Supporting Information

Naphthalene-Based Heterobimetallic Triazolylidene Ir^{III}/Pd^{II} Complex: Regioselective to Regiospecific C–H Activation, Tandem Catalysis and Copper-Free Sonogashira Reaction

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Figure S57. Diffraction and refinement data plots.

Table S1. Selected bond lengths in Å

Table S2. Selected bond lengths in Å

Table S3. Selected bond angles in °

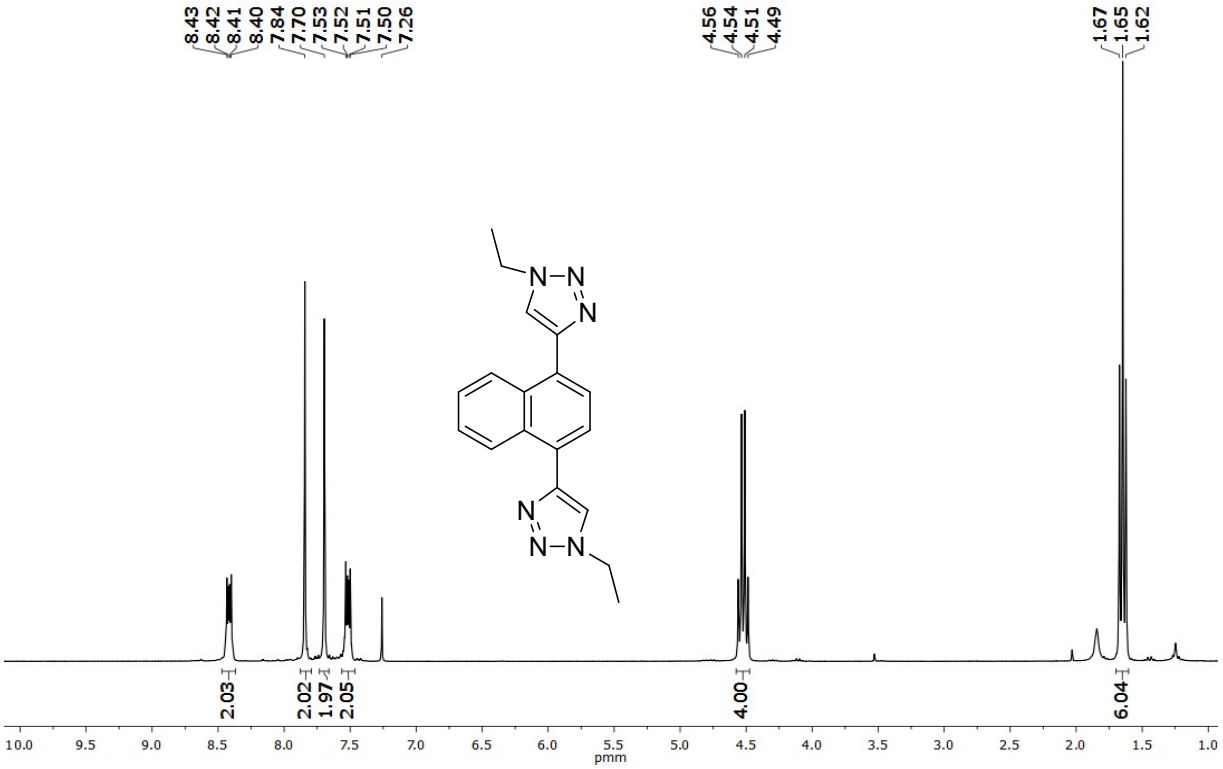


Figure S1. ^{1}H NMR spectrum of bis-triazole in $CDCl_3$.

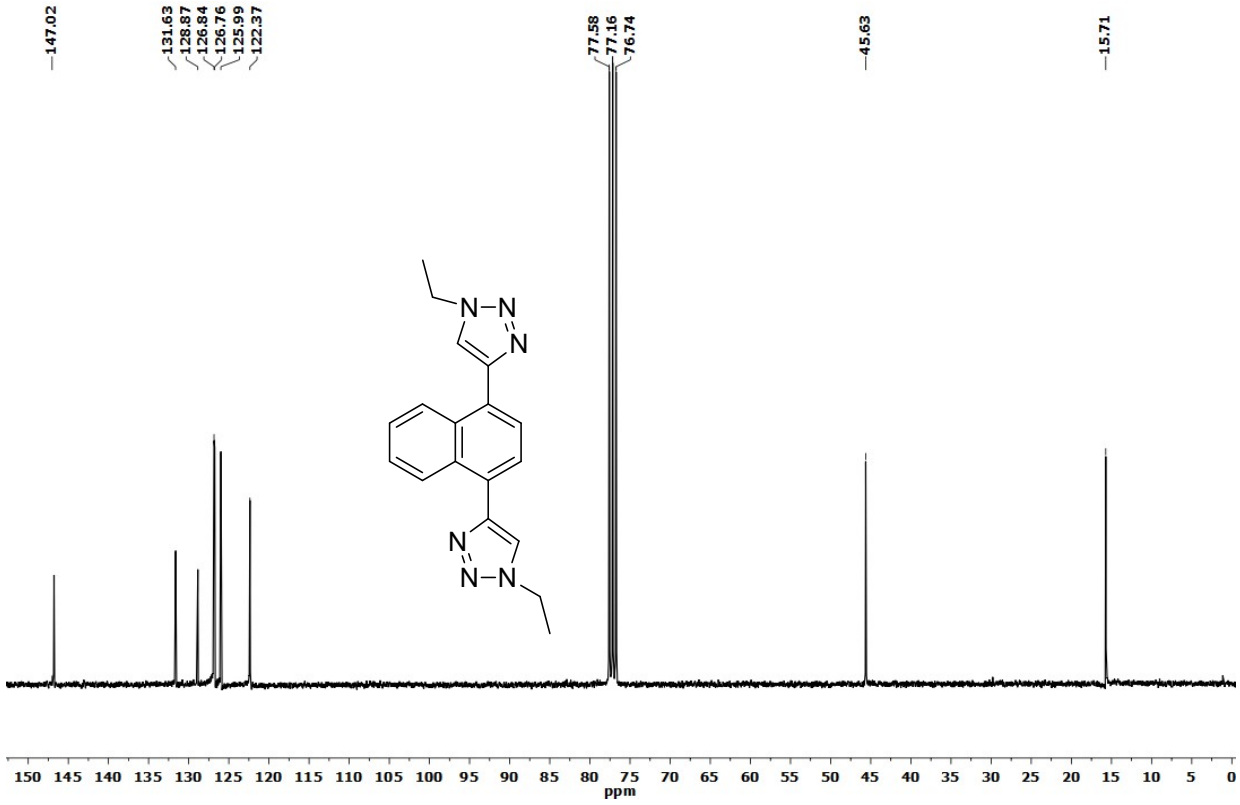


Figure S2. $^{13}C\{^{1}H\}$ NMR spectrum of bis-triazole in $CDCl_3$.

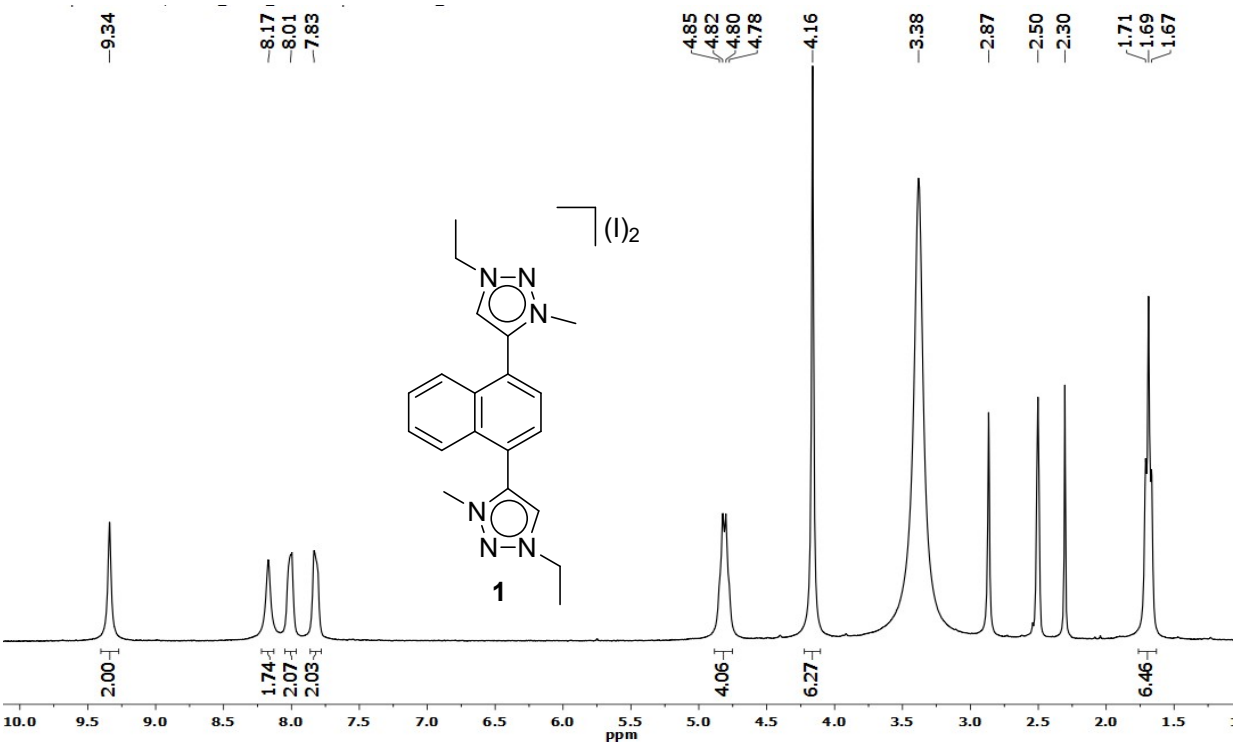


Figure S3. ^{1}H NMR spectrum of **1** in DMSO-d_6.

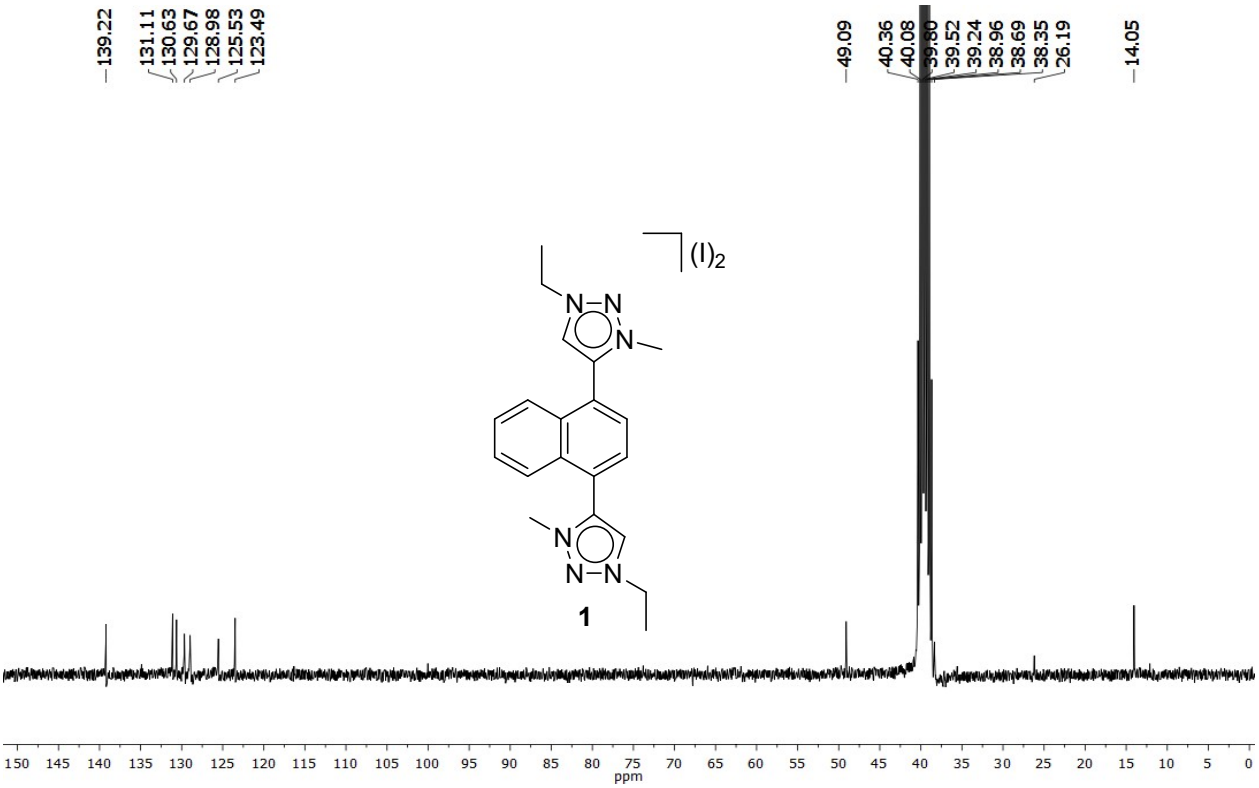


Figure S4. ^{13}C{^{1}H} NMR spectrum of **1** in DMSO-d_6.

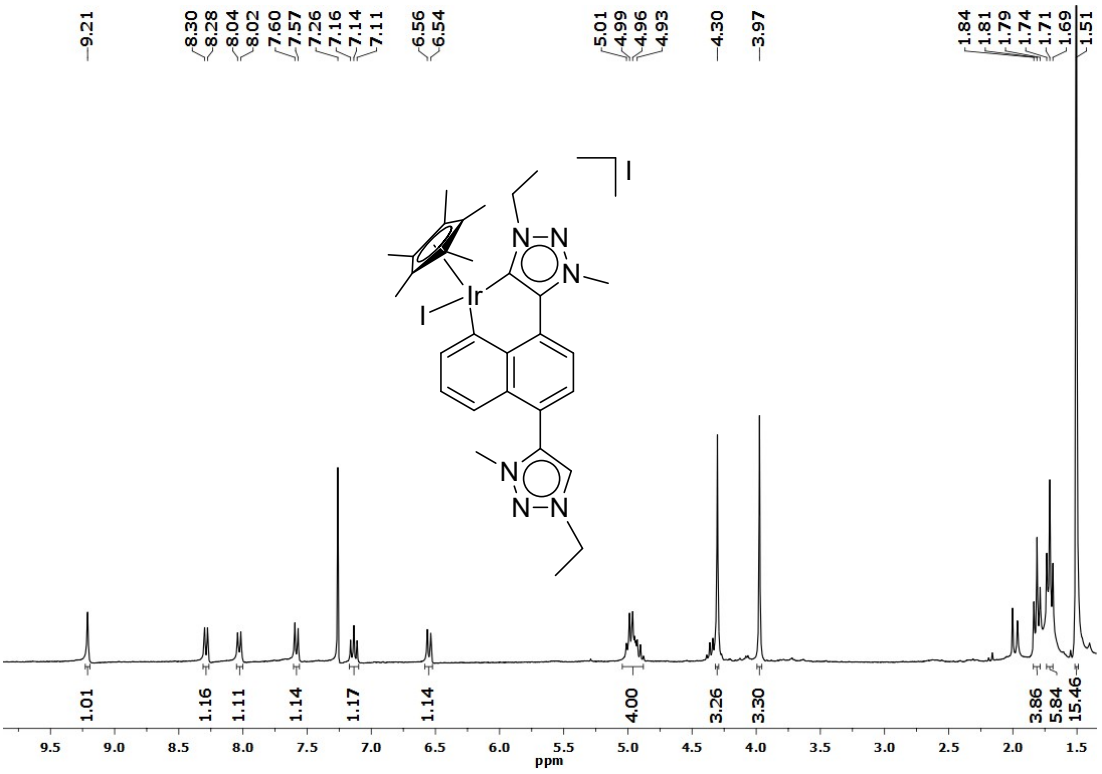


Figure S5. ^{1}H NMR spectrum of [**2**] in $CDCl_3$.

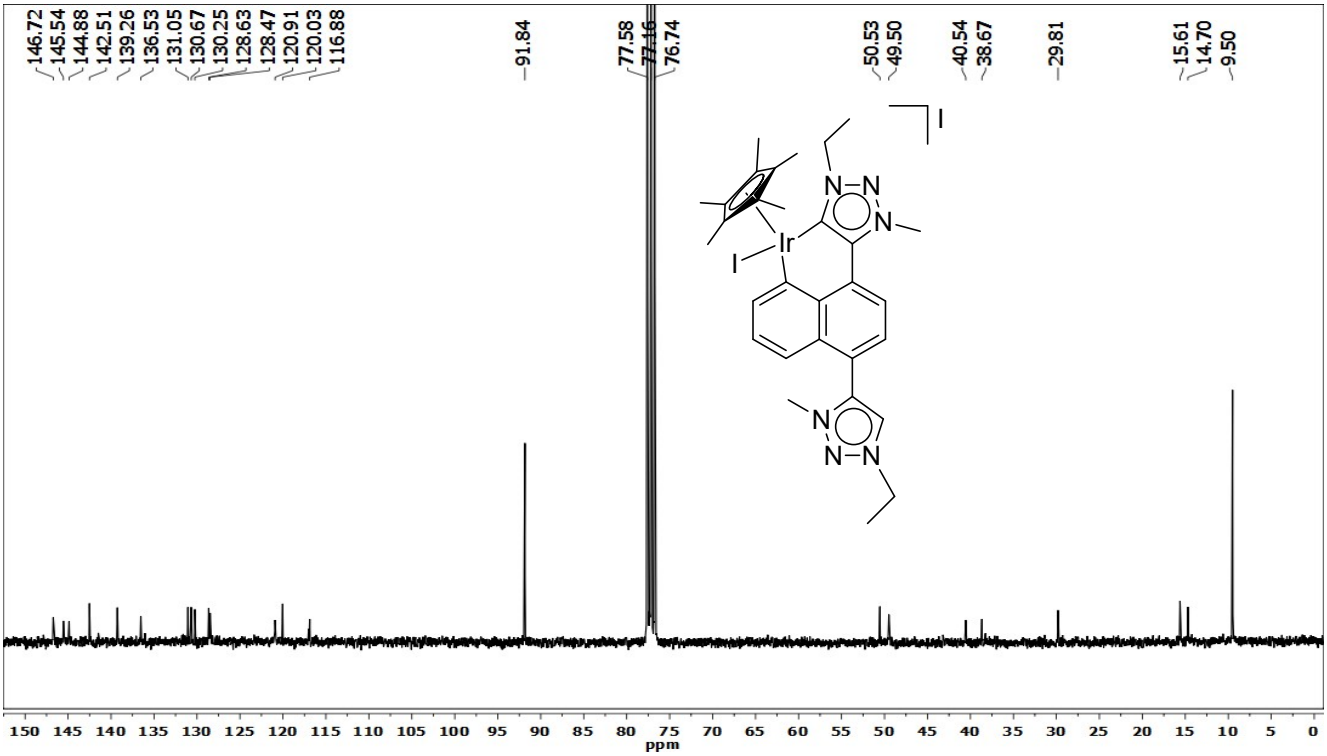


Figure S6. $^{13}C\{^{1}H\}$ NMR spectrum of [**2**] in $CDCl_3$.

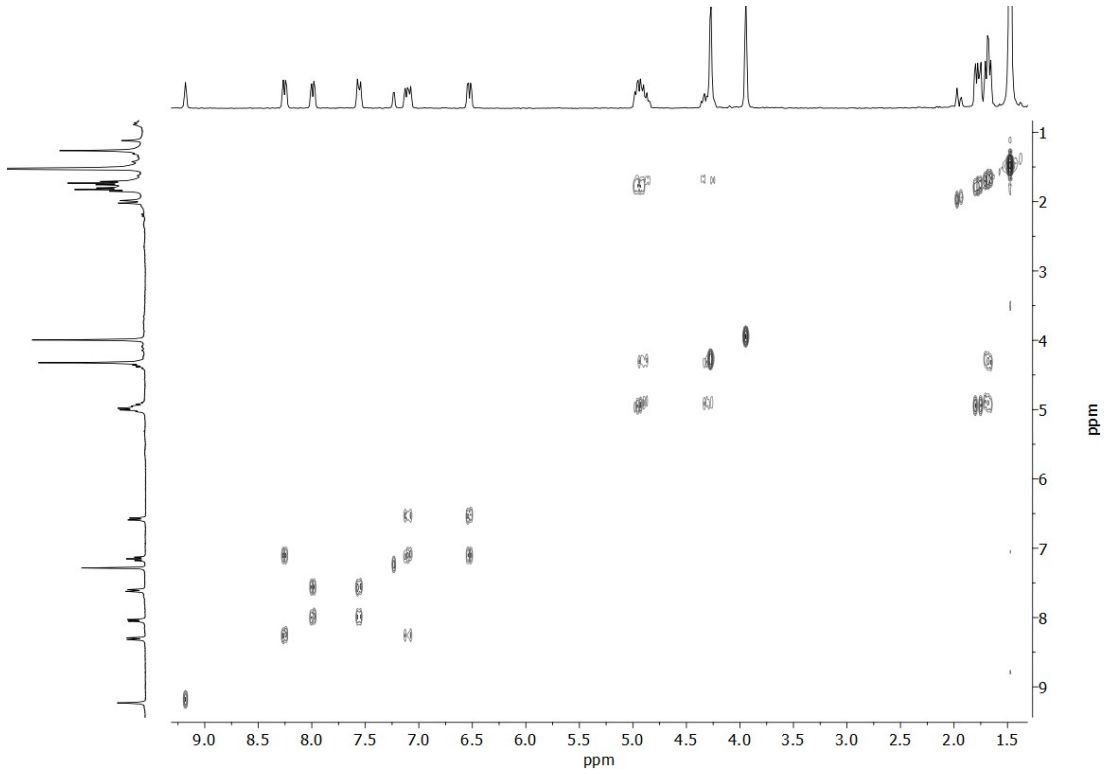


Figure S7. COSY NMR spectrum of [**2**] in $CDCl_3$.

