Electronic Supplementary Material (ESI) for New Journal of Chemistry.

Bimetallic Pd^{II} Complexes with NHC/Py/PCy_3 Donor Set Ligands: Applications in α-Arylation, Suzuki-Miyaura and Sonogashira Coupling Reactions

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Supporting Information

Index

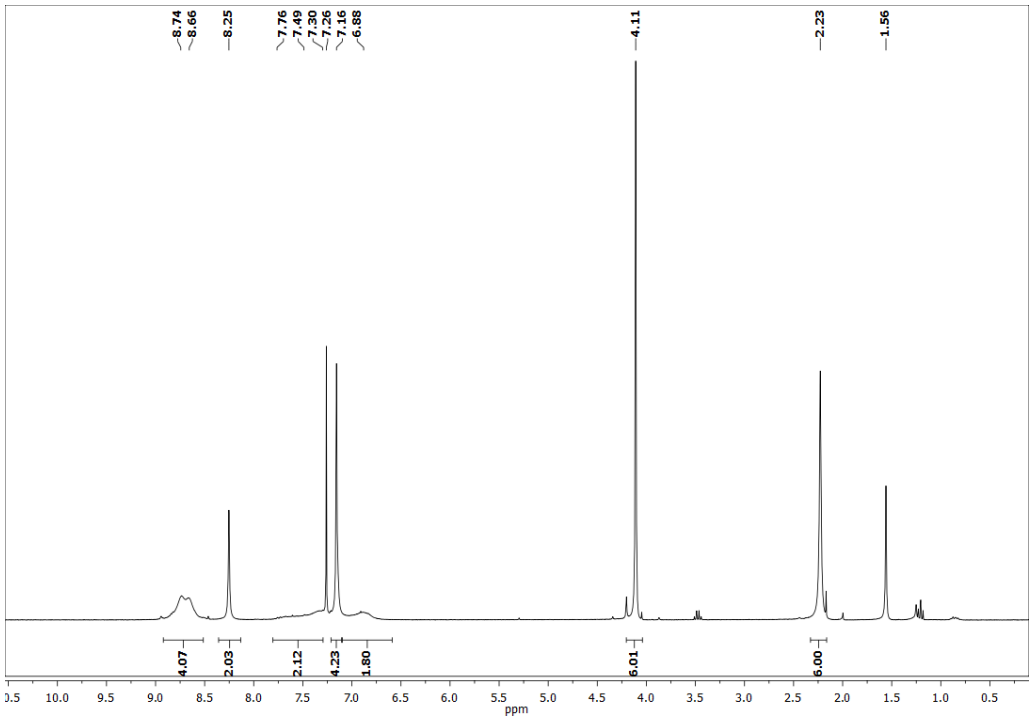


Figure S1. ^{1}H NMR spectrum of [**2**] in $CDCl_3$.

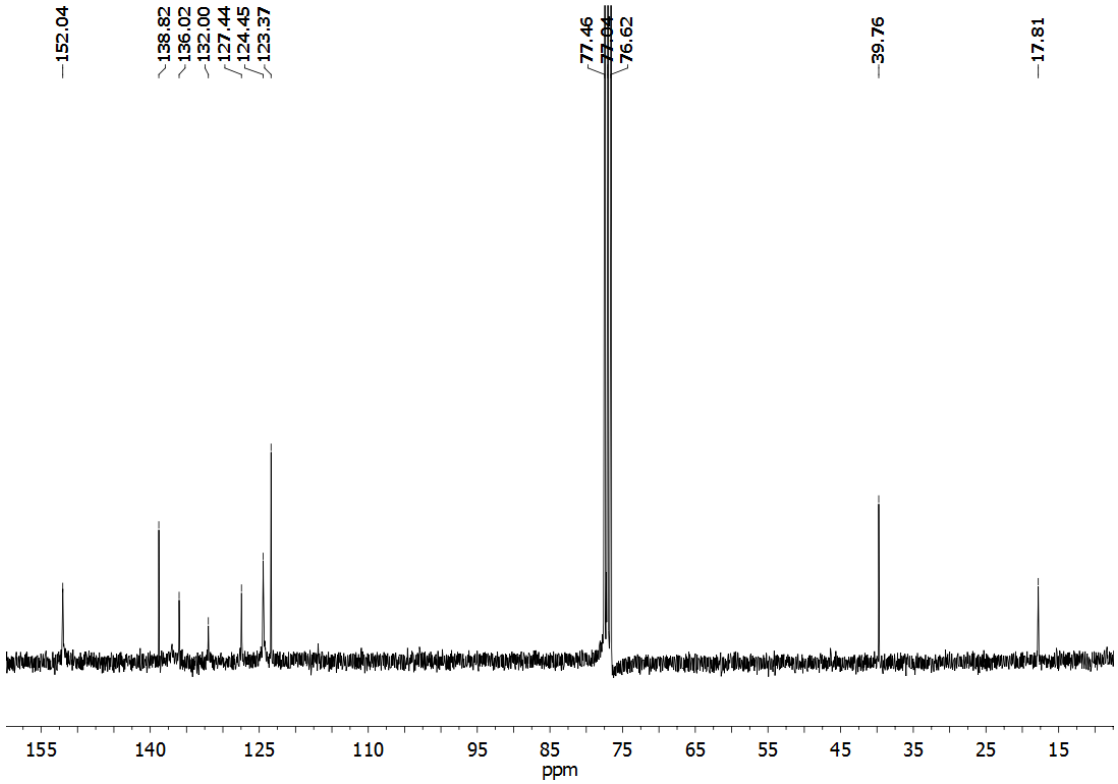


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of [**2**] in $CDCl_3$.

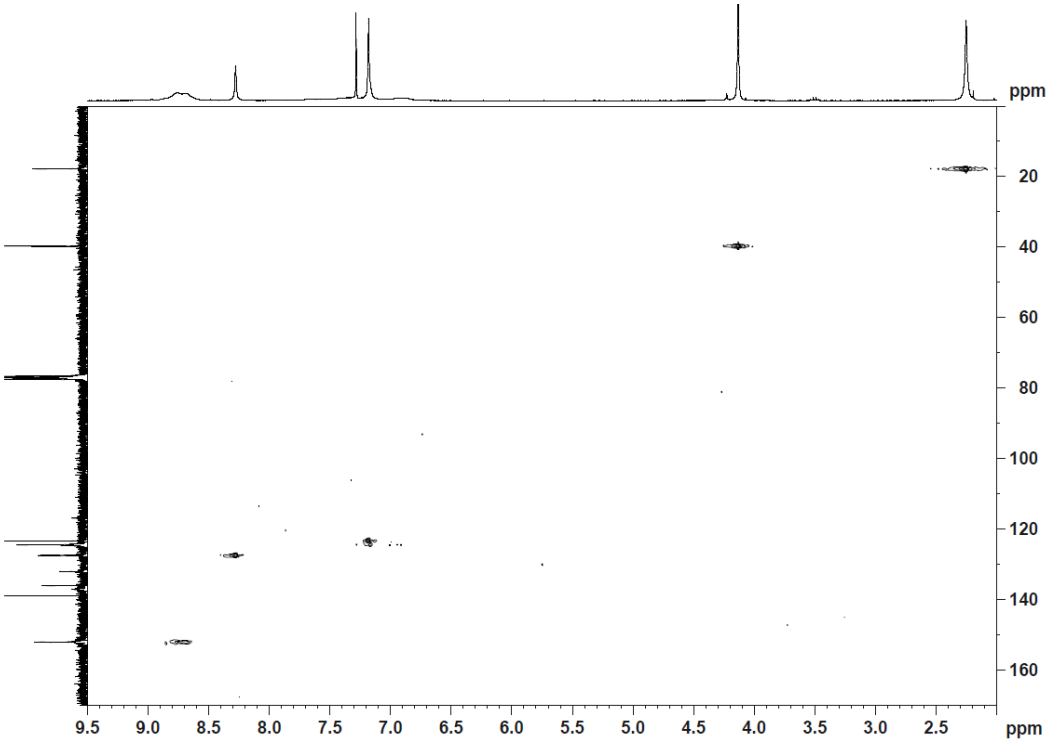


Figure S3. HSQC NMR spectrum of [**2**] in $CDCl_3$.

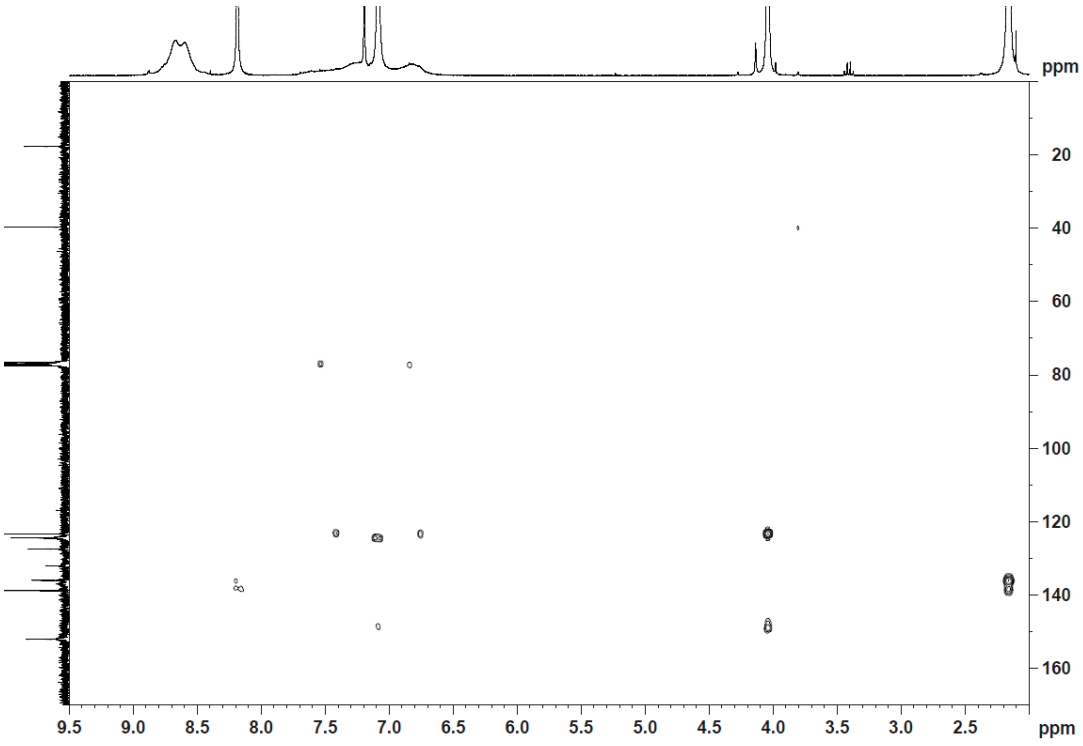


Figure S4. HMBC NMR spectrum of [**2**] in $CDCl_3$.

