Electronic Supplementary Material (ESI) for Analyst.

Supporting Information

Analysis of 1-aminoisoquinoline using the Signal Amplification by Reversible Exchange Hyperpolarization technique

Hye Jin Jeong,[a] Sein Min[b] and Keunhong Jeong*[a]

[a]Department of Chemistry, Korea Military Academy, Seoul 01805, South Korea

[b]Department of Chemistry, Seoul Women's University, Seoul 01797, South Korea

*Corresponding author: Keunhong Jeong

doas1mind@kma.ac.kr

Contents

1. List of figures

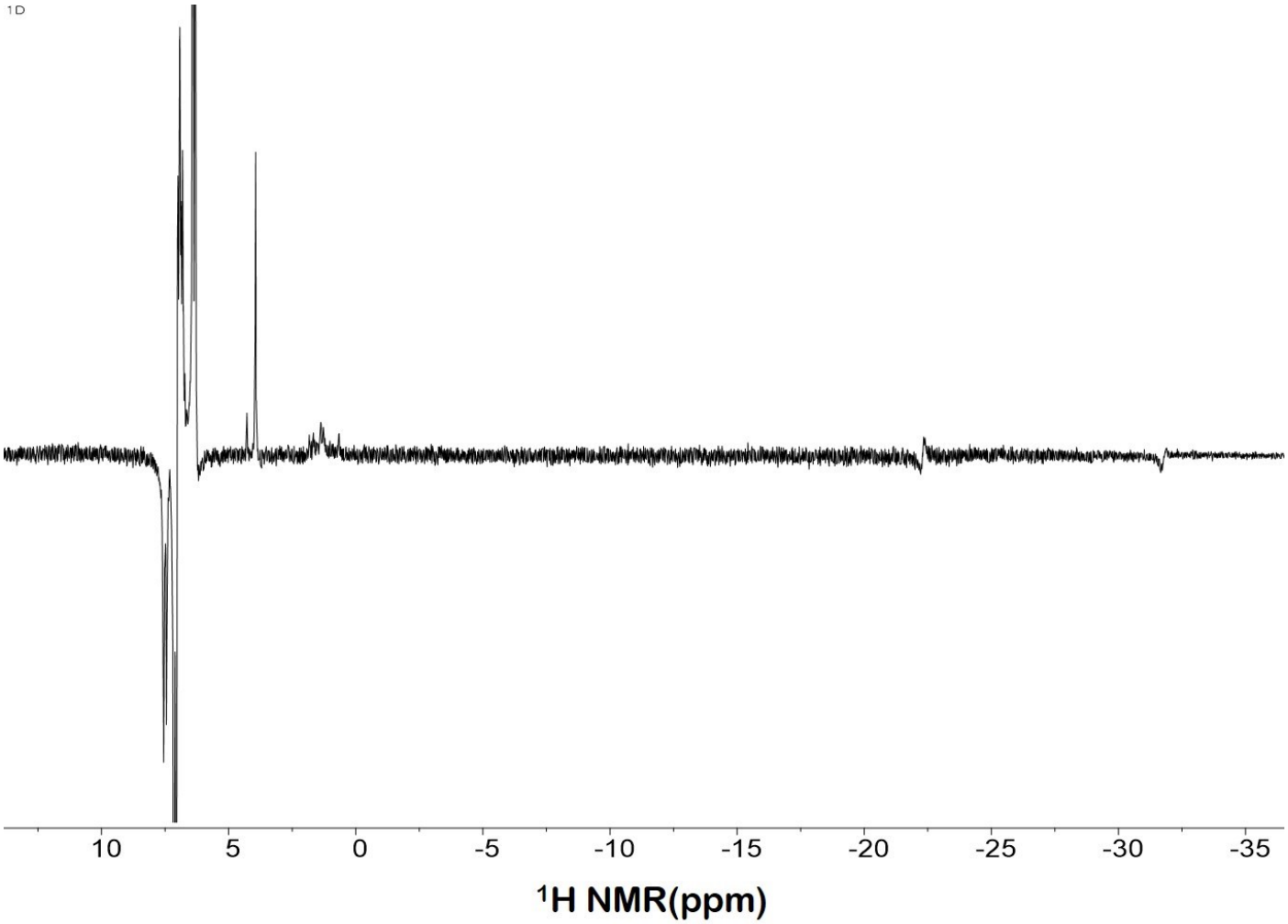

Figure S1 Hyperpolarized ^{1}H NMR spectrum at earth's magnetic field(0.65G) containing signal of hydride region.

