Electronic Supplementary Information (ESI)

Palladium dichloride adduct of *N,N*-bis-(diphenylphosphanylmethyl)-2-aminopyridine: synthesis, structure and catalytic performance in the decarboxylative cross-coupling of 4-picolinic acid with aryl bromide

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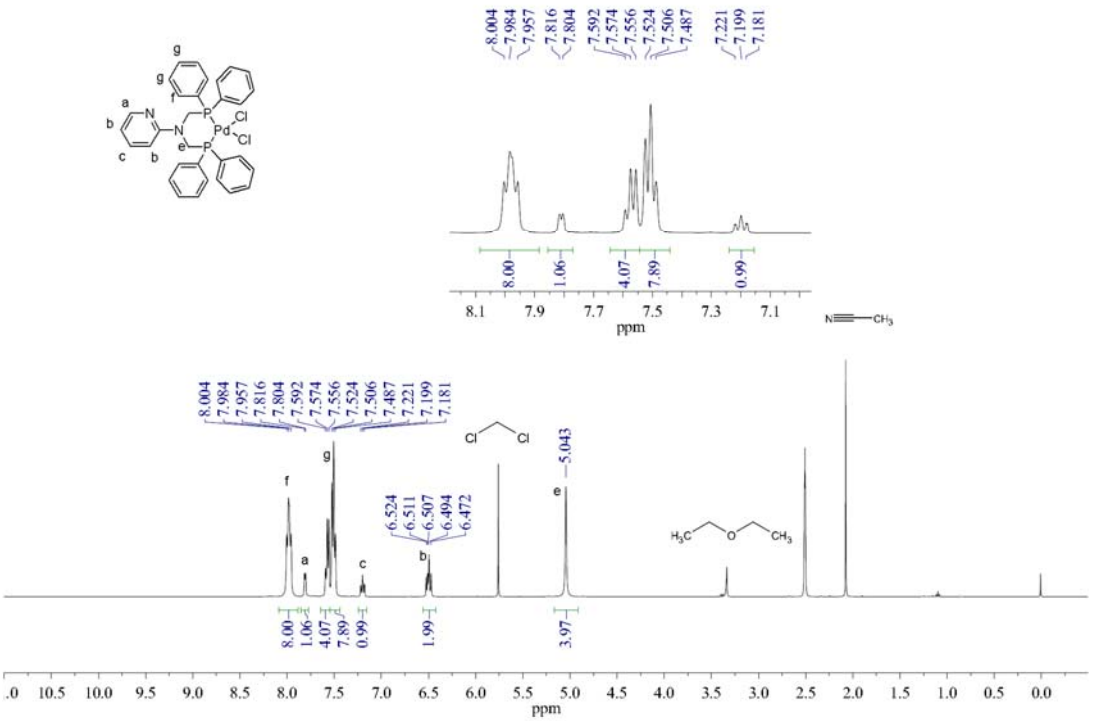
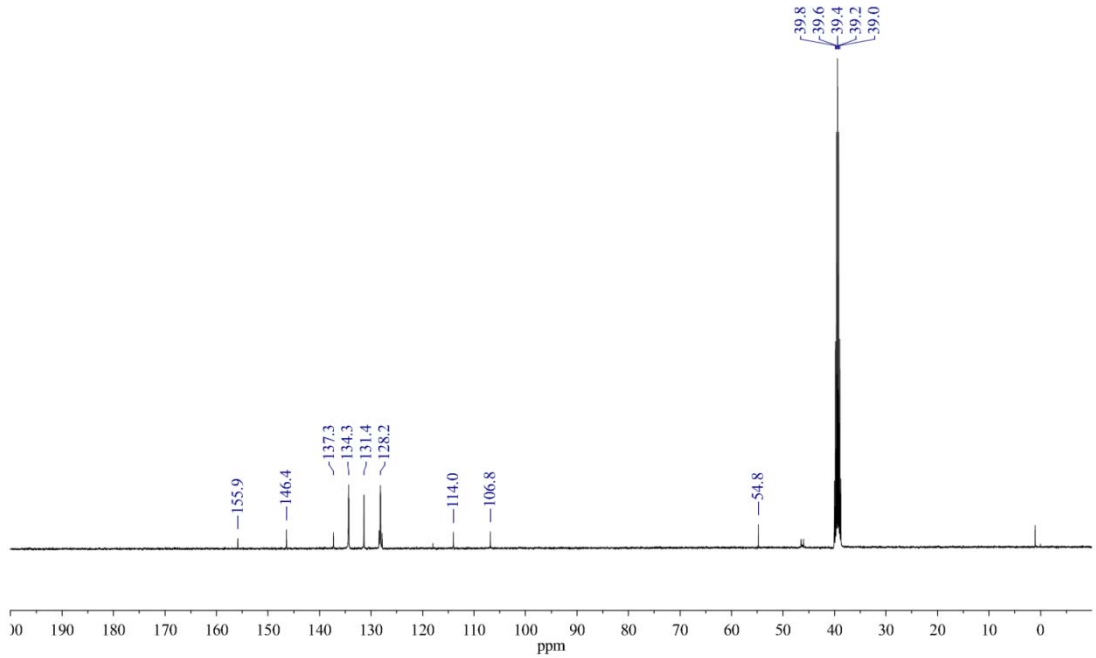
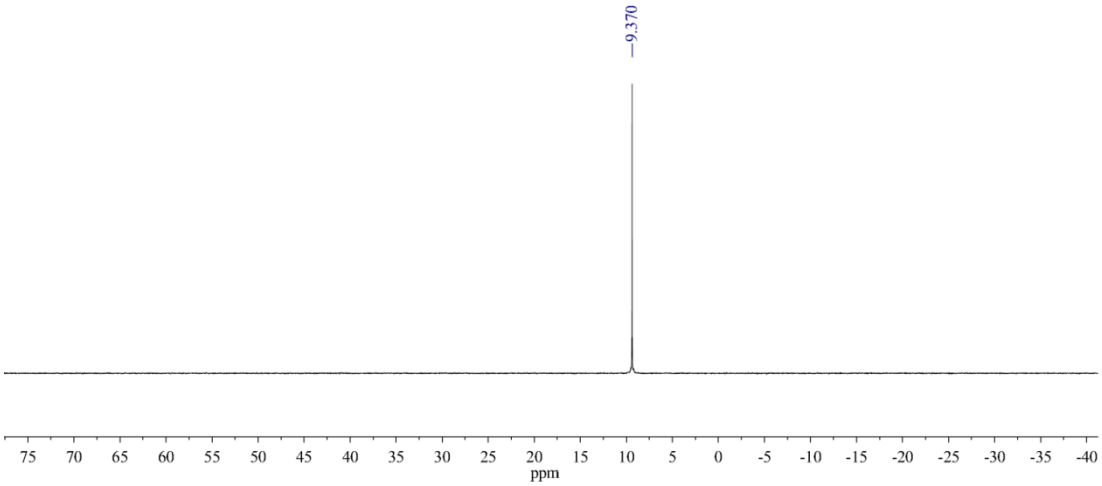
Figure S1. ^{1}H NMR (a), ^{13}C NMR (b) and ^{31}P NMR (c) spectra of **1**.



(a)



(b)


9.370
75 70 65 60 55 50 45 40 35 30 25 20 15 10 5 0 -5 -10 -15 -20 -25 -30 -35 -40
ppm

(c)

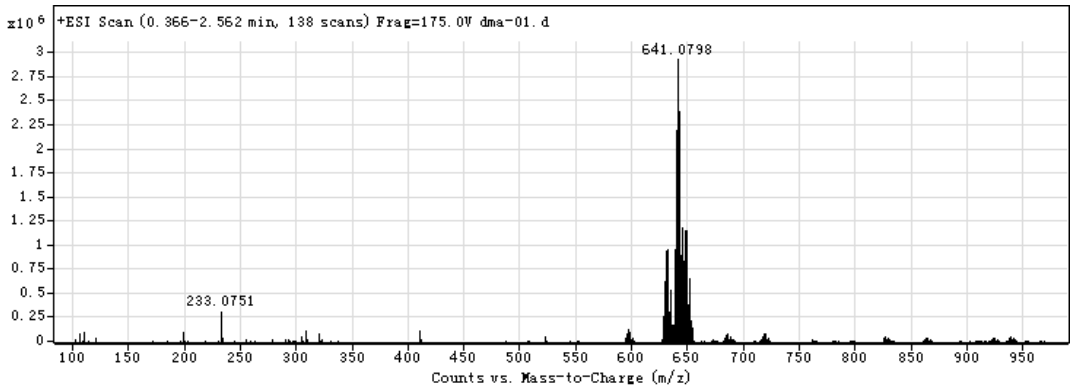


Figure S2 Positive-ion ESI-MS of the mixture of $PdCl_2$ and bdppmapy in DMA.

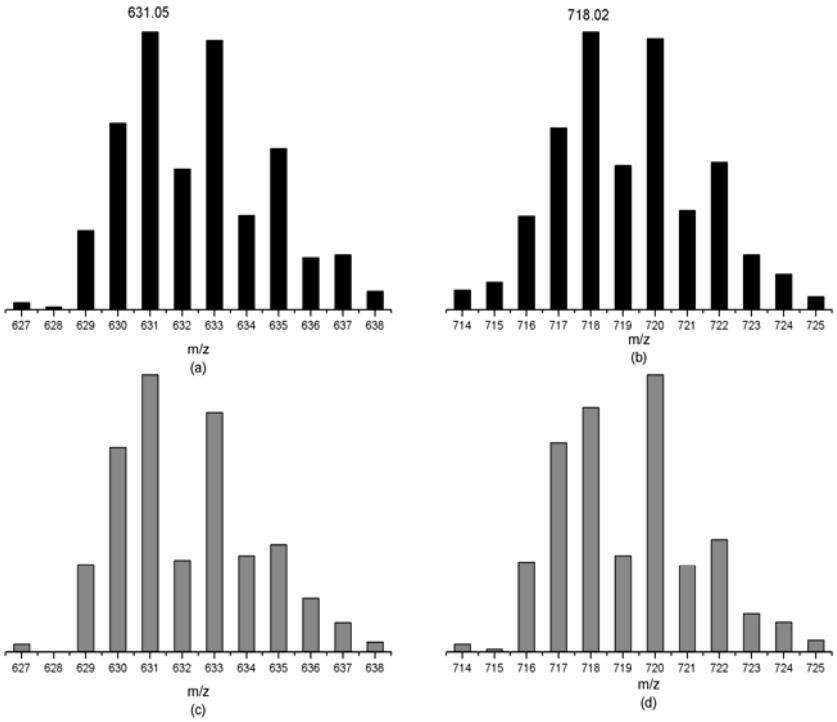


Figure S3. Observed (a and b) and calculated (c and d) isotopic patterns for the $[(bdppmapy)PdCl]^+$ cation and the $\{[(bdppmapy)PdCl]\cdot DMA\}^+$ cation in the mixture of $PdCl_2$ and bdppmapy in DMA.