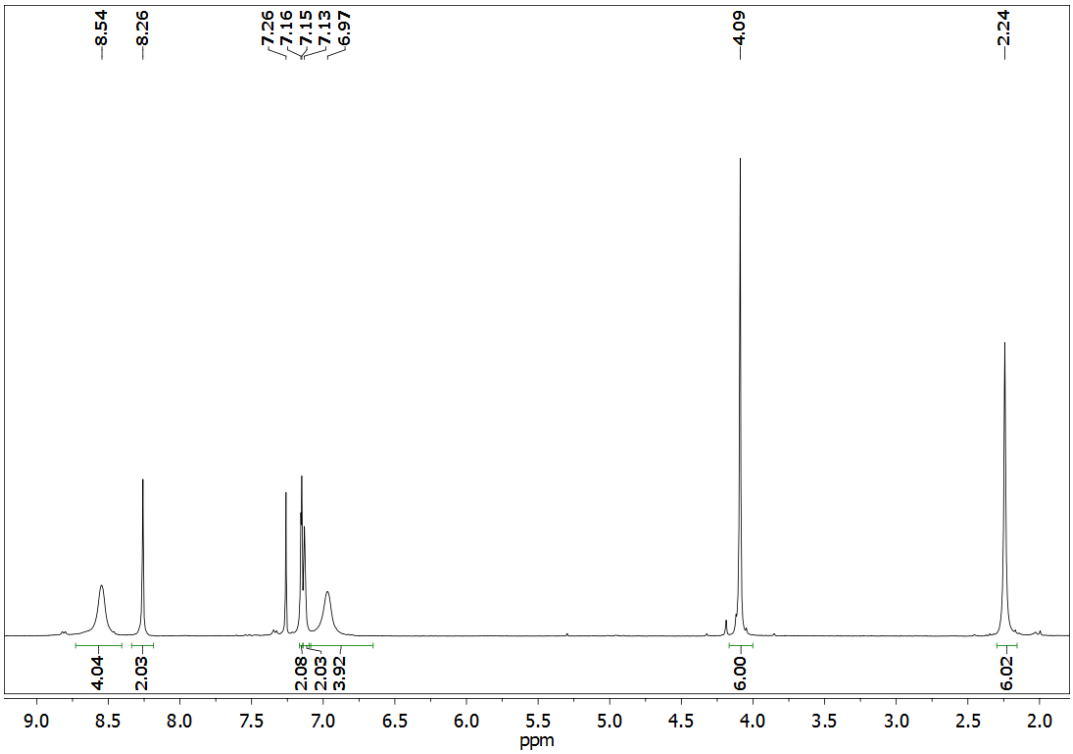


Figure S5. ^1H NMR spectrum of [**3**] in $CDCl_3$.

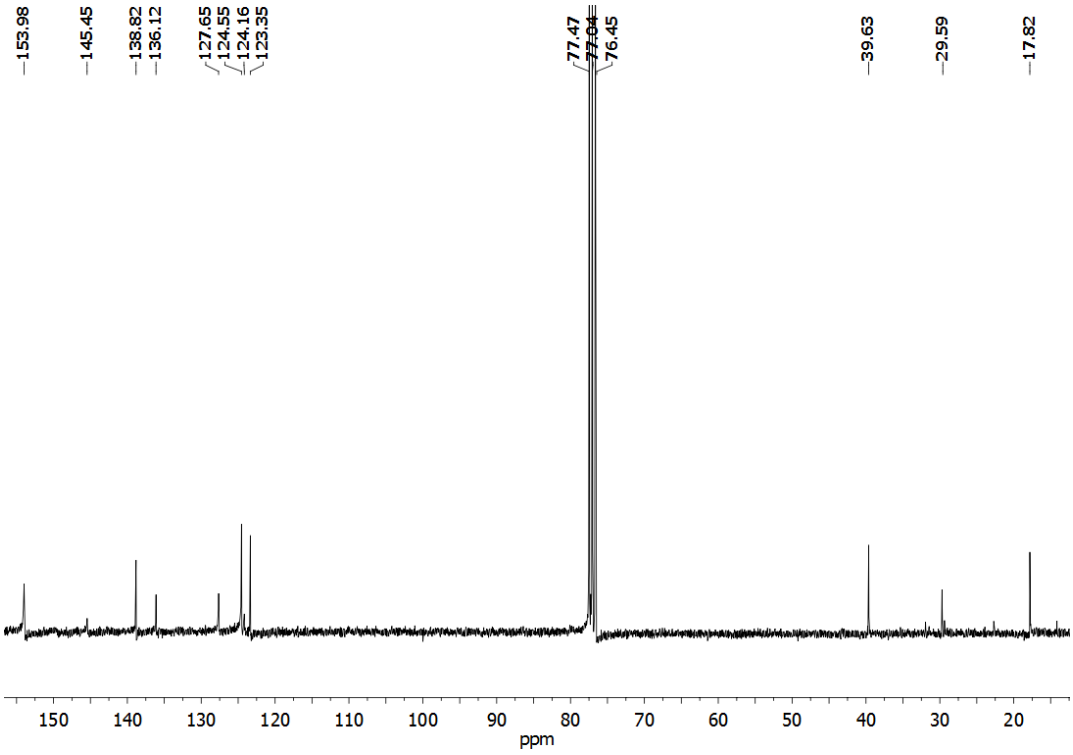


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of [**3**] in $CDCl_3$.

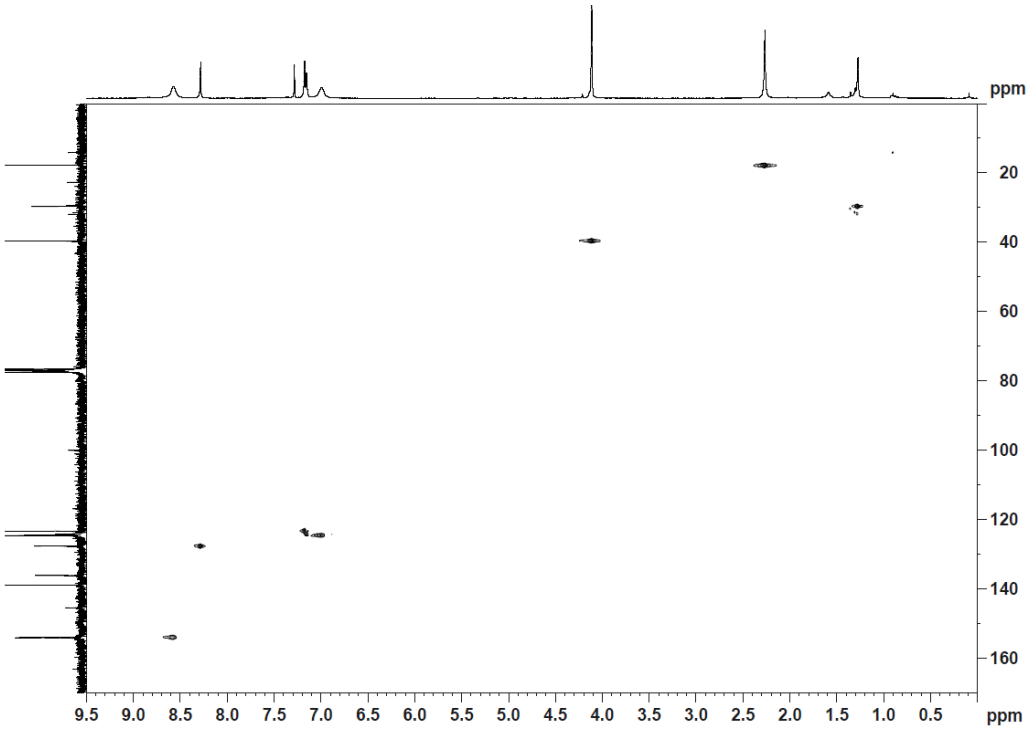


Figure S7. HSQC NMR spectrum of [**3**] in $CDCl_3$.

