	5.23034400	-0.66911100	0.09053200
H	5.82960600	0.16379100	-0.28861800

H	5.54005900	-0.84394800	1.12729000
H	5.47187900	-1.56407700	-0.48702600
C	-0.92394700	1.83505200	-0.28542800
H	-0.24875400	2.66350500	-0.45158000
O	-3.28262900	-1.43244900	0.24953100
C	-4.71951400	-1.41707200	0.24892800
H	-5.01444600	-2.44859100	0.42918000
H	-5.09399200	-0.77604500	1.05069700
H	-5.09419200	-1.08464300	-0.72193700

1n-H$^+$

C	2.59810100	-2.11963200	-0.25595800
C	0.85060100	-0.49526800	-0.09495900
C	1.81751900	0.52121200	0.05102300
C	3.16842100	0.17806200	0.03824900
C	3.55856400	-1.14775300	-0.11615500
H	2.80146300	-3.17349800	-0.38860200
H	0.61122800	-2.48258500	-0.37620100
H	3.92548600	0.94286500	0.16053300
H	4.60630800	-1.41938000	-0.12777300
C	-0.60057200	-0.29310900	-0.05766200
C	-1.20541300	0.77917300	-0.72324500
C	-1.40918600	-1.20401600	0.63326800
C	-2.58393000	0.91979900	-0.70410600
H	-0.60003100	1.49104900	-1.27111000
C	-2.78605700	-1.04582100	0.65402600
H	-0.95885000	-2.02646900	1.18173200
C	-3.39902400	0.01772500	-0.01338500
H	-3.03982600	1.74773700	-1.23911700
H	-3.39570600	-1.75630200	1.20439600

N	1.30703900	-1.75281000	-0.24225000
C	-4.88409300	0.20443800	0.03642800
H	-5.15943000	0.83198000	0.89242600
H	-5.25412700	0.69982500	-0.86468000
H	-5.40264000	-0.75071400	0.15072400
O	1.34907000	1.75591800	0.22558900
C	2.28114700	2.82038500	0.41493500
H	2.89616100	2.64838300	1.30366300
H	2.91653000	2.94460400	-0.46727100
H	1.67514100	3.71368000	0.55757300

1o-H$^+$

C	-3.85514000	-1.11418800	0.45968600
C	-1.85023100	0.07063100	-0.01573500
C	-2.59828000	1.15050300	-0.46358800
C	-3.98440700	1.08174400	-0.44829600
C	-4.62530700	-0.06395700	0.01435700
H	-4.25850800	-2.03906400	0.85097700
H	-1.98026500	-1.79738900	0.79568400
H	-2.08725600	2.02670300	-0.84270000
H	-5.70437600	-0.14452700	0.03518400
C	-0.38055400	0.03709100	-0.01378000
C	0.33138600	1.19608300	0.30982700
C	0.30611600	-1.13687100	-0.33992400
C	1.71580000	1.18430000	0.31804700
H	-0.19846700	2.10332500	0.57749900
C	1.69091600	-1.15847200	-0.33488000
H	-0.23019000	-2.03376600	-0.63359200
C	2.37136300	0.00404800	-0.00331000
H	2.27895400	2.07239600	0.57591600

H	2.23455800	-2.05830000	-0.59385500
N	-2.51812000	-1.01396500	0.43146000
H	-4.56696100	1.92321700	-0.80738000
N	3.84149500	-0.01484900	0.00364800
O	4.41952800	1.01614100	0.28597800
O	4.39533400	-1.06068700	-0.27321700

1p-H$^+$

C	1.20026100	0.58624300	-0.84689100
C	2.57649800	0.72133500	-0.85234400
C	3.39162000	-0.12045700	-0.08559100
C	2.78143700	-1.11933500	0.67564000
C	1.40328600	-1.27507700	0.68108200
C	0.60111000	-0.41588600	-0.07524400
H	0.59582500	1.23933700	-1.46912200
H	3.03187900	1.49343100	-1.46514400
H	3.39402000	-1.77992400	1.28127000
H	0.95297100	-2.04122900	1.30519600
C	-0.85115800	-0.58950600	-0.07125700
C	-1.81957000	0.40676200	0.04351000
C	-3.17400600	0.12791900	-0.01582100
C	-2.63498700	-2.17334800	-0.23897000
C	-3.59226700	-1.19012600	-0.14639000
H	-3.89485800	0.93403800	0.07006600
H	-2.85811000	-3.22695600	-0.35009400
H	-4.64249200	-1.44815400	-0.17593300
N	-1.33525300	-1.84239900	-0.21272200
N	-1.43186900	1.80071300	0.31005600
O	-2.00967300	2.65478900	-0.32762900
O	-0.60272700	1.99395000	1.16956900

C	4.87674400	0.06532700	-0.07614800
H	5.26813500	0.15212600	-1.09410200
H	5.14064900	0.98944300	0.45041800
H	5.38221600	-0.76368000	0.42348400
H	-0.65499400	-2.58964900	-0.34236400

1r-H$^+$

C	-0.03112800	3.63038900	-0.49947300
C	-0.23515300	6.38839200	-0.80498600
H	-1.62359700	3.88688900	0.74952600
H	-0.33930600	7.46078200	-0.90817300
C	-0.02137100	2.17568200	-0.29026300
C	1.19737000	1.50148100	-0.20774800
C	-1.21836800	1.46423700	-0.19477100
C	1.22153600	0.12365100	-0.01428600
H	2.12914800	2.05058200	-0.28155900
C	-1.19842000	0.08351300	-0.01321600
H	-2.17138700	1.97112100	-0.30746000
N	-0.98018600	4.36218200	0.12160700
C	0.87018100	4.30631600	-1.31190100
H	1.63082900	3.74486500	-1.83890400
C	-1.10954500	5.69203200	-0.00339300
H	-1.91380100	6.14952400	0.55815000
C	0.76848600	5.68137300	-1.46230800
H	1.46993600	6.20305600	-2.10441600
C	0.02284400	-0.58153800	0.08243100
H	0.04135700	-1.65286900	0.25114100
C	2.51245900	-0.59084000	0.09839100
C	3.47643000	-0.22071000	1.03152500
C	2.81844900	-1.67057100	-0.72484600

C	4.68362700	-0.88822400	1.14805400
C	4.02013300	-2.35146400	-0.62979200
C	4.95634500	-1.95883100	0.31258600
C	-2.46478600	-0.67750600	0.06647300
C	-2.71369700	-1.76354300	-0.76832900
C	-3.46378500	-0.34614000	0.97696700
C	-3.89278300	-2.48633400	-0.70505400
C	-4.64892600	-1.05619100	1.06234000
C	-4.86435500	-2.13171500	0.21639900
F	1.95168900	-2.06440000	-1.65764100
F	4.28483200	-3.36976700	-1.44048900
F	6.10933900	-2.60397900	0.41289100
F	5.57490200	-0.51537500	2.05992000
F	3.24424100	0.79252200	1.86725100
F	-3.28863700	0.67342400	1.81990000
F	-5.57413100	-0.71887700	1.95403200
F	-5.99610300	-2.81682800	0.28672000
F	-4.10144500	-3.50889400	-1.52637100
F	-1.81303400	-2.12226800	-1.68269600

1s-H^+

G: -714.73013

N	-2.72709900	-1.20119900	0.55392400
C	-0.65522700	-0.09689600	-0.03470800
C	0.10656800	-1.27115800	-0.09328100
C	1.76958900	3.41926900	-1.07307300
C	1.68964900	3.30547300	1.44289300
C	2.10793700	0.03965300	0.01553900
C	2.06561800	2.56424800	0.15964700
C	1.37354600	1.22185200	0.07016800

C	2.32088600	-2.47973200	-0.14519900
C	-4.05709300	-1.38165100	0.60002000
C	-4.31608500	0.64450000	-0.61665400
C	-2.93954900	0.79422600	-0.65159400
C	-4.88955500	-0.45941400	0.01329300
C	-0.01859500	1.14170400	0.04061300
C	1.49473900	-1.21459400	-0.06979700
C	-2.11992300	-0.15637100	-0.04933400
H	-4.40200600	-2.26509700	1.12166500
H	-5.96148500	-0.60330400	0.04993000
H	-4.94846300	1.38552600	-1.09353800
H	-2.48434800	1.63131500	-1.16520900
H	-0.60912700	2.04991800	0.10461400
H	2.31726400	4.36571800	-1.02240900
H	2.06133800	2.90542100	-1.99414900
H	0.70164000	3.65386200	-1.14010300
H	0.62136800	3.54717800	1.46113200
H	1.91680600	2.70721500	2.33061500
H	2.24475800	4.24615600	1.51518000
H	3.19333500	0.09848900	0.03639100
H	3.14343000	2.36745400	0.18576700
C	3.16560700	-2.66589400	1.11562400
H	3.89981900	-1.86012300	1.22030800
H	2.54355400	-2.67491600	2.01605400
H	3.71370400	-3.61238800	1.07047500
C	3.19625400	-2.49968900	-1.39867700
H	2.59511300	-2.39360400	-2.30694000
H	3.92847900	-1.68537700	-1.38132900
H	3.74774900	-3.44310600	-1.46301900
H	1.61875500	-3.31945900	-0.20895100