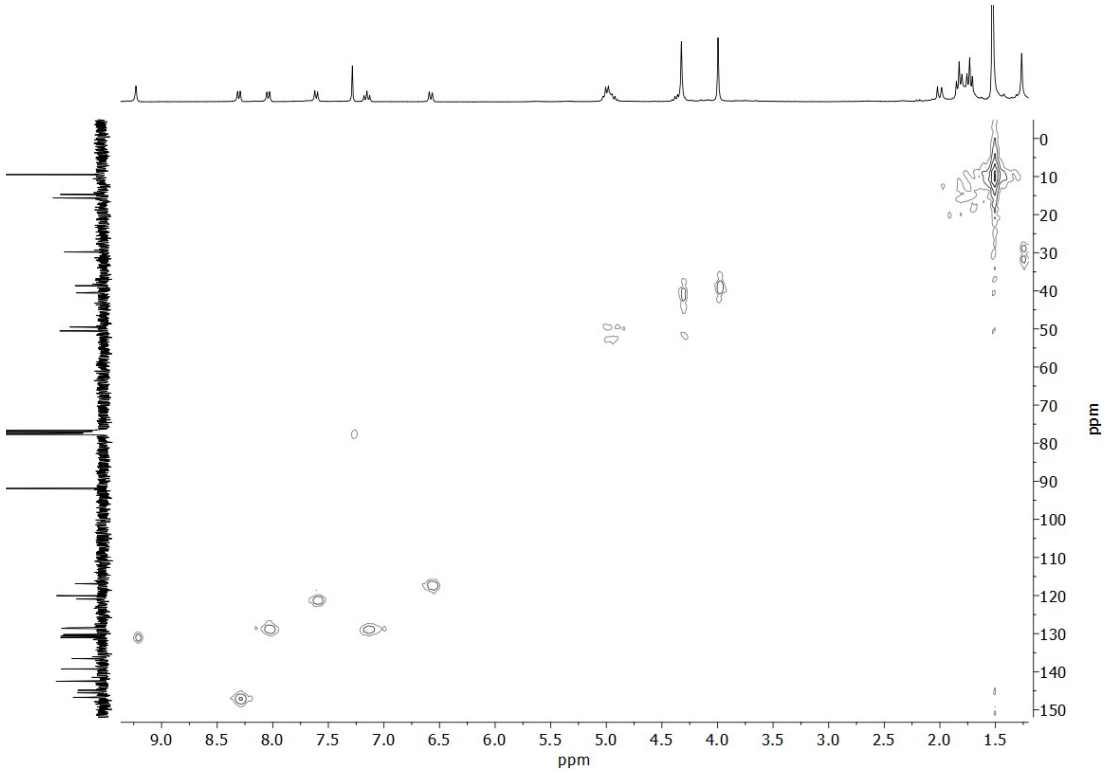


Figure S8. HMQC NMR spectrum of [**2**] in $CDCl_3$.

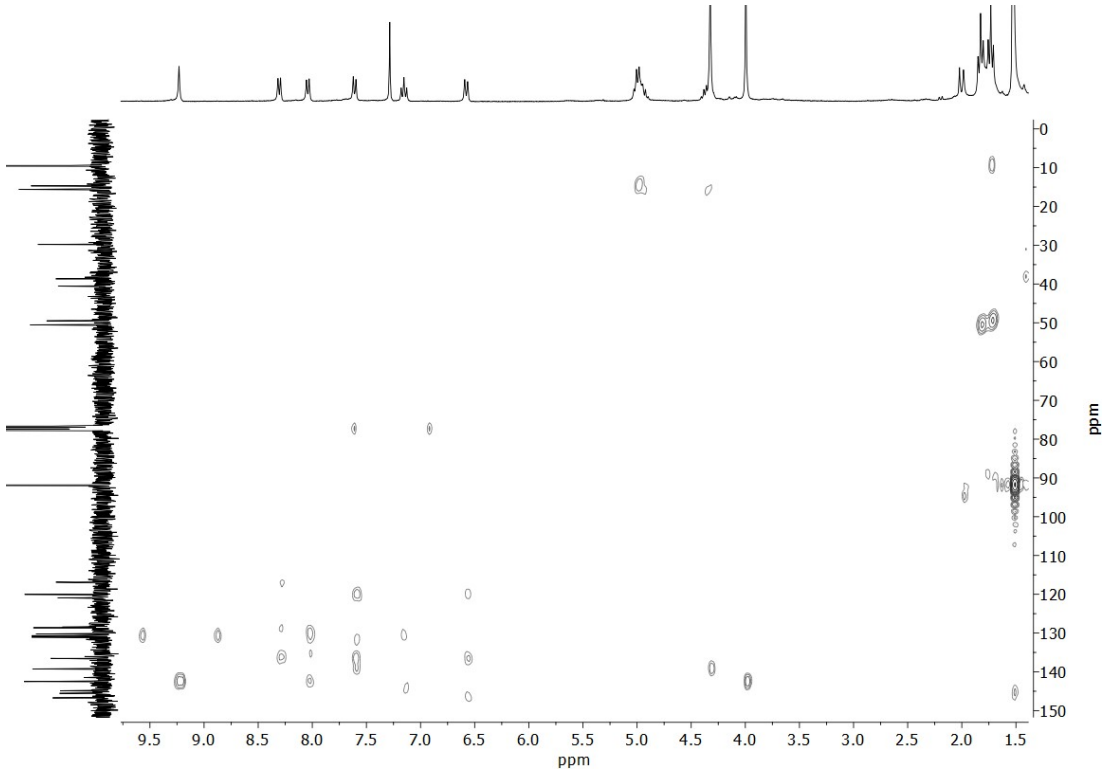


Figure S9. HMBC NMR spectrum of [**2**] in $CDCl_3$.

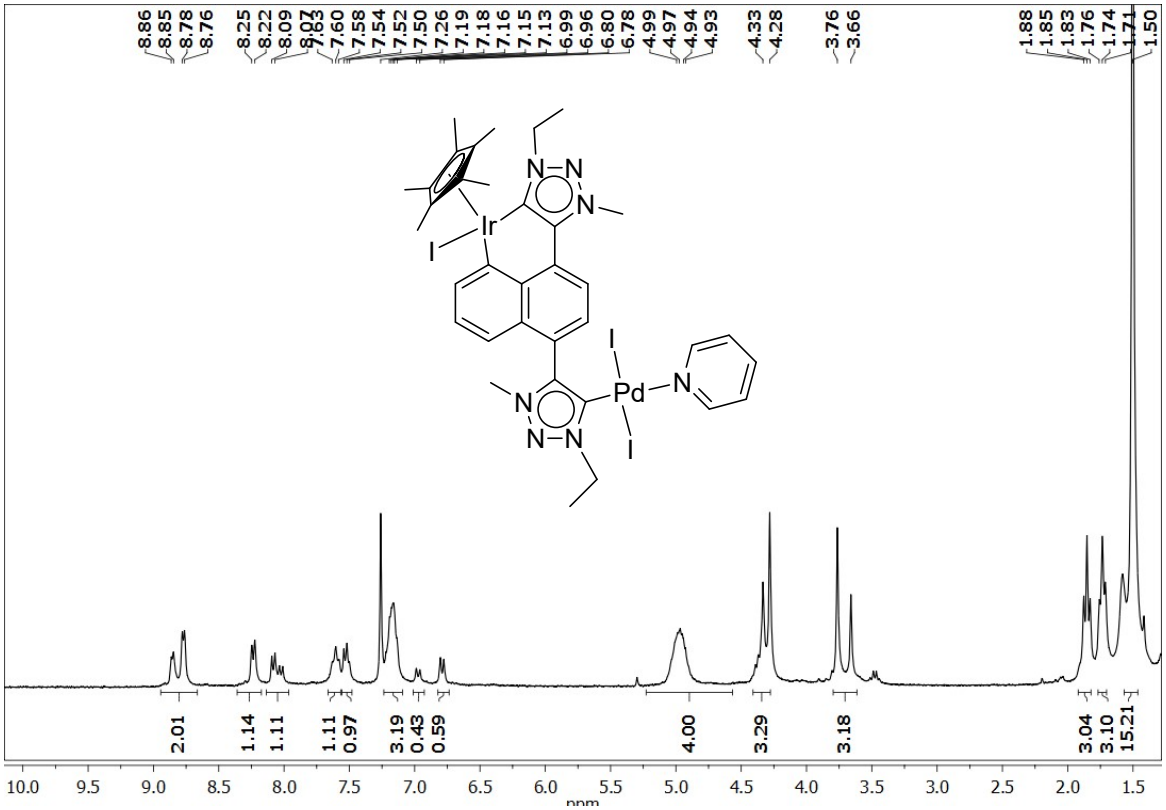


Figure S10. ^1H NMR spectrum of [**3**] in $CDCl_3$.

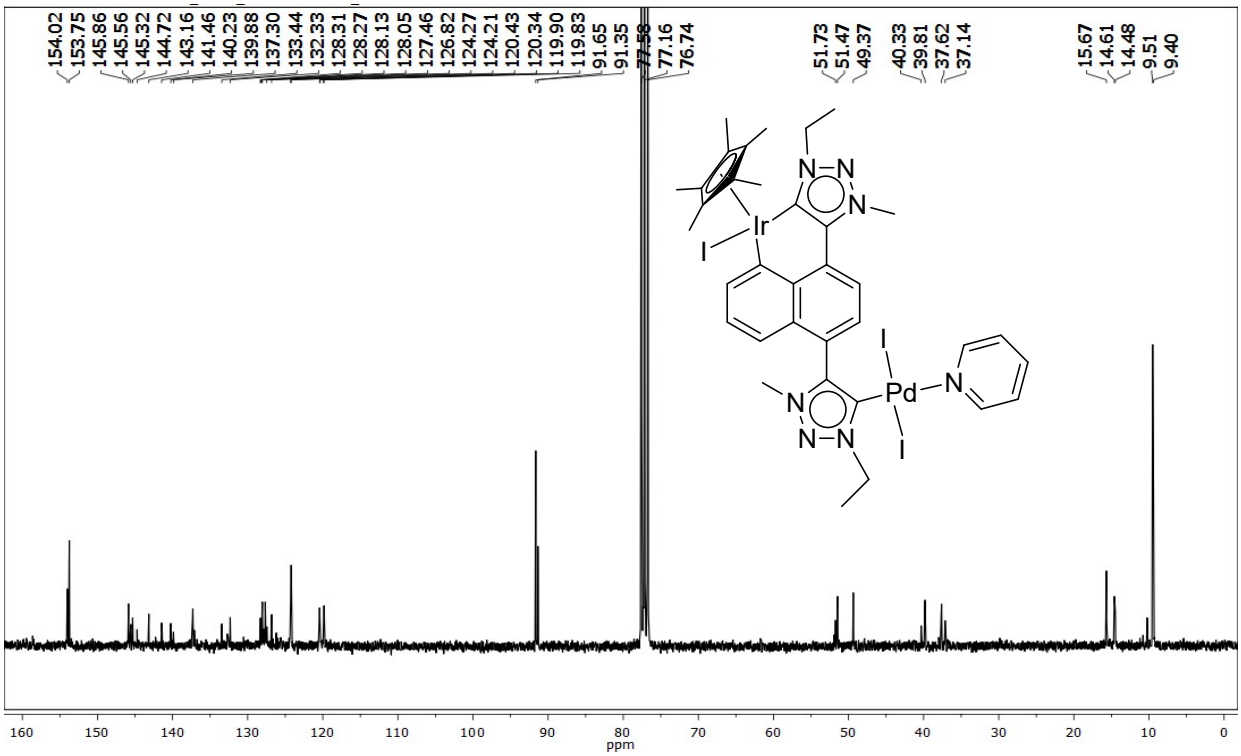


Figure S11. $^{13}C\{^{1}H\}$ NMR spectrum of [**3**] in $CDCl_3$.

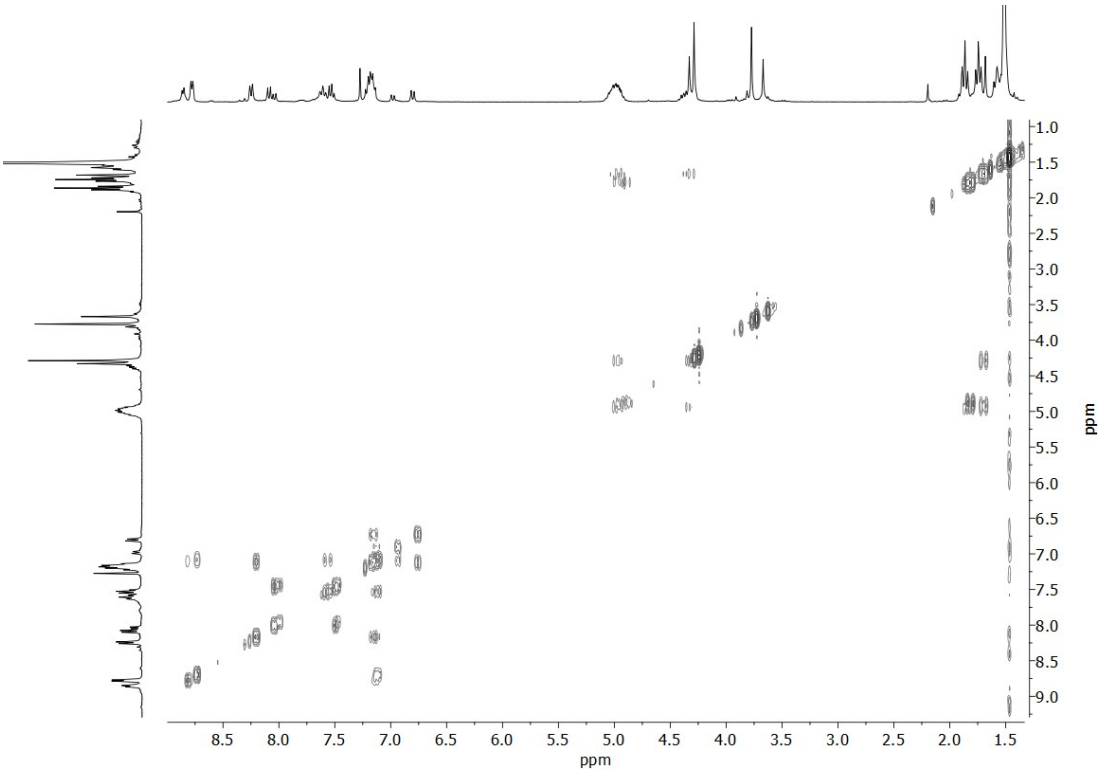


Figure S12. COSY NMR spectrum of [**3**] in $CDCl_3$.

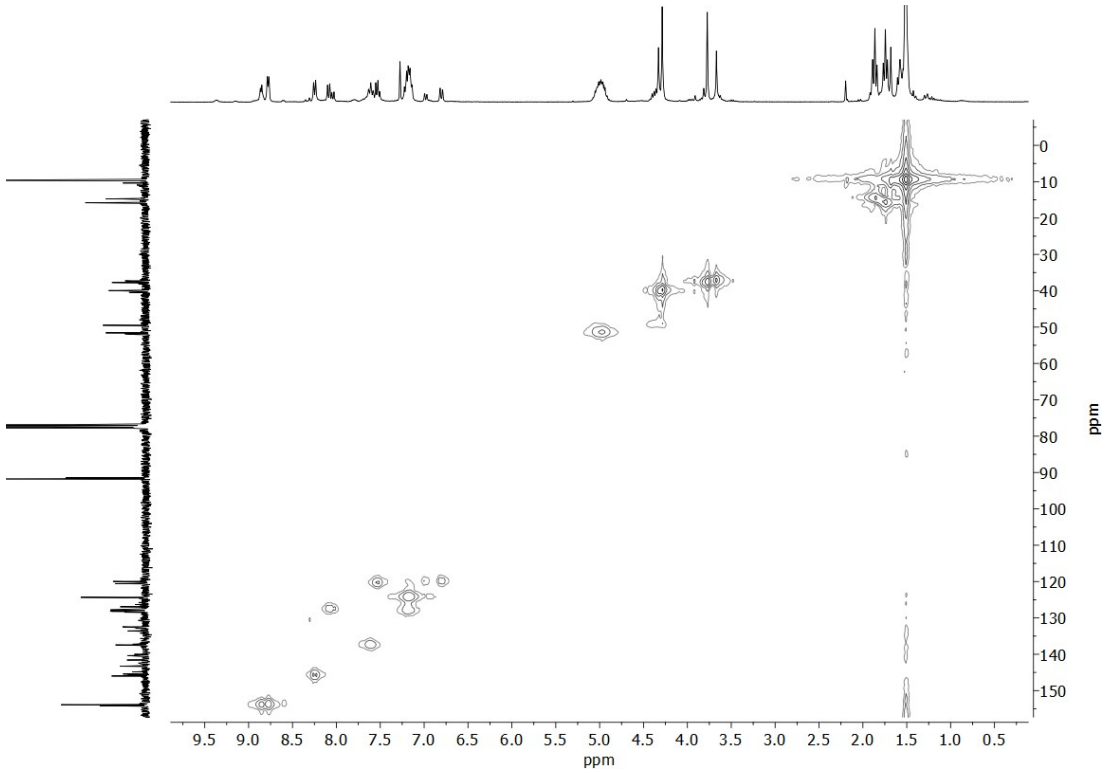


Figure S13. HMQC NMR spectrum of [**3**] in $CDCl_3$.

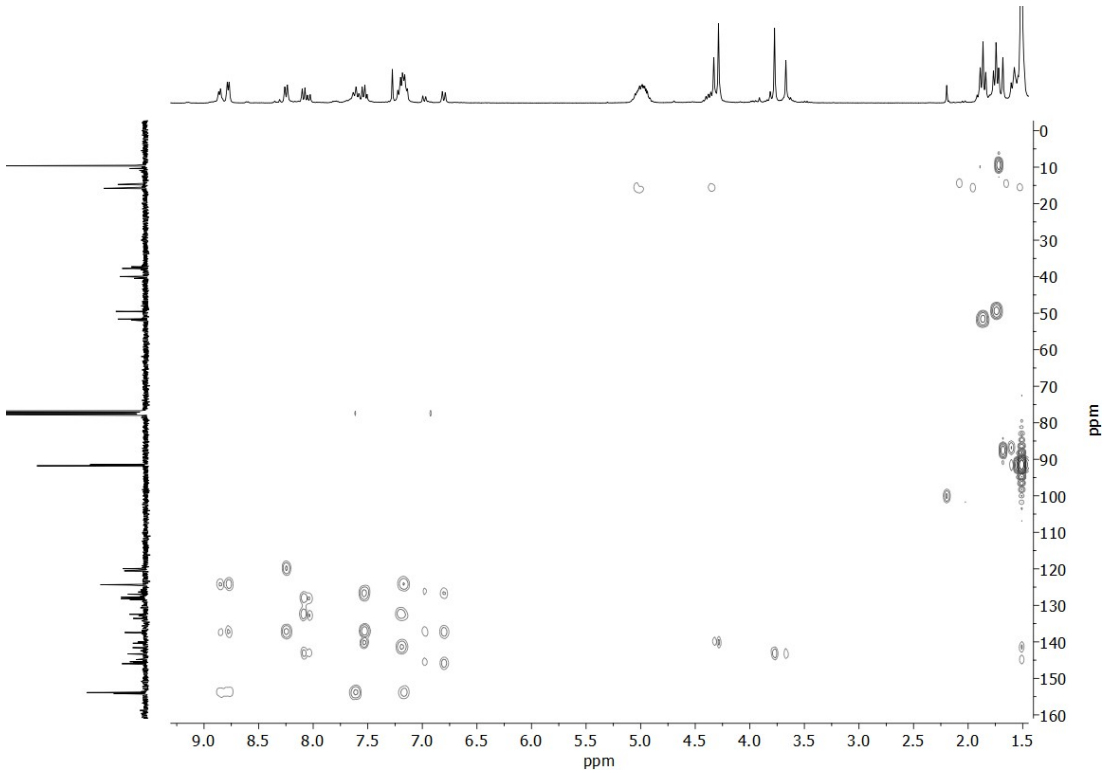


Figure S14. HMBC NMR spectrum of [**3**] in $CDCl_3$.