Computational details

Density functional theory calculations were performed using Gaussian 09[1] with spin-restricted method. All structure optimizations were performed using the B3LYP functional[2] with the standard Pople all-electron basis set 6-31G(d) for all the atoms except for Pd and Br (which were described by LANL2DZ basis set and effective core potential implemented[3]). Frequency analysis was conducted at the same level of theory to verify the stationary points to be real minima and to get the zero-point energy (ZPE) corrections. Single-point calculations were performed with a large basis set, *i.e.* SDD for Pd, Br atoms and 6-311+G(2d,p) for the rest atoms. Basis set superposition errors were corrected for the [Cu]-[Pd] intermediates at the larger basis set level.

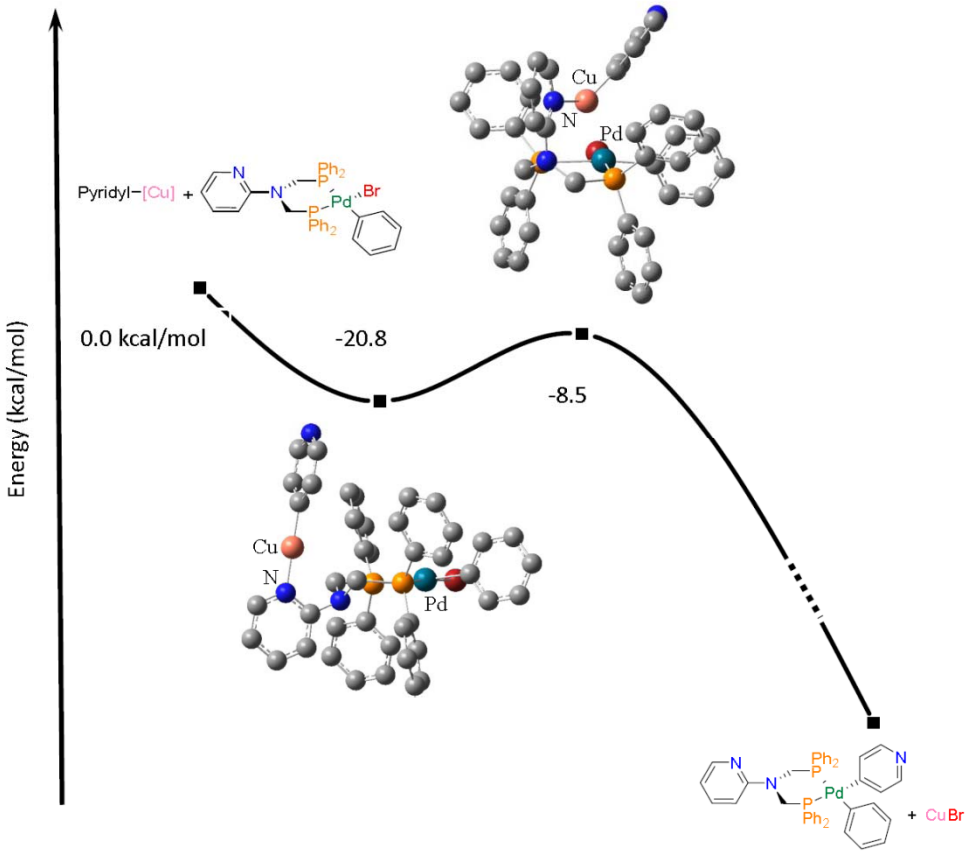
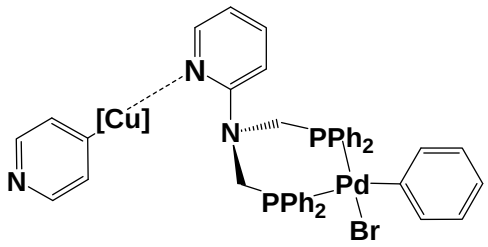


Figure S4 Structures and energies calculated by DFT (B3LYP/DZVP/TZVP). Gibbs free energy (G) in kcal·mol^{-1}.

Coordinates and energies of computed structures



TS for the Palladium(II)-Copper(I) complex (minimum)

E = -4252.15516689 a.u.
ZPE correction = 0.683472 a.u.
BSSE correction = 0.045704154 a.u.

Pd	-1.74898677	0.42778128	-0.57492605
Cu	3.85926514	-0.93702709	0.52641392
Br	-3.00200116	2.33125424	-1.79111236
P	0.16741494	1.90651300	-0.29441828
P	-0.85682280	-1.33279364	0.62216206
N	4.63776782	-2.59468544	-3.84916852
N	3.52373461	-0.34311675	2.28397727
N	1.29210977	0.18161653	1.60804962
C	-2.78392427	-0.52842940	4.16554334
C	-2.60423453	-1.69357130	4.91254616
C	-2.28678968	-0.44827792	2.86274625
C	-1.92057184	-2.77764844	4.35593493
C	-1.59959572	-1.53114374	2.29541546
C	-1.41687064	-2.69679517	3.05750391
C	-5.58196049	-2.40392746	-1.57593230
C	-5.52155348	-1.74788263	-0.34604662
C	4.84730487	-1.31001623	-3.53146203
C	4.63857617	-0.77653032	-2.25824650
C	-4.53775831	-2.24466738	-2.49015714
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C	4.20704866	-3.37955961	-2.85302779
C	4.17898513	-1.58029217	-1.19256206
C	3.97219730	-2.93041090	-1.55198712
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C	-2.01968651	-5.08487948	-0.63140866
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C	-1.34835992	3.62223746	1.33116121
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C	-0.50995796	5.60147078	2.44428635
C	-0.08722113	3.39236641	0.76393716
C	4.47984886	-0.39193919	3.23627809
C	4.25679738	0.01778096	4.54505642

C	2.99367546	0.49737401	4.89193890
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C	2.00077962	0.55107160	3.91446053
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C	1.70109141	1.68060216	-2.64423824
C	1.66494908	1.11658511	0.52419305
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C	0.95706781	4.29323647	1.03571410
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C	0.91642480	2.53523801	-1.85123228
C	0.74749451	5.38931743	1.87127535
C	0.62769996	3.82483689	-2.32227897
C	0.16158620	-3.38938412	-1.01743103
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H	4.84148702	0.28324671	-2.11134327
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H	5.05954733	-0.04155411	5.27211932
H	2.81927183	1.44437277	-4.46185974
H	2.78382936	0.82408644	5.90611531
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H	2.28517884	0.59705298	-0.22252487
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H	1.91895796	0.66465315	-2.32820698
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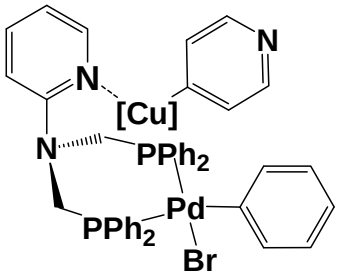

TS for the palladium(II)-copper(I) complex (minimum)

E = -4252.135951 a.u.
ZPE correction = 0.683225 a.u.
BSSE correction = 0.061643586 a.u.

Pd	-0.07245200	0.59270400	-0.75022500
Cu	0.28799900	-1.92093100	0.23698100
Br	1.33257300	0.84205000	-2.92080700
P	2.03991200	0.73175700	0.50794800
P	-1.51973900	0.83713600	1.06404000
N	-0.91009800	-4.92783200	-3.26151700
N	0.79492800	-2.15545200	2.10119500
N	0.58632000	0.07083100	2.90291800
C	-3.88538600	4.07610600	2.11810400
C	-3.41833200	2.77103500	1.95267600
C	-3.20338300	5.14621700	1.53566500
C	-2.26395000	2.52057100	1.19356000
C	-2.05095700	4.90752800	0.78445600
C	-1.58502900	3.60317000	0.61203700
C	-1.42353600	-4.97665200	-2.02588100
C	-1.11943100	-4.05868600	-1.01817700
C	-0.22389000	-2.98854300	-1.24344100
C	-0.06803700	-3.91139400	-3.50068300
C	-5.17181600	-0.97811200	0.51375500
C	-5.13743500	-2.06816300	1.38550300
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C	-4.01091300	-2.28034000	2.18012400
C	-3.96748400	0.88388500	-3.66397000
C	-3.50223000	-0.35871800	-3.23096200
C	-3.31600500	2.04387900	-3.24045200

C	-2.95224800	-0.30242400	1.23667100
C	-2.92578200	-1.40442700	2.10614700
C	-2.40270600	-0.44529100	-2.36877100
C	-2.20937800	1.96033700	-2.38722500
C	-1.75187400	0.71588200	-1.94044700
C	-0.65407700	0.80019400	2.77597600
C	0.28918200	-2.94822800	-2.55548300
C	5.64982700	-1.26905400	0.77514400
C	5.49899100	-2.29921000	-0.15825700
C	4.62171100	-0.34717500	0.96926000
C	4.45129900	3.82993500	-0.80079300
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C	3.90978600	4.94739700	-0.16406600
C	3.42685100	-0.44735100	0.23503600
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H	4.33543800	1.70587400	-1.09707300
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H	4.19669900	-3.19192100	-1.63097900
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H	2.37958200	-1.55261700	-1.28893200
H	2.37678300	5.65523800	1.18046100
H	1.40048100	3.43548900	1.54676100
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H	0.34111100	-3.54389400	5.70245400
H	0.20906400	-1.07978700	5.24117000

Reference:

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2. (*a*) A. D. Becke, *J. Chem. Phys.*, 1993, **98**, 5648; (*b*) C. T. Lee, W. T. Yang and R. G. Parr, *Phys Rev B*, 1988, **37**, 785.
3. P. J. Hay and W. R. Wadt, *J. Chem. Phys.*, 1985, **82**, 270.