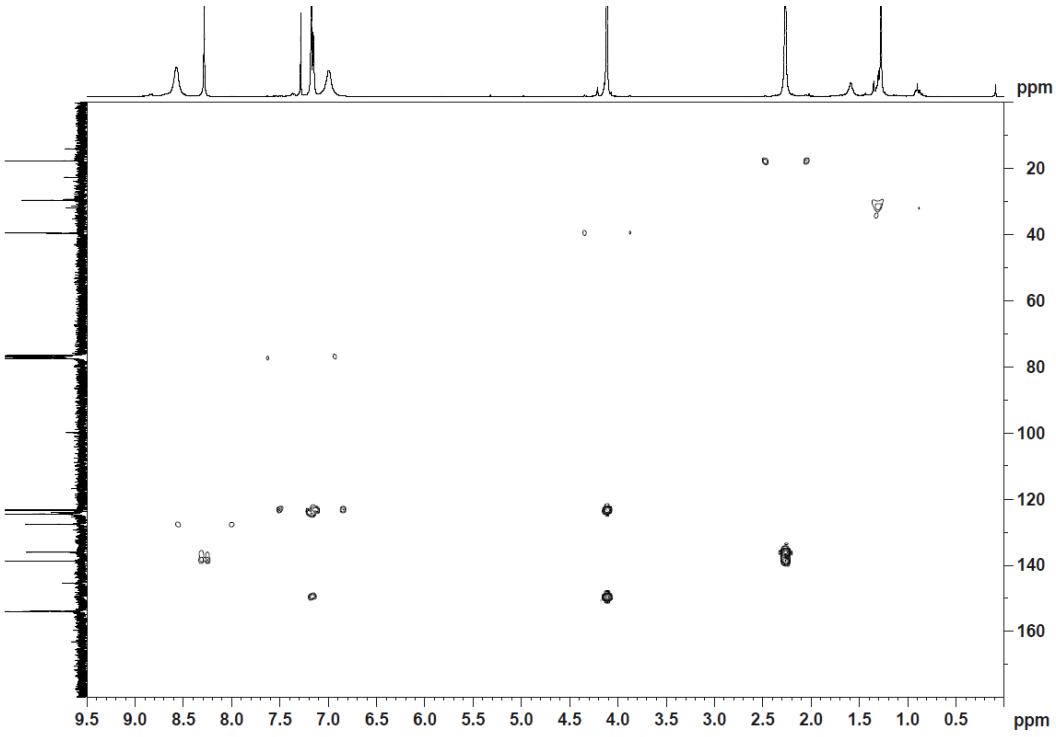


Figure S8. HMBC NMR spectrum of [**3**] in $CDCl_3$.

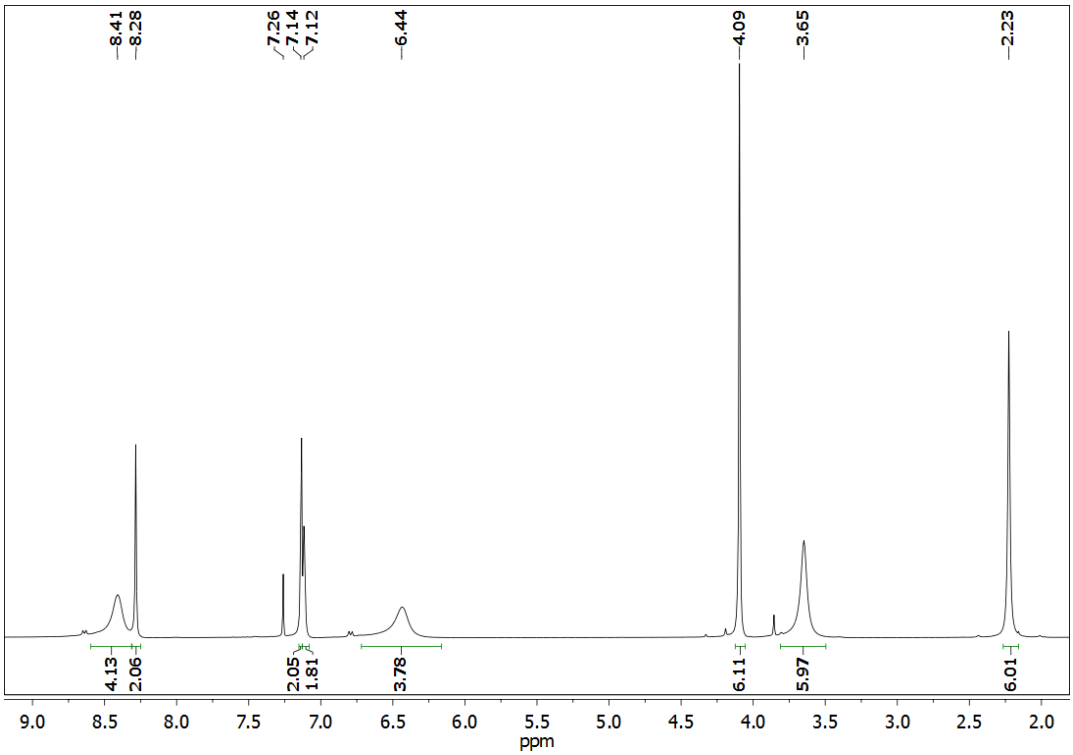


Figure S9. ^{1}H NMR spectrum of [**4**] in $CDCl_3$.

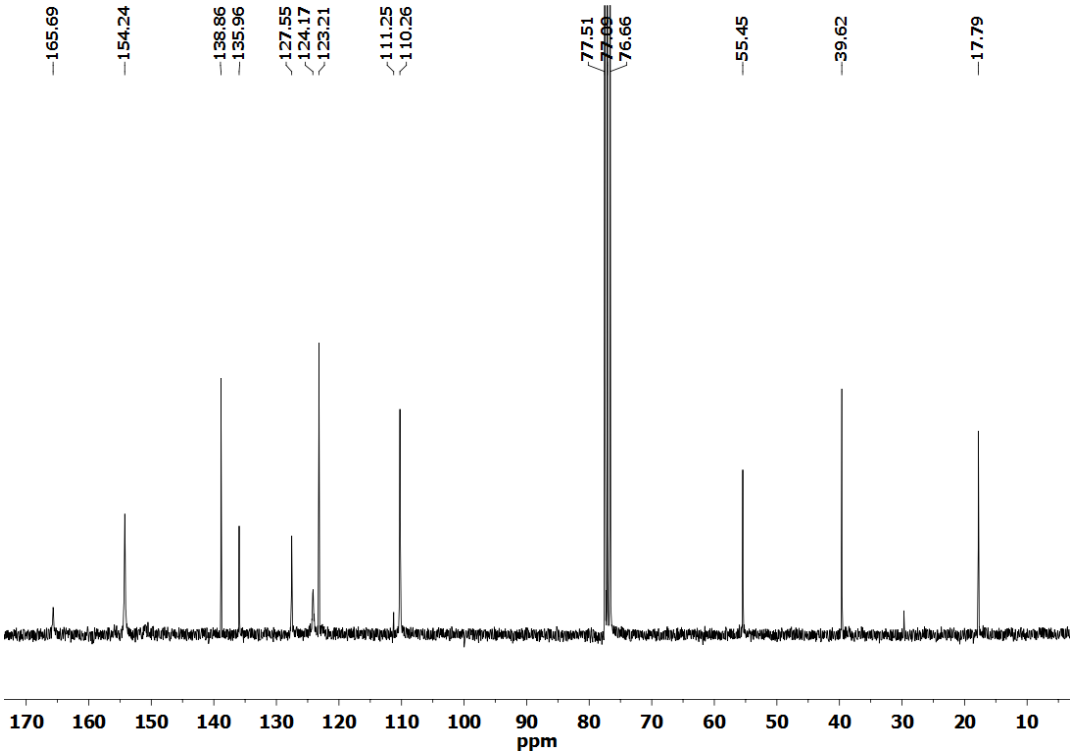


Figure S10. $^{13}C\{^{1}H\}$ NMR spectrum of [**4**] in $CDCl_3$.

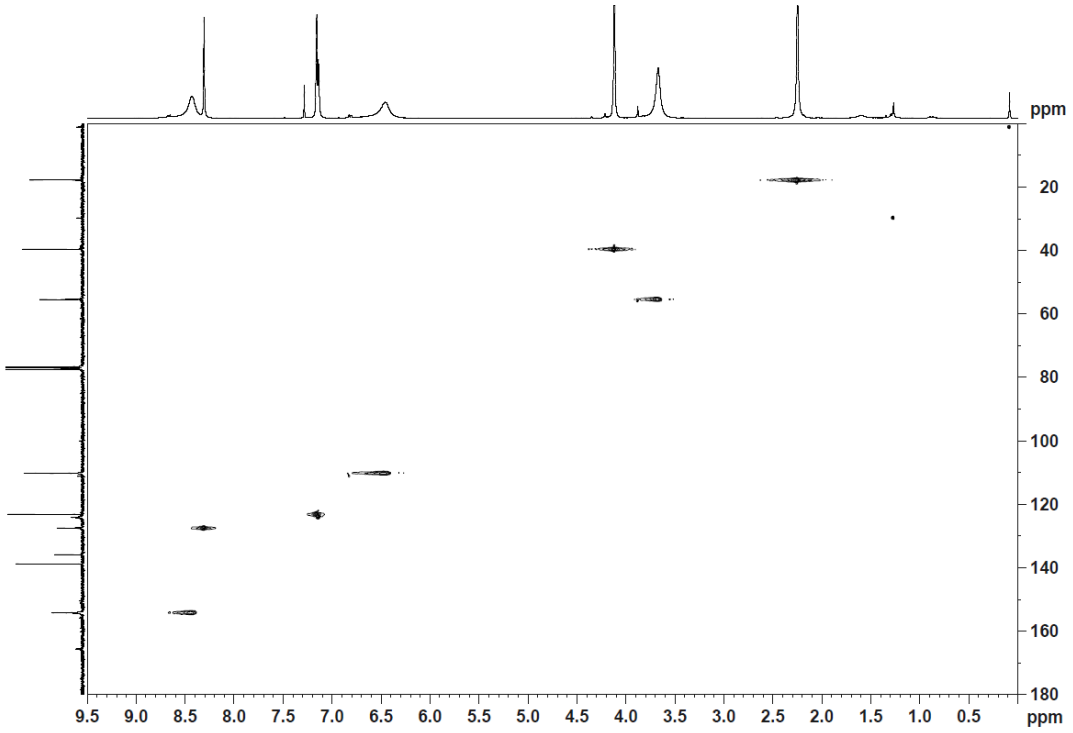


Figure S11. HMQC NMR spectrum of [**4**] in $CDCl_3$.