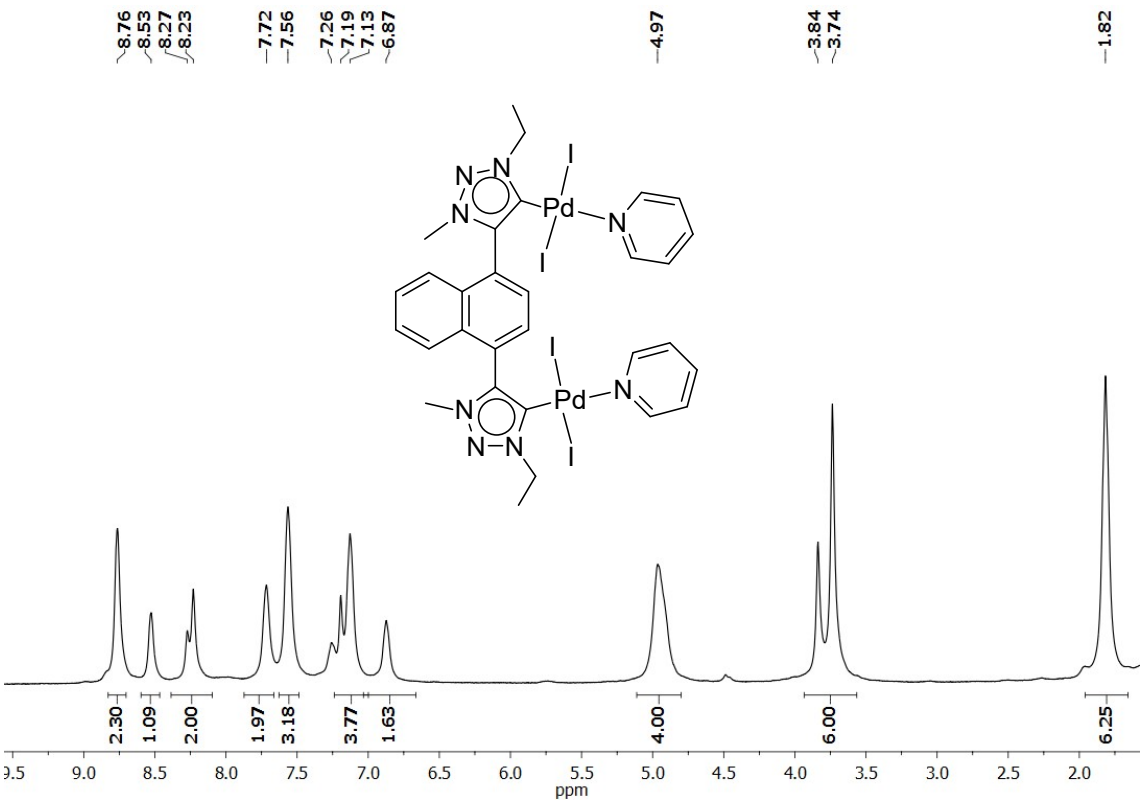


Figure S15. ^{1}H NMR spectrum of [**4**] in $CDCl_3$.

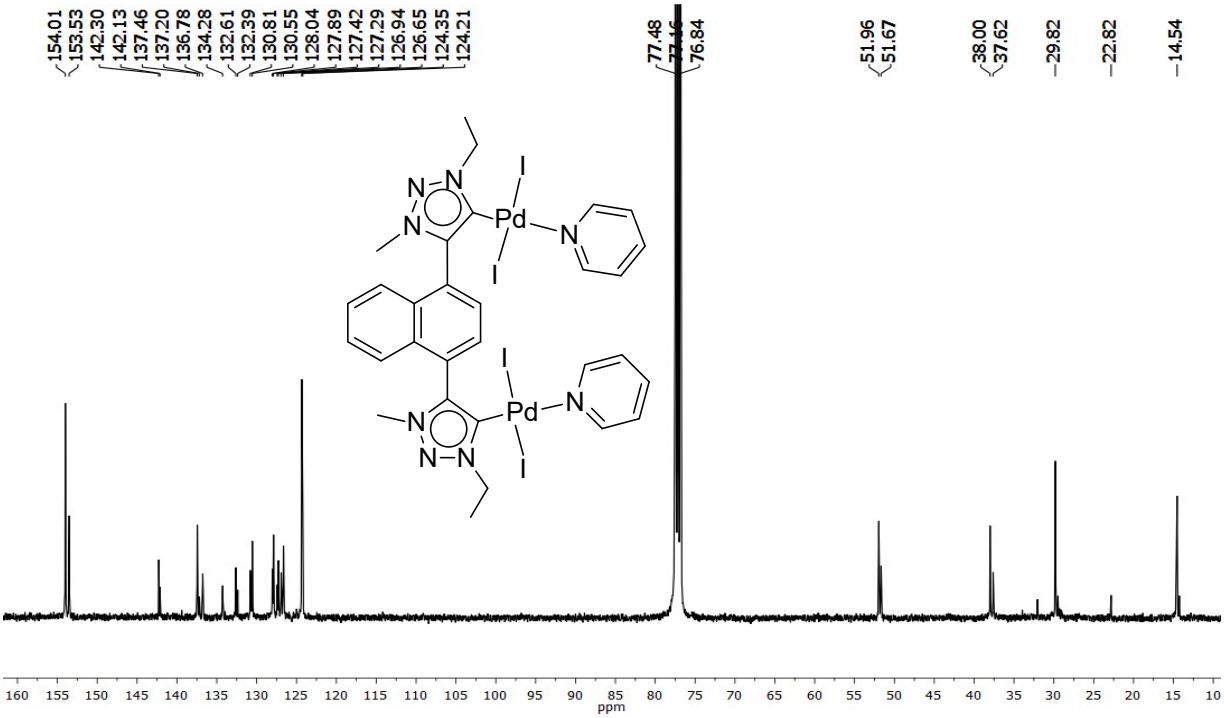


Figure S16. $^{13}C\{^{1}H\}$ NMR spectrum of [**4**] in $CDCl_3$.

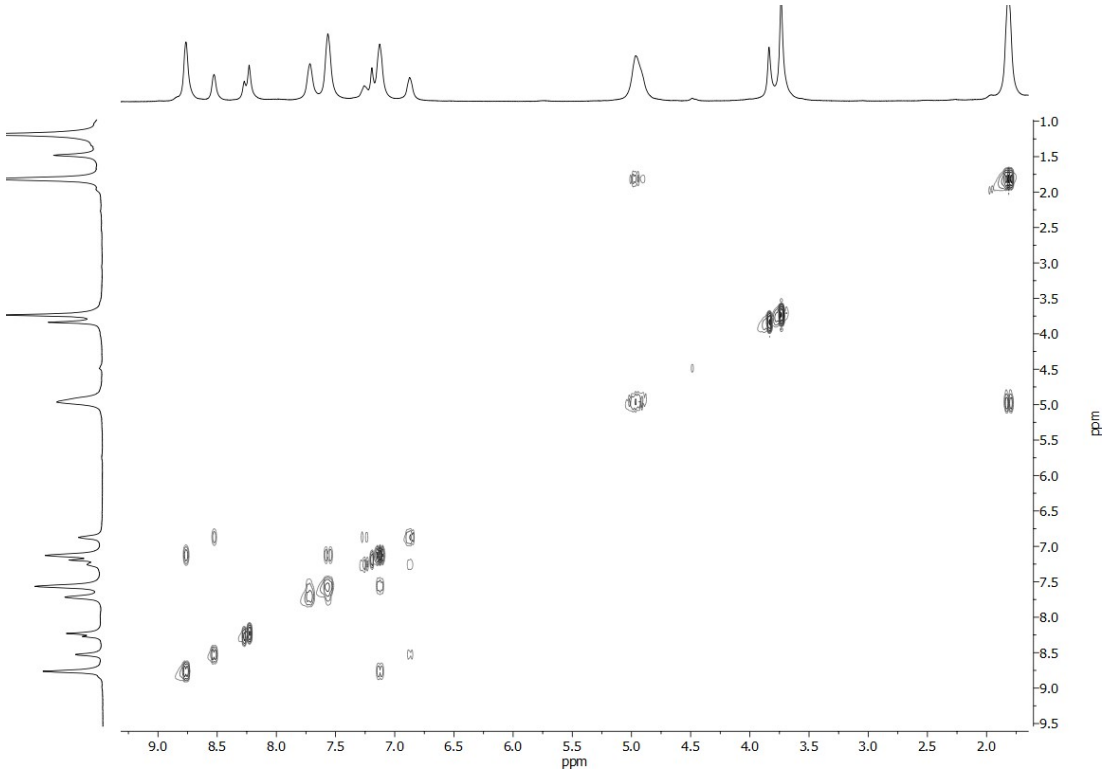


Figure S17. COSY NMR spectrum of [**4**] in $CDCl_3$.

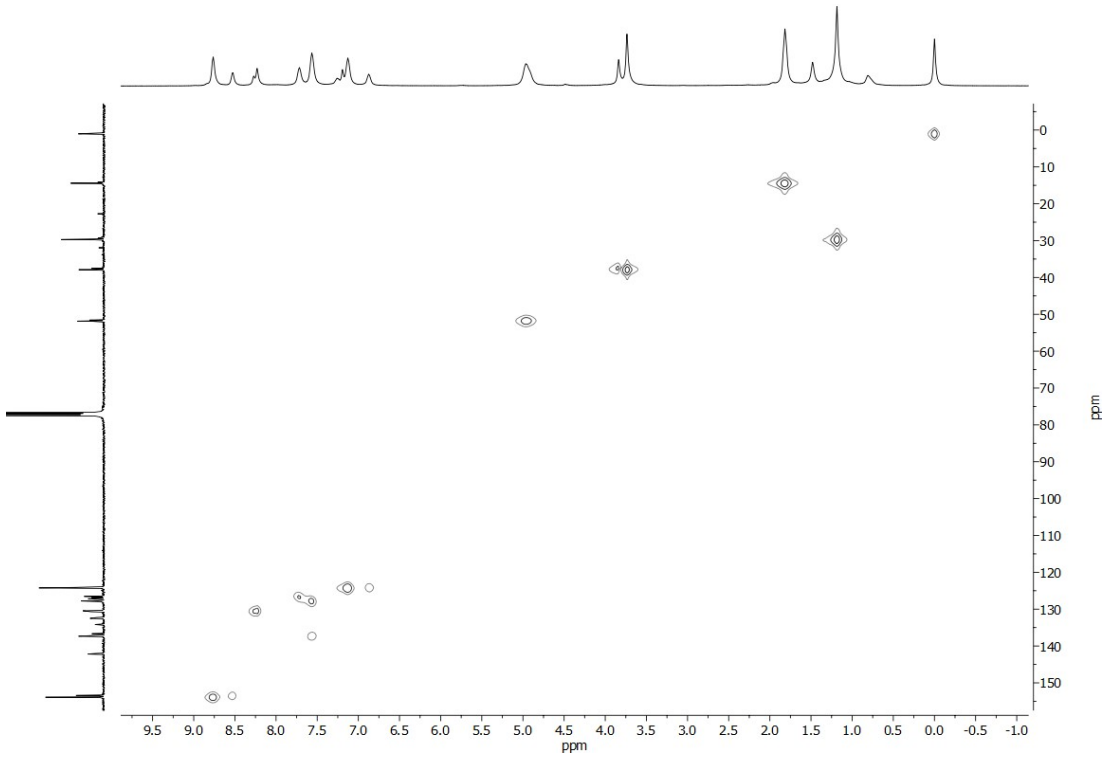


Figure S18. HMQC NMR spectrum of [**4**] in $CDCl_3$.

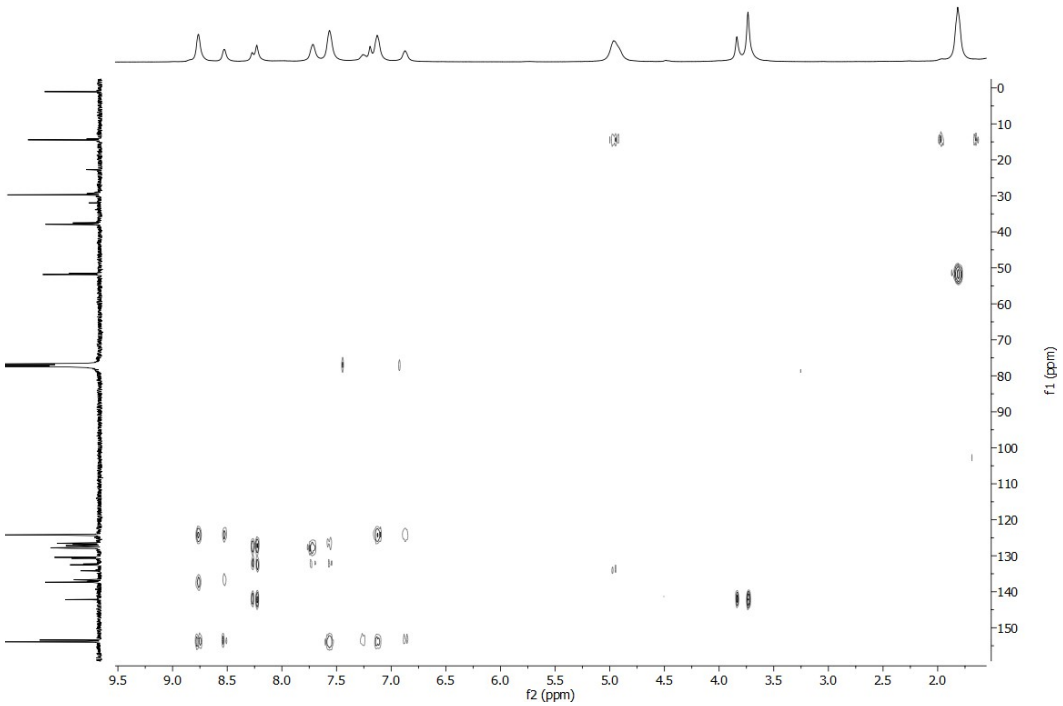


Figure S19. HMBC NMR spectrum of [**4**] in $CDCl_3$.

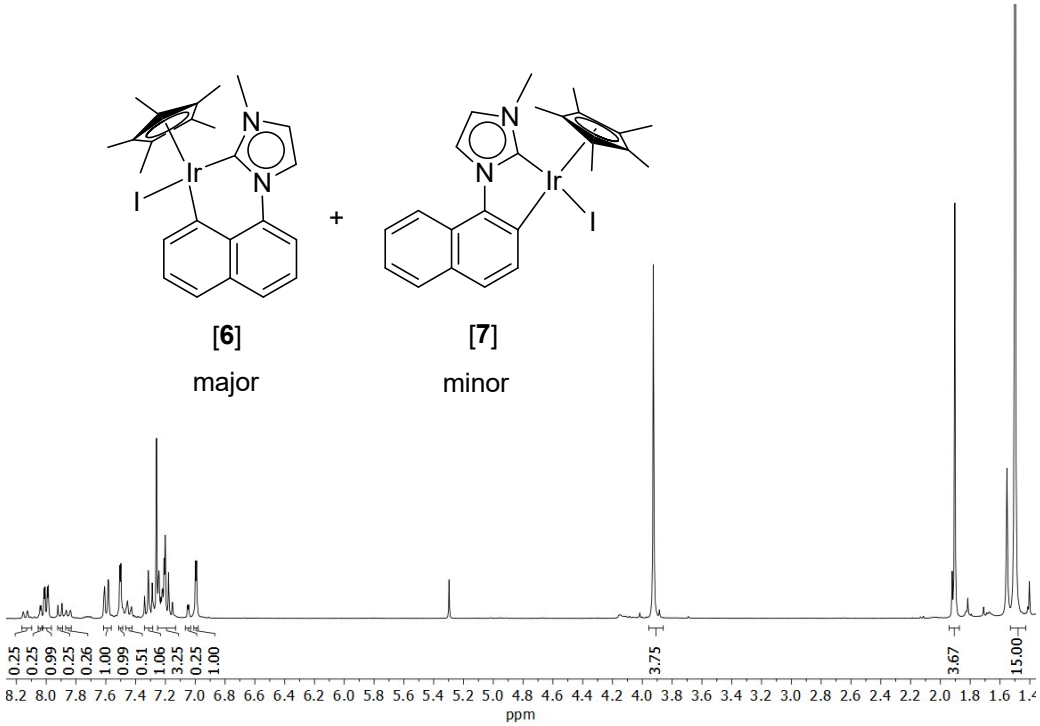


Figure S20. ^1H NMR spectrum of crude mixture of [**6**] and [**7**] in $CDCl_3$.

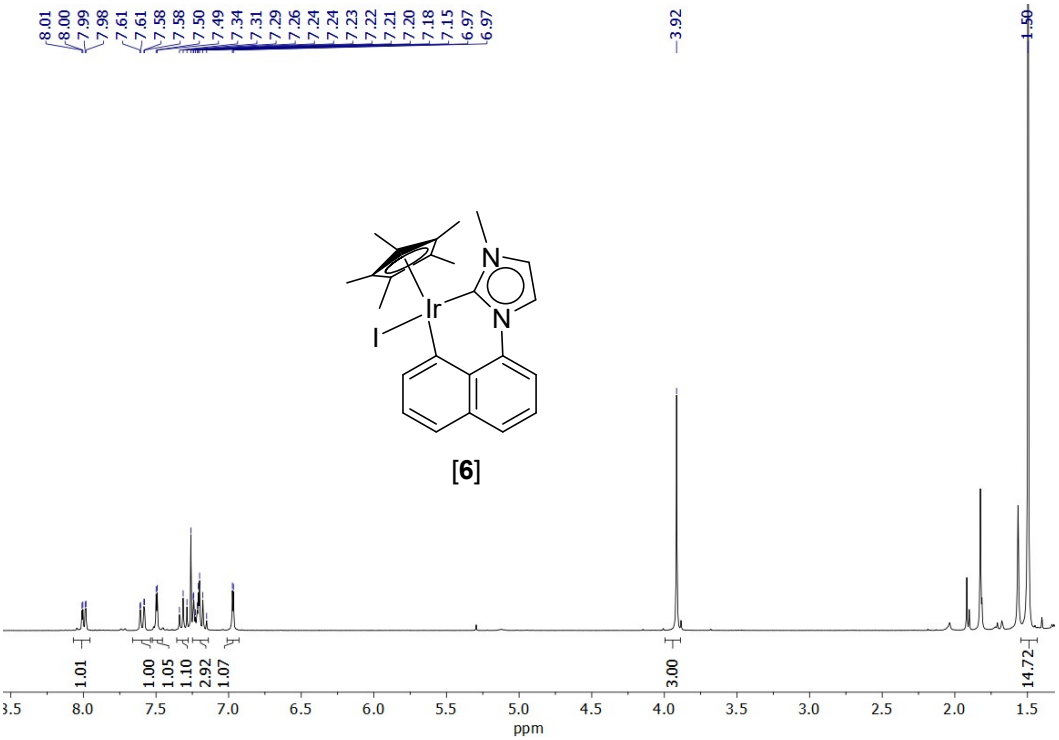


Figure S21. ^{1}H NMR spectrum of [**6**] in $CDCl_3$.

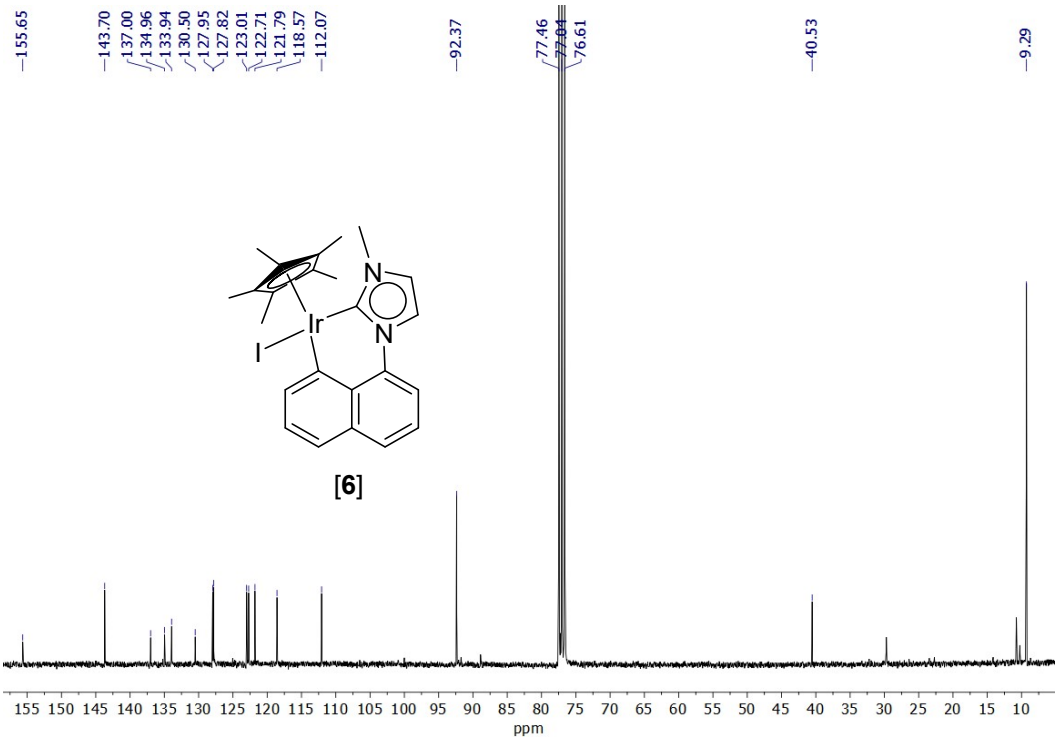


Figure S22. $^{13}C\{^{1}H\}$ NMR spectrum of [**6**] in $CDCl_3$.