4-(2,4-Dimethoxyphenyl)-pyridine (4a):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.61 (s, 2H), 7.61 (d, J = 4.8 Hz, 2H), 7.34 (J = 8.4 Hz, 1H), 6.64 (J = 2.0 Hz, 1H), 6.60 (s, 1H), 3.87 (d, J =11.2 Hz, 6H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 162.1, 158.0, 148.4, 147.1, 131.3, 124.5, 119.5, 105.4, 99.1, 55.6. MS (*m/z*) calcd. for $C_{13}H_{13}NO_2$: 215.25, found 215.26.

2-(2,4-dimethoxyphenyl)pyridine (4b):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.57 (d, J = 4.6 Hz, 1H), 7.88 (t, J = 9.7 Hz, 2H), 7.70 (td, J = 2.0, 7.4 Hz, 1H), 7.18 (ddd, J = 1.4, 4.8, 7.4 Hz, 1H), 6.65 (m, 2H), 3.88 (s, 3H), 3.85 (s, 3H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 163.1, 156.0, 148.7, 147.5, 131.3, 128.5, 119.5, 115.4, 99.1, 55.6. MS (*m/z*) calcd. for $C_{13}H_{13}NO_2$: 215.25, found 215.26.

4-(4-Methoxylphenyl)-pyridine (6a):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.60 (d, J = 6.0 Hz, 2H), 7.59 (d, J = 8.8 Hz, 2H), 7.46 (d, J = 6.0 Hz, 2H), 7.00 (d, J = 8.8 Hz, 2H), 3.86 (s, 3H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 160.8, 150.2, 148.1, 130.5, 128.4, 121.3, 114.8, 55.6. MS (*m/z*) calcd. for $C_{12}H_{11}ON$: 185.08, found: 185.08.

4-(3-Methoxylphenyl)-pyridine (6b):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.66 (d, J = 6.0 Hz, 2H), 7.50 (d, J = 6.0 Hz, 2H), 7.40 (t, J = 8.0 Hz, 1H), 7.22 (d, J = 7.6 Hz, 1H), 7.15 (s, 1H), 6.99 (d, J = 8.0 Hz, 1H), 3.85 (s, 3H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 160.2, 150.0, 148.5, 139.5, 130.2 121.8, 119.4, 114.4, 112.8, 55.4. MS (*m/z*) calcd. for $C_{12}H_{11}ON$: 185.08, found: 185.08.

4-(2-Methoxylphenyl)-pyridine (6c):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.62 (d, J = 6.0 Hz, 2H), 7.47 (d, J = 4.4 Hz, 2H), 7.38 (t, J = 8.0 Hz, 1H), 7.33 (d, J = 7.6 Hz, 1H), 7.05 (t, J = 7.6 Hz, 1H), 6.99 (d, J = 8.4 Hz, 1H), 3.82 (s, 3H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 156.6, 149.3, 146.6, 130.5, 130.2, 127.6, 124.4, 121.1, 111.5, 55.6. MS (*m/z*) calcd. for $C_{12}H_{11}ON$: 185.08, found: 185.08.

4-(2-Methylphenyl)-pyridine (6d):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.64 (d, J = 4.8 Hz, 2H), 7.27 (m, 5H), 7.19 (d, J = 7.2 Hz, 1H), 2.27 (s, 3H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 149.9, 149.5, 139.0, 135.0, 130.7, 129.3, 128.4, 126.1, 124.3, 20.3. MS (*m/z*) calcd. for $C_{12}H_{10}N$: 168.08, found: 168.08.

4-(3-Methylphenyl)-pyridine (6e):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.61 (d, J = 6.0 Hz, 2H), 7.43 (m, 2H), 7.39 (s, 1H), 7.37 (s, 1H), 7.32 (t, J = 7.2 Hz, 1H), 7.22 (d, J = 7.6 Hz, 1H), 2.41 (s, 3H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 150.0, 138.7, 137.9 129.7, 128.9, 127.6, 124.0, 121.5, 21.4. MS (*m/z*) calcd. for $C_{12}H_{11}N$: 169.09, found: 169.09.

4-(4-Methylphenyl)-pyridine (6f):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.64 (d, J = 6.0 Hz, 2H), 7.54 (d, J = 8.0 Hz, 2H), 7.50 (d, J = 6.0 Hz, 2H), 7.29 (d, J = 7.6 Hz, 2H), 2.41 (s, 3H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 150.2, 148.7, 139.6, 135.3, 130.1, 127.1, 121.7, 21.5. MS (*m/z*) calcd. for $C_{12}H_{11}N$: 169.09, found: 169.09.

4-(2,4,6-Trimethyl-phenyl)-pyridine (6g):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.68 (d, J = 5.6 Hz, 2H), 7.16 (t, J = 4.4 Hz, 2H), 6.96 (s, 2H), 2.34 (s, 3H), 1.99 (s, 6H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 150.6, 149.0, 137.8, 135.0, 128.4, 125.1, 21.1, 20.6, 14.2. MS (*m/z*) calcd. for $C_{14}H_{15}N$: 197.21, found: 197.20.

4-(3,5-Dimethylphenyl)-pyridine (6h):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.65 (d, J = 6.0 Hz, 2H), 7.50 (d, J = 6.0 Hz, 2H), 7.26 (s, 2H), 7.10 (s, 1H), 2.41 (s, 6H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 150.0, 148.8, 138.8, 138.1, 130.8, 124.9, 121.8, 21.4. MS (*m/z*) calcd. for $C_{13}H_{13}N$: 183.24, found: 183.24.

4-(4-Fluoro-phenyl)-pyridine (6i):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.66 (d, J = 6.0 Hz, 2H), 7.64 (dd, J = 5.6 Hz, 3.2 Hz, 2H), 7.43 (d, J = 6.0 Hz, 2H), 7.18 (t, J = 8.8 Hz, 2H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 164.7, 162.3, 150.1, 147.5, 134.2, 128.9, 128.8, 121.5, 116.3, 116.1. MS (*m/z*) calcd. for $C_{11}H_8NF$: 173.06, found: 173.06.

4-(Pyridin-4-yl)-benzonitrile (6j):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.72 (d, J = 5.6 Hz, 2H), 7.78 (d, J = 8.4 Hz, 2H), 7.73 (d, J = 8.4 Hz, H), 7.50 (d, J = 6.0 Hz, 2H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 150.5, 146.5, 142.6, 132.9, 127.8, 121.7, 118.4, 112.9. MS (*m/z*) calcd. for $C_{12}H_8N_2$: 180.07, found: 180.07.

4-(4-Trifluoromethylphenyl)-pyridine (6k):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.69 (d, J = 6.4 Hz, 2H), 7.72 (s, 4H), 7.49 (d, J = 6.0 Hz, 2H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 150.5, 147.0, 141.8, 131.3, 130.0, 127.5, 126.2, 126.1, 122.7, 121.8. MS (*m/z*) calcd. for $C_{12}H_8NF_3$: 223.06, found: 223.05.

4-Biphenyl-4-yl-pyridine (6l):
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.69 (d, J = 6.0 Hz, 2H), 7.73 (s, 4H), 7.64 (d, J = 7.2 Hz, 2H), 7.60 (d, J = 6.0 Hz, 2H), 7.48 (t, J = 7.2 Hz, 2H), 7.39 (t, J = 7.2 Hz, 1H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ = 149.4, 148.7, 142.3, 140.1, 136.5, 129.0, 127.9, 127.9, 127.5, 127.1, 121.7. MS (*m/z*) Calcd. for $C_{17}H_{13}N_1$: 231.11, found: 231.11.

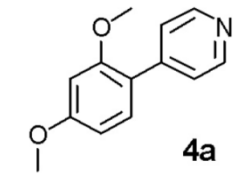
4-(Naphthalen-1-yl)-pyridine (6m):

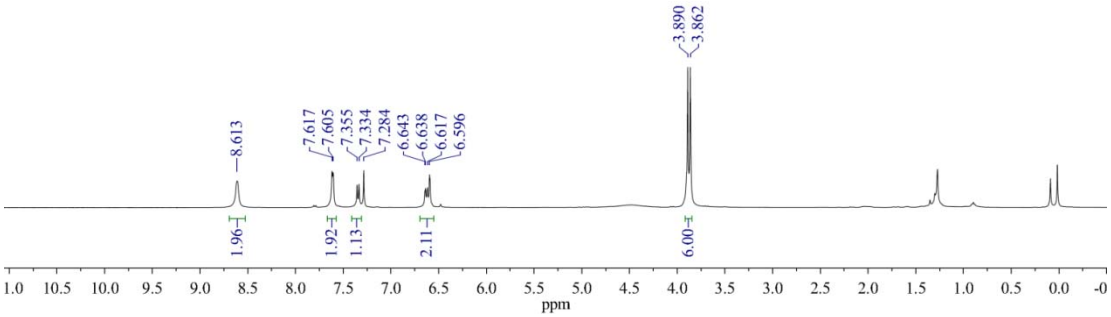
^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.73 (d, J = 5.2 Hz, 2H), 7.92 (m, 2H), 7.84 (d, J = 8.4 Hz, 1H), 7.48 (m, 6H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 149.7, 148.8, 137.3, 133.8, 130.7, 128.9, 128.6, 126.9, 126.7, 126.2, 125.4, 125.2, 125.1. MS (*m/z*) calcd. for $C_{15}H_{11}N$: 205.09, found: 205.08.

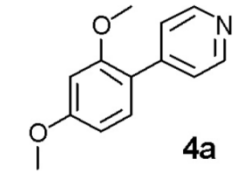
4-(Naphthalen-2-yl)-pyridine (6n):

^{1}H NMR (400 MHz, $CDCl_3$, ppm): δ 8.75 (d, J = 6.4 Hz), 8.10 (m, 1H), 7.63 (m, 2H), 7.56 (d, J = 6.4 Hz, 2H), 7.46 (m, 5H). ^{13}C NMR (400 MHz, $CDCl_3$, ppm): δ 149.7, 148.8, 137.3, 133.8, 130.7, 128.9, 128.6, 126.9, 126.7, 126.2, 125.4, 125.2, 125.1. MS (*m/z*) calcd. for $C_{15}H_{11}N$: 205.09, found: 205.09.