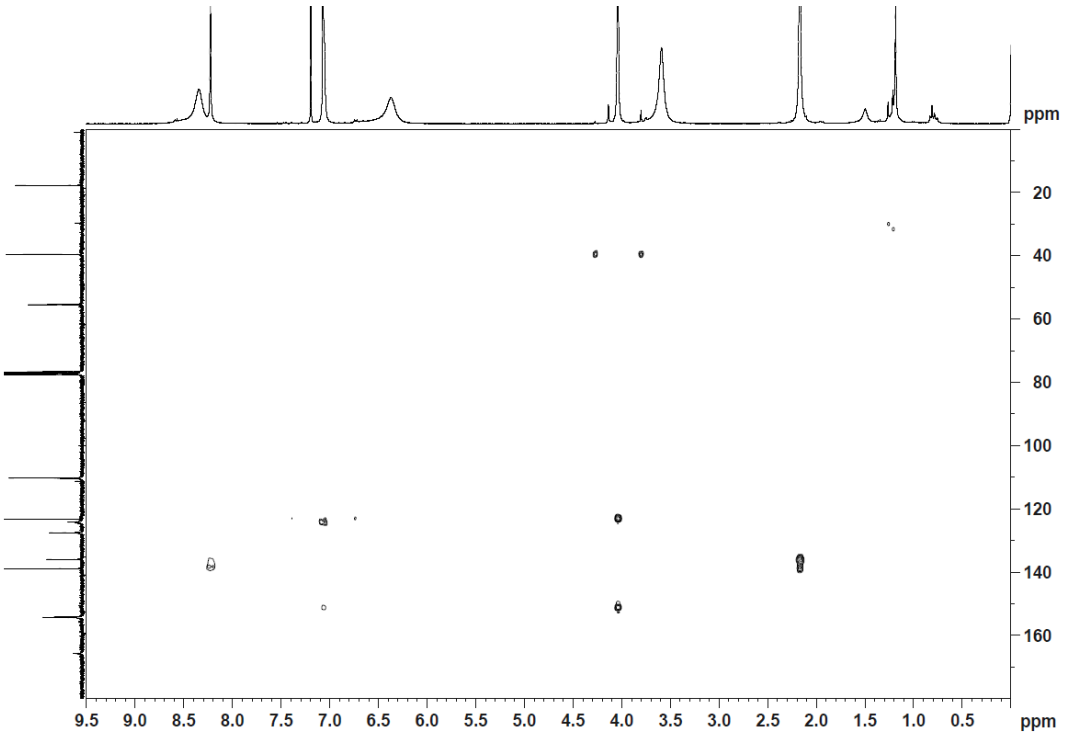


Figure S12. HMBC NMR spectrum of [**4**] in $CDCl_3$.

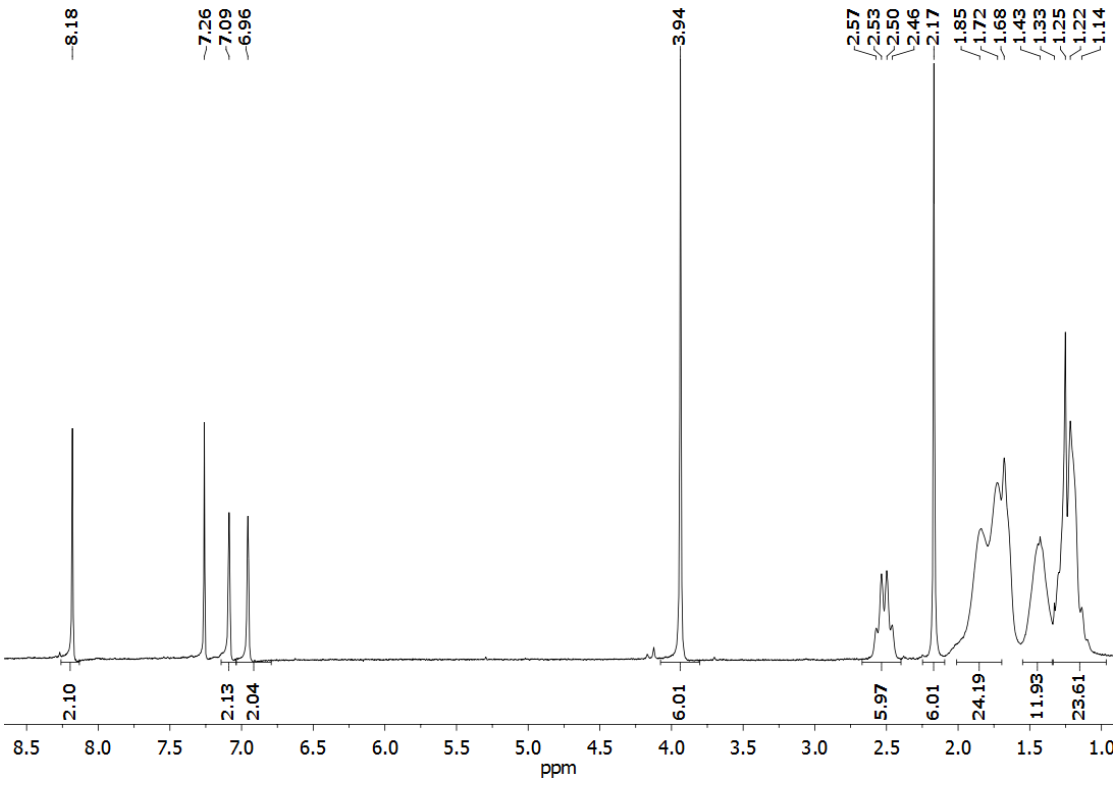


Figure S13. ^{1}H NMR spectrum of [**5**] in $CDCl_3$.

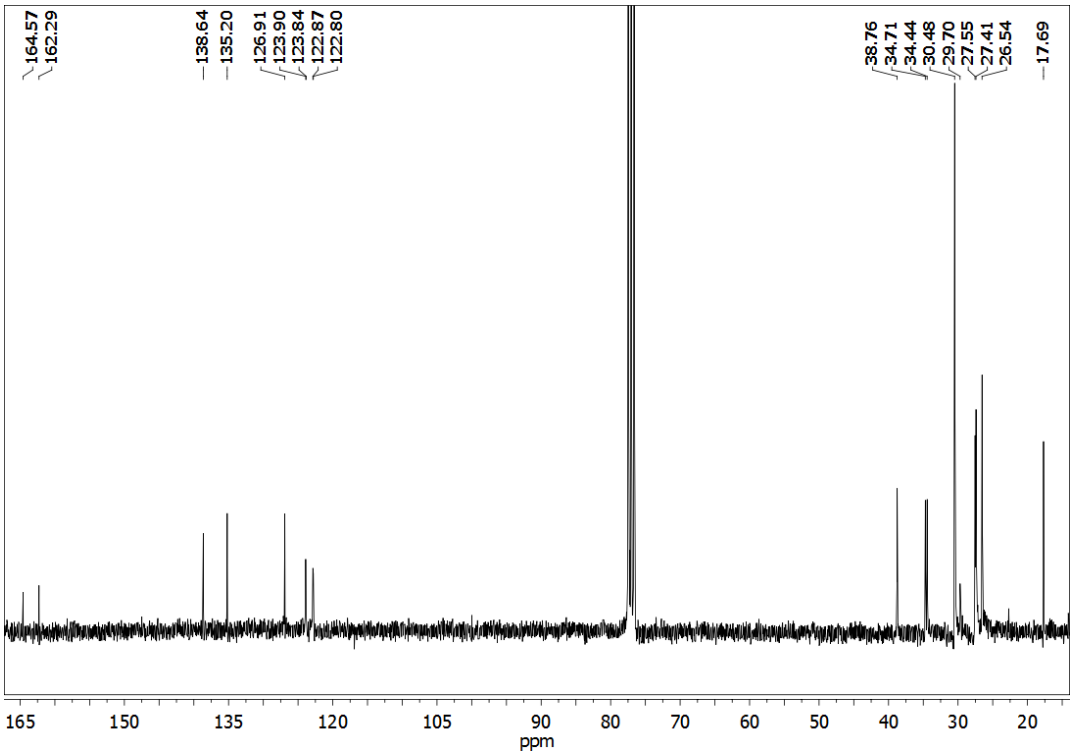


Figure S14. $^{31}P\{^{1}H\}$ NMR spectrum of [**5**] in $CDCl_3$.

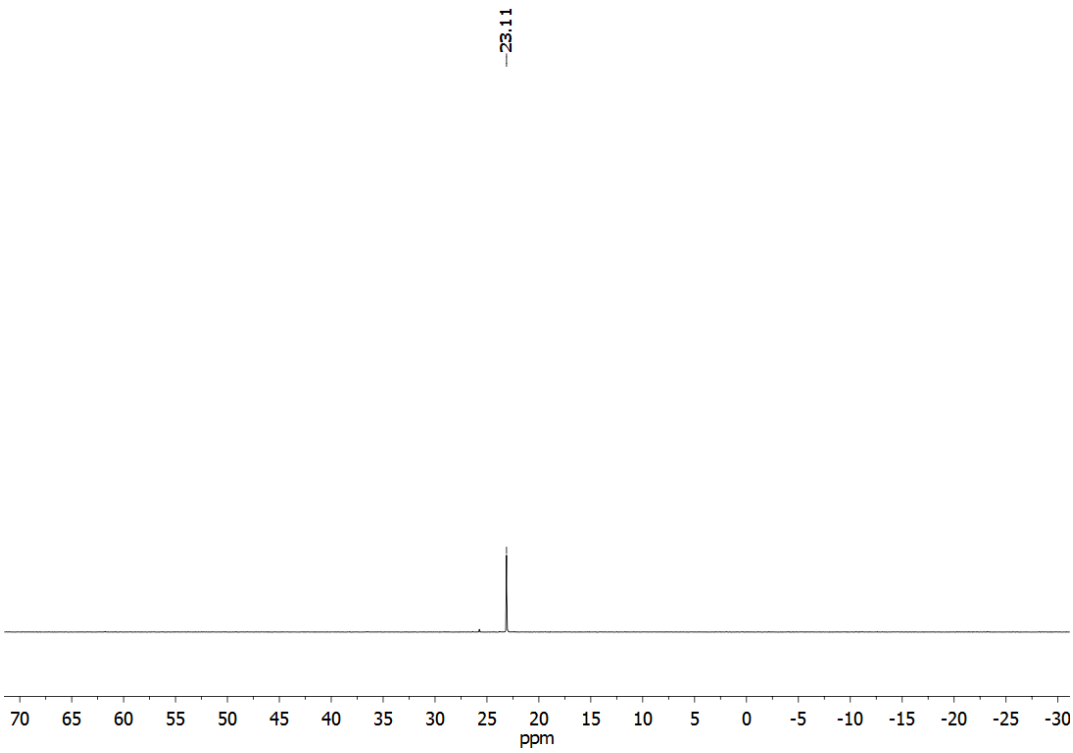


Figure S15. $^{31}P\{^{1}H\}$ NMR spectrum of [**5**] in $CDCl_3$.