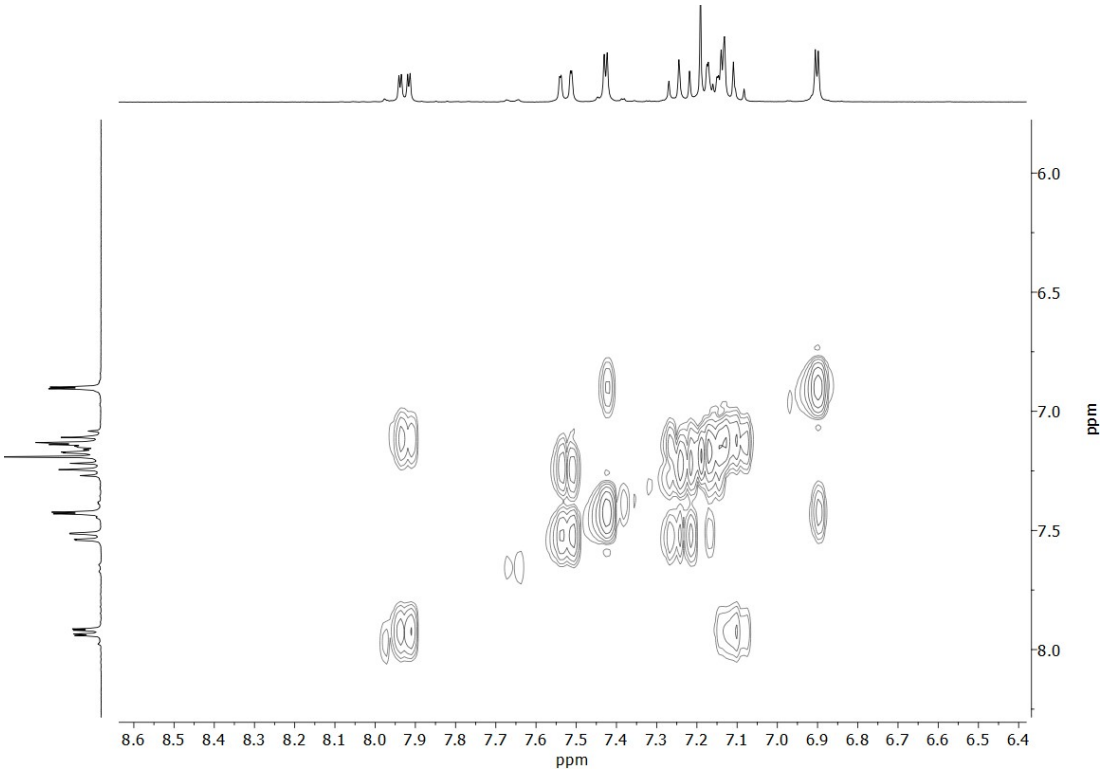


Figure S23. COSY NMR spectrum of [**6**] in $CDCl_3$.

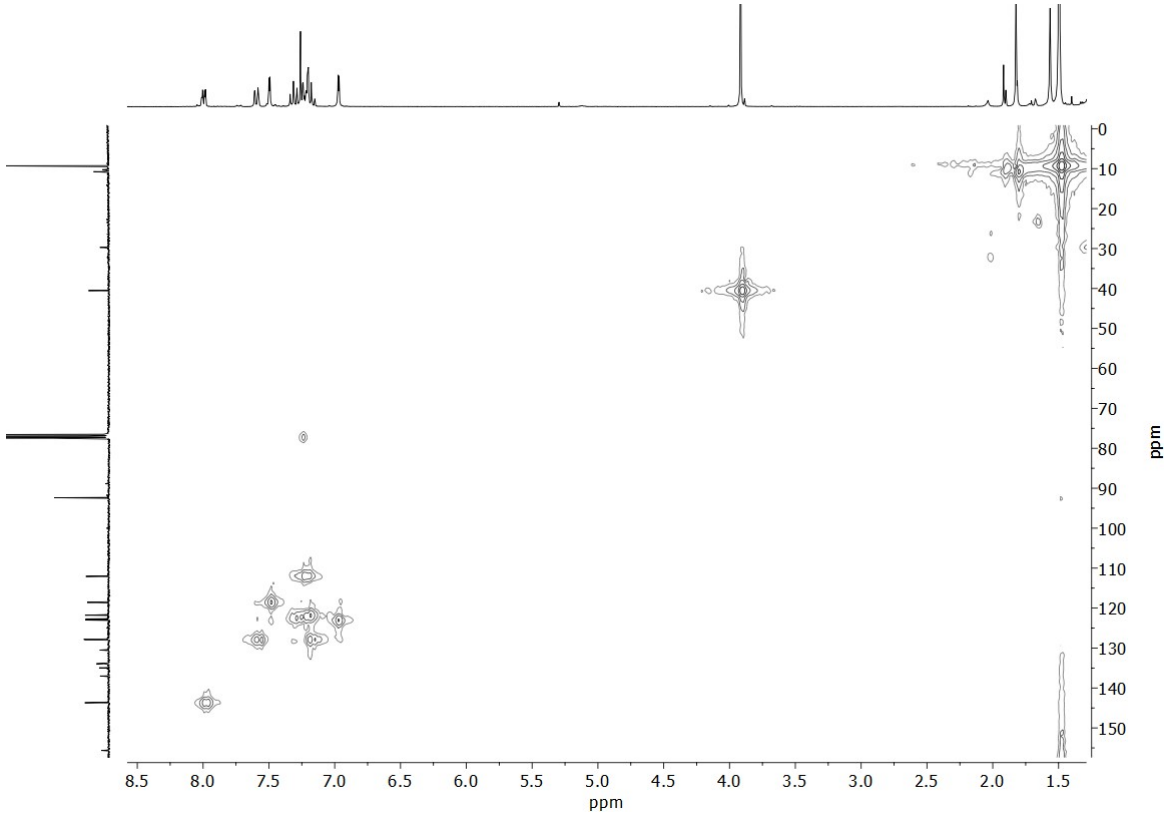


Figure S24. HMQC NMR spectrum of [**6**] in $CDCl_3$.

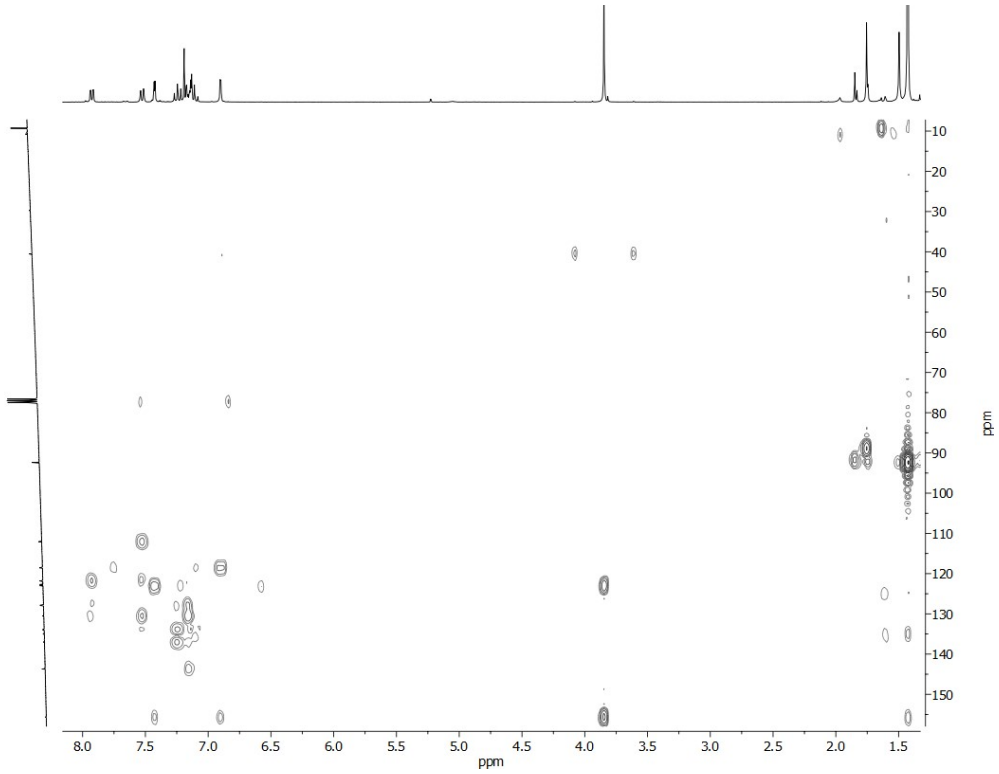
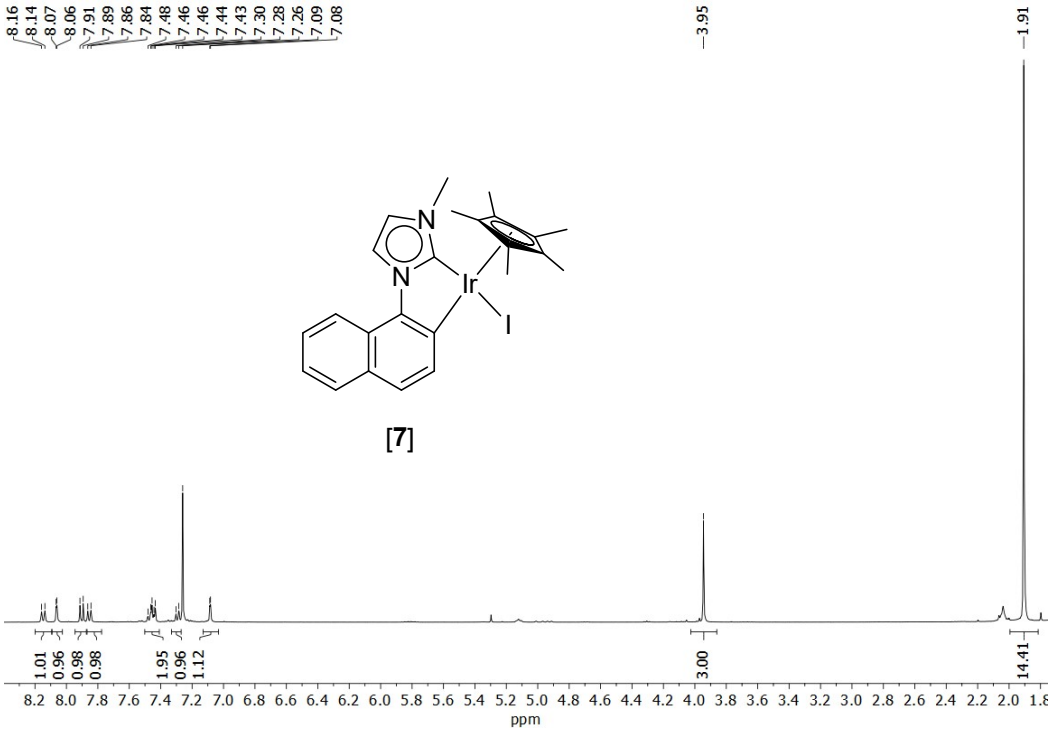


Figure S25. HMBC NMR spectrum of [**6**] in $CDCl_3$.



[**7**]

Figure S26. ^1H NMR spectrum of [**7**] in $CDCl_3$.

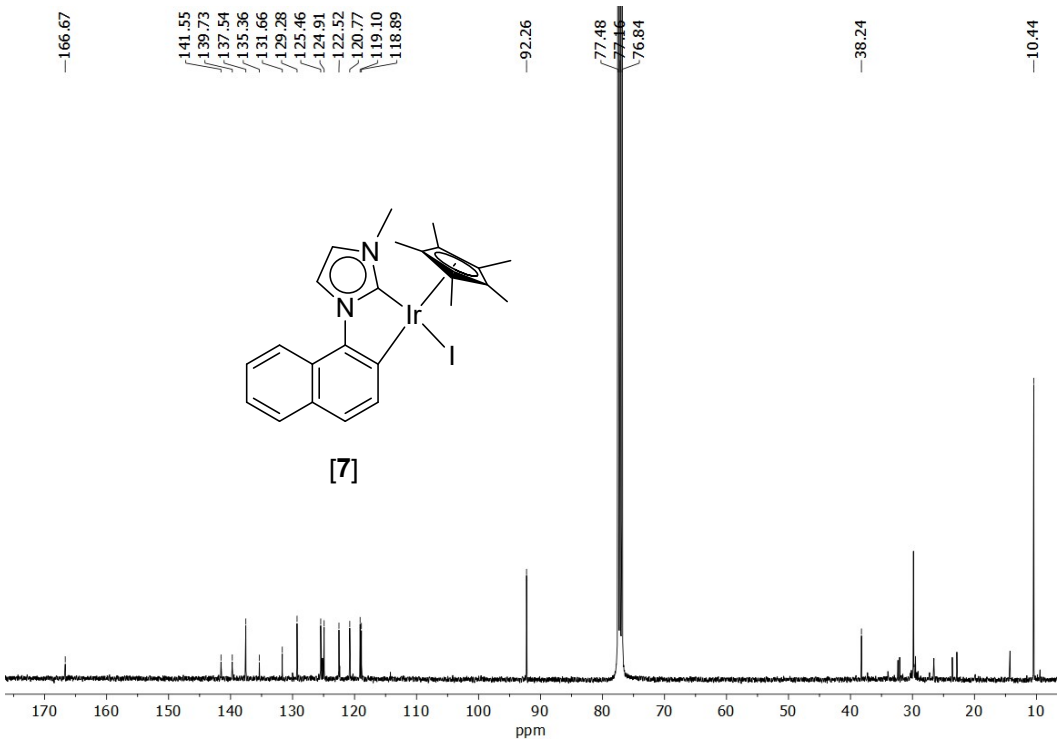


Figure S27. $^{13}C\{^{1}H\}$ NMR spectrum of [**7**] in $CDCl_3$.

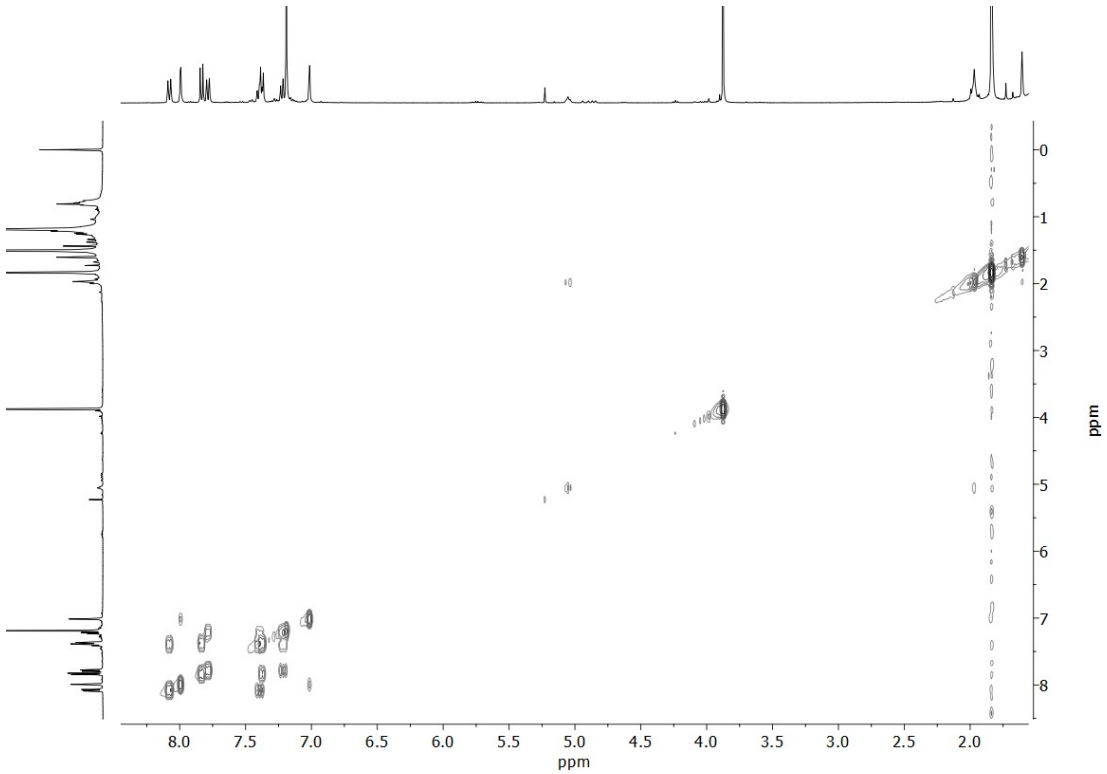


Figure S28. COSY NMR spectrum of [**7**] in $CDCl_3$.

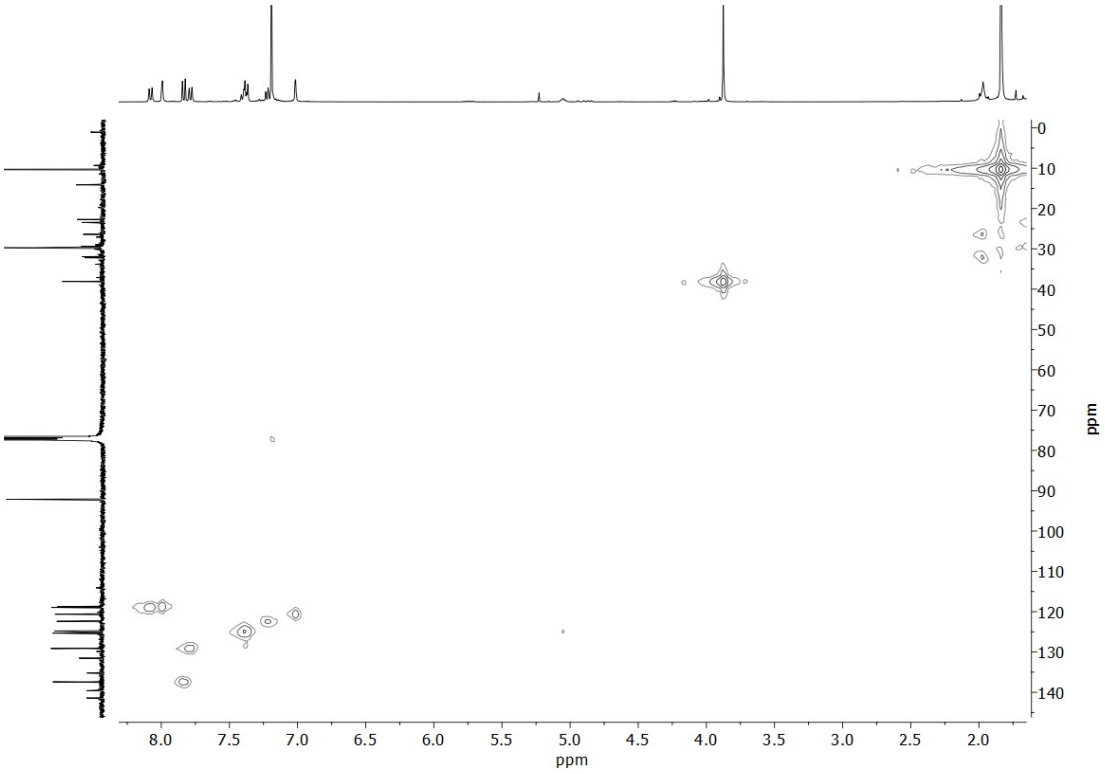


Figure S29. HMQC NMR spectrum of [**7**] in $CDCl_3$.

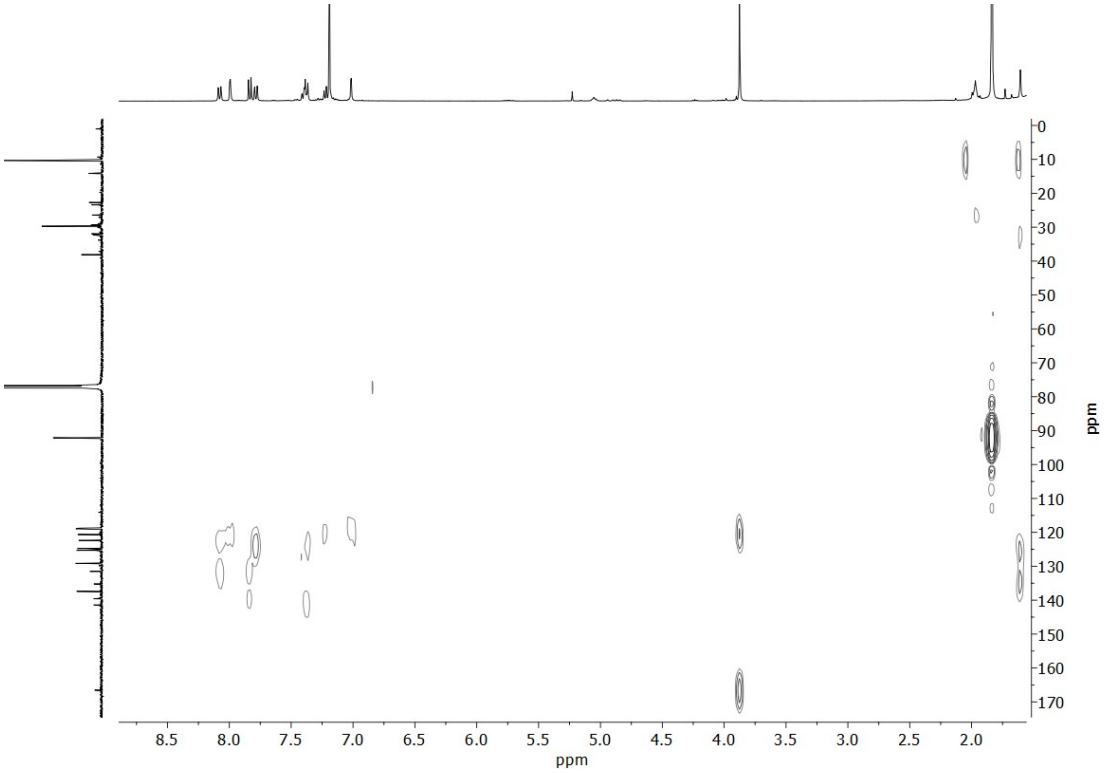


Figure S30. HMBC NMR spectrum of [**7**] in $CDCl_3$.