Figure S5. ^{1}H NMR, ^{13}C NMR spectra of 4-(2,4-dimethoxyphenyl)-pyridine (**4a**).







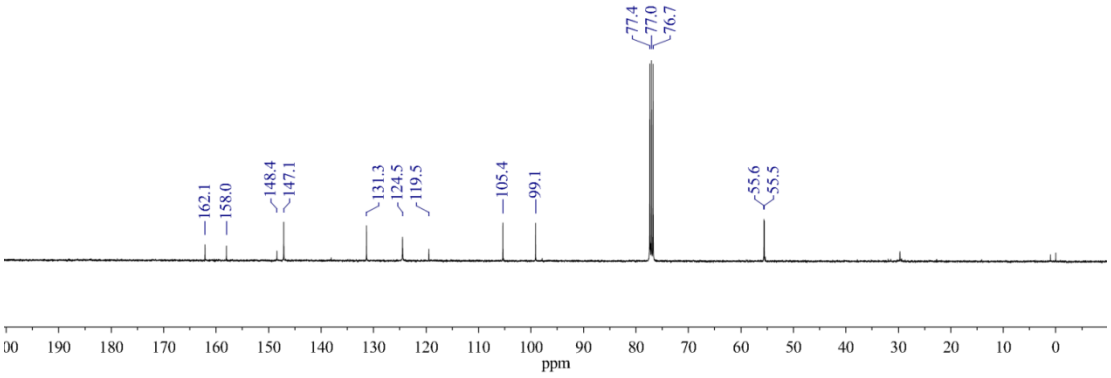
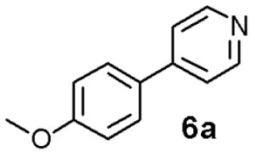
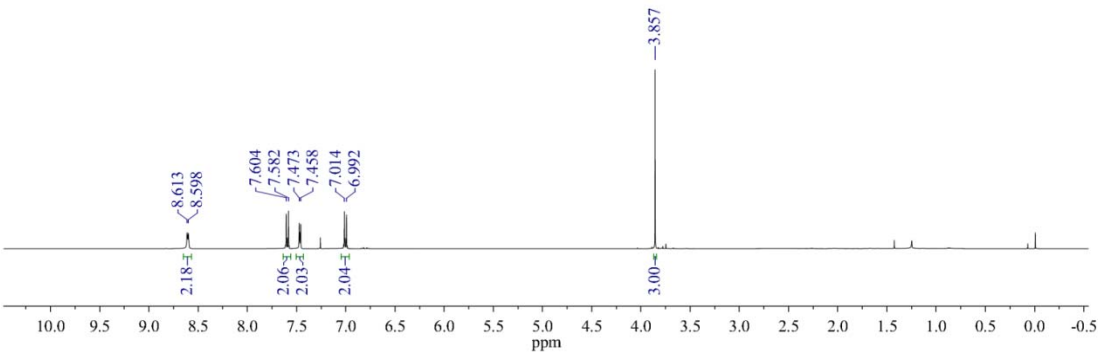
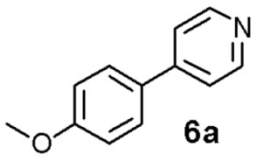


Figure S6. ^{1}H NMR, ^{13}C NMR spectra of 4-(4-methoxylphenyl)-pyridine (**6a**)







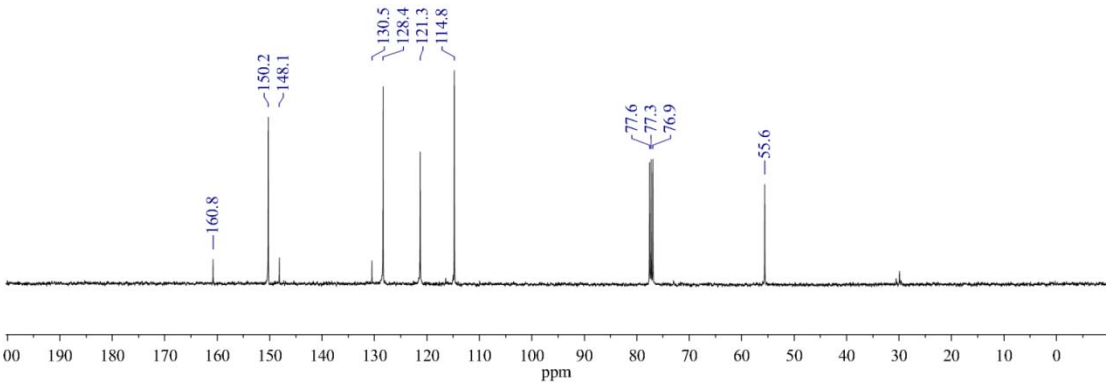
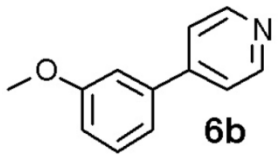
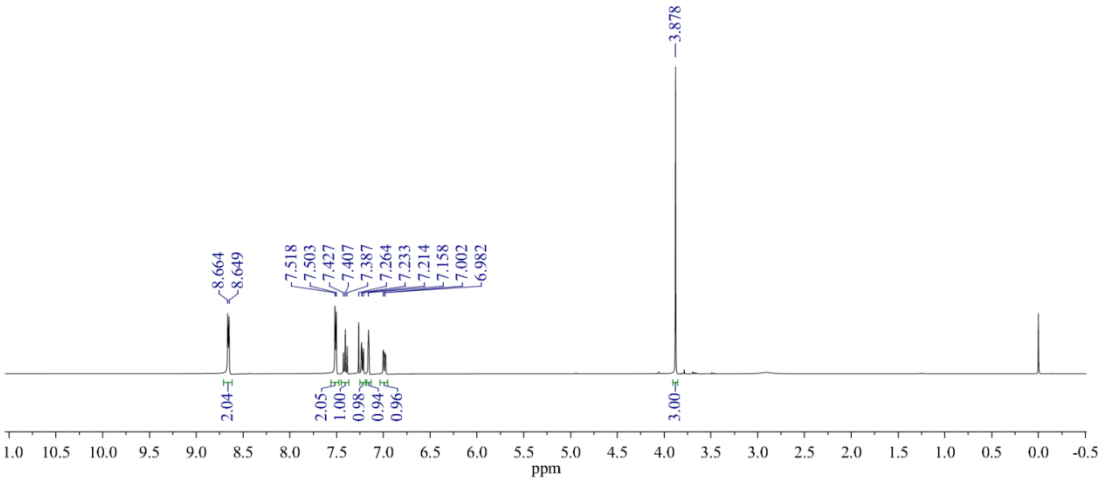
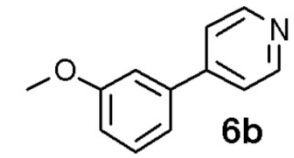


Figure S7. ^{1}H NMR, ^{13}C NMR spectra of 4-(3-methoxylphenyl)-pyridine (**6b**)







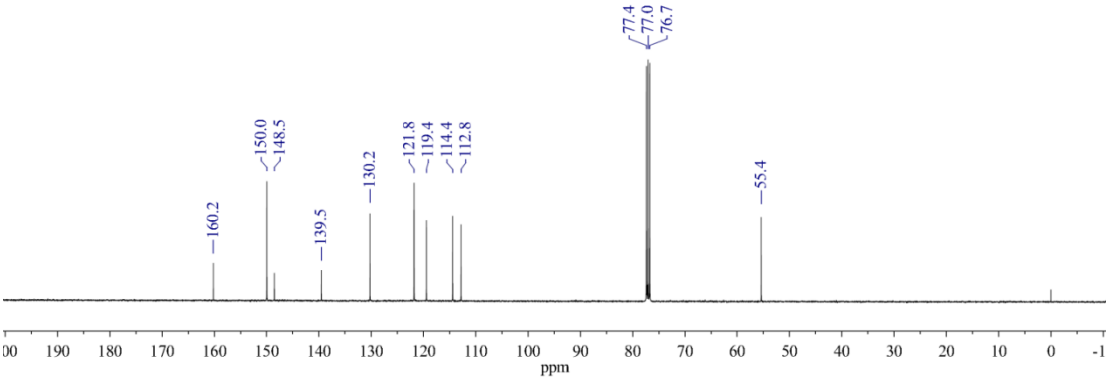
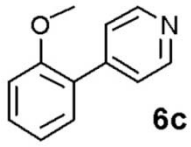
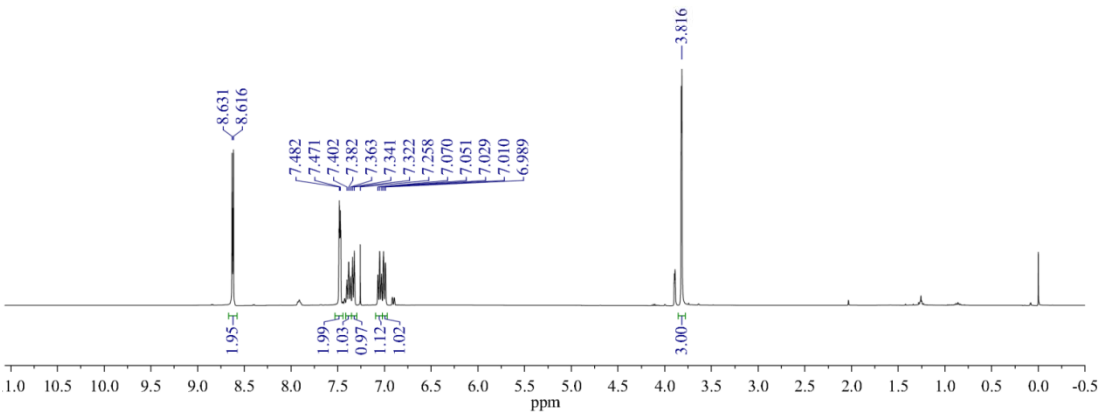
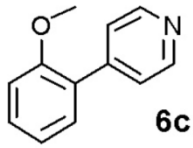


Figure S8. ^{1}H NMR, ^{13}C NMR spectra of 4-(2-methoxylphenyl)-pyridine (**6c**)