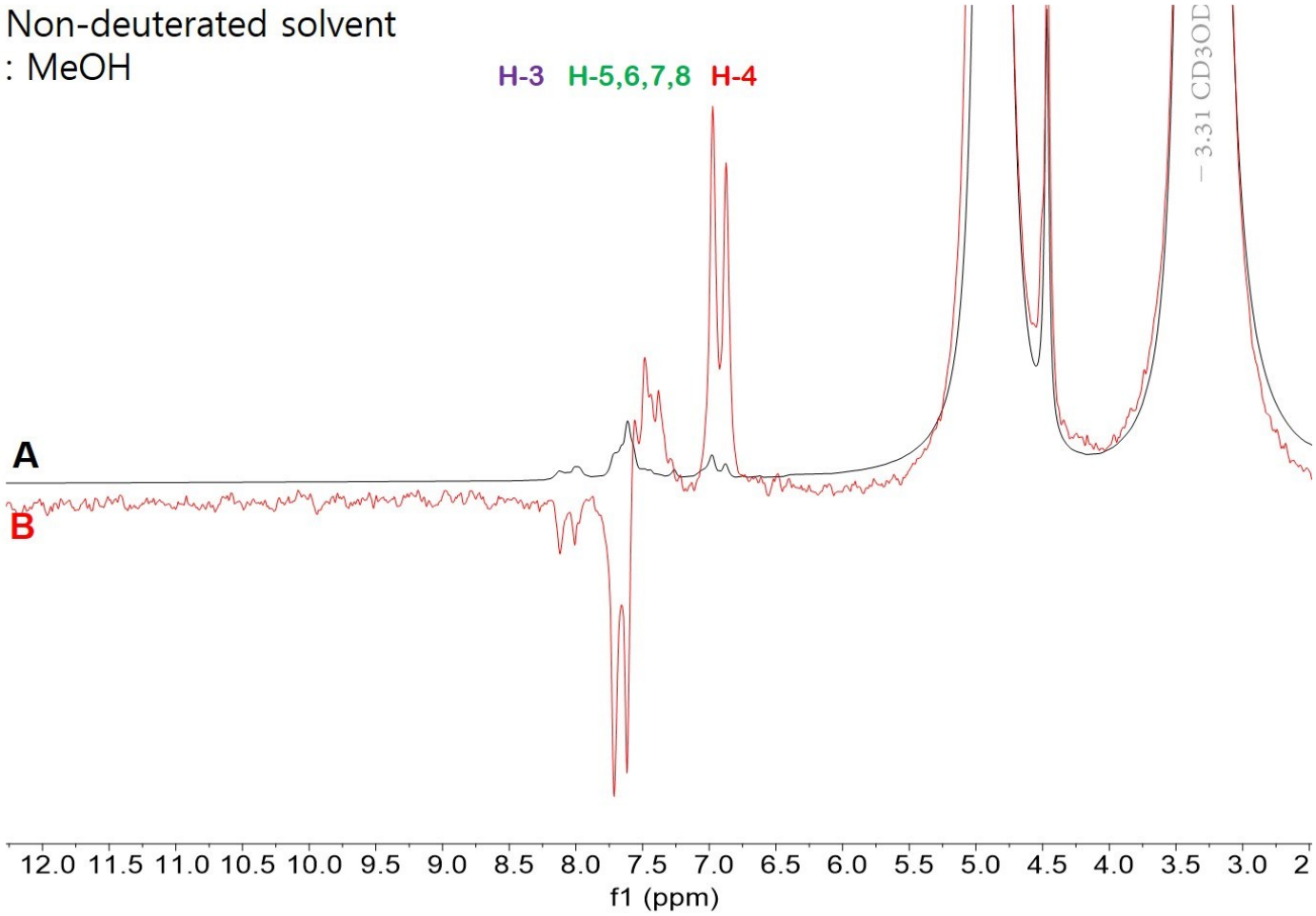

Figure S2 (A) Thermal ^{1}H NMR spectrum of the solution containing catalyst [Ir(IMes)(COD)Cl] (3.5mM) and 1-AIQ (35mM) in methanol; (B) Hyperpolarized ^{1}H NMR spectrum of the solution containing catalyst [Ir(IMes)(COD)Cl] (3.5mM), 1-AIQ (35mM) in methanol.