H	-0.37555700	-2.24061100	-0.19486300
H	-2.14262200	-1.88502700	1.02802900

$[AuOAc^{F}{}_{4}]^{-}$

G: -2239.234711

Au	0.02447800	-0.53983700	-0.54376100
F	4.97376200	-1.08577000	1.02387600
F	4.54632600	-1.44800800	-1.06055000
F	4.53540200	0.57184800	-0.28726000
O	2.01535000	-0.43983700	-0.68523500
O	2.34512000	-1.25706500	1.39674500
C	2.71233700	-0.83530200	0.33166700
C	4.22158100	-0.69721700	-0.00106200
O	-0.01994900	1.28485600	0.27091600
C	-0.08554700	2.29704500	-0.53381600
O	-0.11132100	2.32013600	-1.73641200
C	-0.14946600	3.60607600	0.29603800
F	0.87495000	3.69174000	1.15141300
F	-1.28289700	3.65443400	1.00841300
F	-0.11570500	4.67421500	-0.49503500
O	-1.97100900	-0.54862900	-0.64582000
C	-2.63035800	-0.97734200	0.38247900
O	-2.22544000	-1.38606200	1.43883600
C	-4.14994500	-0.90098100	0.07811300
F	-4.46090600	-1.64469500	-0.99029600
F	-4.86586900	-1.34177000	1.10807800
F	-4.52345300	0.35849500	-0.17724900
O	0.08182200	-2.45135600	-1.12294800
C	0.00060800	-2.68625300	-2.39381900
C	0.07673800	-4.21646900	-2.63694500

F	-0.92279200	-4.85027900	-2.01235100
F	1.22985700	-4.71554700	-2.17590300
F	-0.00394700	-4.49834700	-3.93370100
O	-0.11395600	-1.91346700	-3.30863900

1s-Au(OAc^{F})$_3$

G: -2427.535229

Au	-0.88679700	-0.05602000	-0.64643200
F	3.57341600	-2.85649300	-0.75067400
F	2.21079200	-3.06984400	-2.41162100
F	3.33302600	-1.23957600	-2.15967800
O	0.80305300	-0.85910200	-1.35398700
O	1.38770800	-2.00935300	0.50630100
N	-0.28887200	1.67499900	-1.50566700
C	1.71322700	1.77915000	-0.08660700
C	3.08368600	1.58220300	-0.28282600
C	3.29221400	0.87679400	1.99859100
C	1.52506700	-1.65755100	-0.63340900
C	1.93273400	1.07365900	2.21897300
C	-1.08749100	2.14432800	-2.48284800
C	0.48366400	3.86105200	-2.97269400
C	2.68806400	-2.20937000	-1.50252200
C	1.28531300	3.37635700	-1.95485500
C	-0.73247500	3.24161800	-3.23536100
C	1.14660200	1.53900700	1.16305400
C	3.88706000	1.12889900	0.75728200
C	0.88713900	2.27275800	-1.20219900
H	-2.01537700	1.61198700	-2.65360500
H	-1.40056100	3.58869000	-4.01359000
H	0.09419900	1.74589100	1.33391700

O	-1.57979900	-1.68887700	0.28951200
C	-1.55254000	-2.84439400	-0.28636200
O	-1.19716500	-3.14530400	-1.39630600
C	-2.09027700	-3.91474600	0.70070300
F	-3.35423500	-3.64430600	1.05315100
F	-1.35458800	-3.95338500	1.81676600
F	-2.06834000	-5.12544100	0.15073900
H	3.51962300	1.75931900	-1.26176400
O	-2.69221800	0.74086000	-0.28811000
C	-2.92402800	1.54576900	0.69800200
O	-2.18838300	1.96542700	1.55253700
C	-4.41288600	1.98415300	0.64444500
F	-5.23304200	0.93004000	0.64012600
F	-4.72358800	2.74782300	1.68594700
F	-4.64566600	2.69054200	-0.47150800
H	0.79756000	4.72508500	-3.54829200
H	2.22105200	3.85933800	-1.70104900
H	3.90552000	0.51435800	2.81959200
C	5.37317500	0.93537000	0.54797500
H	5.56568100	1.07496300	-0.52246800
C	1.30774800	0.79264200	3.56710300
H	2.09920800	0.38701900	4.20816900
C	6.16609300	1.99722900	1.31286800
H	6.00441400	1.90167700	2.39212500
H	7.23873100	1.88659200	1.12250000
H	5.86938200	3.00807500	1.01599600
C	5.83487800	-0.46986400	0.93080100
H	5.70571500	-0.65345100	2.00241700
H	5.27565600	-1.23703700	0.38832900
H	6.89762400	-0.59500800	0.69959600

C	0.78298300	2.07554300	4.21352300
H	1.57467300	2.82428100	4.31745200
H	-0.02301000	2.51294000	3.61476200
H	0.38045500	1.86420800	5.20961600
C	0.19840200	-0.25518600	3.45738600
H	-0.64433400	0.12717700	2.87180900
H	0.55717500	-1.16854300	2.97536600
H	-0.17993700	-0.51298600	4.45199500

1s-Au-TSA

G: -2427.500884

Au	-0.68907100	0.43351700	0.03238200
F	3.50678800	-1.09489400	-3.37838400
F	2.05168200	0.31056700	-4.12636800
F	3.53275400	0.94851400	-2.68410100
O	1.01326000	0.55513200	-1.58050800
O	1.81447600	-1.55017300	-1.38260200
N	-0.45843100	2.42621900	0.11033300
C	1.52980100	1.72223400	1.16242300
C	2.86663000	1.59319700	0.85973800
C	2.84716200	-0.63192400	1.81251300
C	1.74964600	-0.43221000	-1.86114900
C	1.51295300	-0.52576500	2.17851600
C	-1.31424200	3.28974900	-0.44726600
C	0.18449200	5.08215800	0.06120300
C	2.72206600	-0.07279100	-3.02715700
C	1.06470900	4.16914400	0.62343200
C	-1.01898300	4.63972800	-0.47649400
C	0.83468700	0.66972200	1.83272600
C	3.54122400	0.40714600	1.18220600

C	0.71646600	2.82816000	0.64518700
H	-2.22468200	2.87696600	-0.86421700
H	-1.72978100	5.32524900	-0.92098900
H	-0.07681800	0.92252900	2.37697400
O	-0.84936100	-1.54728900	0.14489100
C	-1.05881100	-2.21701900	-0.94242200
O	-1.25084200	-1.82992800	-2.06395000
C	-1.07897500	-3.72992800	-0.59944200
F	-2.10084400	-4.00960200	0.22472700
F	0.04738500	-4.11446700	0.01028900
F	-1.22543400	-4.46767300	-1.69631000
H	3.37981500	2.37583900	0.31034400
O	-2.72968100	0.56233800	-0.49410900
C	-3.55699800	0.34691400	0.46467300
O	-3.35000200	0.11727500	1.63207600
C	-5.01332600	0.43877300	-0.06900400
F	-5.21644700	-0.41471900	-1.07761400
F	-5.89959400	0.16620300	0.88478900
F	-5.26762600	1.67624100	-0.52265500
H	0.43555100	6.13699700	0.04204300
H	2.01171700	4.47723200	1.04996700
H	3.38345900	-1.54741100	2.03548200
C	5.00357700	0.25820200	0.84890900
H	5.28598200	1.12220800	0.23751800
C	0.81556700	-1.65099000	2.90800900
H	0.70863600	-2.44995000	2.16003400
C	5.83589900	0.29272200	2.13540400
H	5.59131100	-0.55776600	2.78037200
H	6.90114800	0.23728200	1.89099600
H	5.66181600	1.21228800	2.70209400

C	5.28992300	-1.01072100	0.04600200
H	5.08135800	-1.91199200	0.63068800
H	4.68971200	-1.05451700	-0.86561600
H	6.34648500	-1.03536100	-0.23730800
C	1.66625200	-2.19337100	4.06067100
H	2.63996800	-2.56205300	3.73061000
H	1.83157600	-1.41761700	4.81615900
H	1.14442600	-3.02645000	4.54009700
C	-0.57922000	-1.29819900	3.40895500
H	-0.54268800	-0.49514900	4.15466300
H	-1.25505700	-0.99574400	2.60678500
H	-1.02207700	-2.17390700	3.89128500

2s-Au(OAc^{F})$_2$

G: -1901.123359

Au	-0.24793700	0.34439900	-0.15350200
F	-5.04380600	1.78611000	1.64976900
F	-4.44623300	2.75308600	-0.18544600
F	-4.95617500	0.64970200	-0.18305100
O	-2.23283600	1.09554200	-0.29878100
O	-2.47101800	1.17657700	1.94232200
N	0.58566000	2.15395100	-0.37064800
C	2.55262200	0.90250100	-0.03589700
C	1.69956000	-0.22396400	-0.05940100
C	6.76058600	-0.12482700	-0.75070600
C	6.44493800	-0.08536000	1.74901100
C	3.63178500	-1.60692500	0.17704900
C	-2.86809600	1.25771400	0.79996400
C	5.97421800	-0.69683800	0.42909200
C	4.48509400	-0.51256600	0.24332800

C	1.42707000	-2.78466700	-0.02845600
C	-0.14379600	3.25176300	-0.61114500
C	1.83642000	4.57698900	-0.56216400
C	-4.35173200	1.61524000	0.52406900
C	2.57585400	3.43092200	-0.32367800
C	0.45678900	4.48984800	-0.71514800
C	3.92656100	0.75526300	0.12089100
C	2.24005300	-1.50698800	0.01593600
C	1.93039900	2.20229000	-0.23231400
H	-1.21171100	3.11107200	-0.71949000
H	-0.15435100	5.36187000	-0.91137900
H	2.33595500	5.53685900	-0.63534600
H	3.65147300	3.48095800	-0.21589300
H	4.56566200	1.63215100	0.14326100
H	7.83079800	-0.31785800	-0.62495700
H	6.44227200	-0.57294600	-1.69694400
H	6.62458500	0.95938100	-0.82738400
H	6.29213500	0.99943500	1.75568900
H	5.90231700	-0.50774900	2.60024300
H	7.51314700	-0.27315800	1.89795200
H	4.06877900	-2.59799900	0.25130300
O	-1.22091800	-1.39269700	0.21426500
C	-1.86367700	-1.92098400	-0.76864800
O	-1.78073500	-1.69756600	-1.95224000
C	-2.85005100	-2.99123200	-0.23600000
F	-3.73227800	-2.44352100	0.61018400
F	-2.20179200	-3.96170500	0.42349700
F	-3.53304200	-3.56031300	-1.22670700
H	6.16037000	-1.77629600	0.46925400
C	1.02156900	-3.19045000	1.38963500