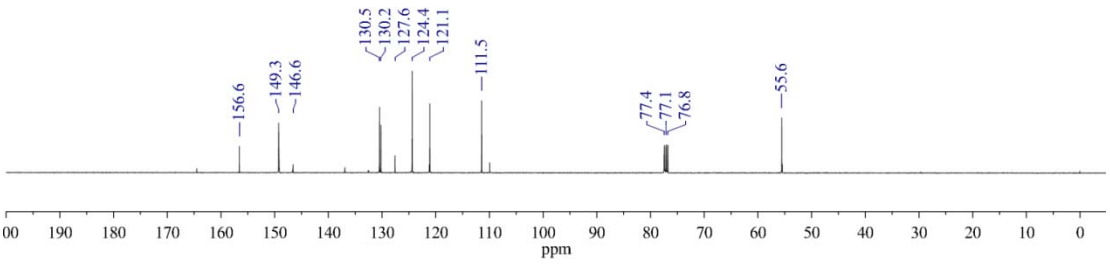
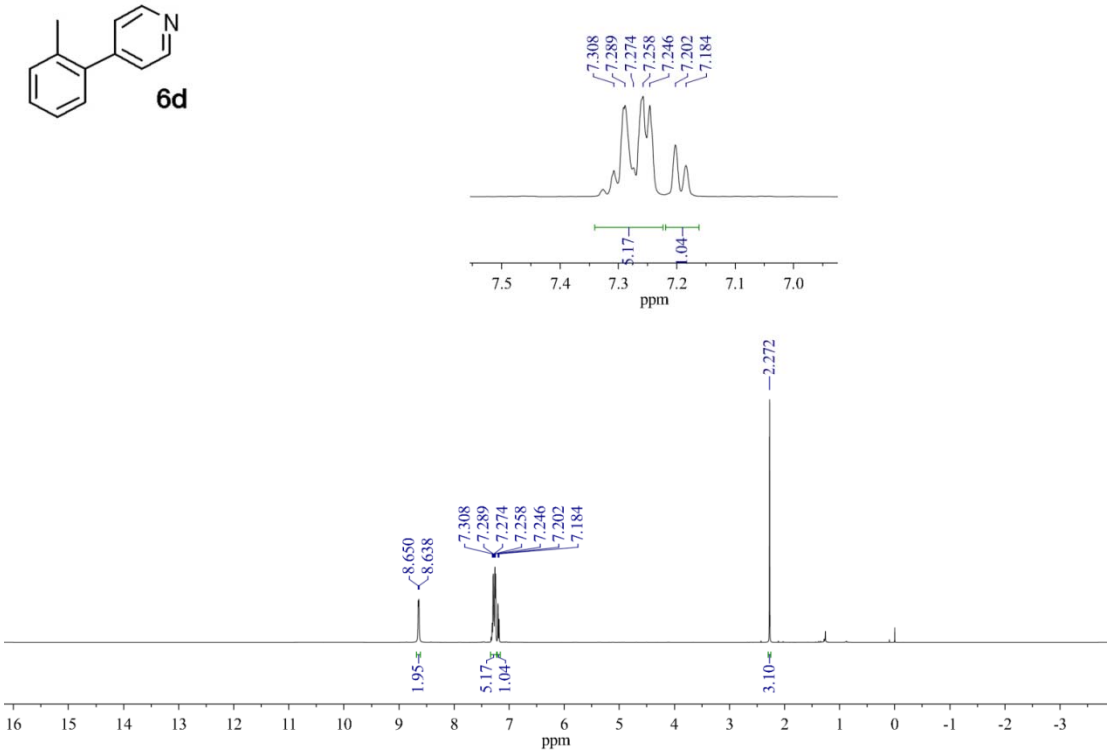


Figure S9. ^{1}H NMR, ^{13}C NMR spectra of 4-(2-methylphenyl)-pyridine (**6d**)



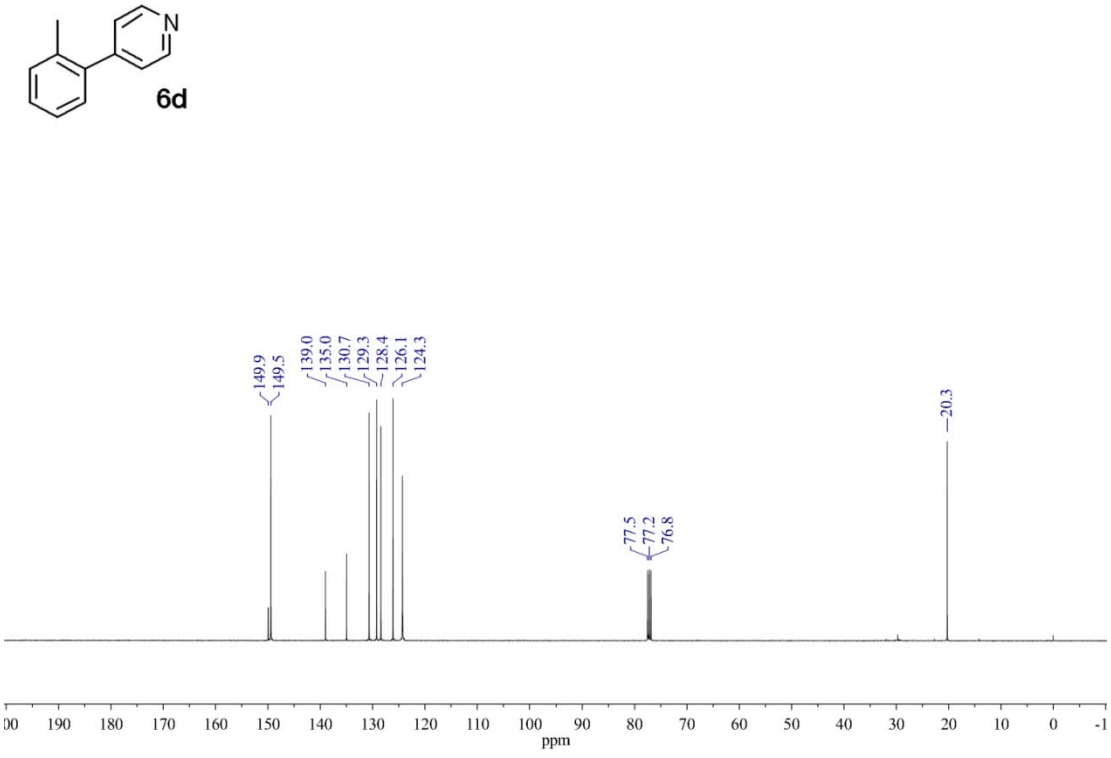


Figure S10. ^{1}H NMR, ^{13}C NMR spectra of 4-(3-methylphenyl)-pyridine (**6e**)

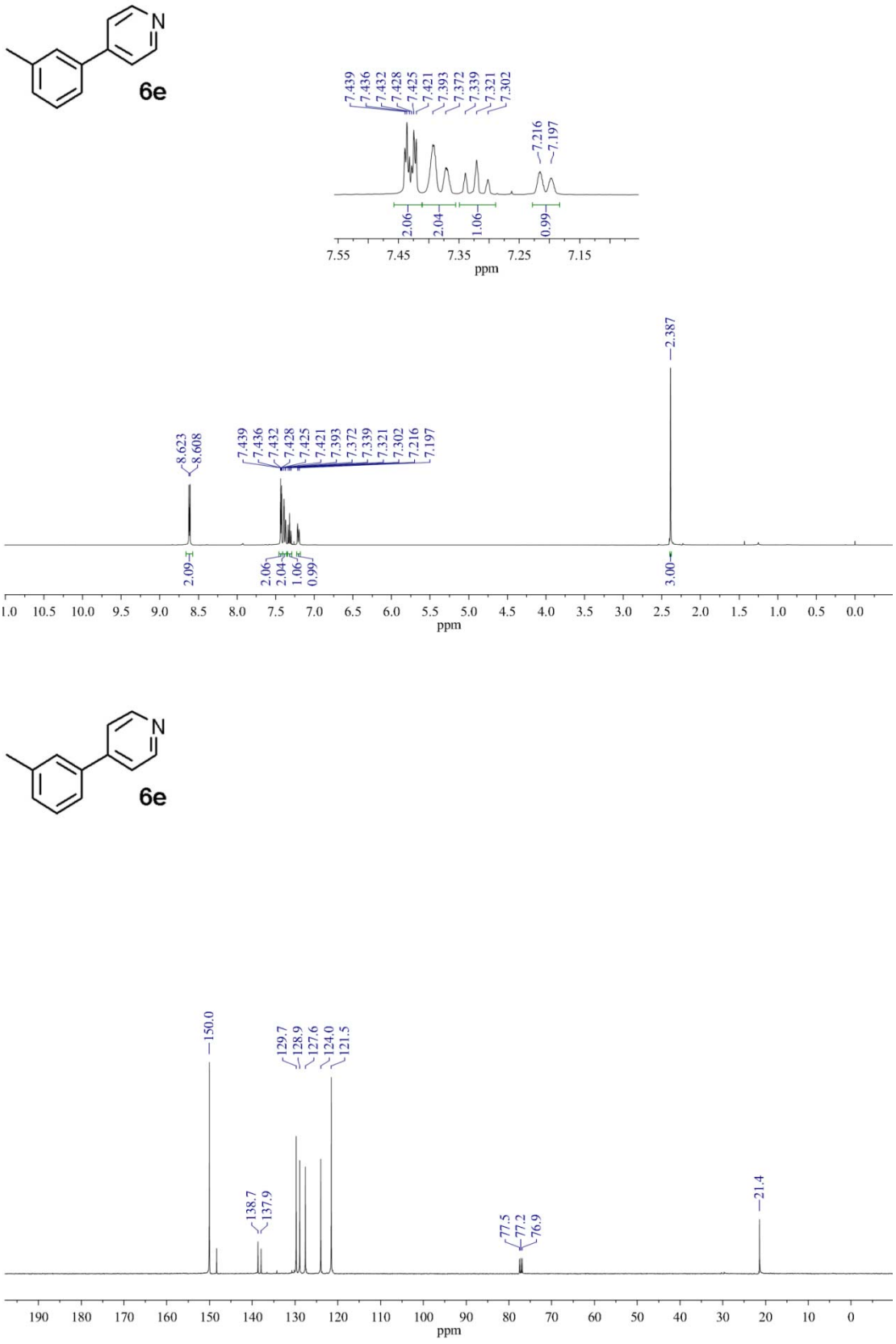


Figure S11. ^{1}H NMR, ^{13}C NMR spectra of 4-(4-methylphenyl)-pyridine (**6f**)