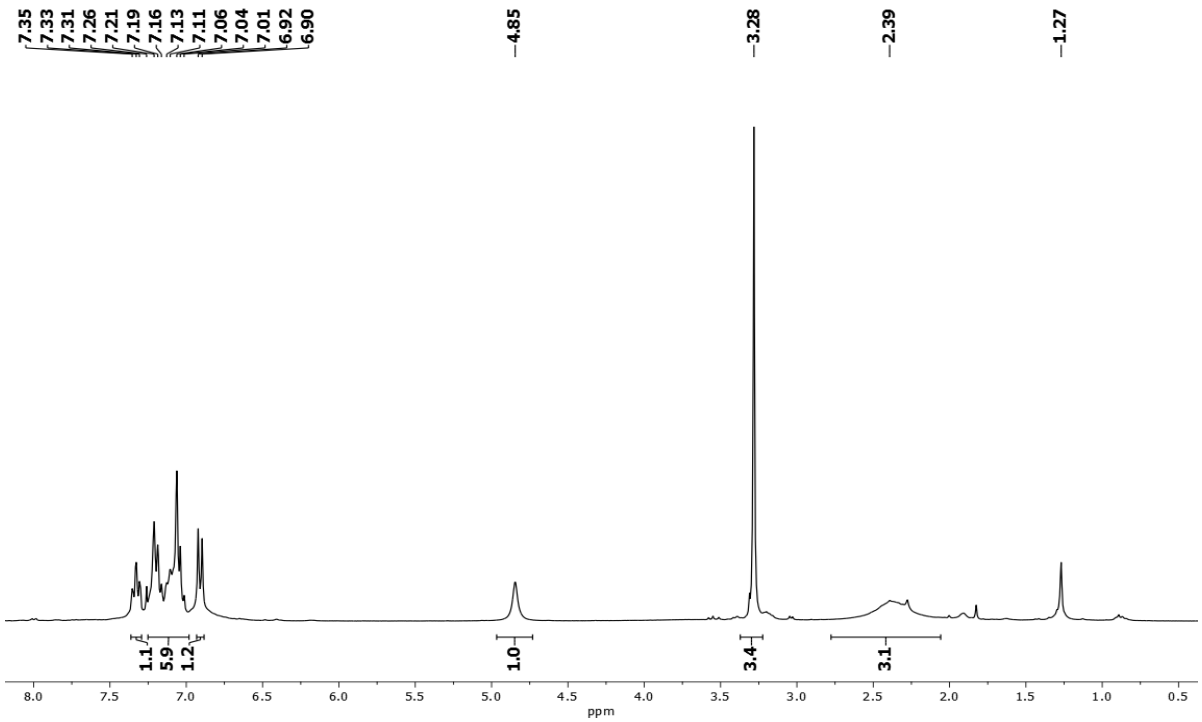


Figure S16. ^{1}H NMR spectrum of 1-methyl-3-(o-tolyl)indolin-2-one in $CDCl_3$.

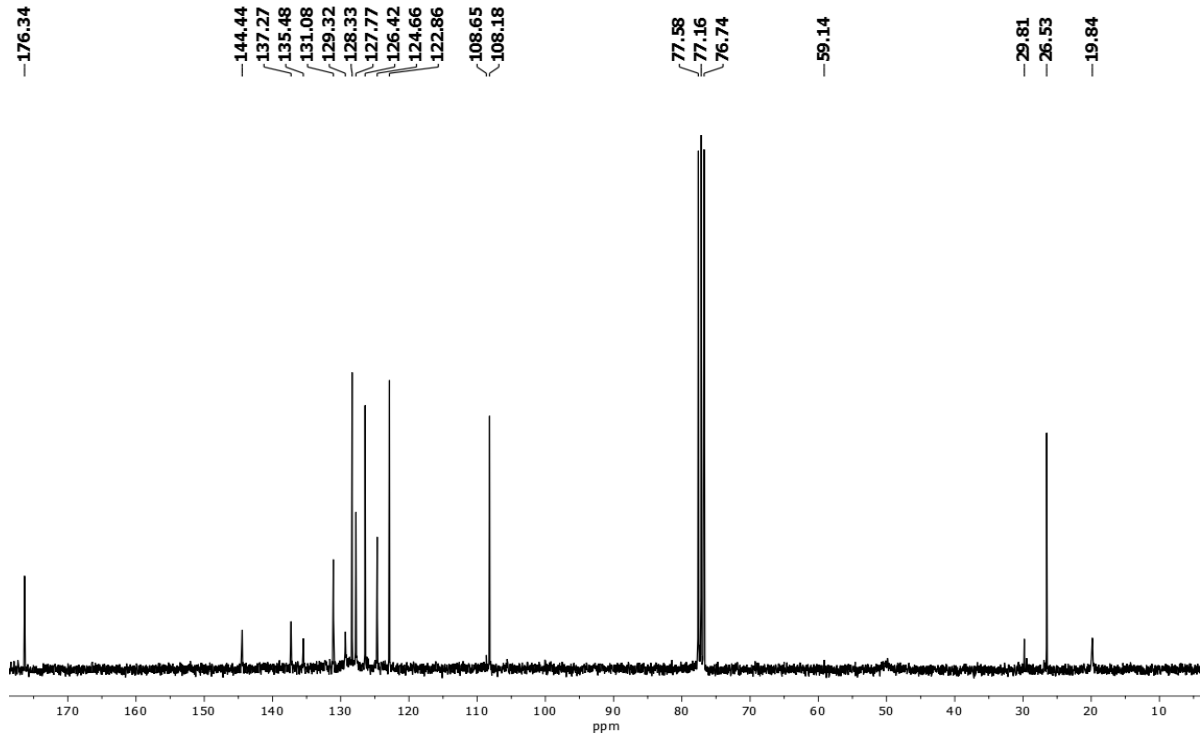


Figure S17. $^{13}C\{^{1}H\}$ NMR spectrum of 1-methyl-3-(o-tolyl)indolin-2-one in $CDCl_3$.

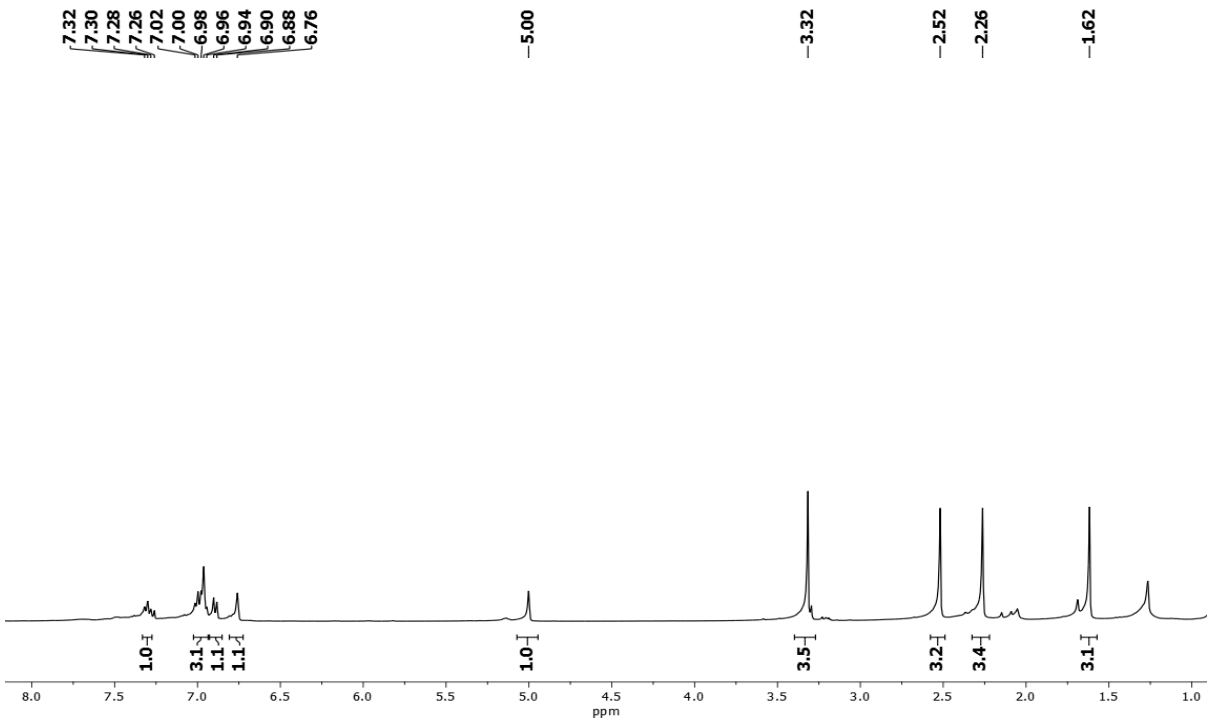


Figure S18. ^{1}H NMR spectrum of 3-mesityl-1-methylindolin-2-one in $CDCl_3$.