H	1.91190700	-3.40637100	1.99101000
H	0.45506500	-2.39845100	1.88482400
H	0.39947300	-4.09042300	1.36825800
C	2.13490000	-3.93649400	-0.73894100
H	2.50201000	-3.63825700	-1.72587500
H	2.97882100	-4.32714200	-0.16194600
H	1.42877400	-4.76116200	-0.87650500
H	0.52752100	-2.57157800	-0.60251400

2s-Au-TS1

G: -1901.085076

Au	-0.13914400	-0.40749500	-0.30246400
F	-5.06522900	-1.58324500	-1.94575800
F	-4.33921900	-2.77704500	-0.29961700
F	-4.86205400	-0.70186800	0.01310700
O	-2.12854800	-1.11947300	-0.11954800
O	-2.51640800	-0.92621400	-2.32930700
N	0.66700400	-1.98477500	0.69748200
C	2.63588000	-0.74313900	0.30967700
C	1.77155000	0.10927100	-0.38887600
C	6.77650200	-0.14282800	-1.02479200
C	0.90170500	3.32394200	-1.16959100
C	6.46686100	1.26215600	1.04481000
C	0.02051100	1.23350000	-2.29589600
C	3.59177500	1.44861200	-1.09296300
C	-2.83863400	-1.14745600	-1.18065200
C	5.96439700	0.97527600	-0.37024000
C	4.48536500	0.65566000	-0.37412800
C	1.25653700	2.03988400	-1.92026700
C	-0.07730400	-2.98286900	1.18305600

C	1.86590700	-3.93324000	2.19028400
C	-4.29899600	-1.55179100	-0.85535000
C	2.62081000	-2.88590500	1.68568400
C	0.50008000	-3.98711600	1.93701600
C	3.99698400	-0.45251600	0.32117600
C	2.21470600	1.19296000	-1.12622000
C	2.00441500	-1.89779300	0.92890800
H	-1.13629500	-2.95305700	0.95528400
H	-0.12139600	-4.78873100	2.31622200
H	2.34272200	-4.70619900	2.78313700
H	3.68572600	-2.82565000	1.87498600
H	4.68216900	-1.09391400	0.86667600
H	7.83645300	0.12800600	-1.06344400
H	6.69086700	-1.07573900	-0.45696300
H	6.43675100	-0.33707600	-2.04674300
H	5.90328700	2.07607900	1.51083700
H	6.37291300	0.37711600	1.68342100
H	7.52355100	1.54715100	1.02322200
H	-0.67826200	1.08176500	-1.39770400
H	-0.70051200	1.79630400	-2.89838800
H	0.25353300	0.31253600	-2.83262500
H	1.79791700	3.92192200	-0.98311400
H	0.20135700	3.92700200	-1.75527500
H	0.43995000	3.09125200	-0.20632600
H	3.97458000	2.29183700	-1.66337400
O	-2.55858100	1.98389200	-0.39429900
C	-1.98991100	2.03739800	0.69041300
O	-0.94800800	1.45932000	1.09132000
C	-2.59741700	2.97177000	1.77741100
F	-1.73984000	3.96187300	2.09632200

F	-3.73859100	3.55242300	1.39188900
F	-2.86032700	2.30113900	2.91383400
H	6.09670500	1.88444400	-0.96783700
H	1.75070200	2.31611100	-2.85976300

[2s-AuOAc^{F}]$^{+}$[OAc^{F}]$^{-}$

G: -1901.08866

Au	0.06767100	0.41761500	-0.55335100
F	5.19825800	0.90221700	-2.00157000
F	4.43236600	2.48573700	-0.75013900
F	4.71733800	0.50208900	0.06448800
O	2.06362200	1.11937500	-0.48973000
O	2.65717900	0.28138300	-2.49510500
N	-0.60211200	1.88376900	0.68060100
C	-2.63859200	0.74198500	0.30626300
C	-1.83607300	-0.08419700	-0.48445400
C	-6.84755600	0.15315200	-0.80483300
C	-1.02597400	-3.31495200	-1.22610200
C	-6.42564600	-1.26663400	1.23497000
C	-0.07118200	-1.21273200	-2.25364000
C	-3.67952800	-1.43967300	-1.07419000
C	2.87675800	0.80099700	-1.42160800
C	-6.00121400	-0.96951200	-0.20327300
C	-4.52429900	-0.64988600	-0.29221700
C	-1.33952100	-2.01577100	-1.96887200
C	0.20331200	2.80631700	1.21381000
C	-1.65453500	3.75366100	2.37323300
C	4.32876200	1.17428700	-1.02848400
C	-2.47644200	2.78516600	1.81642100
C	-0.29761300	3.76628000	2.07355800

C	-3.99437400	0.44282300	0.40198300
C	-2.30981300	-1.17422600	-1.18686000
C	-1.93426600	1.83524500	0.96239600
H	1.24943000	2.75285700	0.93581200
H	0.37457300	4.50394100	2.49370500
H	-2.07295200	4.49624400	3.04399500
H	-3.53577300	2.75713400	2.04063100
H	-4.64315300	1.05630900	1.01968300
H	-7.90849200	-0.11594700	-0.78442100
H	-6.72799400	1.08332200	-0.23861200
H	-6.56647700	0.35199600	-1.84361900
H	-5.83430900	-2.08065200	1.66504000
H	-6.30324900	-0.38561600	1.87414100
H	-7.48058300	-1.55703600	1.26740000
H	0.62305800	-1.16391300	-1.29796600
H	0.70848500	-1.77132500	-2.78454100
H	-0.24648900	-0.31600700	-2.85495600
H	-1.93817900	-3.89377300	-1.05984200
H	-0.32819900	-3.92748900	-1.80459000
H	-0.56947200	-3.10219300	-0.25479900
H	-4.09695900	-2.28606800	-1.61443200
O	2.01517800	-1.98213900	-0.01631600
C	1.79907200	-1.70266900	1.17354100
O	0.95784700	-0.94557300	1.68175000
C	2.73611900	-2.45061600	2.16846100
F	2.61586400	-2.03834700	3.43832000
F	2.47573500	-3.77592400	2.16510600
F	4.03175000	-2.30892900	1.83504100
H	-1.78300400	-2.26552200	-2.94026500
H	-6.16825000	-1.87447500	-0.79850000

2s-Au-TS2

G: -1901.089371

Au	-0.00119400	0.40701300	-0.48764200
F	5.09471700	1.17835300	-1.97836900
F	4.21451200	2.74240900	-0.77837700
F	4.65768800	0.81773900	0.10462900
O	1.96852300	1.18044000	-0.43451300
O	2.60073800	0.37516600	-2.44255100
N	-0.74552800	1.92686300	0.66436800
C	-2.73413000	0.69491000	0.29501000
C	-1.87999200	-0.15361900	-0.41148600
C	-6.87507800	-0.09485400	-0.91723300
C	-0.92196800	-3.38721800	-0.85178800
C	-6.48785300	-1.38973600	1.20975800
C	0.02422000	-1.29206600	-1.93000500
C	-3.65051300	-1.61774500	-0.96867400
C	2.79052600	0.92071300	-1.37649000
C	-6.01945400	-1.15774200	-0.22685800
C	-4.54954600	-0.79904400	-0.28047200
C	-1.22648800	-2.14978800	-1.69767100
C	0.00649000	2.90642100	1.17290800
C	-1.91645900	3.84281200	2.22962200
C	4.21189900	1.41738700	-1.00871700
C	-2.68581200	2.81763800	1.69884700
C	-0.55258200	3.89061000	1.96785900
C	-4.08294400	0.35598900	0.35801500
C	-2.28807500	-1.30984100	-1.04435000
C	-2.08342400	1.84784900	0.90976700
H	1.06216300	2.87841300	0.92842700

H	0.07925000	4.67305400	2.36935700
H	-2.38135800	4.60159400	2.84983300
H	-3.74953900	2.75954900	1.89575800
H	-4.77665900	0.98706700	0.90515300
H	-7.92761200	-0.39584400	-0.92186600
H	-6.80474200	0.86594500	-0.39567200
H	-6.56014700	0.05972100	-1.95382800
H	-5.88986500	-2.16112300	1.70445000
H	-6.41353200	-0.47186800	1.80292600
H	-7.53468900	-1.70972700	1.22163600
H	0.80510900	-1.25934900	-0.91039400
H	0.87424100	-1.86199000	-2.32879400
H	-0.12580500	-0.51223500	-2.68409700
H	-1.81789600	-4.00341800	-0.73774300
H	-0.14453400	-3.99399600	-1.32499100
H	-0.57426900	-3.10038700	0.14506500
H	-4.02078100	-2.51543400	-1.45802100
O	1.99361300	-1.90632900	-0.08968300
C	2.00568300	-1.71725600	1.15238800
O	1.25290000	-1.05652400	1.86206900
C	3.16057500	-2.48508900	1.85899400
F	3.30121900	-2.14751900	3.14594200
F	2.93416800	-3.81493000	1.82346000
F	4.34565800	-2.27439000	1.26344600
H	-1.57568400	-2.48287900	-2.68279700
H	-6.13889900	-2.09815500	-0.77700900