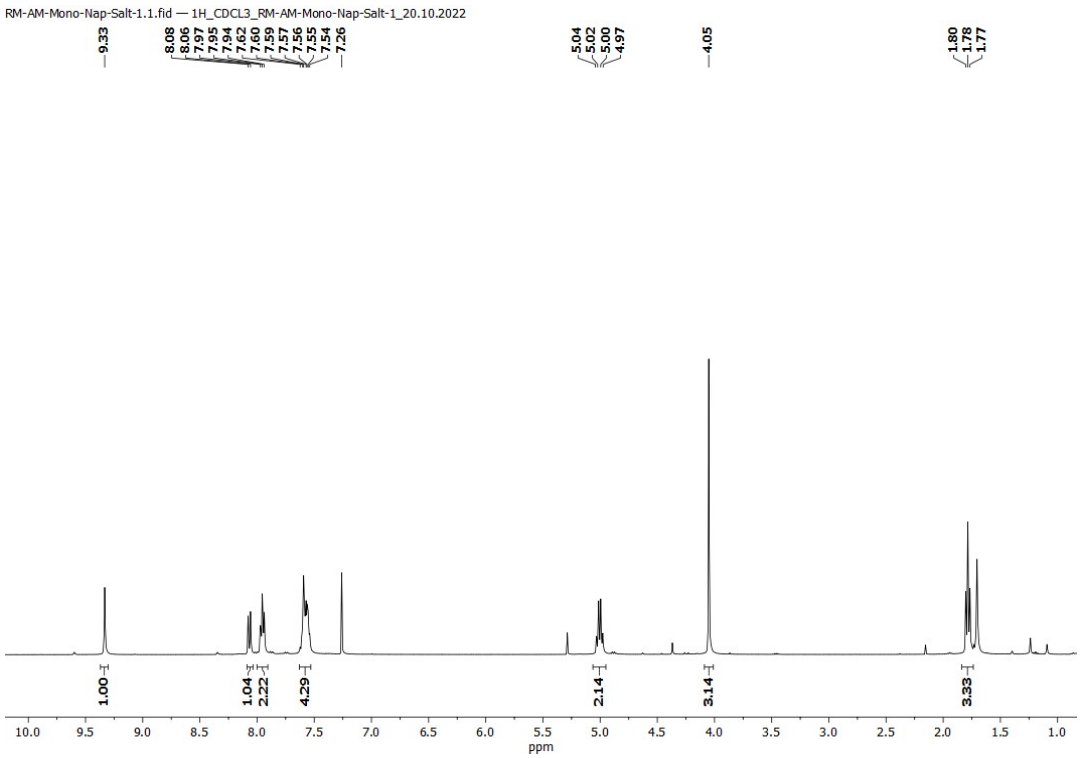


Figure S31. ^{1}H NMR spectrum of **8** in $CDCl_3$.

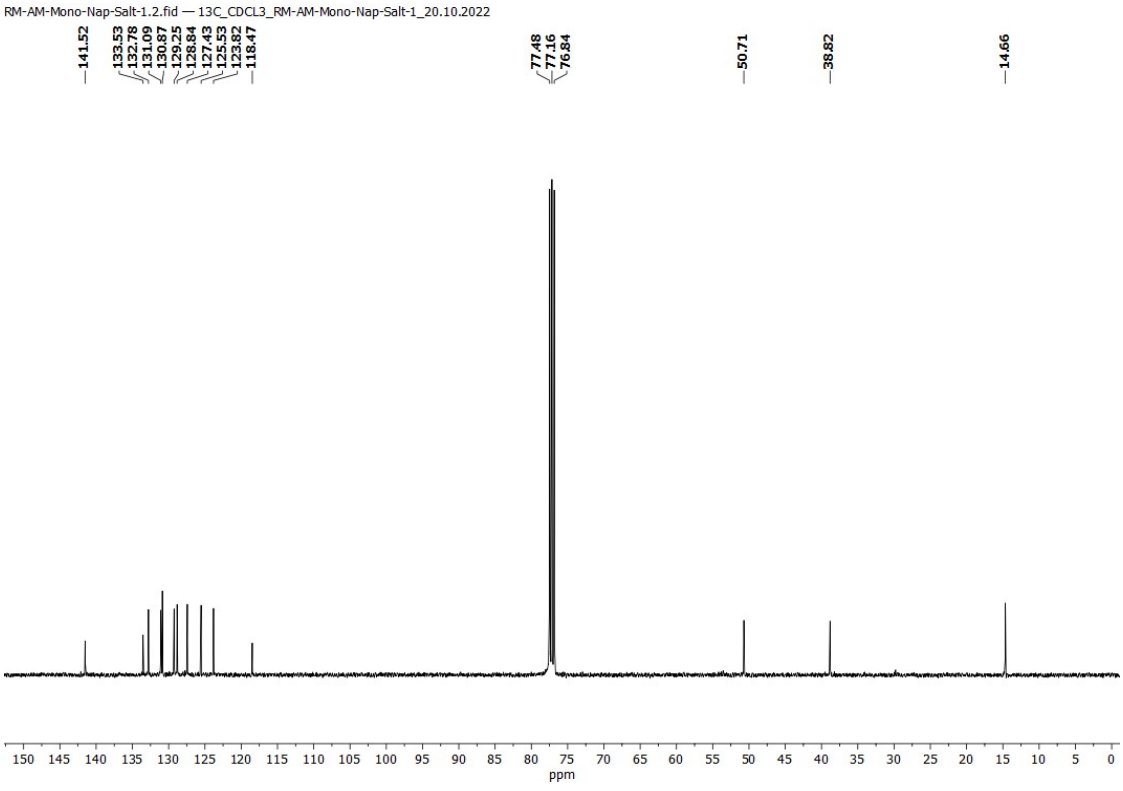


Figure S32. $^{13}C\{^{1}H\}$ NMR spectrum of **8** in $CDCl_3$.

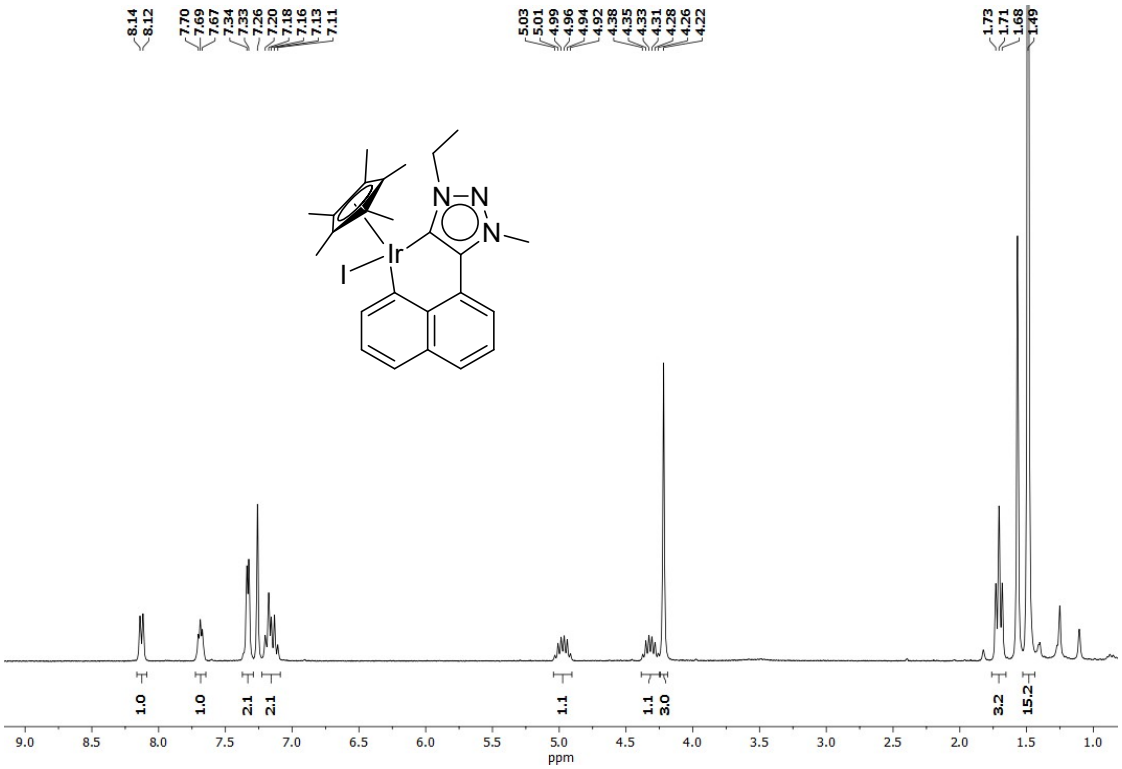


Figure S33. ^{1}H NMR spectrum of [**9**] in $CDCl_3$.

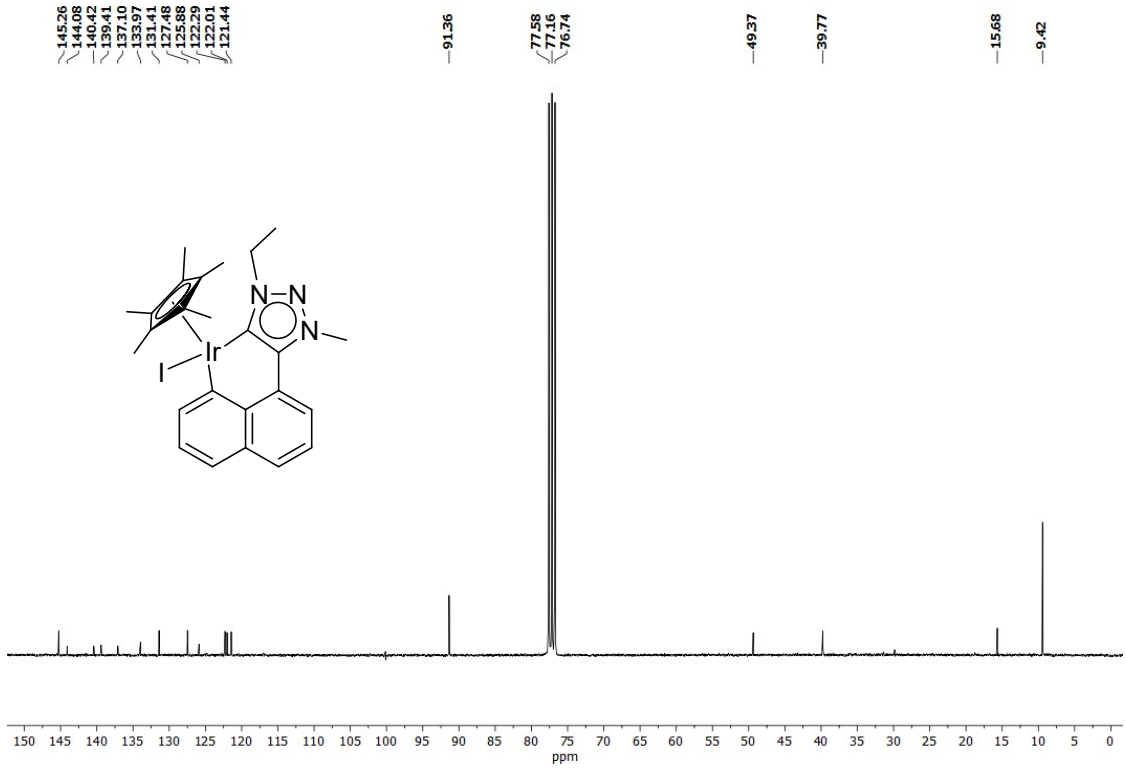


Figure S34. $^{13}C\{^{1}H\}$ NMR spectrum of [**9**] in $CDCl_3$.

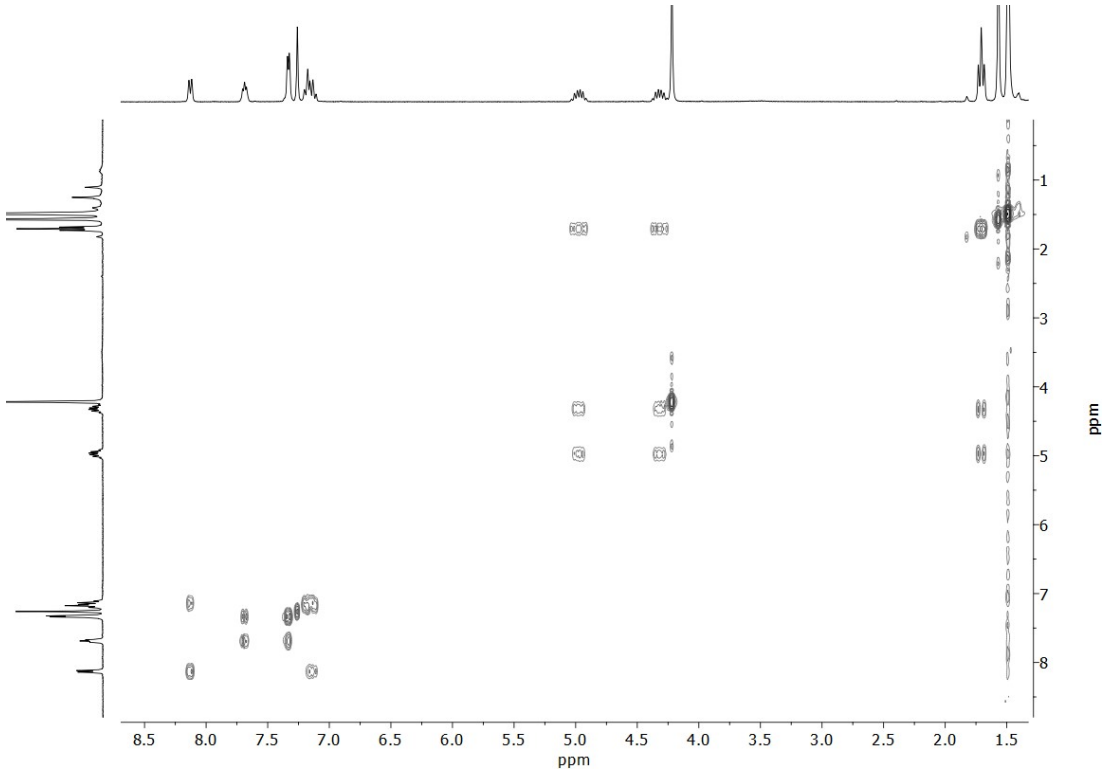


Figure S35. COSY NMR spectrum of [**9**] in $CDCl_3$.

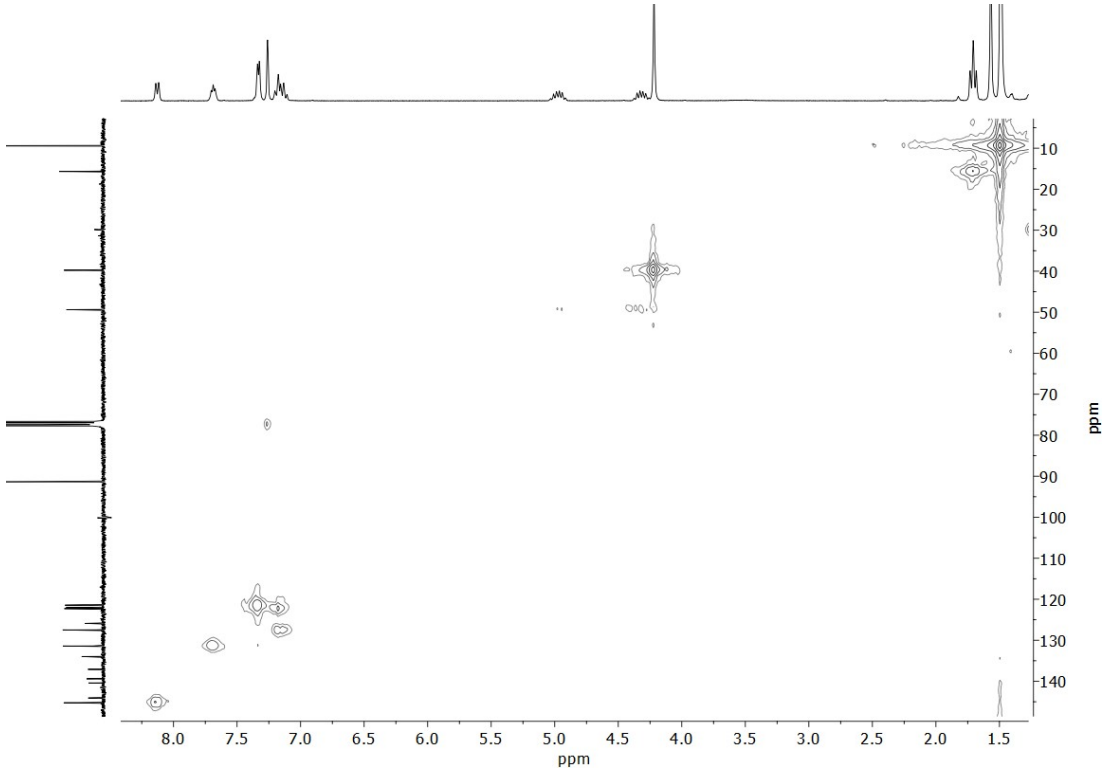


Figure S36. HMQC NMR spectrum of [**9**] in $CDCl_3$.

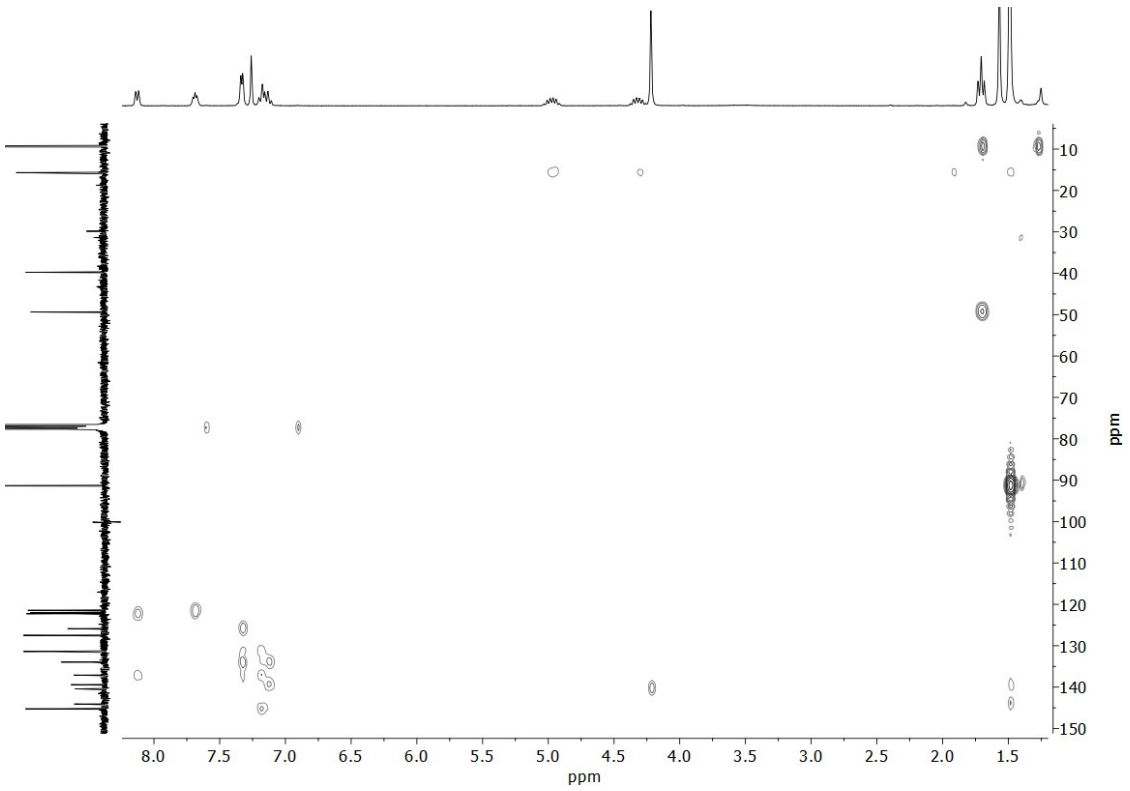


Figure S37. HMBC NMR spectrum of [**9**] in $CDCl_3$.

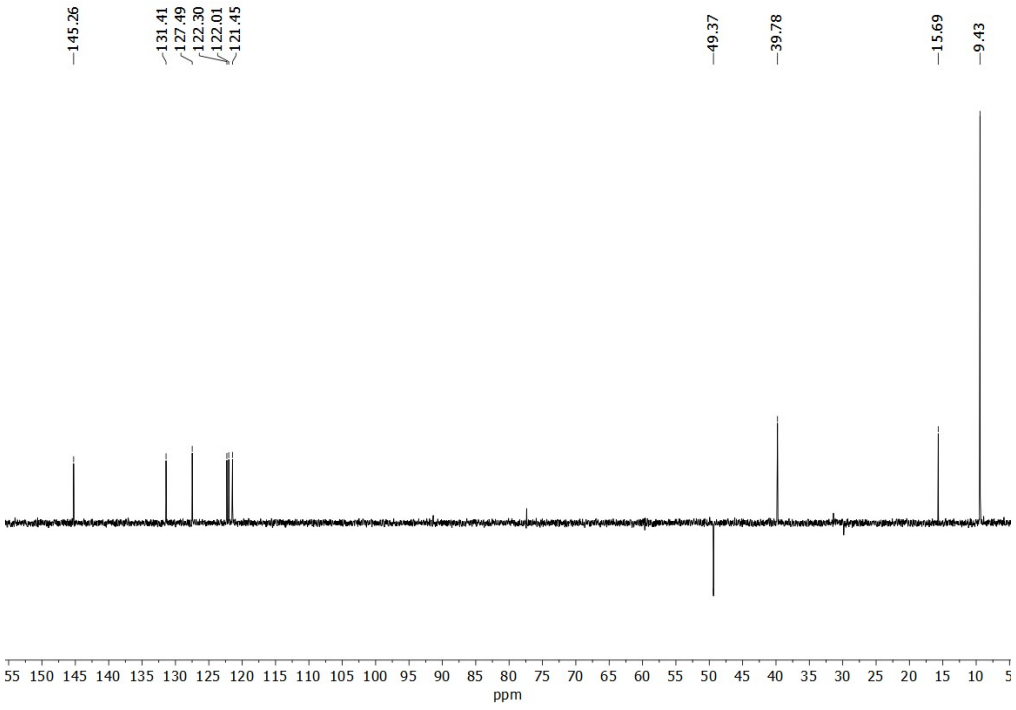


Figure S38. DEPT-135 NMR spectrum of [**9**] in $CDCl_3$.