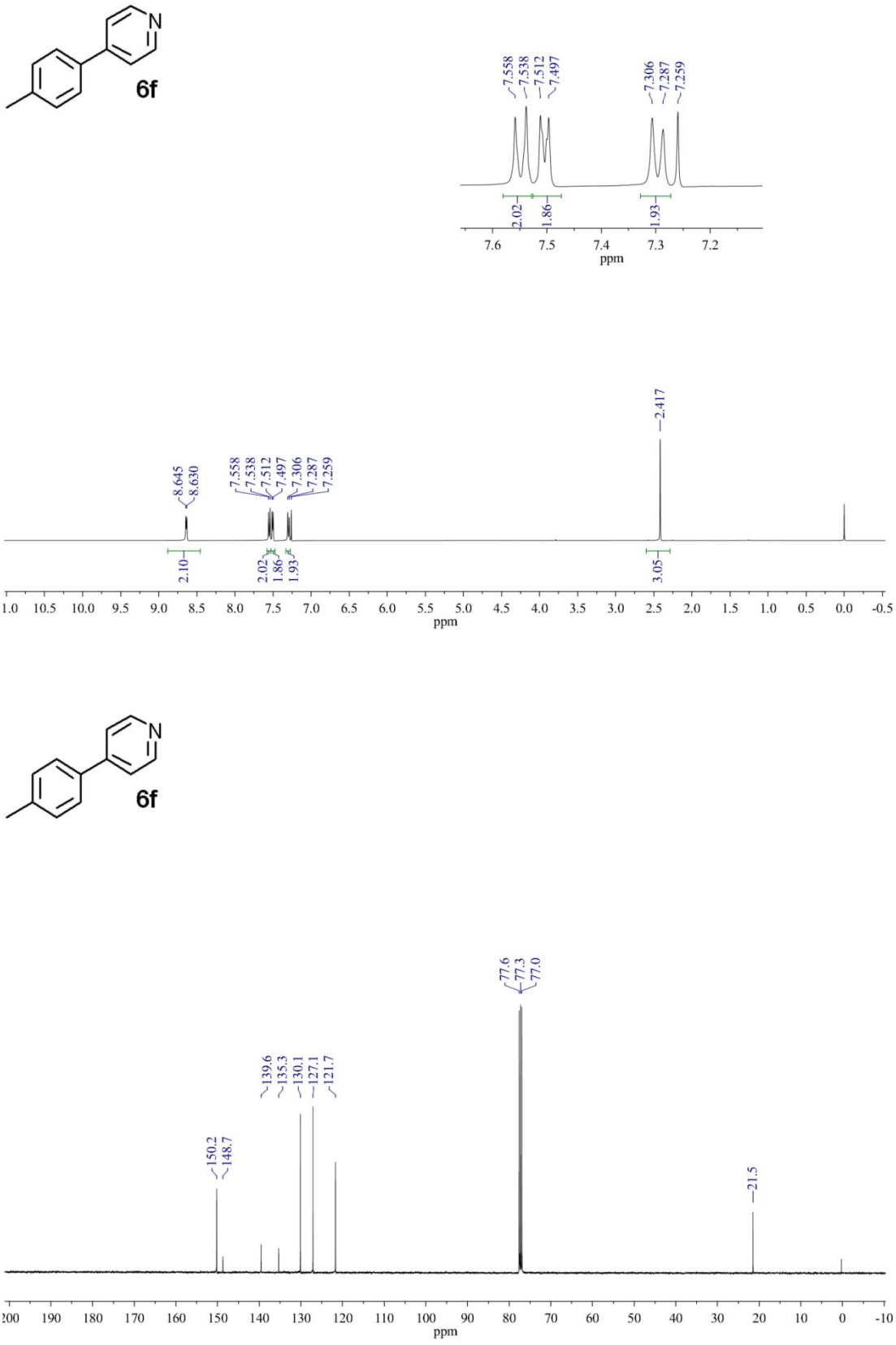
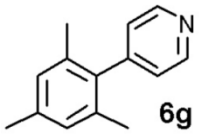
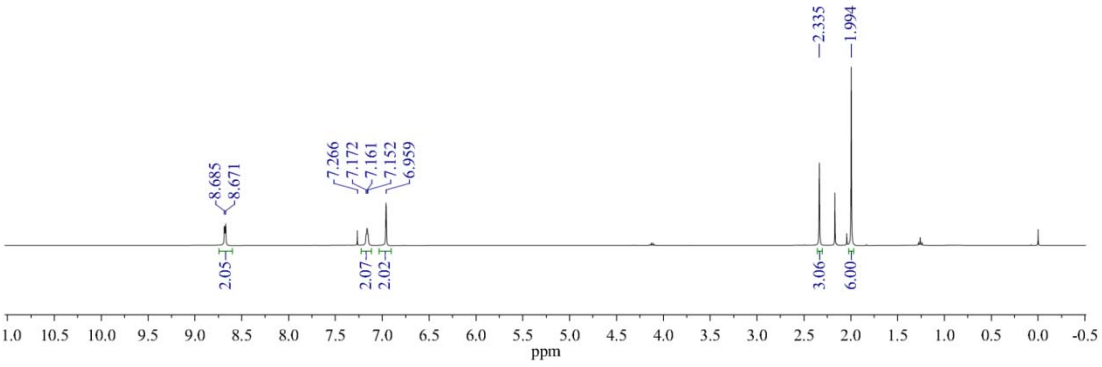
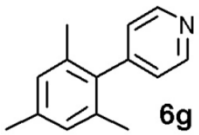


Figure S12. ^{1}H NMR, ^{13}C NMR spectra of 4-(2,4,6-trimethyl-phenyl)-pyridine (**6g**)







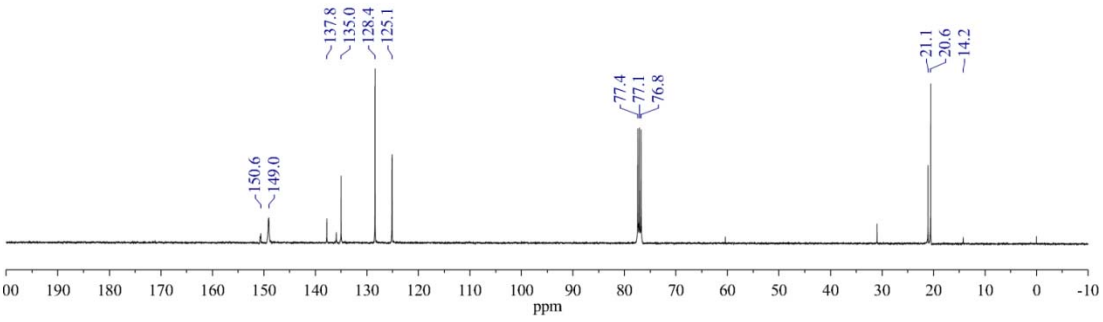
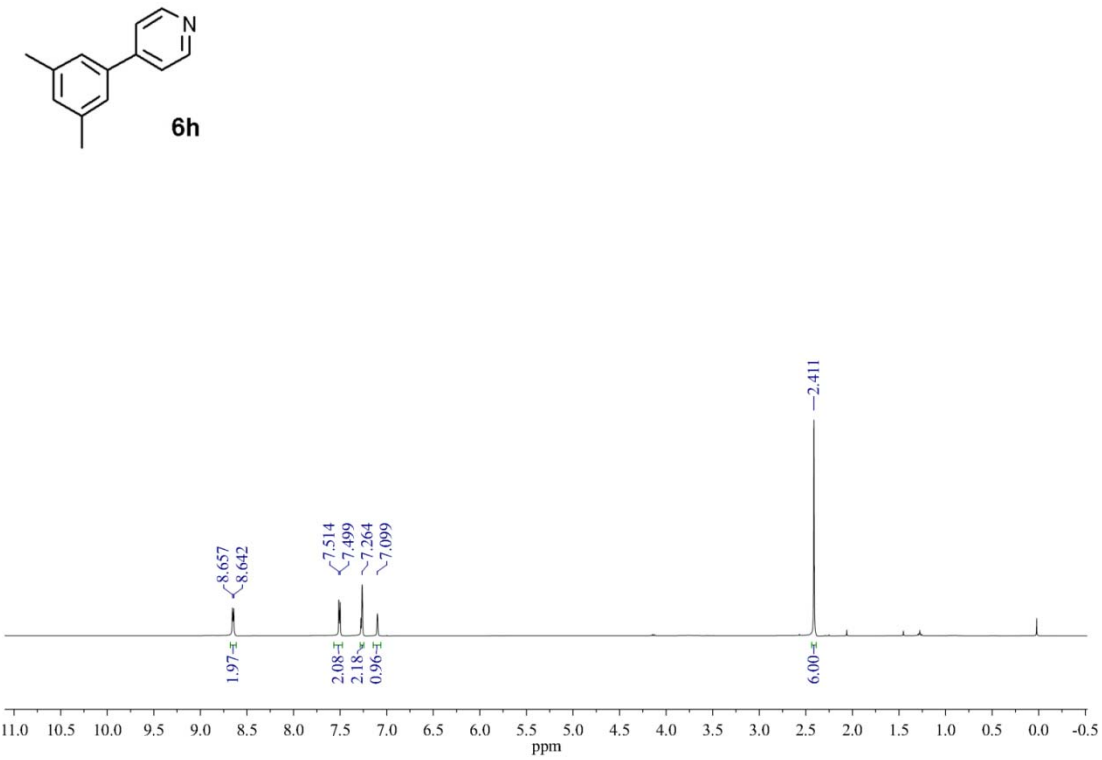


Figure S13. ^{1}H NMR, ^{13}C NMR spectra of 4-(3,5-dimethyl-phenyl)-pyridine (**6h**)