3s-AuOAc^{F}

G: -1374.70172

Au	-0.56176300	-0.38491900	-0.13176000

F	-5.72975900	-0.06026700	1.26747800
F	-5.15615400	0.93092100	-0.56178600
F	-5.28405900	-1.22802600	-0.49092500
O	-2.67696600	-0.31399500	-0.40560300
O	-3.12893800	-0.15660900	1.79891100
N	-0.11793900	1.74256300	-0.28776000
C	2.05090500	0.79676100	0.02052600
C	1.37778300	-0.42665800	0.01595200
C	6.08174200	0.27696800	1.68153500
C	1.23903300	-3.40939500	-1.45622100
C	6.31526000	0.12645000	-0.82248000
C	-0.34242000	-2.39073100	0.24383200
C	3.40819000	-1.64350700	0.25074500
C	-3.42228400	-0.21192000	0.61995700
C	5.63117900	-0.45357300	0.41615400
C	4.12308400	-0.44070300	0.27239900
C	1.11117400	-2.84133000	-0.04115900
C	-0.98546600	2.74158900	-0.44572200
C	0.76956000	4.34629700	-0.30910300
C	-4.91792000	-0.14375600	0.21185400
C	1.67098600	3.30493500	-0.14116000
C	-0.58248700	4.06698000	-0.46638100
C	3.43989800	0.77458400	0.14624500
C	2.01883000	-1.65165200	0.11295100
C	1.20845300	1.99262800	-0.13594500
H	-2.02666400	2.45729200	-0.55761800
H	-1.31576500	4.85321400	-0.59932400
H	1.12235800	5.37223800	-0.31529500
H	2.72775300	3.50621300	-0.01142500
H	4.00412000	1.70235600	0.14055500

H	7.16790200	0.20442600	1.79979000
H	5.82177100	1.34017000	1.63702600
H	5.61268300	-0.14711500	2.57472100
H	6.01862600	-0.41018400	-1.72899300
H	6.05777300	1.18267500	-0.95683200
H	7.40392500	0.05826900	-0.72680200
H	-1.07470700	-2.96526700	-0.33001500
H	-0.58584900	-2.47957600	1.30787000
H	2.26977300	-3.70392000	-1.67573500
H	0.59774400	-4.28830100	-1.57734900
H	0.93440900	-2.65824500	-2.19376500
H	3.95159500	-2.58186600	0.33627800
H	1.38693100	-3.63125800	0.66981300
H	5.93444300	-1.50311400	0.50723100

2t-Au(OAc^{F})$_2$

G: -1822.622881

Au	-0.00000700	0.27629500	-0.08744500
F	-4.74290200	1.87291300	1.71576700
F	-4.11938600	2.80455500	-0.12874500
F	-4.69207400	0.71746300	-0.10689800
O	-1.94807000	1.11561000	-0.23038800
O	-2.20271800	1.13614400	2.01010600
N	0.92255300	2.03344900	-0.37215000
C	2.83240500	0.67138200	-0.15188500
C	1.91317500	-0.38726200	0.01031000
C	6.66350200	-0.93995800	1.69193000
C	3.76801000	-1.86801500	0.29822000
C	-2.58709700	1.26582900	0.86778800
C	6.16791300	-1.10026500	0.25517300

C	4.69175600	-0.84131900	0.13487600
C	1.51789800	-2.90658200	0.39629900
C	0.24405500	3.17038900	-0.57696200
C	2.29833200	4.35689700	-0.80549400
C	-4.05791700	1.67141600	0.59065300
C	2.98401200	3.17178700	-0.59868200
C	0.90776000	4.36050700	-0.79566900
C	4.20444700	0.44091900	-0.08997500
C	2.37811600	-1.68148200	0.24574900
C	2.27543600	1.99553100	-0.37894300
H	-0.83600200	3.09926600	-0.56720700
H	0.33574700	5.26555300	-0.95725600
H	2.84736900	5.27626200	-0.97803600
H	4.06618500	3.15093900	-0.61218900
H	4.90157000	1.26414800	-0.21255900
H	6.47911300	0.07434800	2.06018900
H	6.15257100	-1.63771400	2.36293500
H	7.73865400	-1.13375800	1.75556400
H	4.13270400	-2.87711000	0.47826400
O	-1.02332500	-1.43613800	0.24261300
C	-1.73962800	-1.88506000	-0.73014400
O	-1.75004200	-1.56724800	-1.89410500
C	-2.70572400	-2.97630900	-0.20349400
F	-2.06153500	-3.90946200	0.50897300
F	-3.33765600	-3.59042200	-1.20112300
F	-3.63307600	-2.42540700	0.59368300
H	6.38657800	-2.11387300	-0.09612400
C	1.14875300	-3.50673700	-0.95915000
H	0.48015700	-4.36409000	-0.83627600
H	0.64914400	-2.77304300	-1.59750500

H	2.04365000	-3.84817800	-1.48939600
H	0.61708600	-2.67205500	0.96084200
H	6.71119600	-0.41020000	-0.39881600
H	2.07863900	-3.64565700	0.97646000

2t-Au-TS1

G: -1822.58297

Au	0.01150000	-0.42618700	-0.33538300
F	-5.00094700	-1.50254600	-1.82423200
F	-4.19809300	-2.75921200	-0.26345000
F	-4.68911600	-0.69412900	0.15236500
O	-1.96041900	-1.16899000	-0.14742900
O	-2.48854300	-0.77107700	-2.30090600
N	0.82857300	-1.91549600	0.78478000
C	2.76919200	-0.62899100	0.39496500
C	1.89732400	0.16228600	-0.35606100
C	6.78717500	0.63012900	-1.37052400
C	0.13604100	1.17872400	-2.30779800
C	3.65153400	1.61971200	-0.98008800
C	-2.73688400	-1.09733900	-1.15991800
C	6.01676600	1.24678500	-0.20374800
C	4.55986500	0.87116600	-0.22612800
C	1.29063100	2.05747200	-1.85925800
C	0.10282000	-2.91346000	1.29727300
C	2.04961100	-3.76377300	2.38463900
C	-4.17854700	-1.51566300	-0.77538400
C	2.78619700	-2.71761800	1.85067200
C	0.69153000	-3.86718800	2.10651300
C	4.11175400	-0.25841400	0.45824800
C	2.29721400	1.28342600	-1.06317800

C	2.15904400	-1.78161300	1.03906500
H	-0.95105100	-2.92540700	1.04502500
H	0.08485700	-4.66967800	2.50715900
H	2.53461900	-4.49699700	3.01986100
H	3.84444800	-2.61557800	2.05912200
H	4.81372400	-0.84542400	1.04309400
H	7.84195100	0.91930900	-1.33493600
H	6.73376100	-0.46296600	-1.34238000
H	6.37741600	0.96115300	-2.33010600
H	-0.60847000	0.96313500	-1.45122100
H	-0.60459700	1.70410500	-2.91948800
H	0.45128800	0.29069400	-2.85756700
H	4.00692500	2.49078800	-1.52555600
O	-2.30288400	2.04545000	-0.36313800
C	-1.61353700	2.21568900	0.63914800
O	-0.59509000	1.60129200	1.03609100
C	-2.01029200	3.38140700	1.59245300
F	-1.04368500	4.32176200	1.62852700
F	-3.14043900	3.99883300	1.23076800
F	-2.18369300	2.95173300	2.85567400
H	6.10905500	2.33708200	-0.24048700
H	1.76337300	2.50313500	-2.73959800
H	6.46016500	0.91970900	0.74219000
H	0.90866900	2.88639800	-1.25250300

[2t-AuOAc^{F}]$^{+}$[OAc^{F}]$^{-}$

G: -1822.585519

Au	-0.18720100	0.28825500	-0.54063300
F	4.86047000	1.00881800	-2.19420100
F	4.02208200	2.59576600	-0.99455000

F	4.48726000	0.68545700	-0.09233000
O	1.77952500	1.06599600	-0.56419200
O	2.35589900	0.18201200	-2.55483300
N	-0.84988300	1.70920700	0.74719700
C	-2.85024100	0.47732800	0.47619400
C	-2.06050400	-0.29588600	-0.37693100
C	-7.03953900	-0.60672700	-0.83085400
C	-0.31344900	-1.33816100	-2.21916400
C	-3.86208200	-1.74570500	-0.86537500
C	2.57681000	0.76687700	-1.51605300
C	-6.14326400	-1.37851600	0.13663600
C	-4.69295100	-1.00818500	-0.01776700
C	-1.55566900	-2.16697900	-1.91913900
C	-0.05767700	2.66108700	1.24749400
C	-1.88302300	3.50007100	2.53490300
C	4.00941900	1.26737500	-1.20172400
C	-2.69105700	2.50162300	2.01141500
C	-0.54957300	3.58309700	2.15279900
C	-4.18037700	0.10488300	0.65434300
C	-2.51937200	-1.40648600	-1.06098000
C	-2.15871400	1.59276700	1.10819700
H	0.97134100	2.66073300	0.90759900
H	0.11183700	4.34548500	2.54498700
H	-2.29368700	4.21077700	3.24389200
H	-3.73164200	2.41734000	2.30031600
H	-4.82348600	0.67080000	1.32222800
H	-8.08795700	-0.89114500	-0.69904900
H	-6.95805800	0.47247800	-0.66590500
H	-6.76109200	-0.80901100	-1.87001600
H	0.39647300	-1.29027300	-1.27247600

H	0.47161200	-1.86882300	-2.76876500
H	-0.52162800	-0.44484000	-2.81639500
H	-4.26852500	-2.60989300	-1.38528400
O	1.75587900	-2.10298900	-0.04691700
C	1.71534700	-1.73861100	1.14104700
O	0.94428100	-0.95890500	1.71663500
C	2.81996100	-2.39433300	2.02293200
F	2.86031500	-1.92269100	3.27684000
F	2.63171300	-3.72823200	2.11619400
F	4.04620200	-2.21189100	1.49924100
H	-2.02173100	-2.46422100	-2.86375300
H	-6.26174700	-2.45351200	-0.03167300
H	-6.45921900	-1.17897500	1.16589500
H	-1.26570400	-3.09057900	-1.40612700