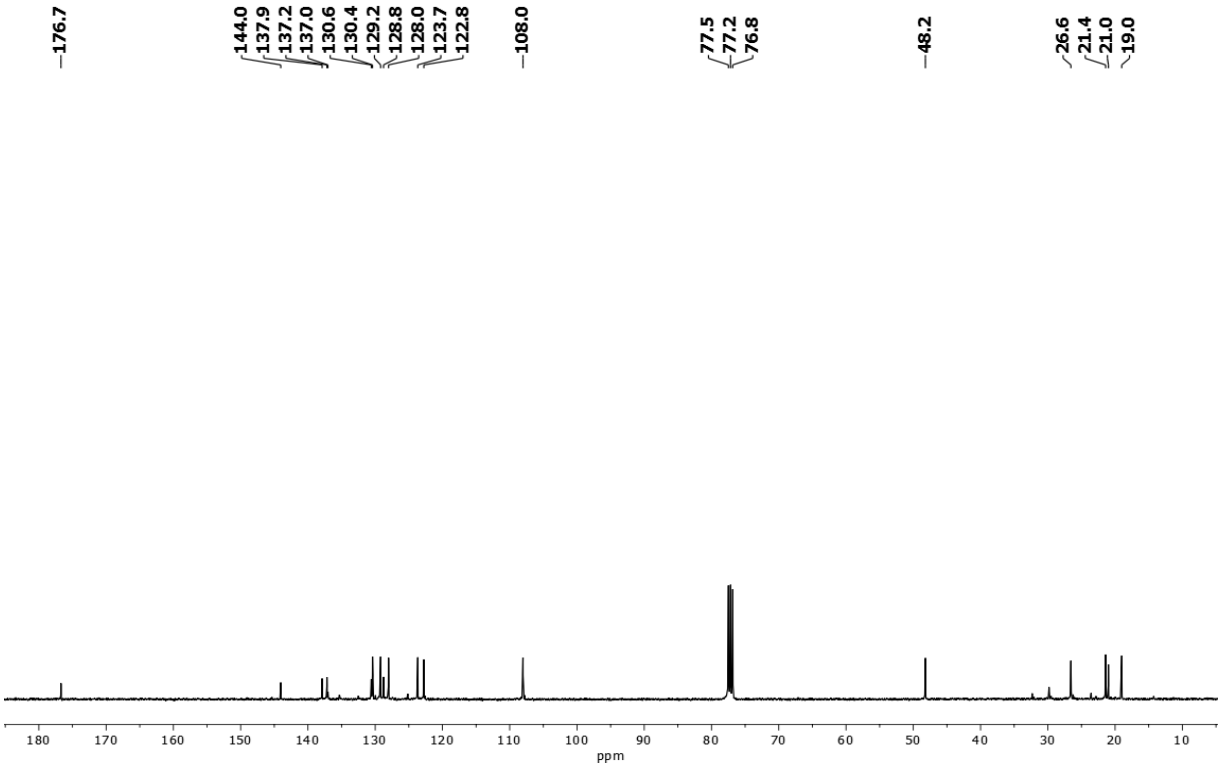


Figure S19. $^{13}C\{^{1}H\}$ NMR spectrum of 3-mesityl-1-methylindolin-2-one in $CDCl_3$.

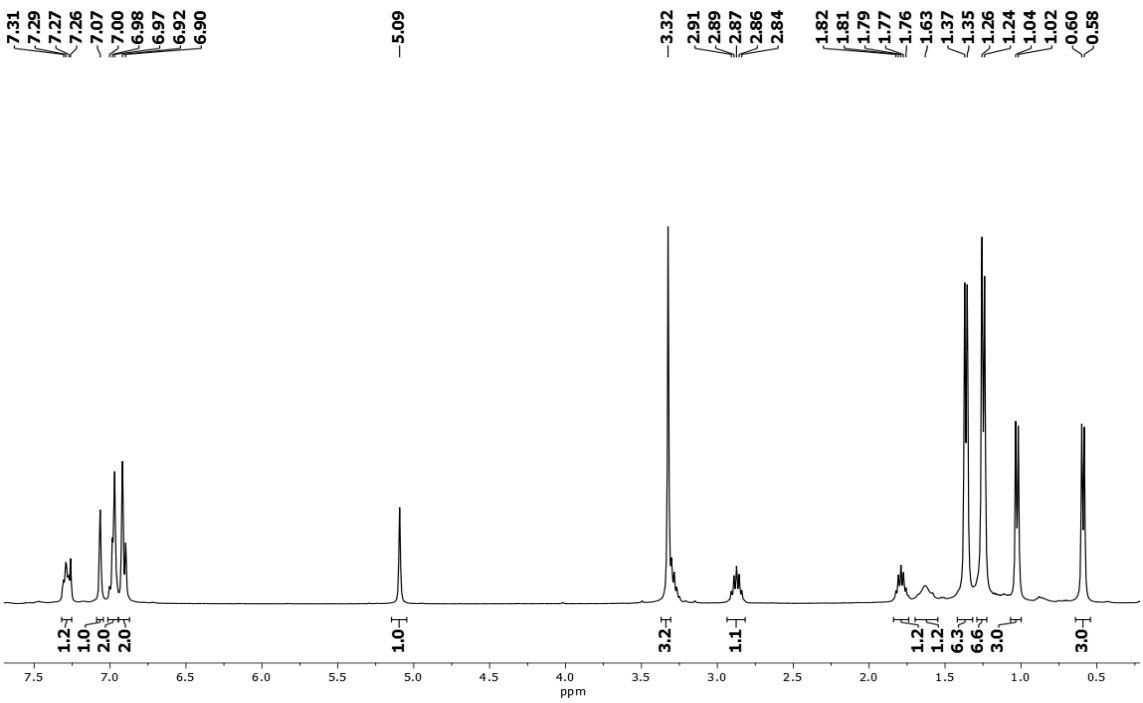


Figure S20. ^{1}H NMR spectrum of 1-methyl-3-(2,4,6-triisopropylphenyl)indolin-2-one in $CDCl_3$.

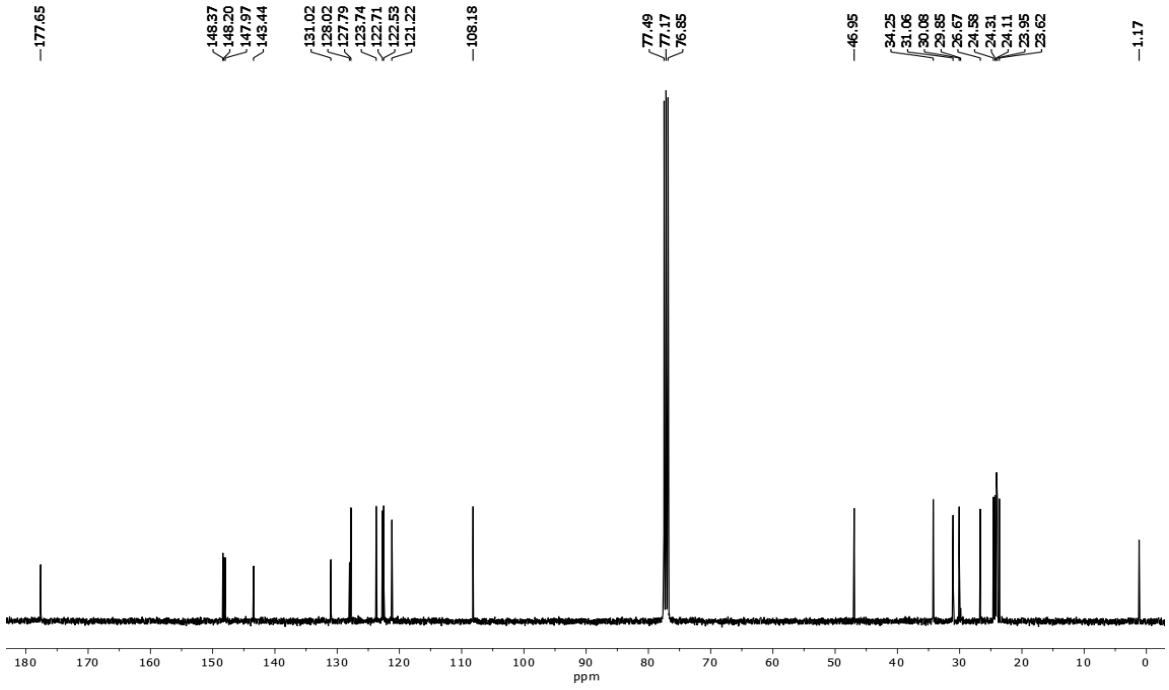


Figure S21. $^{13}C\{^{1}H\}$ NMR spectrum of 1-methyl-3-(2,4,6-triisopropylphenyl)indolin-2-one in $CDCl_3$.

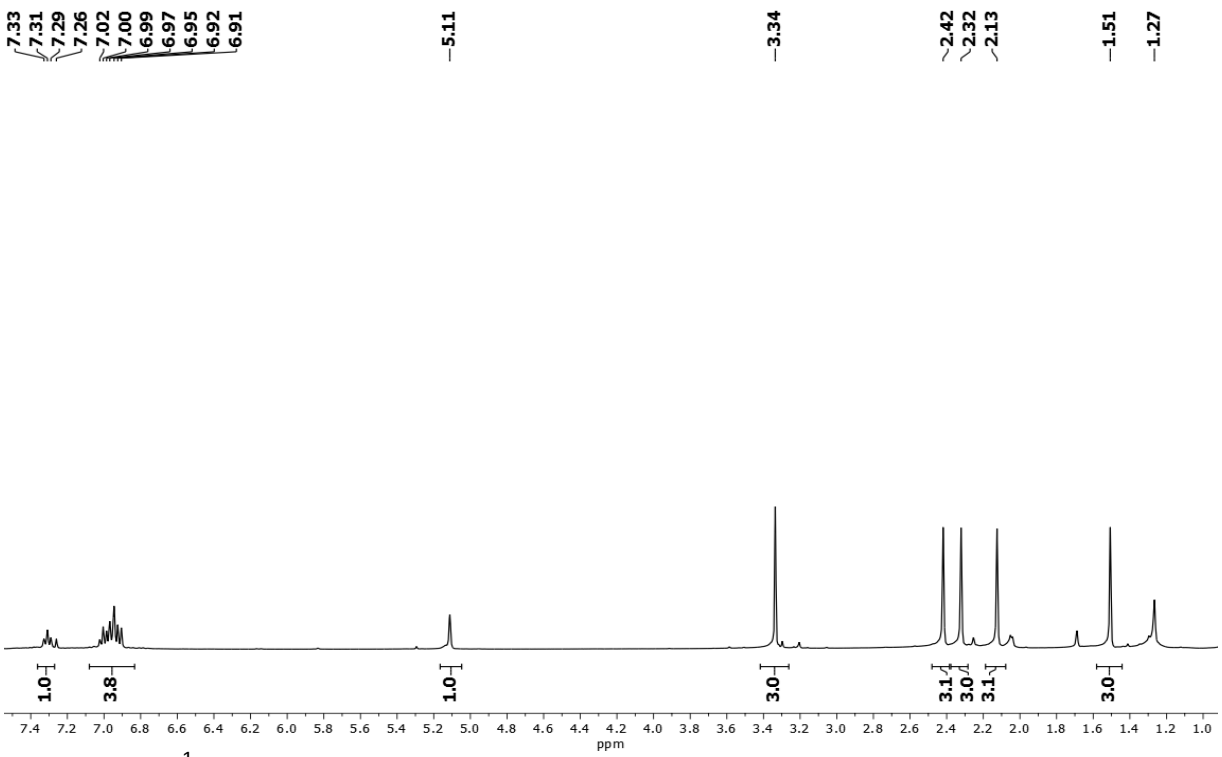


Figure S22. ^{1}H NMR spectrum of 1-methyl-3-(2,3,5,6-tetramethylphenyl)indolin-2-one in $CDCl_3$.