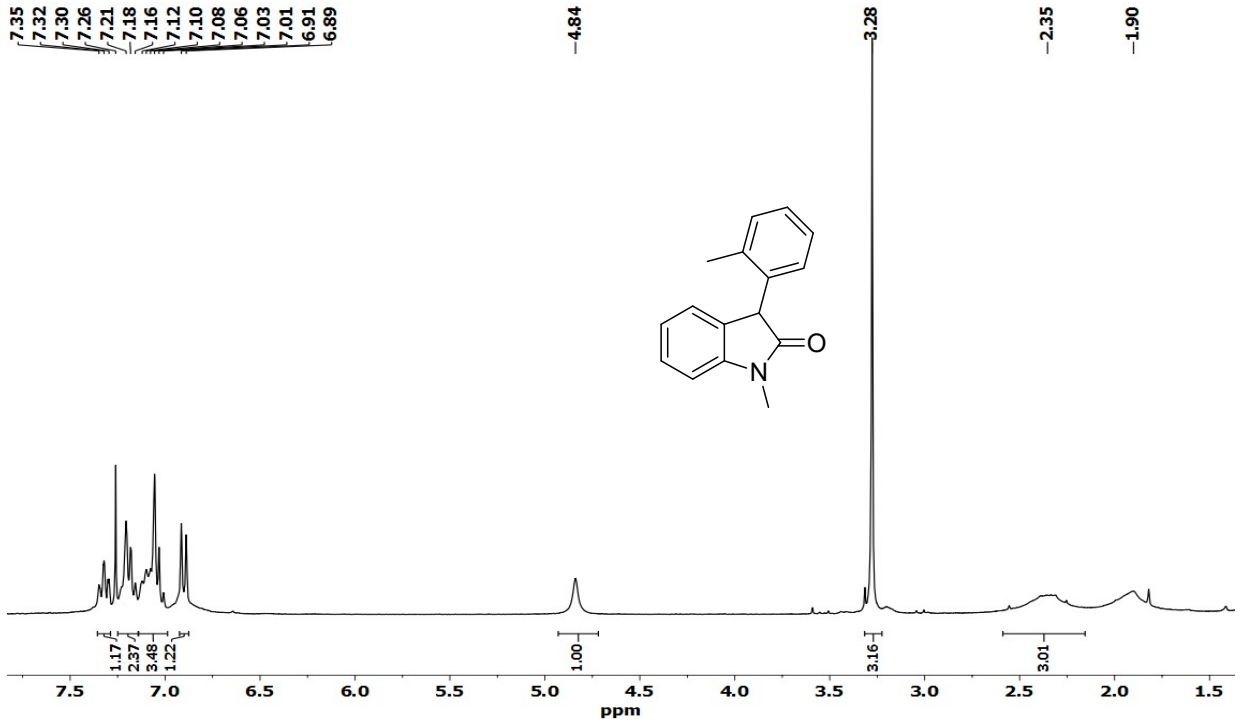


Figure S39. ^{1}H NMR spectrum of 1-methyl-3-(o-tolyl)indolin-2-one in $CDCl_3$.

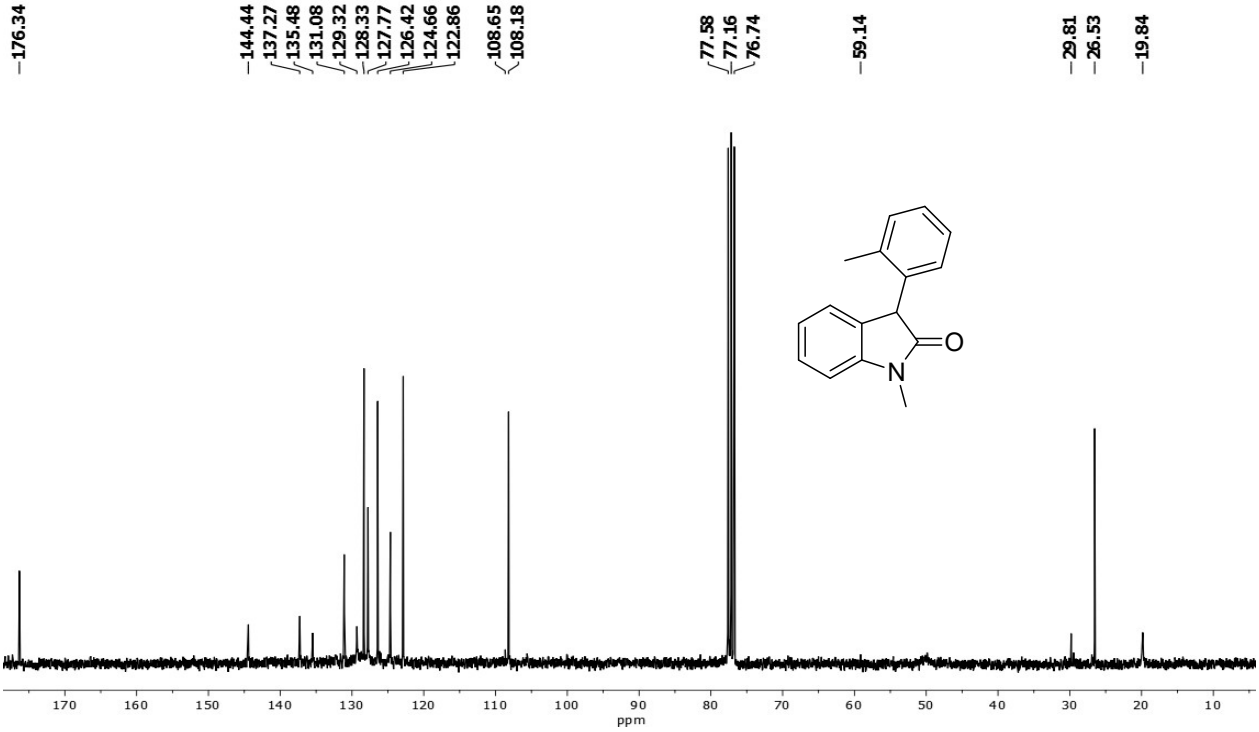


Figure S40. $^{13}C\{^{1}H\}$ NMR spectrum of 1-methyl-3-(o-tolyl)indolin-2-one in $CDCl_3$.

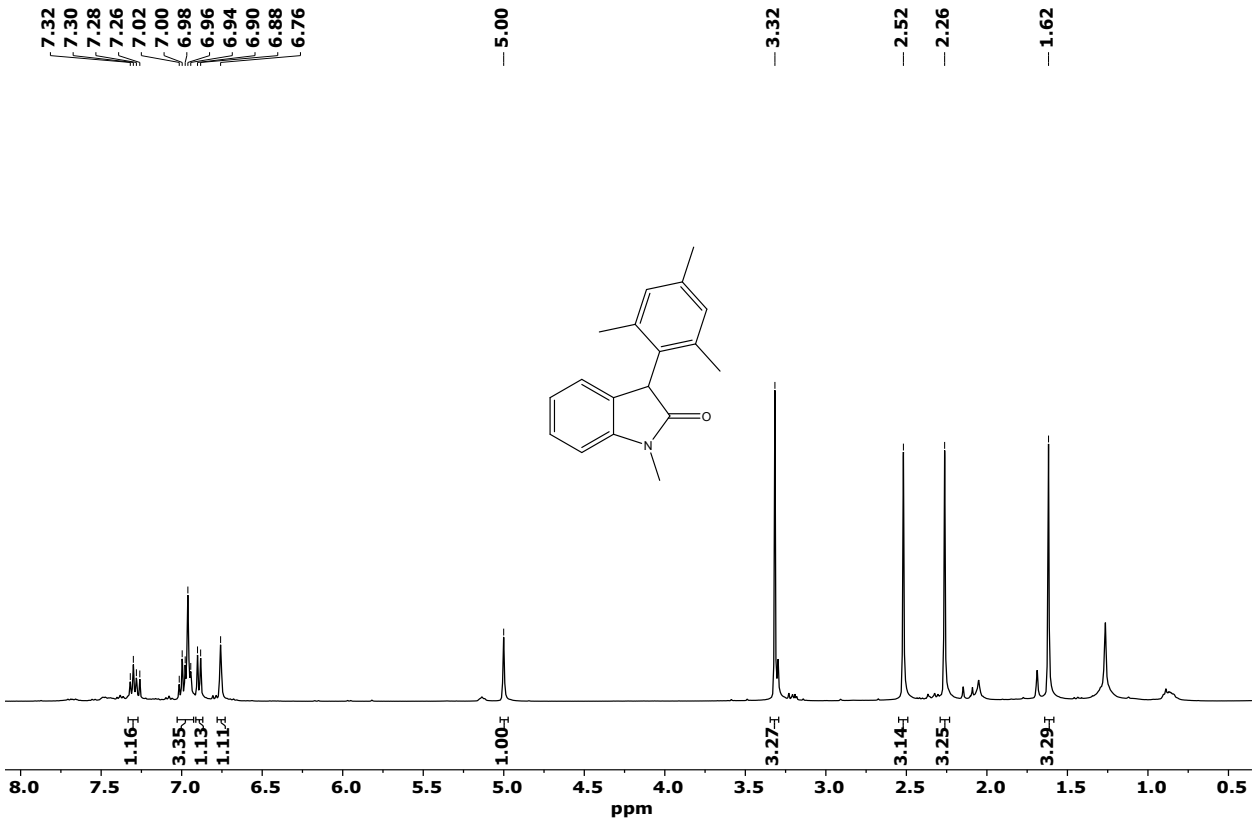


Figure S41. ^{1}H NMR spectrum of 3-mesityl-1-methylindolin-2-one in $CDCl_3$.

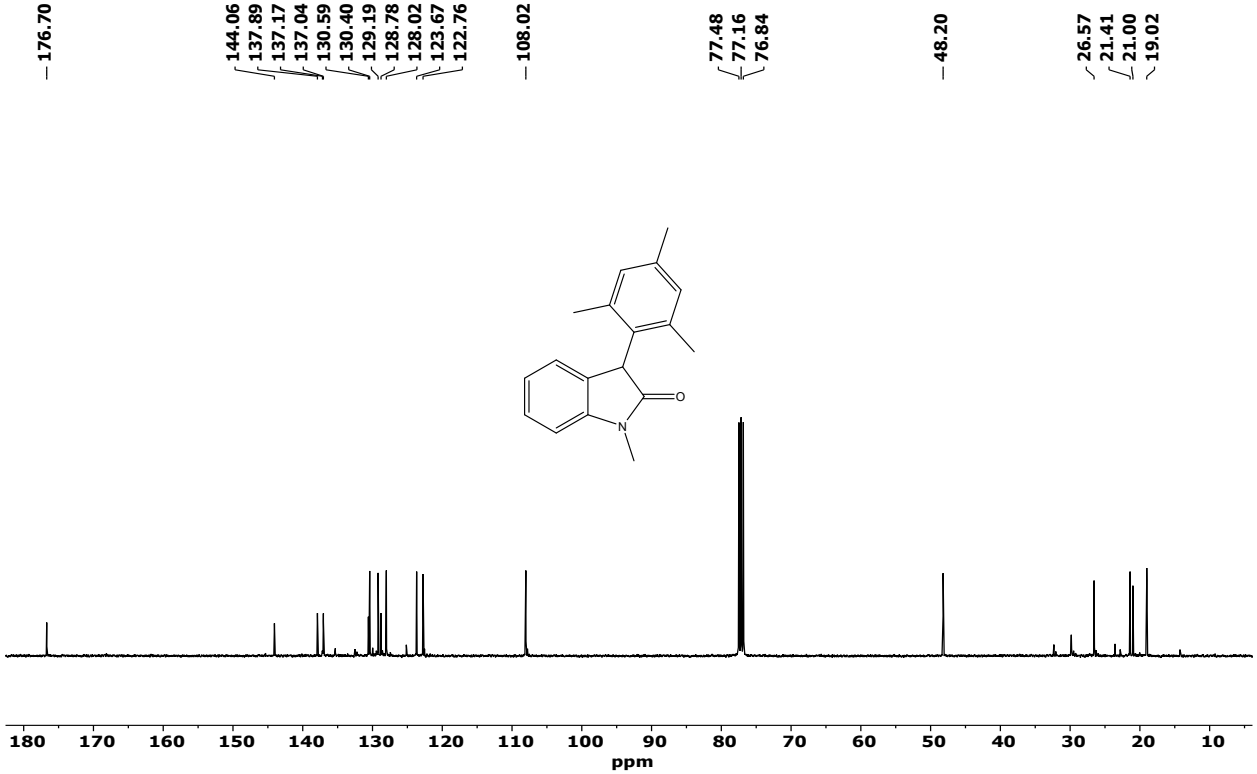


Figure S42. $^{13}C\{^{1}H\}$ NMR spectrum of 3-mesityl-1-methylindolin-2-one in $CDCl_3$.

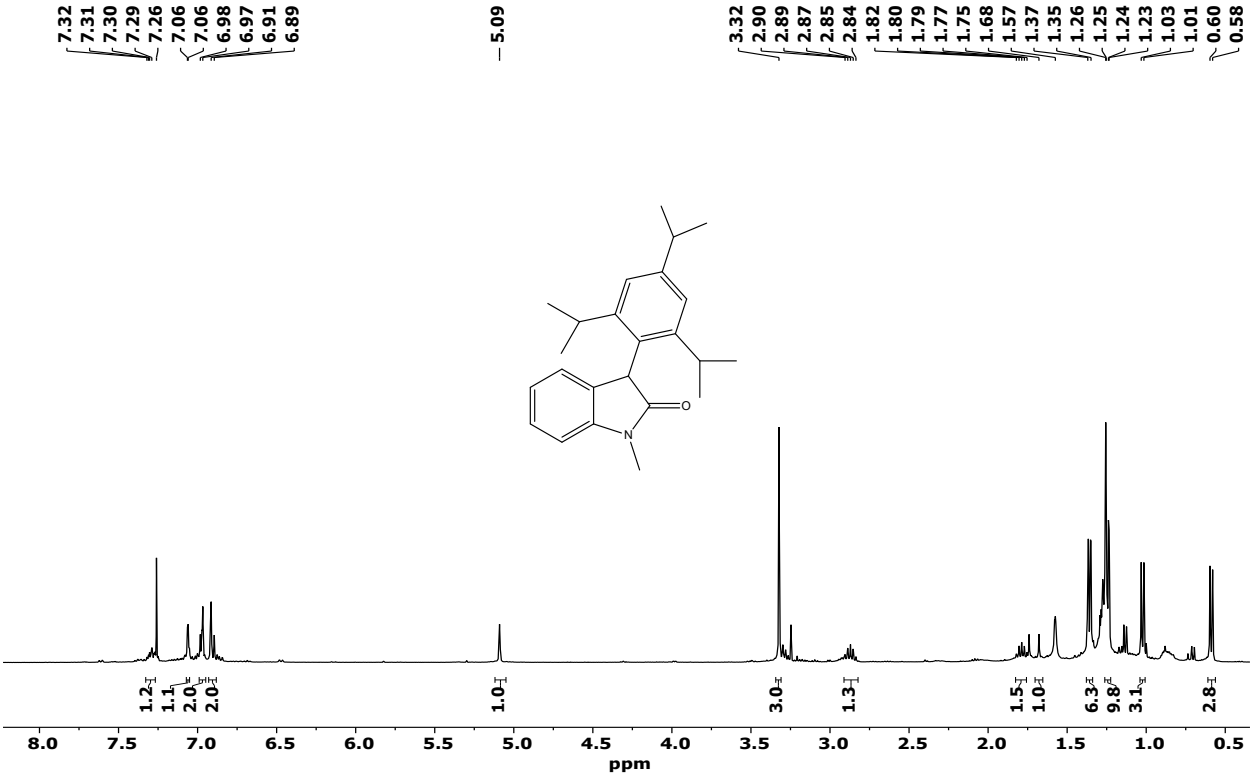


Figure S43. ^{1}H NMR spectrum of 1-methyl-3-(2,4,6-triisopropylphenyl)indolin-2-one in $CDCl_3$.

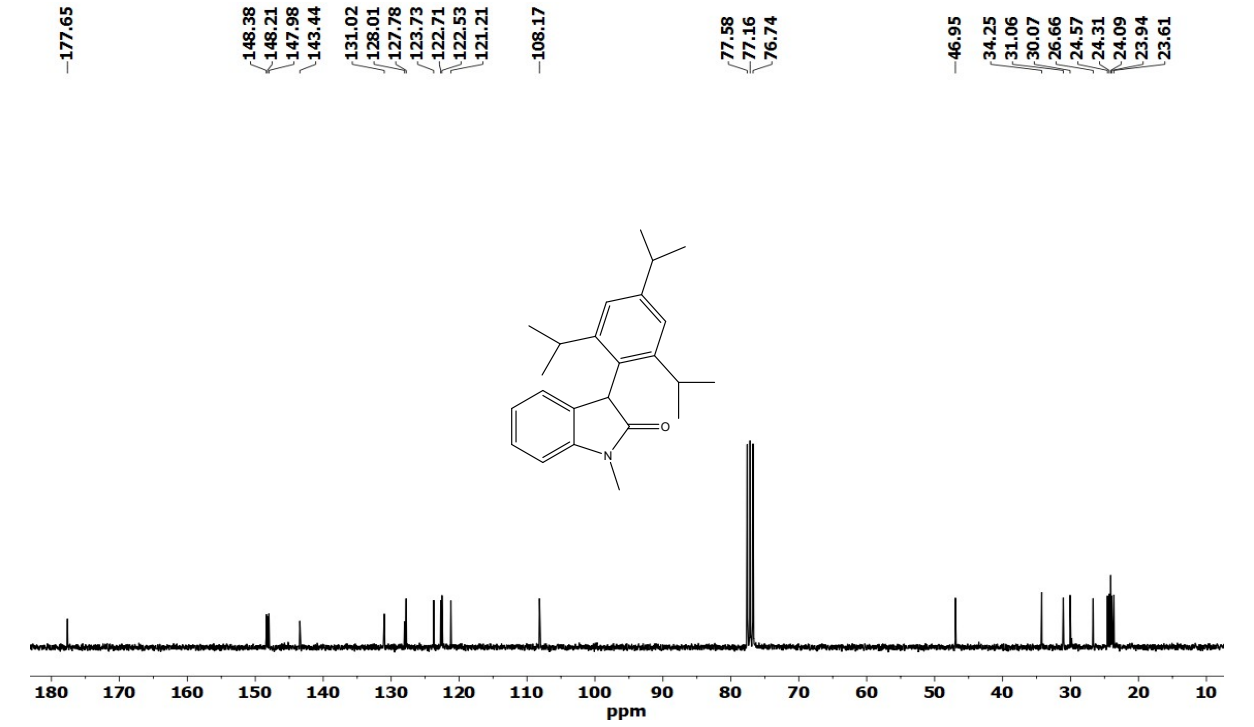


Figure S44. $^{13}C\{^{1}H\}$ NMR spectrum of 1-methyl-3-(2,4,6-triisopropylphenyl)indolin-2-one in $CDCl_3$.

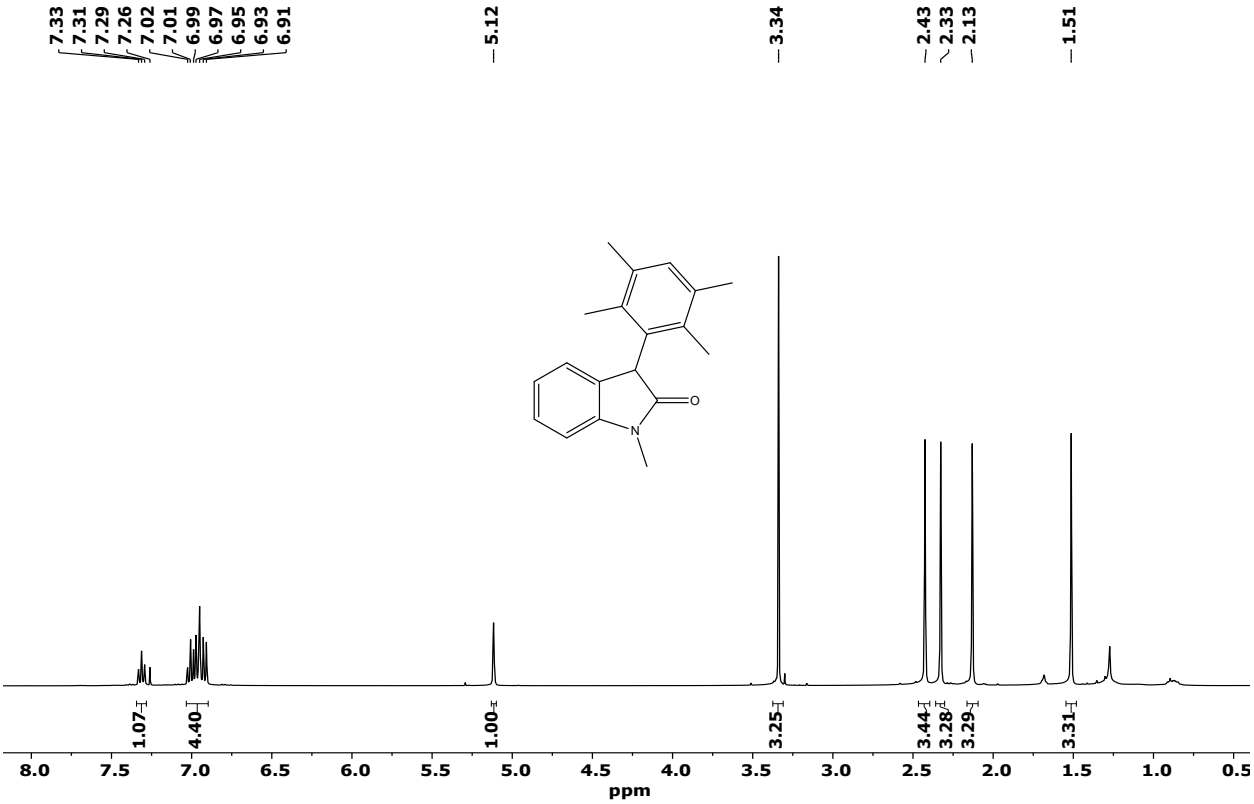


Figure S45. ^{1}H NMR spectrum of 1-methyl-3-(2,3,5,6-tetramethylphenyl)indolin-2-one in $CDCl_3$.