2t-Au-TS2

G: -1822.58554

Au	-0.22691400	0.26541800	-0.47064300
F	4.78214200	1.20677400	-2.18775800
F	3.88460600	2.73782300	-0.95886200
F	4.44008800	0.83682800	-0.08845900
O	1.71234400	1.11253300	-0.53838400
O	2.32028600	0.25649500	-2.53351400
N	-0.96718000	1.77334200	0.69799200
C	-2.92010800	0.45443600	0.46332400
C	-2.07606000	-0.36729800	-0.28353700
C	-6.98764000	-0.91532600	-1.00423100
C	-0.20774000	-1.44838900	-1.89867400
C	-3.81004000	-1.91602000	-0.71456900
C	2.51620700	0.85153800	-1.49537000

C	-6.14925500	-1.51318900	0.12513200
C	-4.69957200	-1.12300700	0.01823900
C	-1.41712100	-2.33301800	-1.59971900
C	-0.22946900	2.79221500	1.14619400
C	-2.12508500	3.66345900	2.30337000
C	3.92768700	1.41357100	-1.18580200
C	-2.87931000	2.59748400	1.83485300
C	-0.78283900	3.76544700	1.95851200
C	-4.24842000	0.05984300	0.61155900
C	-2.47067800	-1.55218600	-0.87672700
C	-2.28349700	1.64176800	1.02419600
H	0.81034400	2.80392900	0.84020300
H	-0.16296100	4.58094600	2.30975300
H	-2.58458500	4.41172400	2.94015800
H	-3.92517600	2.49546000	2.09774800
H	-4.93984700	0.66653800	1.18959900
H	-8.03659600	-1.21210400	-0.90855400
H	-6.94207800	0.17844200	-0.99041700
H	-6.62736500	-1.25314500	-1.98120400
H	0.58094900	-1.39677600	-0.89422800
H	0.64394400	-1.98956300	-2.32912500
H	-0.41767800	-0.67636400	-2.64693800
H	-4.17085700	-2.83627700	-1.16756800
O	1.73961900	-2.07920000	-0.05557500
C	1.86721800	-1.72248700	1.14258300
O	1.18632200	-0.95508300	1.81675600
C	3.08682400	-2.39631500	1.83553000
F	3.29703600	-1.94555600	3.07717600
F	2.90917100	-3.72988200	1.92527500
F	4.22229300	-2.19812600	1.14494900

H	-1.79966300	-2.75292500	-2.53545800
H	-6.23314600	-2.60448000	0.10478900
H	-6.54424200	-1.17939100	1.09019000
H	-1.10775900	-3.18126700	-0.97843800

3t-AuOAc^{F}

G: -1296.197986

Au	-0.31131300	-0.45714400	-0.26118000
F	-5.41138800	-0.26546500	1.38883300
F	-4.93935700	0.81266300	-0.42026800
F	-5.03459600	-1.34897000	-0.43830400
O	-2.43885100	-0.41243400	-0.43491500
O	-2.78742400	-0.32703300	1.79255600
N	0.09083300	1.68240500	-0.20924400
C	2.28619000	0.75386900	-0.10314100
C	1.63330800	-0.47539000	-0.19891500
C	6.33071900	-0.60126200	1.53513700
C	-0.06526000	-2.49015400	-0.14851300
C	3.68981700	-1.67159600	-0.17023300
C	-3.13565200	-0.35149700	0.62748500
C	5.88469600	-0.46166700	0.08013700
C	4.38494000	-0.46038000	-0.05726400
C	1.39973100	-2.87681500	-0.45411000
C	-0.79683900	2.67604400	-0.22584700
C	0.94280800	4.29354000	-0.04495000
C	-4.64994300	-0.29079700	0.29337200
C	1.86560800	3.25759700	-0.02506800
C	-0.41256500	4.00480900	-0.14657100
C	3.68075200	0.74713700	-0.03267700
C	2.29758800	-1.69403300	-0.25050400

C	1.42025700	1.94222800	-0.10820800
H	-1.83909100	2.38558200	-0.30675900
H	-1.16264100	4.78631600	-0.16401800
H	1.28168500	5.32218400	0.01969100
H	2.92611400	3.46445100	0.05521400
H	4.23518700	1.67874800	0.03823800
H	7.42274600	-0.60273700	1.61029300
H	5.94974500	0.22580300	2.14293100
H	5.95978400	-1.53444500	1.97106300
H	-0.77836600	-2.98711300	-0.81055500
H	-0.33135600	-2.72768300	0.88669800
H	4.25198700	-2.60221100	-0.20258200
H	1.70888400	-3.73700800	0.15120500
H	6.30236100	-1.28505000	-0.50898900
H	1.48330400	-3.19365800	-1.50079100
H	6.28893400	0.46623600	-0.33796400

1s

G: -714.292467

N	-2.69275600	-1.34812700	0.49051600
C	-0.68382800	-0.11565300	-0.00049600
C	0.09800000	-1.27601200	-0.04454900
C	1.68248600	3.43083600	-1.10538800
C	1.68285000	3.31235000	1.41025000
C	2.09367300	0.05121100	-0.00398900
C	2.02321300	2.57458700	0.11480700
C	1.34365100	1.22316200	0.04961500
C	2.31944900	-2.47077500	-0.11414700
C	-4.01769300	-1.47756700	0.50024400
C	-4.34459200	0.65708300	-0.50066300

C	-2.96596300	0.80279600	-0.52061500
C	-4.89124800	-0.50762800	0.02408500
C	-0.04935000	1.12549300	0.04826400
C	1.48637000	-1.20822400	-0.05185700
C	-2.16229100	-0.22103500	-0.00539200
H	-4.40365900	-2.40661800	0.91389900
H	-5.96314200	-0.66776300	0.05988400
H	-4.98313900	1.43942600	-0.89895400
H	-2.51526400	1.69125400	-0.94777400
H	-0.64311100	2.03236400	0.10974900
H	2.22501800	4.38153400	-1.07199300
H	1.94710800	2.92010400	-2.03650100
H	0.61150500	3.65854200	-1.13892200
H	0.61275100	3.54008500	1.46439400
H	1.94449300	2.71492800	2.28909900
H	2.22883600	4.25995400	1.46722500
H	3.17885700	0.12327500	-0.00522800
H	3.10406800	2.39018800	0.10647100
C	3.19407200	-2.62716000	1.13031000
H	3.92673100	-1.81599200	1.20178100
H	2.59131000	-2.61805500	2.04372700
H	3.74570700	-3.57256700	1.09546400
C	3.16710700	-2.51952200	-1.38592500
H	2.54458400	-2.43681100	-2.28230300
H	3.89584100	-1.70190300	-1.40558000
H	3.72164900	-3.46220200	-1.44221300
H	1.62003900	-3.31472900	-0.14240200
H	-0.39632600	-2.24176500	-0.08076000

1b-Au(OAc^{F})$_2$

G: -1979.605751

Au	-0.42684100	0.39262900	-0.12016300
F	-5.29723000	1.48691000	1.73181200
F	-4.70759500	2.62383800	-0.00599000
F	-5.14797100	0.51335600	-0.18895100
O	-2.43686500	1.07678400	-0.22189400
O	-2.71493000	0.90994300	2.01082600
N	0.28349900	2.25578400	-0.29571400
C	2.34268900	1.12581300	-0.11705000
C	1.58482300	-0.06228400	-0.02549200
C	6.33366700	-0.74109500	1.58892300
C	2.60741900	-3.80936200	0.43530500
C	6.47569600	-1.05569400	-0.89429500
C	6.60249500	1.22459800	0.08880400
C	0.83734500	-2.96341900	-1.02679400
C	3.65972400	-1.23059900	0.22201200
C	-3.09490100	1.09976900	0.87641800
C	5.94589200	-0.14889000	0.22614300
C	4.42453400	-0.06848800	0.13056400
C	1.59879000	-2.66231500	0.27557300
C	-0.52953300	3.31034900	-0.45333000
C	1.36304600	4.74936900	-0.58763700
C	-4.58562500	1.43377100	0.60677900
C	2.18687900	3.64805500	-0.43416300
C	-0.01728700	4.58249400	-0.59898200
C	3.73700800	1.11833400	-0.04129000
C	0.74498000	-2.69114600	1.55525500
C	2.26270000	-1.28601100	0.15103600
C	1.62763800	2.38126000	-0.28494900
H	-1.59197600	3.10711100	-0.46780500

H	-0.69636900	5.41685100	-0.72164900
H	1.79711500	5.73664000	-0.70300900
H	3.26197300	3.76899100	-0.43469800
H	4.27532900	2.05411300	-0.11176300
H	5.96663400	-0.11329300	2.40738400
H	5.92665900	-1.74728800	1.72486100
H	7.42374700	-0.80658600	1.67173700
H	7.56780400	-1.11671900	-0.83998700
H	6.08065800	-2.07281300	-0.81690800
H	6.20523400	-0.66055900	-1.87892700
H	6.37873500	1.68800700	-0.87766500
H	6.28608500	1.90912400	0.88270800
H	7.68898500	1.11632500	0.15988000
H	1.55261300	-3.26794500	-1.79812800
H	0.12949800	-3.78519900	-0.88223500
H	0.29977500	-2.10575100	-1.42371700
H	3.19484400	-3.72828600	1.35510900
H	2.04551500	-4.74740900	0.48907500
H	3.29132000	-3.88819100	-0.41524700
H	0.16204000	-3.61656000	1.59873700
H	1.40879700	-2.66921500	2.42630400
H	4.18861200	-2.16355500	0.35987500
H	0.05340100	-1.85832900	1.64472400
O	-1.38591500	-1.38641800	0.09156100
C	-2.10617600	-1.79529400	-0.89371400
O	-2.11184800	-1.44508300	-2.04873000
C	-3.07302000	-2.90474500	-0.40473900
F	-2.41155100	-3.91903900	0.16854300
F	-3.78898500	-3.40429500	-1.41015700
F	-3.92859400	-2.41480100	0.50406400