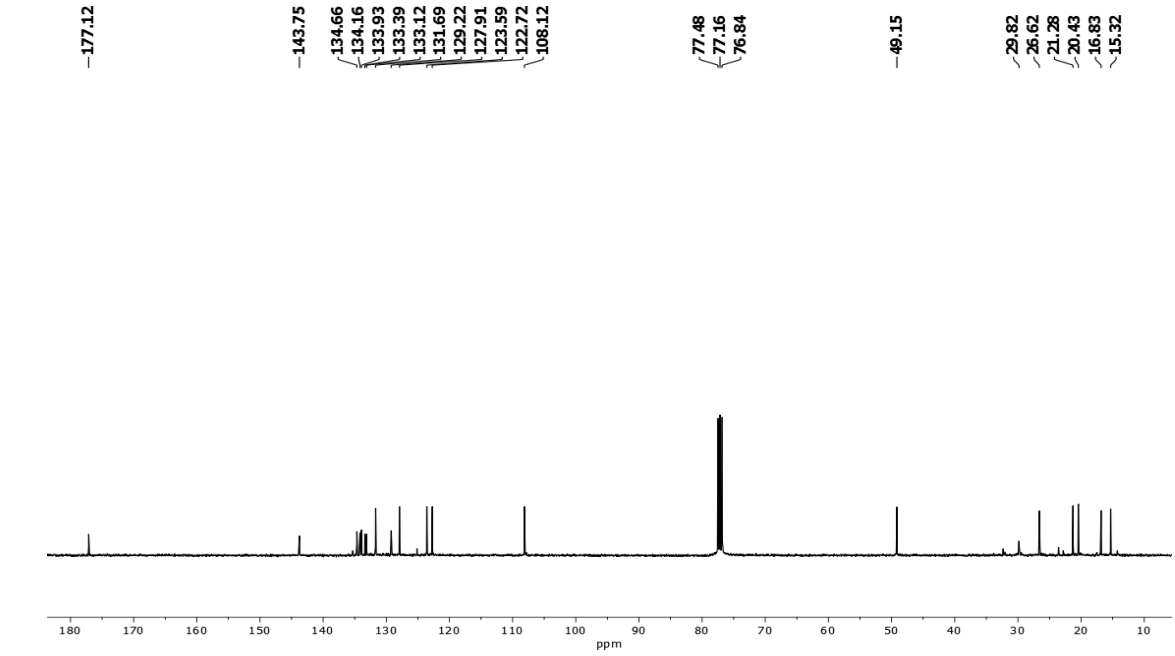


Figure S23. $^{13}C\{^{1}H\}$ NMR spectrum of 1-methyl-3-(2,3,5,6-tetramethylphenyl)indolin-2-one in $CDCl_3$.

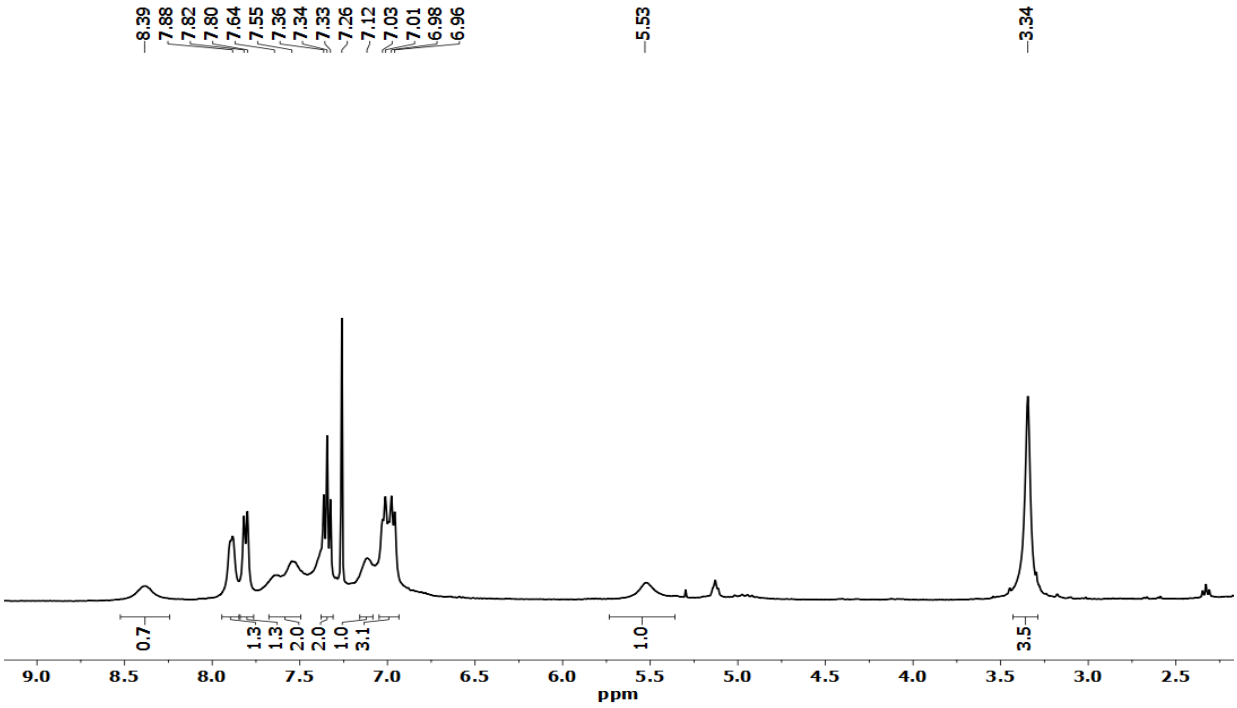


Figure S24. ^{1}H NMR spectrum of 1-methyl-3-(naphthalen-1-yl)indolin-2-one in $CDCl_3$.

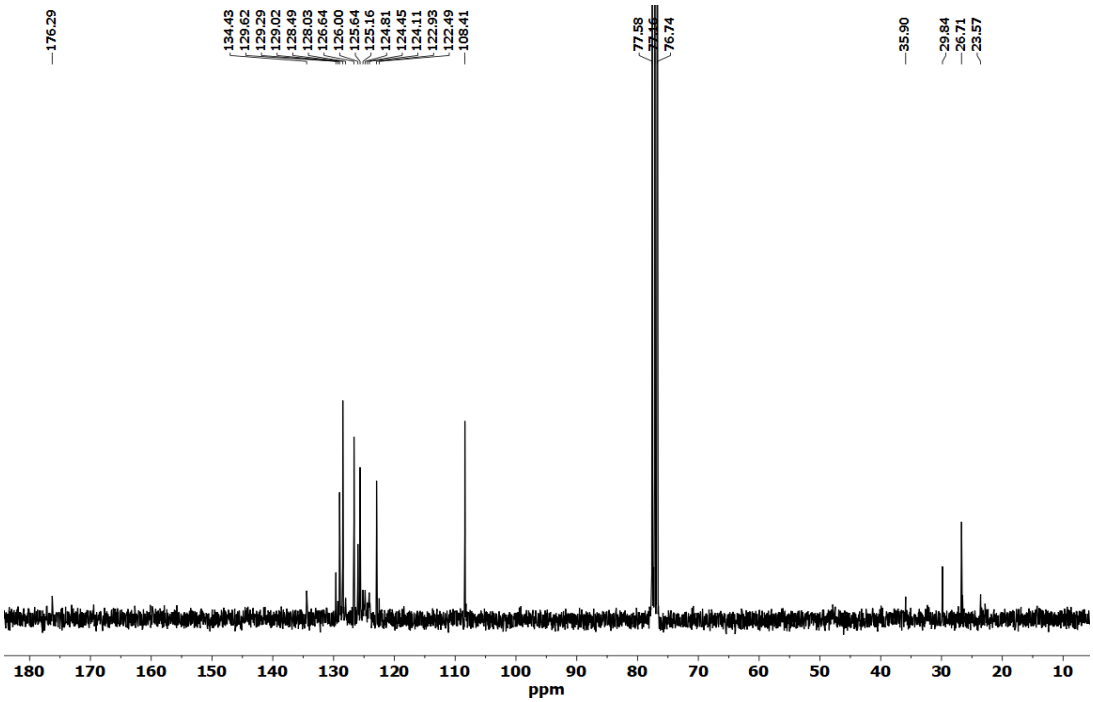


Figure S25. $^{13}C\{^{1}H\}$ NMR spectrum of 1-methyl-3-(naphthalen-1-yl)indolin-2-one in $CDCl_3$.