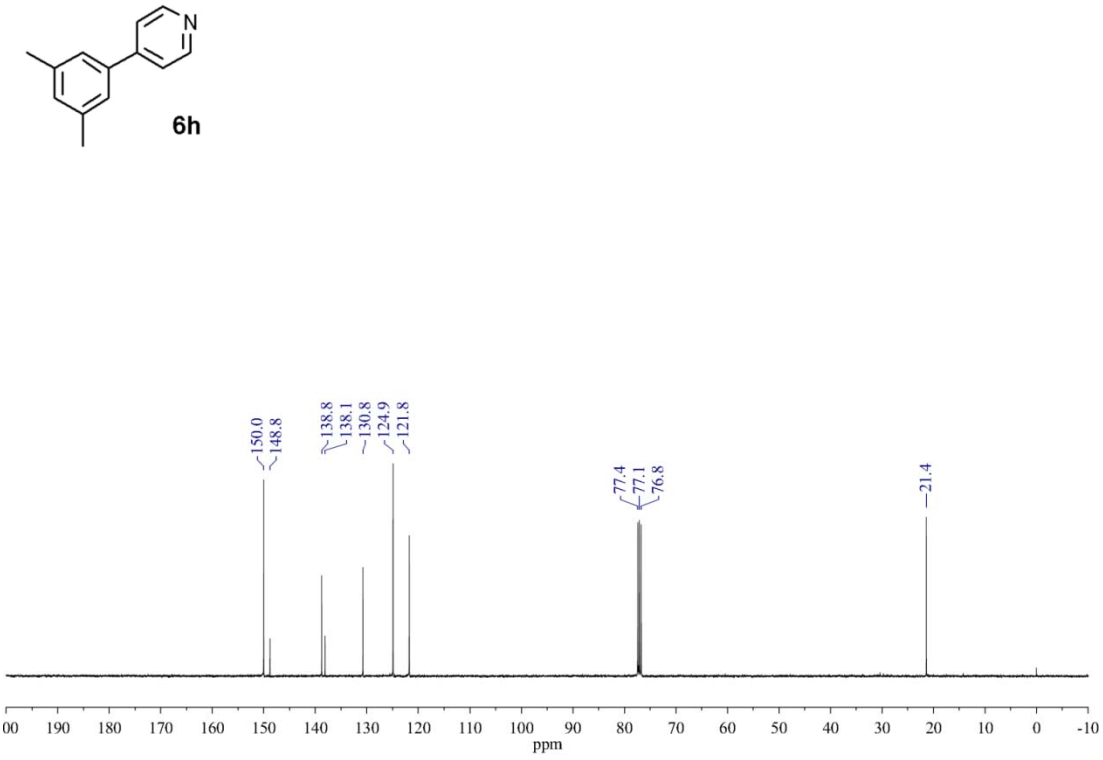
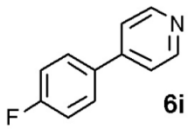
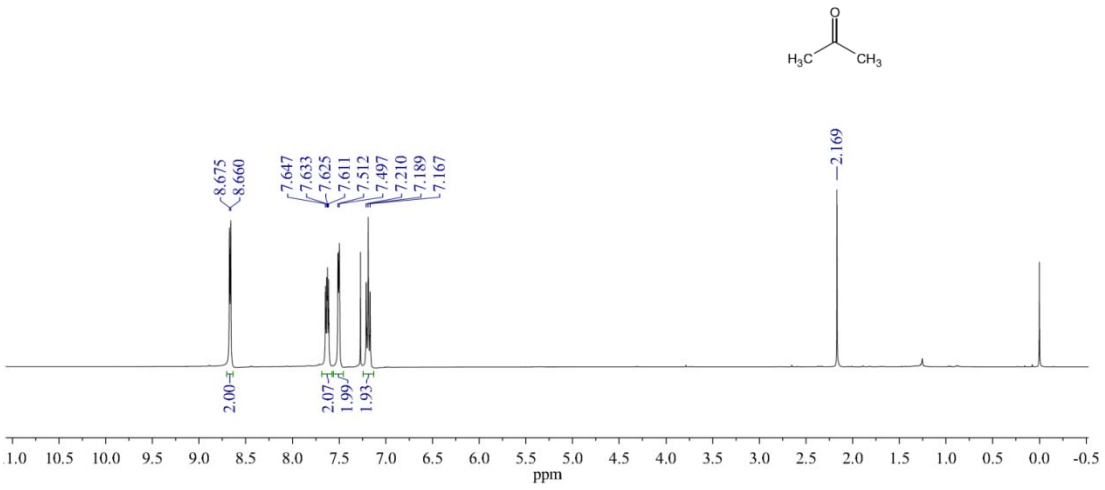
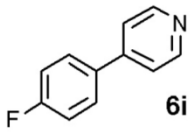


Figure S14. ^{1}H NMR, ^{13}C NMR spectra of 4-(4-fluoro-phenyl)-pyridine (**6i**)







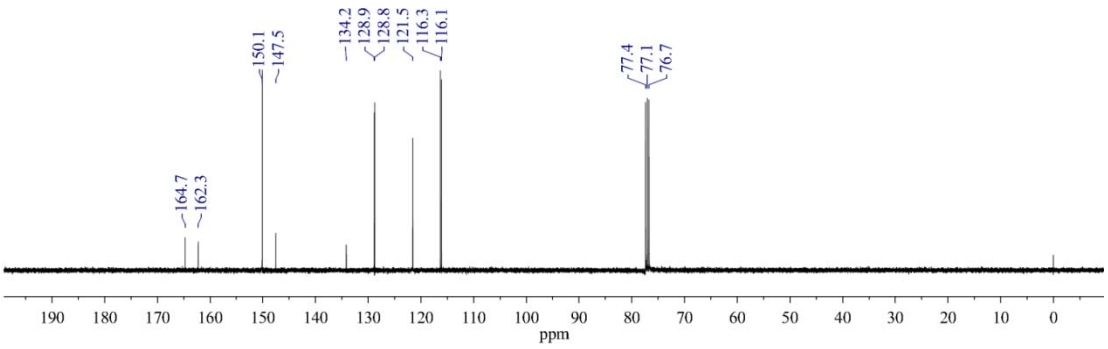
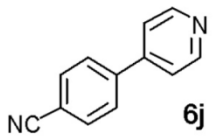
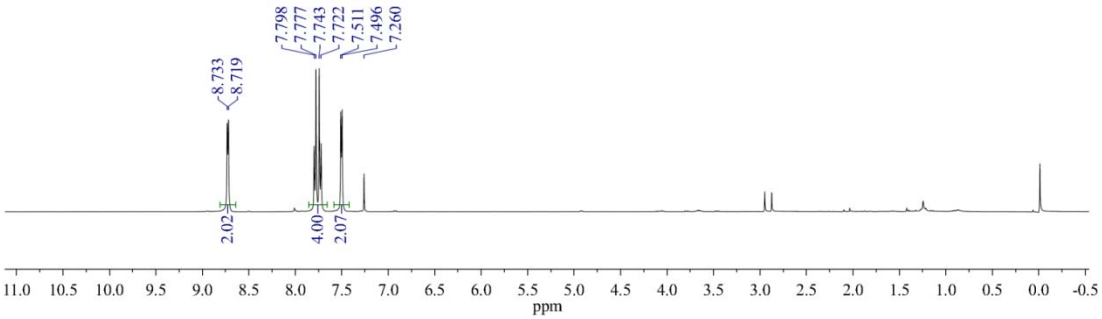
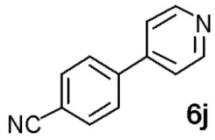


Figure S15. ^{1}H NMR, ^{13}C NMR spectra of 4-(pyridin-4-yl)-benzonitrile (**6j**)







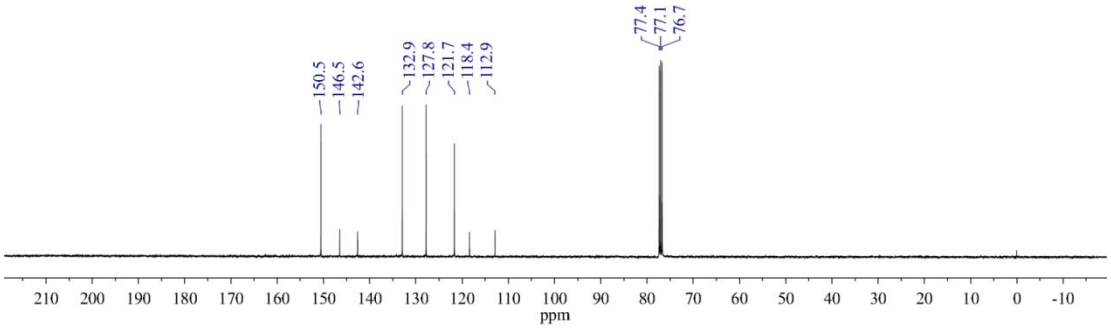
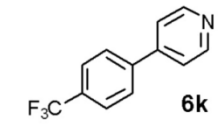
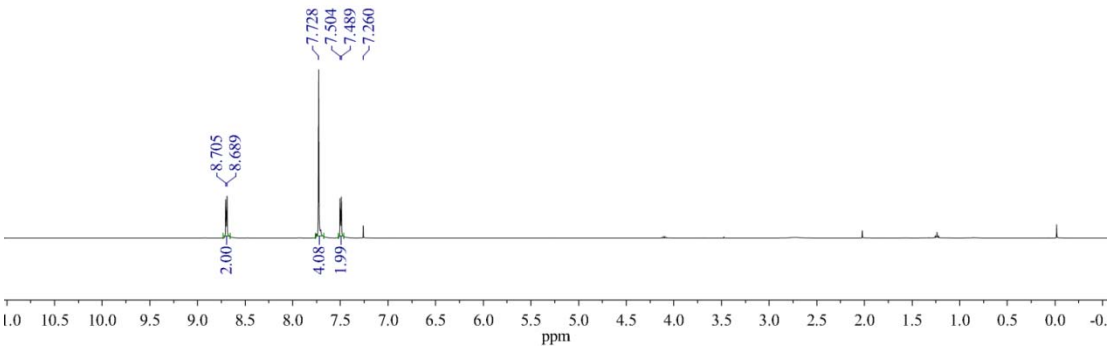
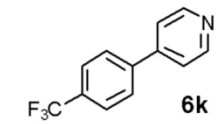


Figure S16. ^{1}H NMR, ^{13}C NMR spectra of 4-(4-trifluoromethylphenyl)-pyridine (**6k**)