1b

G: -792.790646

N	3.04704600	1.06134300	-0.53605000
C	0.95939700	-0.00934100	0.00289000
C	0.26514300	1.20685200	0.03487800
C	-1.50541700	-3.29279100	-1.37207600
C	-1.51155100	-3.39151800	1.13081400
C	-1.81234800	0.01678200	0.00580000
C	-1.89975000	-2.54466600	-0.09012000
C	-1.15536900	-1.20945500	-0.03507200
C	-1.91699100	2.54503700	0.08887300
C	4.37784500	1.09747400	-0.55374300
C	4.55999800	-1.01514300	0.52742000
C	3.17467400	-1.06337100	0.55639500
C	5.18396500	0.08750200	-0.04333700
C	0.24370800	-1.20228200	-0.03281600
C	-1.12329000	1.23845800	0.04235200
C	2.44172900	-0.00669000	0.00327800
H	4.82550500	1.98107000	-1.00333600
H	6.26423700	0.17041800	-0.08822600
H	5.14443900	-1.82407400	0.95461400
H	2.66563200	-1.90060000	1.02000600
H	0.78107600	-2.14340200	-0.08473900
H	-2.03210500	-4.25198400	-1.42544000
H	-1.76817500	-2.71012700	-2.26113600
H	-0.43162700	-3.49862600	-1.40823100
H	-0.43762200	-3.59857400	1.15562300
H	-1.77935000	-2.88090000	2.06173800
H	-2.03728300	-4.35235800	1.10588100

H	-2.89570400	0.03548100	0.00700100
C	-2.80725300	2.55520700	1.34022300
H	-3.51524500	1.72128800	1.34289500
H	-2.20210500	2.48762600	2.25037300
H	-3.38499900	3.48502700	1.38401400
C	-2.79993900	2.64625400	-1.16372500
H	-2.18931000	2.64317800	-2.07264300
H	-3.50871200	1.81564600	-1.23033500
H	-3.37655400	3.57761600	-1.14396000
H	0.84383800	2.12128100	0.06016700
C	-3.41806000	-2.36494600	-0.08702900
H	-3.76753800	-1.86108300	0.81999700
H	-3.76238600	-1.79176400	-0.95397100
H	-3.90004600	-3.34686800	-0.12680400
C	-1.00793400	3.77342900	0.13575300
H	-0.36926900	3.77375500	1.02490400
H	-0.36551000	3.83863800	-0.74817400
H	-1.62185600	4.67917900	0.16758100

1t-*p*-H$^+$

G: -557.722243

N	2.36574500	0.87908000	-0.36377200
C	0.00662000	0.48165300	0.03412900
C	-0.31437100	1.78408400	0.43209700
C	-3.93310200	-1.76641100	0.45904400
C	-2.64512400	1.30789300	0.04713400
C	-3.43119800	-0.96029100	-0.73848800
C	-2.34350500	0.00362600	-0.35274400
C	3.67492600	0.58120500	-0.39430500
C	3.13821700	-1.60424400	0.37258600

C	1.79635500	-1.25964400	0.39855400
C	4.09667900	-0.67307700	-0.02371100
C	-1.01009000	-0.39841900	-0.34818700
C	-1.64199500	2.18791000	0.43807600
C	1.39875600	0.01916800	0.02229100
H	4.33660700	1.37017200	-0.72769300
H	5.15143100	-0.91424800	-0.04810800
H	3.44204700	-2.60093600	0.67386000
H	1.04628200	-1.96484700	0.73288500
H	-0.75817300	-1.40404100	-0.67267100
H	-3.12307600	-2.35187700	0.90578700
H	-4.33757000	-1.10747900	1.23389500
H	-4.72437600	-2.45862500	0.15583000
H	-3.68049700	1.63685300	0.05078700
H	-4.26450600	-0.40599500	-1.18190600
H	-3.05435100	-1.64325400	-1.50685500
H	0.45834600	2.46863100	0.77000300
H	2.09088000	1.80776400	-0.67453800
H	-1.89627500	3.19359200	0.75626400

1t-*p*-Au(OAc^{F})$_3$

G: -2270.526112

Au	0.52088000	-0.07956900	-0.37500200
F	-3.18940500	1.53585100	-3.70800300
F	-3.79074600	1.00151900	-1.70398500
F	-2.68962300	2.83046400	-2.05480300
O	-1.10540600	0.89998000	-1.00382500
O	-0.98520000	0.15591000	-3.13680900
N	-0.38093300	-1.85213400	-0.72201900
C	-1.78213100	-1.49264000	1.24289000

C	-3.06571300	-0.95922400	1.35654300
C	-2.48735600	-0.03098600	3.48964900
C	-1.48778400	0.77268100	-2.23391700
C	-1.21385200	-0.57813500	3.39210500
C	0.02350600	-2.54805300	-1.79980100
C	-1.71428700	-4.13656200	-1.44245400
C	-2.81219500	1.55594200	-2.43381200
C	-2.11065700	-3.41268600	-0.33000500
C	-0.61938800	-3.70585800	-2.18147800
C	-0.85050900	-1.30894600	2.26810800
C	-3.43017800	-0.21121400	2.47428000
C	-1.41946300	-2.26370200	0.03872600
H	0.86000700	-2.14417600	-2.35643200
H	-0.26768900	-4.24204600	-3.05404600
H	-2.94259000	-3.73213900	0.28595600
H	0.14088700	-1.74543700	2.19327600
O	1.50682700	1.65734500	-0.20331400
C	1.14094000	2.48815100	0.71942800
O	0.27787900	2.38072300	1.55004900
C	2.02721700	3.75874000	0.64209800
F	1.92737400	4.34380100	-0.55723300
F	3.31512100	3.45045400	0.84131900
F	1.67033000	4.64740300	1.56441500
H	-3.77744400	-1.10222100	0.54817700
O	2.06654400	-1.01444100	0.49285200
C	3.14388900	-1.17616800	-0.20880900
O	3.35890600	-0.88636500	-1.35623100
C	4.22729500	-1.85600900	0.66872300
F	3.79103800	-3.03399300	1.13331100
F	5.33714600	-2.07361100	-0.02781400

F	4.53757100	-1.09090100	1.72075300
H	-2.75592400	0.55249400	4.36606500
H	-2.24939800	-5.03670200	-1.72509800
C	-4.81884900	0.35180900	2.59933100
H	-4.77679800	1.29435700	3.15486300
H	-5.20592900	0.58517500	1.60205100
H	-0.49541000	-0.43046300	4.19179700
C	-5.76911200	-0.61469800	3.30524600
H	-5.41502500	-0.84540000	4.31508800
H	-6.77156300	-0.18354100	3.38809000
H	-5.85003200	-1.55776500	2.75495900

1t-*p*-Au-TSA

G: -2270.490218

Au	0.56969700	-0.33595700	0.19566100
F	-4.10446400	1.89968300	-1.91804500
F	-2.76515000	1.29368500	-3.50154400
F	-3.71794600	-0.19361000	-2.25452700
O	-1.21462000	0.05741400	-1.34010100
O	-1.78764100	2.12369000	-0.62378500
N	0.17217900	-2.27414000	-0.16300900
C	-1.76592600	-1.68105800	1.04278300
C	-3.11181300	-1.46283400	0.83189500
C	-2.98596000	0.58398100	2.12887800
C	-1.92056100	1.10007100	-1.27443800
C	-1.65009700	0.36858000	2.37451300
C	0.95389500	-3.05558200	-0.91641600
C	-0.65377000	-4.81772400	-0.74652500
C	-3.14604200	1.02255600	-2.23829800
C	-1.46001500	-3.98737100	0.01818900

C	0.56548600	-4.34727800	-1.21967300
C	-1.00917600	-0.77030000	1.84080900
C	-3.73912200	-0.33293800	1.37310500
C	-1.02147700	-2.70455200	0.30515100
H	1.88442000	-2.62777500	-1.26834400
H	1.22062600	-4.96671800	-1.81952000
H	-0.11182900	-1.13711500	2.34808400
O	0.89363400	1.55332400	0.73993000
C	1.10738800	2.42210800	-0.19666800
O	1.25958900	2.26197100	-1.37759000
C	1.21566500	3.83395500	0.43638700
F	2.34996600	3.93403500	1.14981400
F	0.19736700	4.09757900	1.26000000
F	1.24105500	4.77665100	-0.50165100
H	-3.67231200	-2.12773700	0.18279500
O	2.56118500	-0.47084500	-0.46441300
C	3.42416900	-0.71986800	0.45585500
O	3.26475400	-0.94238800	1.63205400
C	4.85249700	-0.72306600	-0.15634200
F	5.13965600	0.45766800	-0.71395600
F	5.77627700	-0.97729100	0.76641600
F	4.95514100	-1.66231400	-1.10843600
H	-0.97541000	-5.82794500	-0.97447900
H	-2.41992200	-4.31609300	0.39792700
H	-3.47459500	1.47003000	2.52103400
C	-5.19963500	-0.10382800	1.15182300
H	-5.50514900	-0.57292700	0.21218900
C	-6.02773800	-0.67591300	2.30735300
H	-5.75512300	-0.20601900	3.25691300
H	-7.09170400	-0.49649200	2.13029800