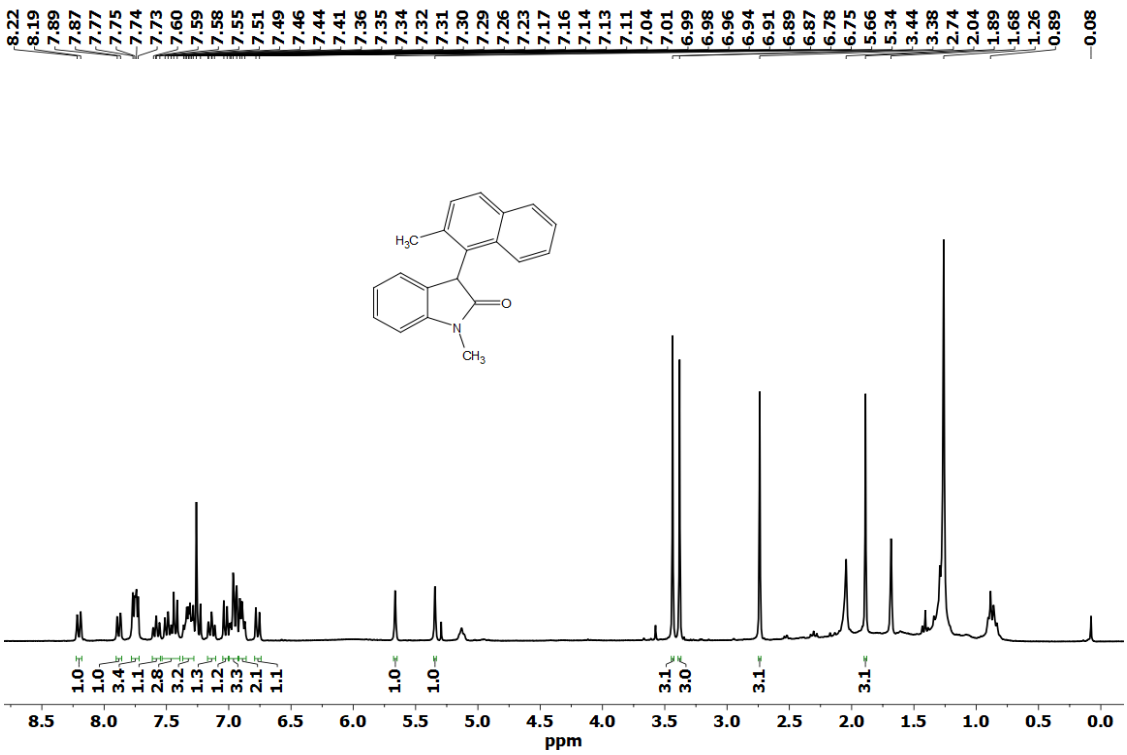


Figure S26. ^{1}H NMR spectrum of 1-methyl-3-(2-methylnaphthalen-1-yl)indolin-2-one in $CDCl_3$.

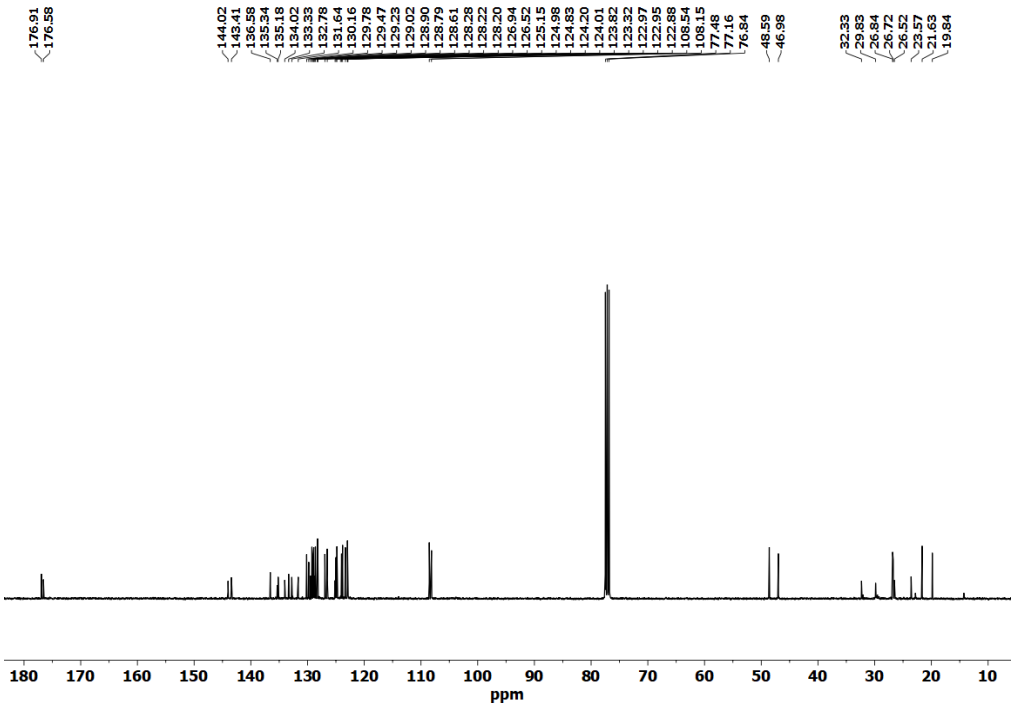


Figure S27. $^{13}C\{^{1}H\}$ NMR spectrum of 1-methyl-3-(2-methylnaphthalen-1-yl)indolin-2-one in $CDCl_3$.

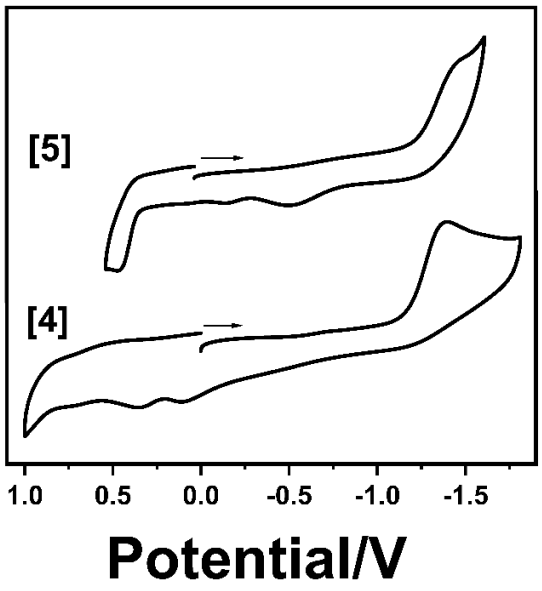


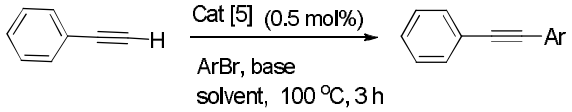
Figure S28. Cyclic voltammograms of the complexes [**4**] and [**5**] in DMF–0.1 M Bu_4NClO_4 at 298 K. Scan rate: 100 mV s−1.

Table S1. Electrochemical data from cyclic voltammetry[a]

complex	E^{red1} / V[b]	E^{ox1} / V[b]	E^{ox2} / V[b]	E^{ox3} / V[b]
[**4**]	-1.38	0.09	0.35	-
[**5**]	-1.53	-0.51	-0.14	0.46

[a] Cyclic voltammograms of the complexes in DMF–0.1 M Bu_4NClO_4 at 298 K. Scan rate: 100 mV s−1.

Table S2. Solvent screening for catalytic copper-free Sonogashira coupling reaction.



Entry	ArBr	Solvent	Base	CuI (2 mol%)	yield (%)
1	4-Bromoacetophenone	DMF	Cs_2CO_3	-	20
2	4-Bromoacetophenone	DMF	Cs_2CO_3	CuI	42
3	4-Bromoacetophenone	DMF	KO*t*Bu	CuI	53
4	4-Bromoacetophenone	Toluene	KO*t*Bu	-	0
5	4-Bromoacetophenone	ACN	KO*t*Bu	-	0
6	4-Bromoacetophenone	DMF	KO*t*Bu	-	84

Table S3. Crystallographic details

	[**4**]
Chemical formula	$C_{28}H_{32}I_4N_6O_2Pd_2$
M_r	1204.99
Crystal system Space group	Monoclinic *P21/n*
a (Å) b (Å) c (Å) α (°) β (°) γ (°)	9.3535(8) 23.046(2) 17.3965(15) 90 102.035(4) 90
V (Å^3)	3667.6(6)
Z	4
Densitiy (g cm^{-3})	2.182
F(000)	2248.0
Radiation Type	CuK_α
μ (mm^{-1})	34.615
Crystal size	0.4 x 0.15 x 0.12
Meas. Refl.	50546
Indep. Refl.	6032
Obsvd. [$I > 2\sigma(I)$] refl.	6391
R_{int}	0.1091
R [$F^2 > 2\sigma(F^2)$] wR(F^2) S	0.0678 0.1807 1.293
$\Delta\rho_{max}$ (e Å^{-3}) $\Delta\rho_{min}$ (e Å^{-3})	1.57 -2.90

Table S4. Selected bond lengths in Å

Atoms	[3]
Pd1 – I1	2.6225(11)
Pd1 – I2	2.6025(11)
Pd2 – I3	2.6046(9)
Pd2 – I4	2.5952(10)
Pd1 – C1	1.950(11)
Pd2 – C14	1.968(11)
Pd1–N3	2.088(9)
Pd2–N6	2.079(9)
N1– C1	1.336(14)
N2– C1	1.365(14)
N4– C14	1.333(14)
N5– C14	1.345(13)
C2– C3	1.339(18)
C12– C13	1.338(16)

Table S5. Selected bond angles in °

Atoms	[3]
I1–Pd1–C1	87.2(3)
I2–Pd1–C1	87.7(3)
I1–Pd1–I2	171.43(4)
I3–Pd2–C14	89.4(3)
I3–Pd2–I4	173.62(4)
N3–Pd1–C1	177.8(4)
N6–Pd2–C14	175.8(4)
N1–C1–N2	105.4(9)
N4–C14–N5	105.3(9)