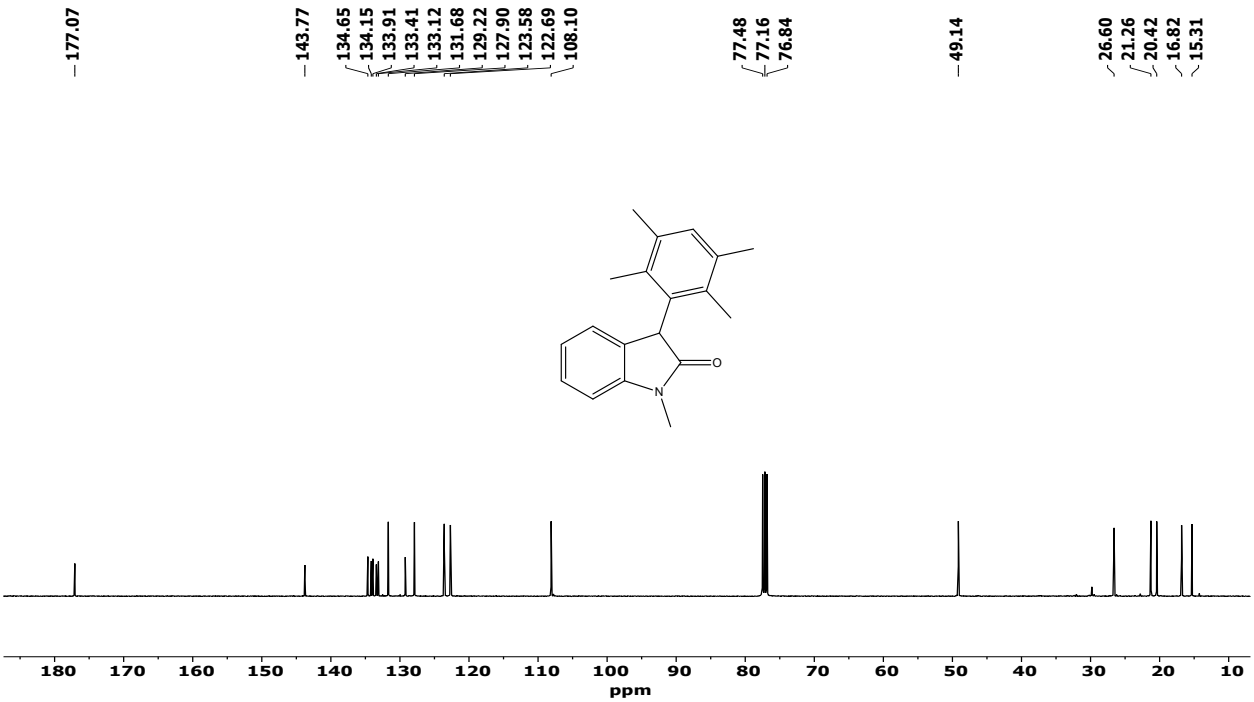


Figure S46. $^{13}C\{^{1}H\}$ NMR spectrum of 1-methyl-3-(2,3,5,6-tetramethylphenyl)indolin-2-one in $CDCl_3$.

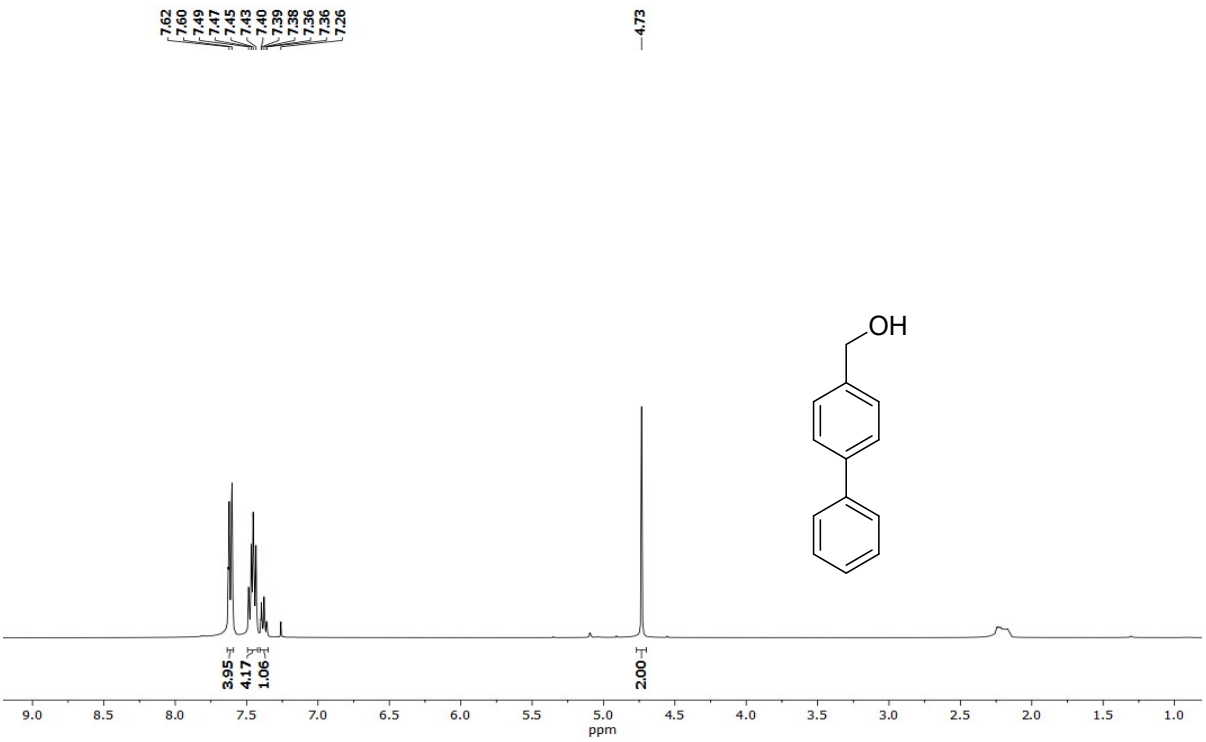


Figure S47. ^{1}H NMR spectrum of biphenyl-4-methanol in $CDCl_3$.

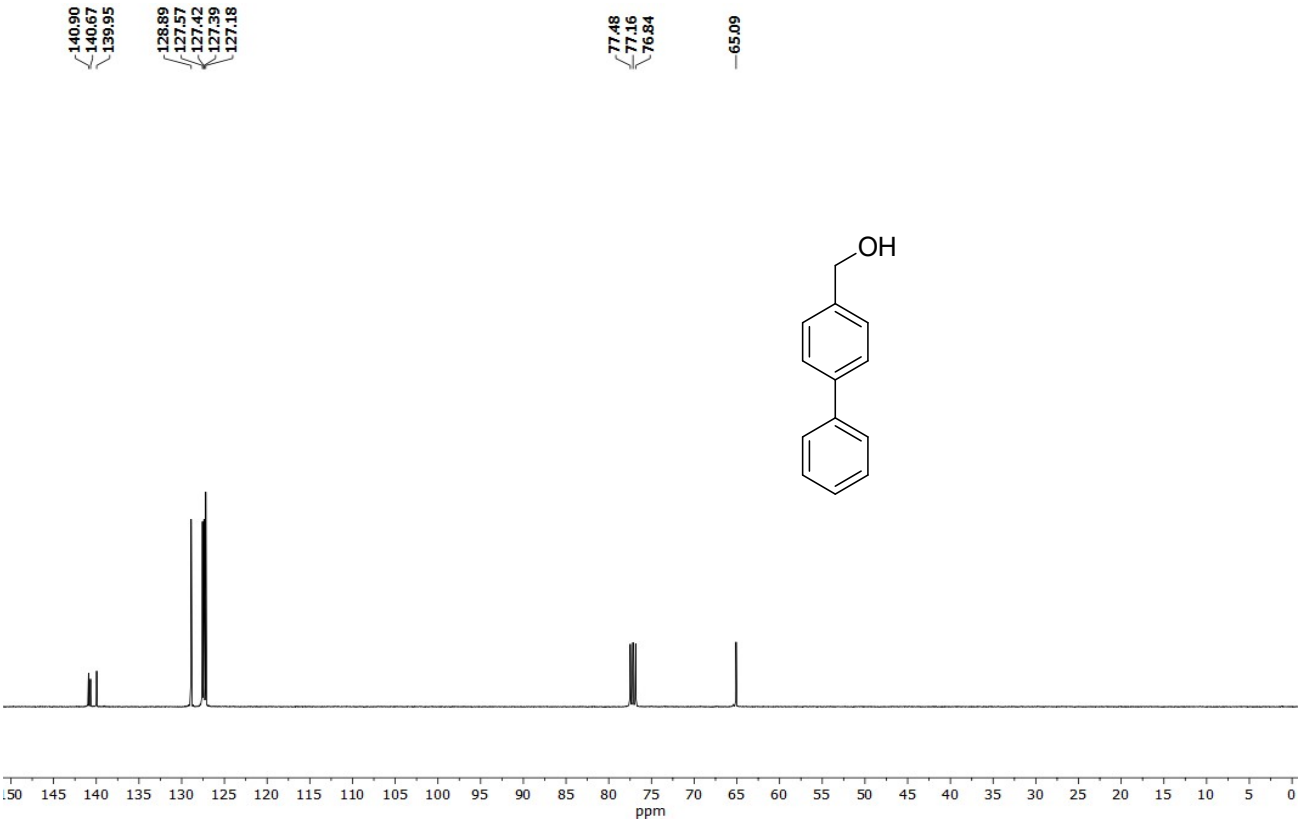


Figure S48. $^{13}C\{^{1}H\}$ NMR spectrum of biphenyl-4-methanol in $CDCl_3$.

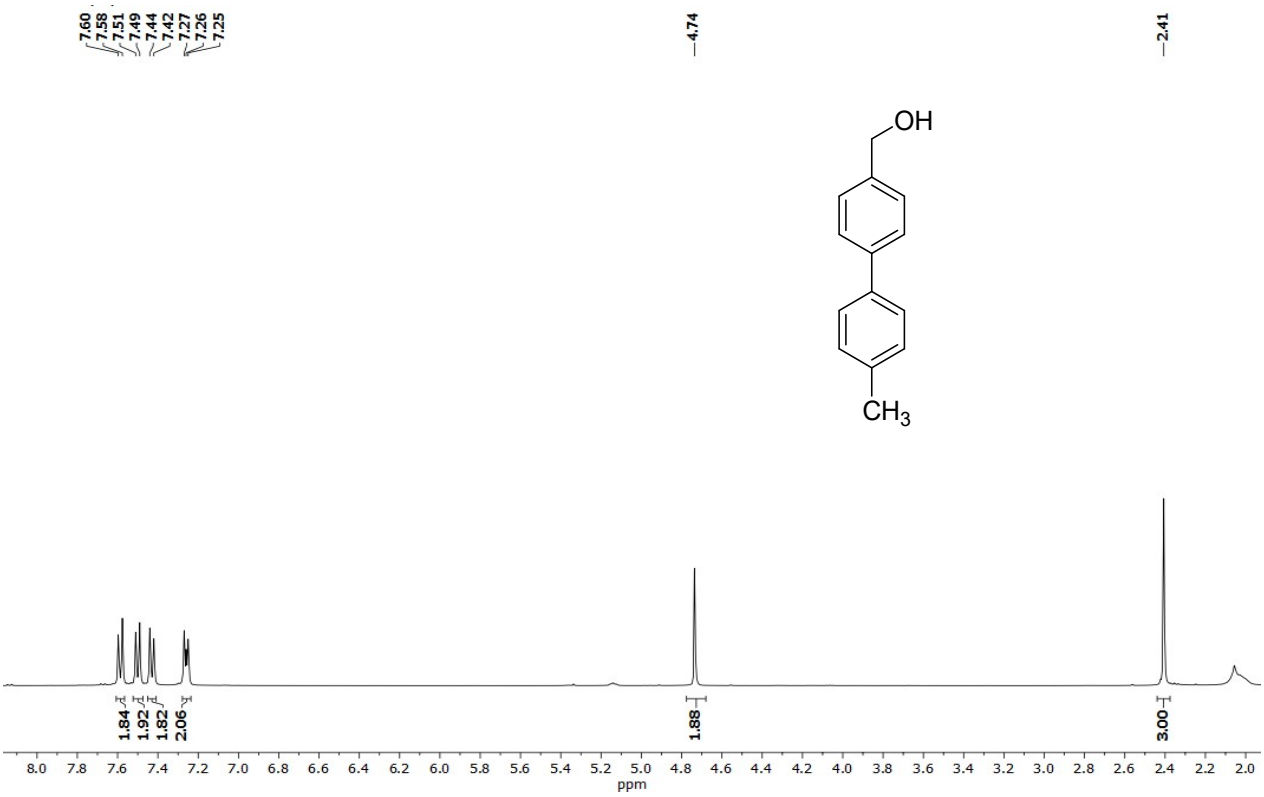


Figure S49. ^{1}H NMR spectrum of 4-(4-methylphenyl)phenylmethanol in $CDCl_3$.

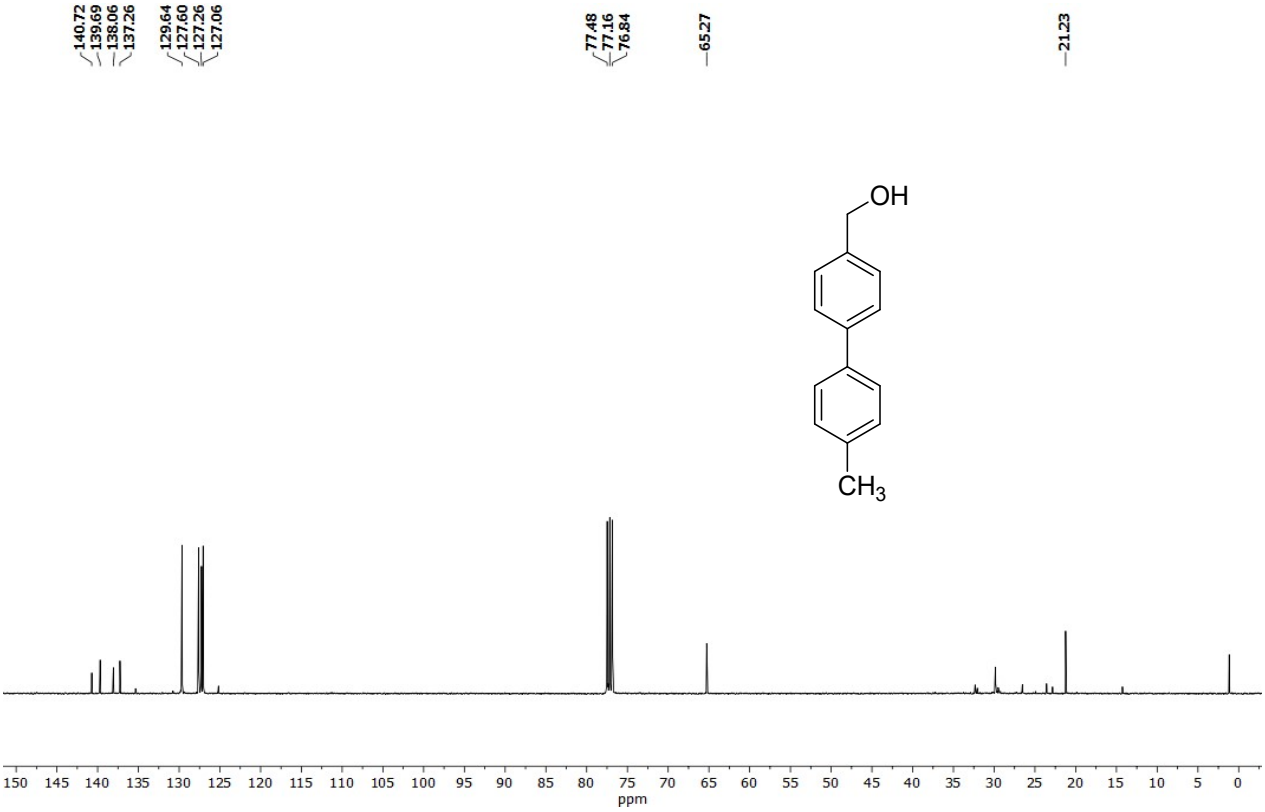


Figure S50. $^{13}C\{^{1}H\}$ NMR spectrum of 4-(4-methylphenyl)phenylmethanol in $CDCl_3$.

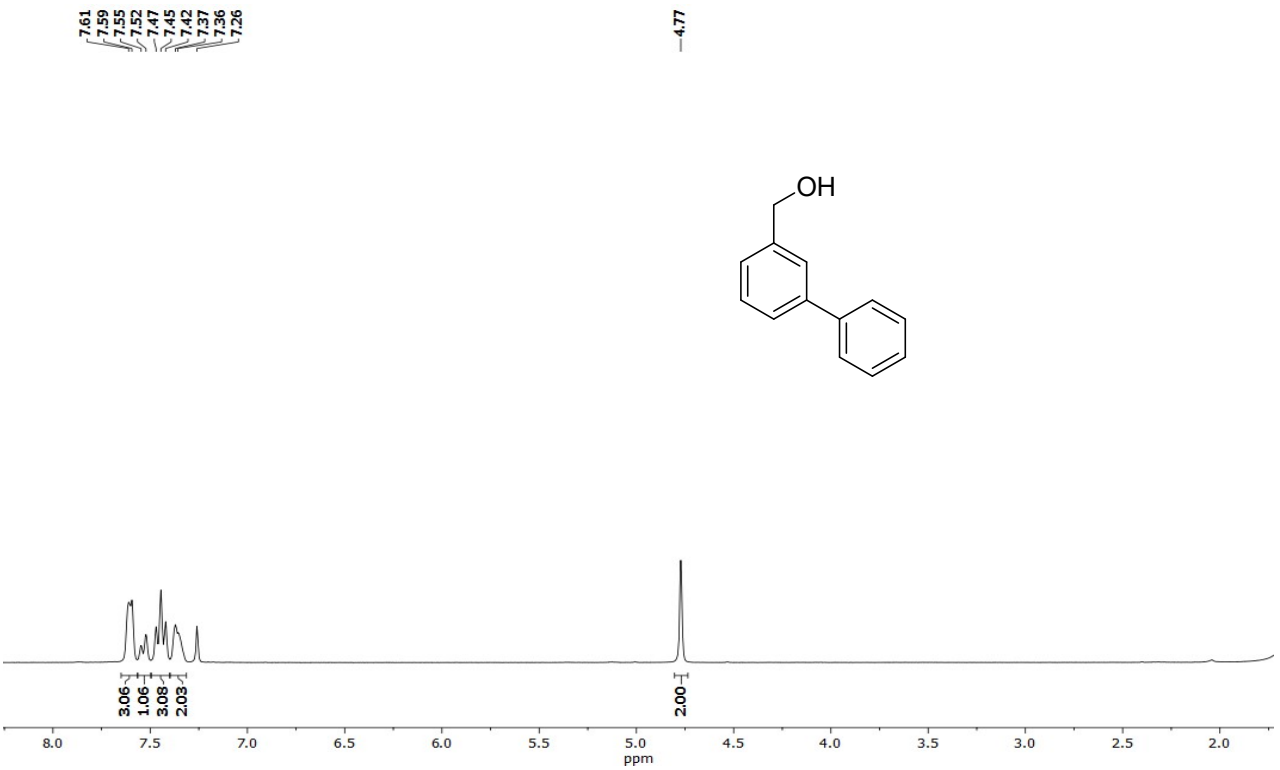


Figure S51. ^{1}H NMR spectrum of 3-biphenylmethanol in $CDCl_3$.