H	-5.87358600	-1.75475600	2.40461000
H	-1.07933900	1.05859000	2.98548100
H	-5.38629700	0.97085000	1.06517700

2t-*p*-Au(OAc^{F})$_2$

G: -1744.124632

Au	-0.06361400	0.19594900	-0.08568600
F	-4.87642400	1.69924600	1.63081100
F	-4.22043800	2.62589000	-0.20511800
F	-4.80053800	0.54105100	-0.18853600
O	-2.06010800	0.89328200	-0.26577600
O	-2.32672200	1.02221400	1.96894900
N	0.80448700	1.99141800	-0.35549700
C	2.74894200	0.66813500	-0.15019900
C	1.83632600	-0.38757100	-0.00181400
C	6.56413500	-1.03829800	1.63103400
C	3.64736200	-1.92697500	0.24125900
C	-2.70622300	1.09323300	0.81913900
C	6.05502400	-1.17584300	0.19652700
C	4.58046400	-0.89859200	0.09299500
C	0.10431200	3.11655400	-0.54009700
C	2.13293200	4.35754800	-0.71000100
C	-4.17389100	1.49304000	0.51737700
C	2.84540900	3.18330500	-0.52361100
C	0.74320100	4.32765800	-0.72188300
C	4.11619400	0.40132400	-0.10363000
C	2.27484300	-1.68222600	0.19535900
C	2.16297300	1.98670100	-0.34783500
H	-0.97428300	3.02048800	-0.54376800
H	0.15260300	5.22319600	-0.86890100

H	2.66143700	5.29448300	-0.84847500
H	3.92815600	3.18653300	-0.51371600
H	4.83350200	1.20832600	-0.22427100
H	6.39447100	-0.02631800	2.01262200
H	6.05076600	-1.73796200	2.29819700
H	7.63745400	-1.24505000	1.68330100
H	3.99605600	-2.94481200	0.39340700
O	-0.80848300	-1.64717000	0.27551300
C	-1.19747000	-2.33474500	-0.74261200
O	-1.14035700	-2.06874700	-1.91815600
C	-1.79984300	-3.68037500	-0.26482300
F	-0.89865500	-4.38532500	0.43524300
F	-2.19242200	-4.42963500	-1.29180100
F	-2.86053000	-3.47813900	0.52685200
H	6.25890500	-2.18747400	-0.16871900
H	6.60085700	-0.48414900	-0.45353900
H	1.57248400	-2.49879000	0.31710600

1t-*o*-H$^+$

G: -557.721222

N	1.87790000	-0.94067600	-0.66325100
C	0.00933900	0.51191600	-0.13707000
C	-0.97140600	-0.48537900	-0.18687000
C	-2.67596800	1.18876600	-0.36079300
C	-1.70953800	2.18690200	-0.30977200
C	-3.37388300	-1.23509500	-0.28166200
C	3.14425300	-1.38462500	-0.60952000
C	3.66764300	0.44956000	0.80917100
C	2.35108800	0.87483900	0.73643000
C	4.07507200	-0.69957900	0.13373600

C	-0.36668400	1.85750900	-0.19248700
C	-2.32132300	-0.16118700	-0.29625400
C	1.42795900	0.15723300	-0.01760700
H	3.36248500	-2.27759400	-1.18100900
H	5.09568800	-1.05657900	0.17843300
H	4.38009700	1.00897400	1.40566600
H	2.01928300	1.74940700	1.28112000
H	0.38583100	2.63855400	-0.17449700
H	-3.72453800	1.45850800	-0.45178800
C	-3.90799000	-1.49437800	1.12660200
H	-4.67525300	-2.27434800	1.11271700
H	-3.10573100	-1.81899900	1.79700000
H	-4.35299200	-0.58853100	1.55018900
H	-2.95598100	-2.16036800	-0.69147400
H	-4.19976000	-0.93796900	-0.93628300
H	-0.69044200	-1.53298300	-0.10482600
H	1.22790300	-1.45189500	-1.25497000
H	-2.00325100	3.22965400	-0.37094800

1t-*o*-Au(OAc^{F})$_3$

G: -2270.525881

Au	0.38684700	0.07534500	-0.61914300
F	-4.62856500	1.30053400	0.22009300
F	-3.76012200	2.32237700	-1.47437200
F	-4.09614200	0.18892600	-1.55012600
O	-1.53974900	0.42094100	-1.02766100
O	-2.04687100	1.41896400	0.93884400
N	0.09488400	-1.79551700	-1.33122400
C	-1.58962100	-2.29063600	0.38813200
C	-2.98293200	-2.40861200	0.38782900

C	-3.02607200	-1.65042400	2.67682000
C	-2.30320900	1.00446200	-0.15890300
C	-1.63674800	-1.54071200	2.69778400
C	0.82664500	-2.11796400	-2.41345200
C	-0.31749200	-4.19465700	-2.59842100
C	-3.72569900	1.19285700	-0.75202200
C	-1.05170100	-3.85471200	-1.47600100
C	0.64802900	-3.31466900	-3.07165100
C	-0.92777900	-1.86938600	1.54127600
C	-3.69368100	-2.07977700	1.53268400
C	-0.83482000	-2.64005000	-0.82863100
H	1.55542400	-1.38859400	-2.74499400
H	1.25454700	-3.53723200	-3.94061000
H	0.15742300	-1.80338500	1.55387000
O	0.79137300	1.87618700	0.16100300
C	0.45292000	2.94314200	-0.48389700
O	-0.06174300	3.05577500	-1.56641700
C	0.82055000	4.18991500	0.36386500
F	2.13769700	4.22941900	0.60449800
F	0.19003300	4.17372000	1.54290900
F	0.48492700	5.31154900	-0.26704600
H	-3.50267300	-2.72301300	-0.51127300
O	2.35578800	-0.29035000	-0.53898200
C	2.89958900	-0.66294600	0.57557800
O	2.39297600	-0.87700100	1.64515100
C	4.42732700	-0.83043200	0.36265700
F	4.98697300	0.32589200	-0.00796400
F	5.02191500	-1.24029500	1.47730500
F	4.67582100	-1.73248800	-0.59617600
H	-0.48803500	-5.14442000	-3.09370000

H	-1.78823600	-4.53221600	-1.06152600
H	-3.59406800	-1.38723600	3.56476200
C	-0.89828600	-1.09983900	3.93126900
H	-1.60516700	-0.63343900	4.62424600
C	-0.17720700	-2.25332100	4.62602400
H	-0.88525900	-3.02619000	4.94232200
H	0.55412700	-2.71926400	3.95810800
H	0.35719900	-1.89821100	5.51242100
H	-4.77695900	-2.14624600	1.53049000
H	-0.16936200	-0.33047800	3.65352600

1t-*o*-Au-TSA

G: -2270.494455

Au	-0.37153700	0.41877600	0.18916500
F	4.34132200	-1.25660200	-2.41360200
F	3.02560600	-0.02508200	-3.60055800
F	4.15231200	0.84645500	-1.97246200
O	1.50127100	0.44880100	-1.30608900
O	2.25008500	-1.62864700	-0.82560300
N	-0.13376200	2.41314500	0.18462800
C	1.76598000	1.76508200	1.41655700
C	3.13313500	1.66323900	1.26608900
C	3.06417000	-0.55924100	2.26661900
C	2.28019400	-0.54011000	-1.37602600
C	1.69523600	-0.47309000	2.47663000
C	-0.93676400	3.24943600	-0.48216100
C	0.50973900	5.06932600	0.07942700
C	3.46424800	-0.24995700	-2.34954100
C	1.33926500	4.18395300	0.75206800
C	-0.64021500	4.59828000	-0.54360100

C	1.03016600	0.70102700	2.02588900
C	3.76899400	0.49722300	1.69305200
C	0.99126500	2.84346900	0.79786800
H	-1.80755100	2.81775000	-0.95965800
H	-1.31087200	5.26093600	-1.07644700
H	0.08018100	0.94503200	2.51285000
O	-0.57441800	-1.55270700	0.36810300
C	-0.64784400	-2.26943200	-0.70936900
O	-0.70807500	-1.92922100	-1.85942900
C	-0.70274000	-3.76780300	-0.31105400
F	-1.83152400	-4.02897400	0.36821700
F	0.32606100	-4.11219200	0.46904000
F	-0.68435700	-4.54937500	-1.38669400
H	3.69215600	2.44552300	0.76580400
O	-2.29905600	0.51277100	-0.64093100
C	-3.25699300	0.39759600	0.20978500
O	-3.21958700	0.30162000	1.41270900
C	-4.62008400	0.40510600	-0.53569300
F	-4.69461900	-0.60522800	-1.40810700
F	-5.63863500	0.29219000	0.31227800
F	-4.77955400	1.54886000	-1.21775300
H	0.75963500	6.12379800	0.03922400
H	2.24668100	4.51268400	1.24441300
H	3.60578700	-1.44743600	2.56883000
C	0.90390600	-1.52136700	3.19473900
H	0.00215700	-1.72394200	2.60751400
C	1.63288200	-2.82082600	3.48623500
H	2.01447900	-3.27737200	2.56843500
H	2.47339100	-2.67456700	4.17152100
H	0.94601700	-3.53240800	3.95150200

H	4.84079300	0.40074600	1.55082200
H	0.54637400	-1.06893300	4.13038900

2t-*o*-Au(OAc^{F})$_2$

G: -1744.116379

Au	-0.40757600	-0.12369600	-0.00698700
F	3.95666000	-2.82119000	1.39316000
F	3.01419200	-3.49364100	-0.42849000
F	4.06504400	-1.60246400	-0.38528600
O	1.29257700	-1.35743500	-0.31869600
O	1.69686500	-1.50974700	1.89441800
N	-1.70012000	-1.63414200	-0.26181900
C	-3.25617900	0.08991100	0.13415500
C	-2.12416600	0.92706300	0.24775000
C	-3.58720800	2.76309300	0.70322200
C	1.95728500	-1.68722400	0.72409700
C	-4.70274400	1.94980600	0.58497900
C	-1.16012100	3.28442600	0.65492100
C	-1.29465600	-2.87981800	-0.54235300
C	-3.56448400	-3.60313900	-0.61586400
C	3.26897000	-2.41266400	0.32751100
C	-3.96672300	-2.30861000	-0.33259800
C	-2.20976400	-3.89650300	-0.72584700
C	-4.54073800	0.60414300	0.30083600
C	-2.27699900	2.28281400	0.54272800
C	-3.01074300	-1.31423600	-0.15627700
H	-0.22660700	-3.03650200	-0.62086200
H	-1.85584200	-4.89498600	-0.94996100
H	-4.30663300	-4.38192200	-0.75383500
H	-5.01792700	-2.06368100	-0.25015300