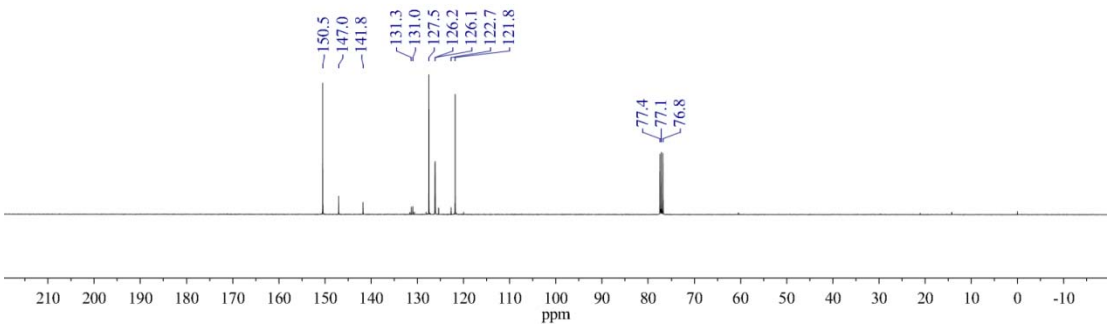
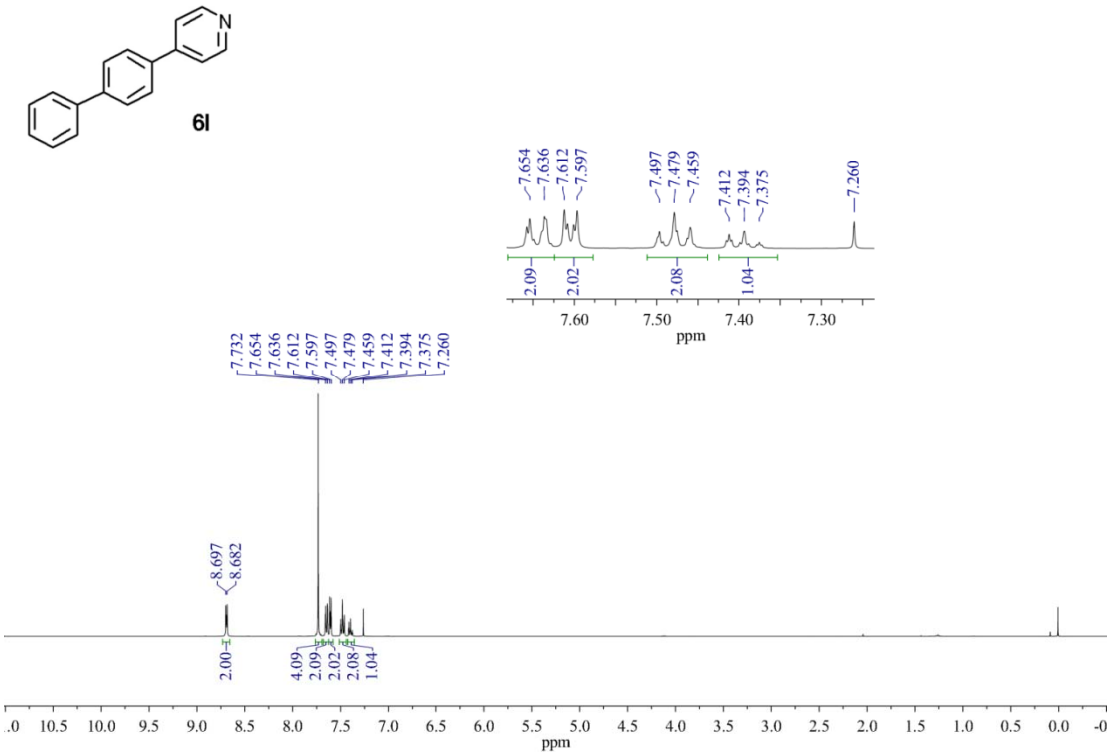


Figure S17. ^{1}H NMR, ^{13}C NMR spectra of 4-biphenyl-4-yl-pyridine (**6l**)



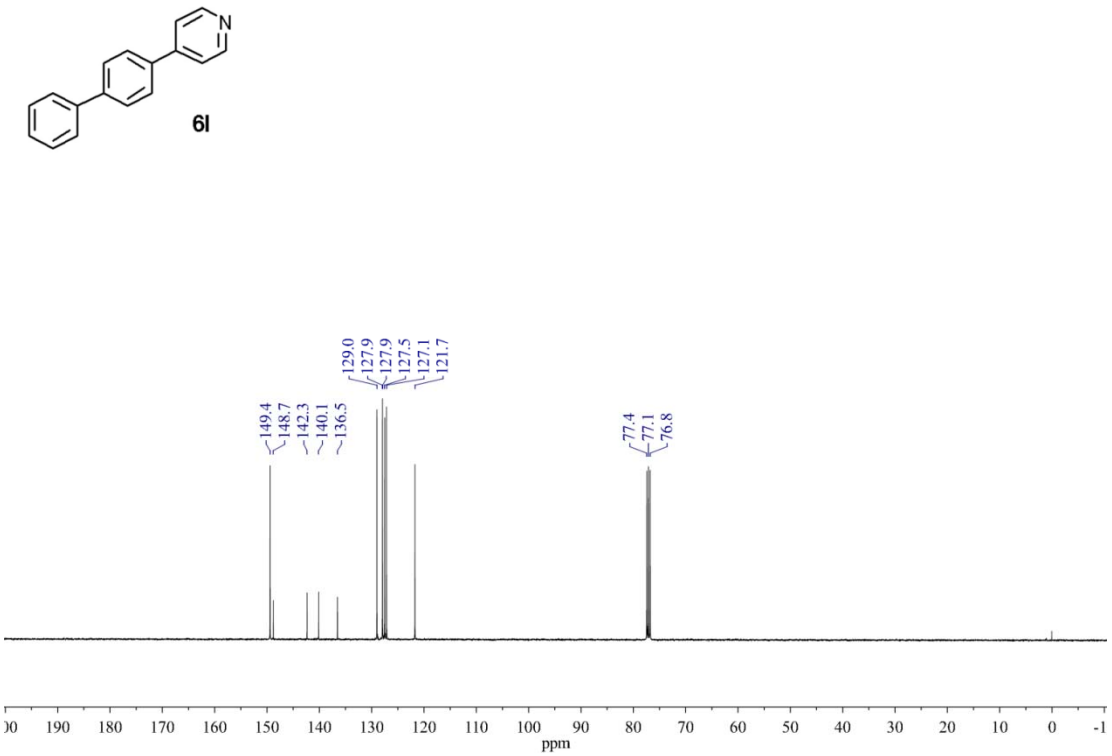
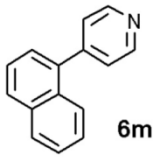
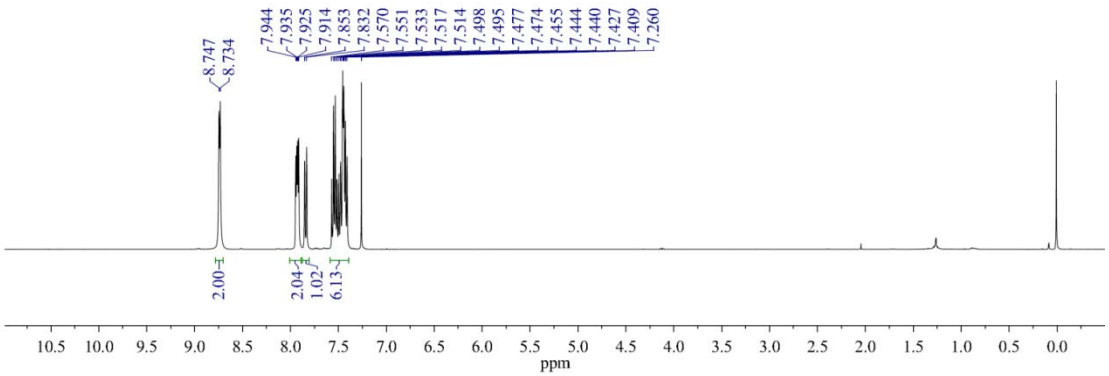
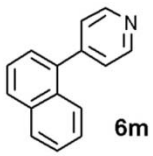


Figure S18. ^{1}H NMR, ^{13}C NMR spectra of 4-(naphthalen-1-yl)-pyridine (**6m**)







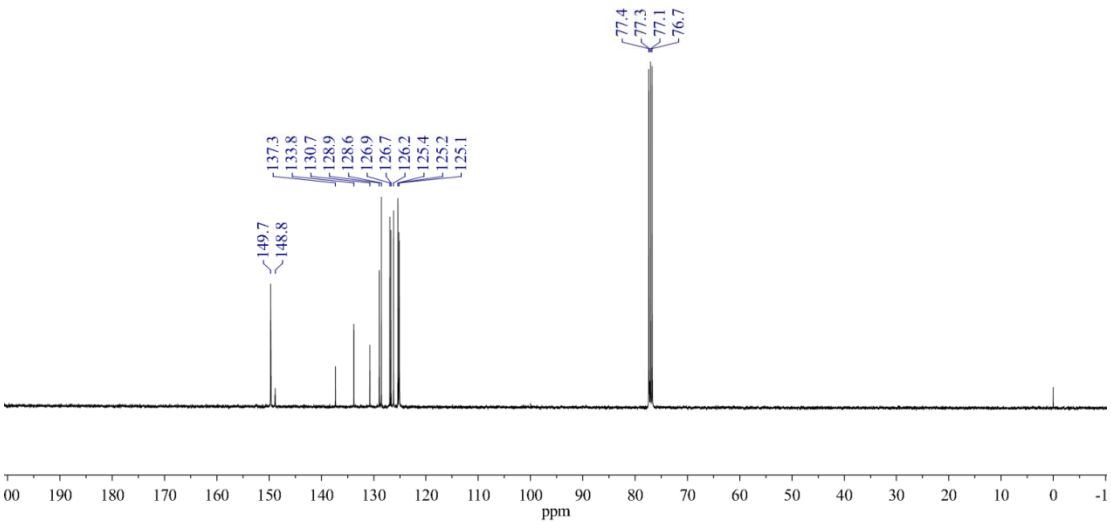


Figure S19. ^{1}H NMR, ^{13}C NMR spectra of 4-(naphthalen-2-yl)-pyridine (**6n**)