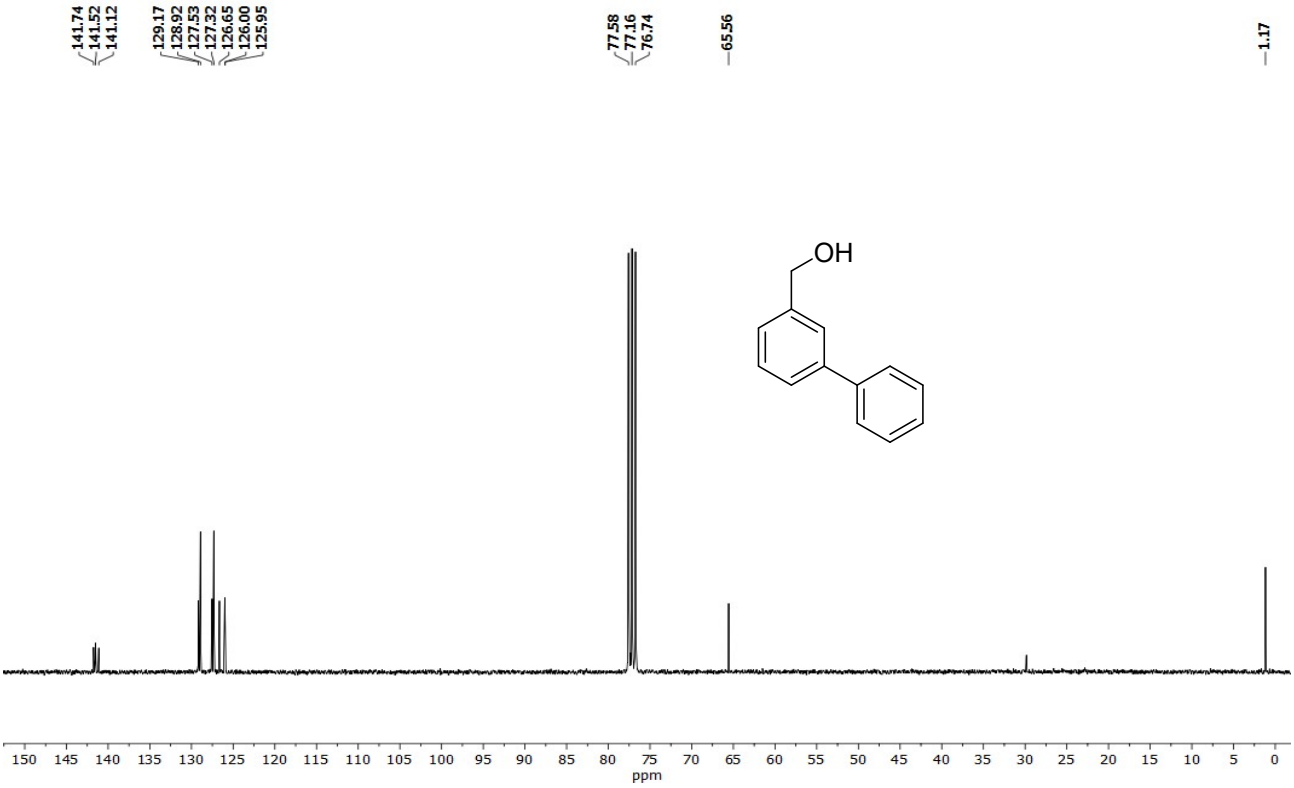


Figure S52. $^{13}C\{^{1}H\}$ NMR spectrum of 3-biphenylmethanol in $CDCl_3$.

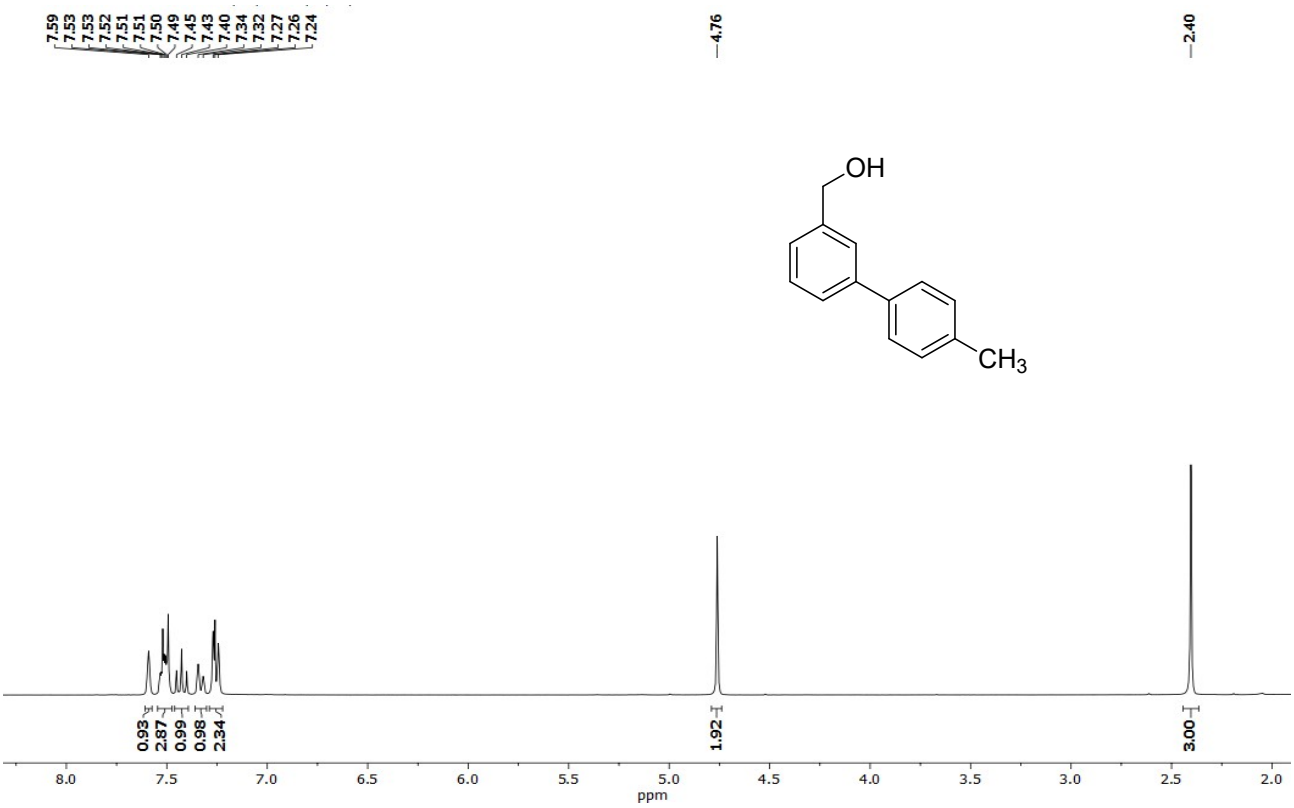


Figure S53. ^{1}H NMR spectrum of 3-(4-methylphenyl)phenylmethanol in $CDCl_3$.

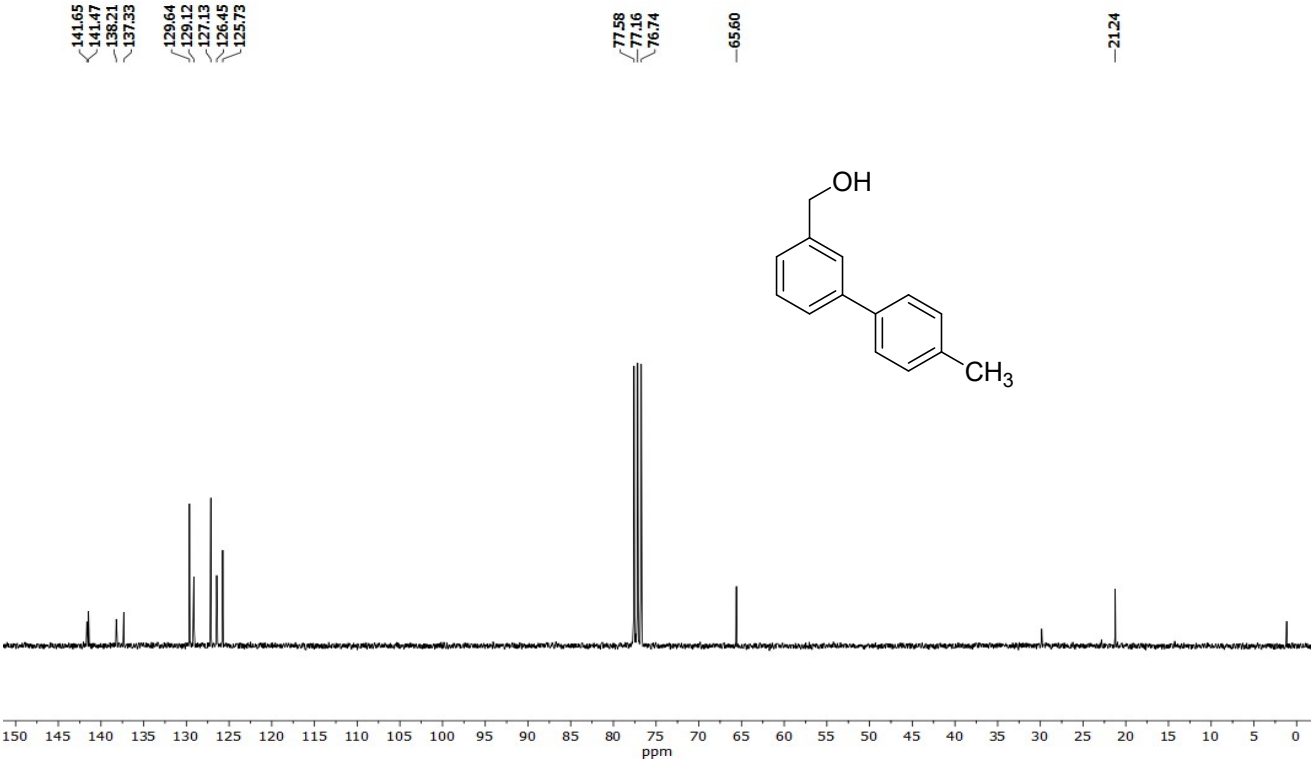


Figure S54. $^{13}C\{^{1}H\}$ NMR spectrum of 3-(4-methylphenyl)phenylmethanol in $CDCl_3$.

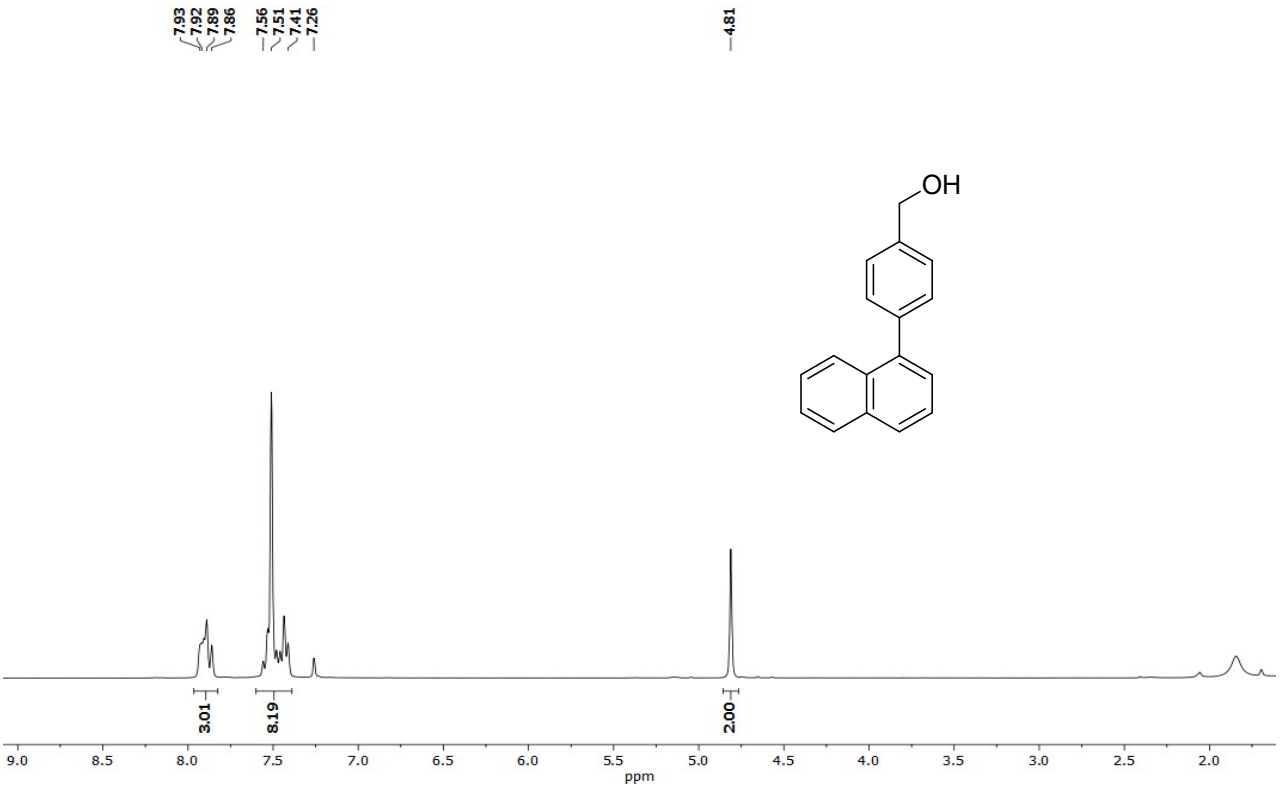


Figure S55. ^{1}H NMR spectrum of 4-(1-naphthalenyl)phenylmethanol in $CDCl_3$.

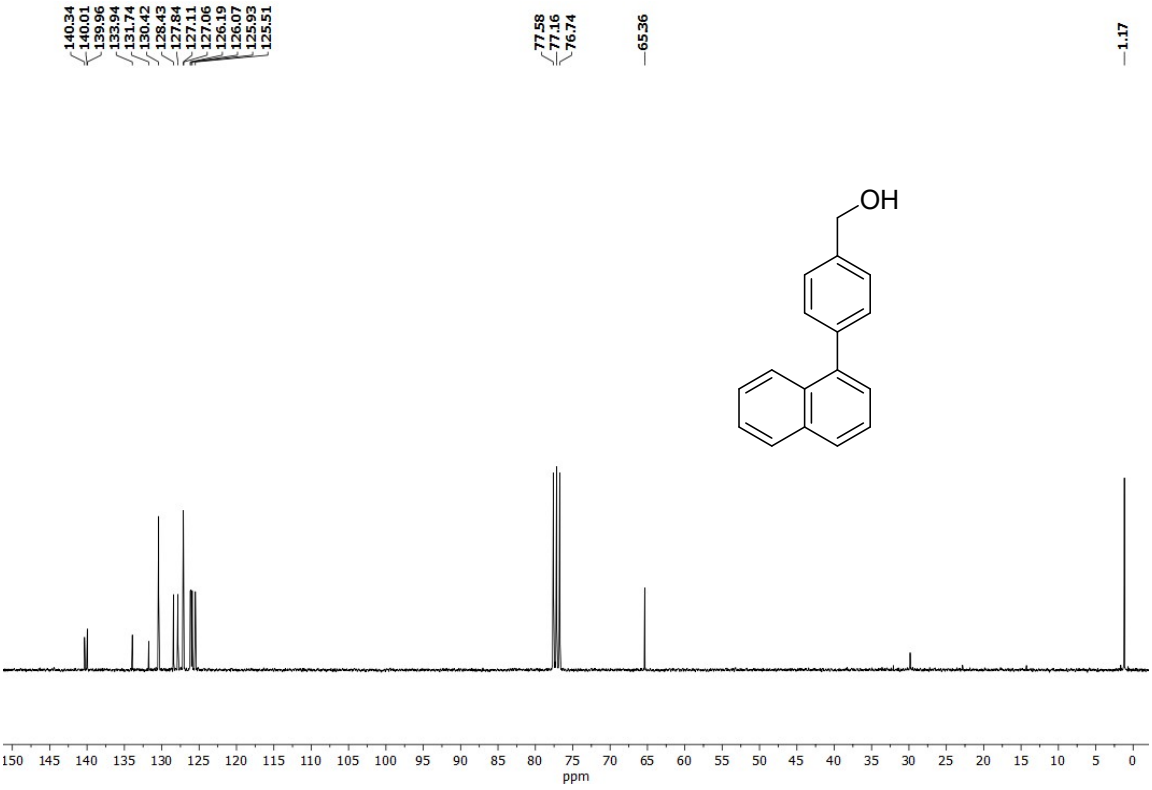


Figure S56. $^{13}C\{^{1}H\}$ NMR spectrum of 4-(1-naphthalenyl)phenylmethanol in $CDCl_3$.

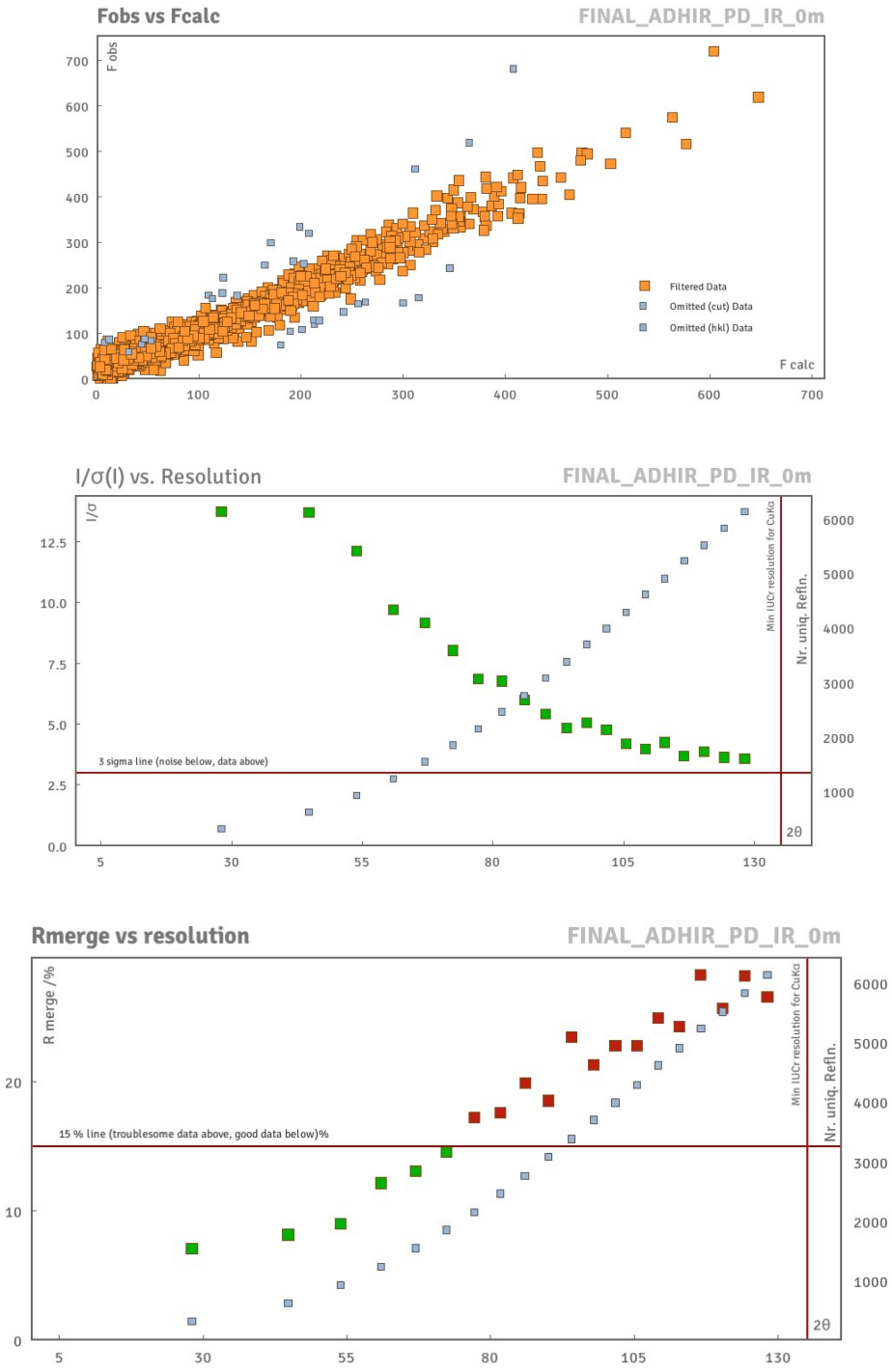


Figure S57. Diffraction and refinement data plots.

Table S1. Selected bond lengths in Å

Compound	**[3]**
Formula	$C_{35}H_{41}I_3IrN_7Pd$
$D_{calc.}$/ g cm^{-3}	2.174
m/mm^{-1}	30.011
Formula Weight	1239.05
Colour	clear orangish orange
Shape	block-shaped
Size/mm^3	0.21×0.12×0.10
T/K	100.00
Crystal System	monoclinic
Space Group	$P2_1/n$
a/Å	14.4972(6)
b/Å	16.5680(6)
c/Å	15.7790(6)
a/°	90
b/°	92.497(2)
g/°	90
V/Å^3	3786.4(3)
Z	4
Z'	1
Wavelength/Å	1.54178
Radiation type	CuK_a
Q_{min}/°	4.054
Q_{max}/°	65.080
Measured Refl's.	25748
Indep't Refl's	6340
Refl's I≥2 s(I)	5090
R_{int}	0.1388
Parameters	433
Restraints	404
Largest Peak	6.603
Deepest Hole	-2.608
GooF	1.079
wR_2 (all data)	0.2485
wR_2	0.2339
R_1 (all data)	0.1241
R_1	0.1010

Table S2. Selected bond lengths in Å

Atoms	[**3**]
Ir1 – I1	2.7114(15)
Ir1 – C11	1.975(18)
Ir1 – C19	2.052(17)
Pd1 – I2	2.603(2)
Pd1 – I3	2.579(2)
Pd1 – N7	2.106(17)
Pd1 – C24	1.94(2)
N1 – C12	1.36(2)
N3 – C11	1.39(2)
N6 – C24	1.37(3)
N4 – C23	1.34(2)

Table S3. Selected bond angles in °

Atoms	[**3**]
I1 – Ir1 – C19	92.3(5)
I1 – Ir1 – C11	92.3(6)
C11 – Ir1 – C19	85.5(7)
I2 – Pd1 – I3	175.51(8)
I2 – Pd1 – N7	91.1(4)
I2 – Pd1 – N6	90.9(5)
I2 – Pd1 – C24	89.1(6)
I3 – Pd1 – C24	89.1(6)
N7 – Pd1 – C24	176.3(7)
N3 – C11 – C12	100.9(15)
N1 – N2– N3	103.4(15)
N4 – N5 – N6	101.6(16)