H	-5.40652500	-0.04306000	0.21419800
H	-3.71609500	3.81758500	0.93198400
O	0.98462800	1.31345800	0.28900800
C	1.71736500	1.63503100	-0.72102900
O	1.57874300	1.37459600	-1.89088300
C	2.93964200	2.45571300	-0.23792400
F	2.58082900	3.45419800	0.57850500
F	3.60518400	2.98594600	-1.26151700
F	3.78595000	1.66338000	0.43716500
C	-0.75524800	3.83229400	-0.71245600
H	0.09436800	4.51580700	-0.62165000
H	-0.47479300	3.02762900	-1.39744500
H	-1.58348900	4.38125600	-1.17203500
H	-0.29902500	2.84047900	1.15149200
H	-1.50593500	4.10889400	1.28563200
H	-5.69633200	2.36379600	0.71967200

2t-*o*-Au-TS1

G: -1744.075103

Au	0.41808500	-0.30665900	-0.40159400
F	-4.37847600	-2.41555400	-1.42340800
F	-3.20311300	-3.44936400	0.06353100
F	-4.06202100	-1.51543200	0.51218700
O	-1.34631000	-1.40683700	-0.02441700
O	-2.09801000	-1.25171900	-2.14247500
N	1.59967500	-1.55118800	0.68895000
C	3.20741700	0.07560100	0.10113000
C	2.13890400	0.64604300	-0.59699800
C	0.05459600	1.16931300	-2.40615700
C	3.50069500	2.39332000	-1.42467000

C	-2.19120800	-1.55404800	-0.97213700
C	4.58138100	1.86441100	-0.72440700
C	1.03529400	2.29081500	-2.10951700
C	1.12979400	-2.65009300	1.28605500
C	3.28669700	-3.05656200	2.22169000
C	-3.48095800	-2.23925000	-0.45424000
C	3.75571900	-1.90858800	1.60121300
C	1.95878900	-3.43570200	2.06496500
C	4.44949100	0.70792100	0.03531300
C	2.24074700	1.78639600	-1.37620800
C	2.89260700	-1.14753400	0.82447900
H	0.08253500	-2.87834600	1.12579300
H	1.55740600	-4.32384600	2.53677900
H	3.95720600	-3.65356100	2.83017400
H	4.78619600	-1.59545100	1.71637700
H	5.30436900	0.30447000	0.56765100
H	-0.56832600	0.87793300	-1.47432600
H	-0.82640500	1.49083000	-2.97111200
H	0.50091600	0.32985800	-2.94165700
H	3.63254900	3.28677000	-2.02818600
O	-2.32715600	1.68891400	-0.32888000
C	-1.62927400	2.01807400	0.62791300
O	-0.49554700	1.61633700	0.97880200
C	-2.18951500	3.11868800	1.57679800
F	-1.39133900	4.20579100	1.57942000
F	-3.41438900	3.53666500	1.23806000
F	-2.25993900	2.68382400	2.84866700
H	1.33185500	2.76469700	-3.05000100
H	0.54200300	3.06359400	-1.50890500
H	5.54584800	2.35763000	-0.78100300

[2t-*o*-AuOAc^{F}]$^{+}$[OAc^{F}]$^{-}$

G: -1744.079928

Au	-0.57321800	0.18791400	-0.55879600
F	4.39828100	1.64170700	-1.94575300
F	3.33793200	3.02376200	-0.67094200
F	3.97296600	1.10541600	0.10170800
O	1.26225600	1.23640600	-0.47819500
O	2.02275100	0.56980100	-2.49262200
N	-1.48809200	1.46628600	0.72387500
C	-3.28215700	-0.02186600	0.32202900
C	-2.35033000	-0.66189600	-0.49846300
C	-0.39261700	-1.36849100	-2.28779200
C	-3.90578600	-2.32251100	-1.14080200
C	2.12906000	1.09759200	-1.40641200
C	-4.85874300	-1.71411300	-0.32807000
C	-1.50519000	-2.38426600	-2.06409900
C	-0.86481100	2.50963600	1.27789900
C	-2.85468100	3.06027400	2.47399500
C	3.48161800	1.72389900	-0.98185200
C	-3.48552700	1.96815900	1.89660100
C	-1.52841300	3.33669700	2.16526900
C	-4.56186100	-0.56946700	0.40599400
C	-2.61159800	-1.79984500	-1.24158600
C	-2.78501000	1.16223000	1.01065200
H	0.17043700	2.65998000	0.99477300
H	-1.00284000	4.17724500	2.60079100
H	-3.39754500	3.69315300	3.16763200
H	-4.51679600	1.73191800	2.12901900
H	-5.31872300	-0.11213300	1.03477300

H	0.27348100	-1.25225800	-1.30911900
H	0.48618500	-1.76086600	-2.81142400
H	-0.70732500	-0.49868100	-2.87191400
H	-4.16657000	-3.21155600	-1.70764800
O	1.68309600	-1.92944800	-0.12099700
C	1.55891400	-1.65316100	1.08559300
O	0.68369300	-1.00574000	1.67489200
C	2.69684800	-2.24187300	1.97265000
F	2.63721700	-1.85114300	3.25307100
F	2.65275500	-3.59144000	1.97607700
F	3.91416700	-1.89493800	1.51608400
H	-1.87627800	-2.72609000	-3.03513000
H	-1.10078700	-3.26511300	-1.55323200
H	-5.85491200	-2.13923300	-0.26720500

2t-*o*-Au-TS2

G: -1744.078266

Au	-0.58054200	0.16004800	-0.53108300
F	4.34061100	1.85606200	-1.88375300
F	3.16122300	3.18686700	-0.65983100
F	3.94048700	1.35031600	0.17651800
O	1.23488100	1.24184700	-0.42392800
O	2.05818400	0.59407300	-2.42029200
N	-1.56534400	1.47974800	0.68312400
C	-3.30957400	-0.07083400	0.27730600
C	-2.33491800	-0.72236100	-0.48105700
C	-0.27016600	-1.42425500	-2.07381800
C	-3.81949000	-2.45645300	-1.10118700
C	2.11521800	1.15121400	-1.34514200
C	-4.81724600	-1.83344200	-0.35451200

C	-1.36407000	-2.47686100	-1.90574700
C	-0.99219100	2.55812600	1.22323600
C	-3.03498200	3.09555900	2.33156300
C	3.41117500	1.89382000	-0.92939000
C	-3.61707200	1.96875200	1.76898600
C	-1.70632800	3.39724900	2.05931300
C	-4.57735200	-0.64933800	0.33811300
C	-2.53748000	-1.90230000	-1.17510100
C	-2.86373200	1.15328200	0.93623700
H	0.04836500	2.72724900	0.97062300
H	-1.21839800	4.26505500	2.48522200
H	-3.61819300	3.73515800	2.98520800
H	-4.64930000	1.71375700	1.97555600
H	-5.37060100	-0.18718400	0.91652400
H	0.43653500	-1.35975800	-1.01392000
H	0.66694400	-1.81482400	-2.48859200
H	-0.54527600	-0.62843100	-2.77429600
H	-4.03746200	-3.37880000	-1.63176300
O	1.59200500	-1.98616800	-0.12232200
C	1.57518800	-1.71091900	1.10329500
O	0.73743500	-1.10540000	1.76678300
C	2.83256100	-2.24455400	1.84841300
F	2.86117800	-1.89884500	3.14010800
F	2.88852200	-3.59008300	1.79887100
F	3.96567400	-1.78415200	1.29062900
H	-1.65392100	-2.86152100	-2.88875900
H	-0.97024400	-3.32848900	-1.33929400
H	-5.80472300	-2.28062500	-0.31068900

3t-AuOAc^{F}

G: -1217.690809

Au	0.10731800	-0.51031000	-0.17590000
F	-5.07789300	0.01307700	1.09674100
F	-4.38777800	1.09500100	-0.63879500
F	-4.63495600	-1.05268200	-0.72571200
O	-1.99270700	-0.33549400	-0.49582700
O	-2.49865800	-0.21098600	1.69925800
N	0.63068800	1.60025800	-0.14715700
C	2.75529200	0.55033800	0.13179000
C	2.03953500	-0.64366200	0.01675600
C	0.21419700	-2.54933300	0.00040100
C	4.00758300	-1.96680000	0.21747900
C	-2.76032200	-0.21752400	0.51173100
C	4.74639100	-0.78985400	0.34772500
C	1.66834900	-3.03399600	-0.19552100
C	-0.19448600	2.64144700	-0.25044600
C	1.61842400	4.16149700	0.02719600
C	-4.23562800	-0.04297500	0.06353400
C	2.47575600	3.07594700	0.13644600
C	0.25997200	3.94782800	-0.17111800
C	4.13981600	0.46355200	0.29868200
C	2.62440300	-1.90425100	0.03889900
C	1.96231400	1.78629900	0.04465200
H	-1.24328200	2.40804100	-0.40180400
H	-0.43975000	4.76989400	-0.26135100
H	2.01080900	5.17057700	0.09739800
H	3.53707700	3.22604000	0.29438600
H	4.74850400	1.35759900	0.38691300
H	-0.48346200	-3.01913600	-0.69690400
H	-0.13466200	-2.74153900	1.02032700

H	4.51380800	-2.92746700	0.25103500
H	1.88254400	-3.89342600	0.45046100
H	1.80105300	-3.38559100	-1.22590200
H	5.82140400	-0.85013200	0.48488100

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