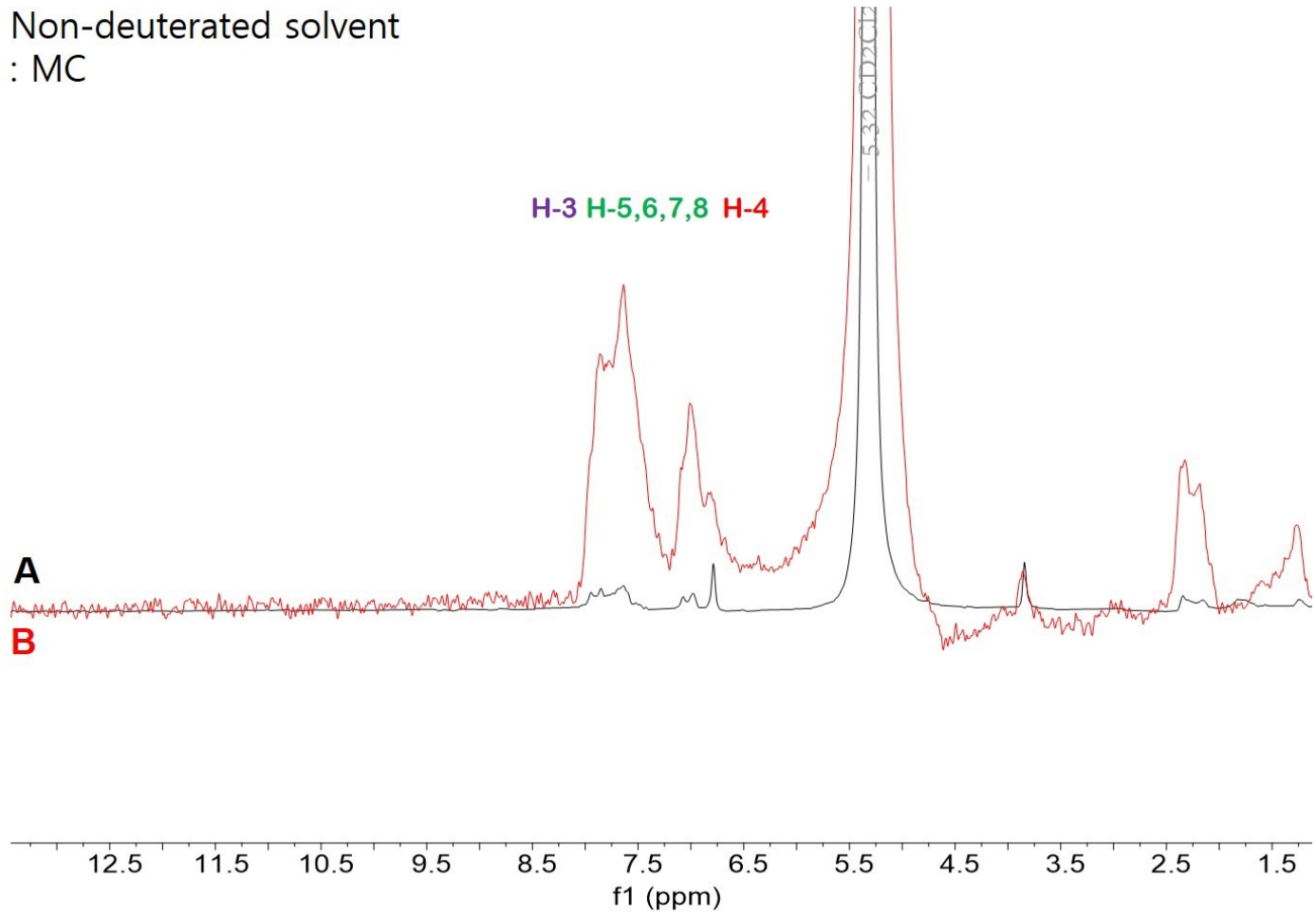

Figure S3 (A) Thermal ^{1}H NMR spectrum of the solution containing catalyst [Ir(IMes)(COD)Cl] (3.5mM) and 1-AIQ (35mM) in methylene chloride; (B) Hyperpolarized ^{1}H NMR spectrum of the solution containing catalyst [Ir(IMes)(COD)Cl] (3.5mM), 1-AIQ (35mM) in methylene chloride.

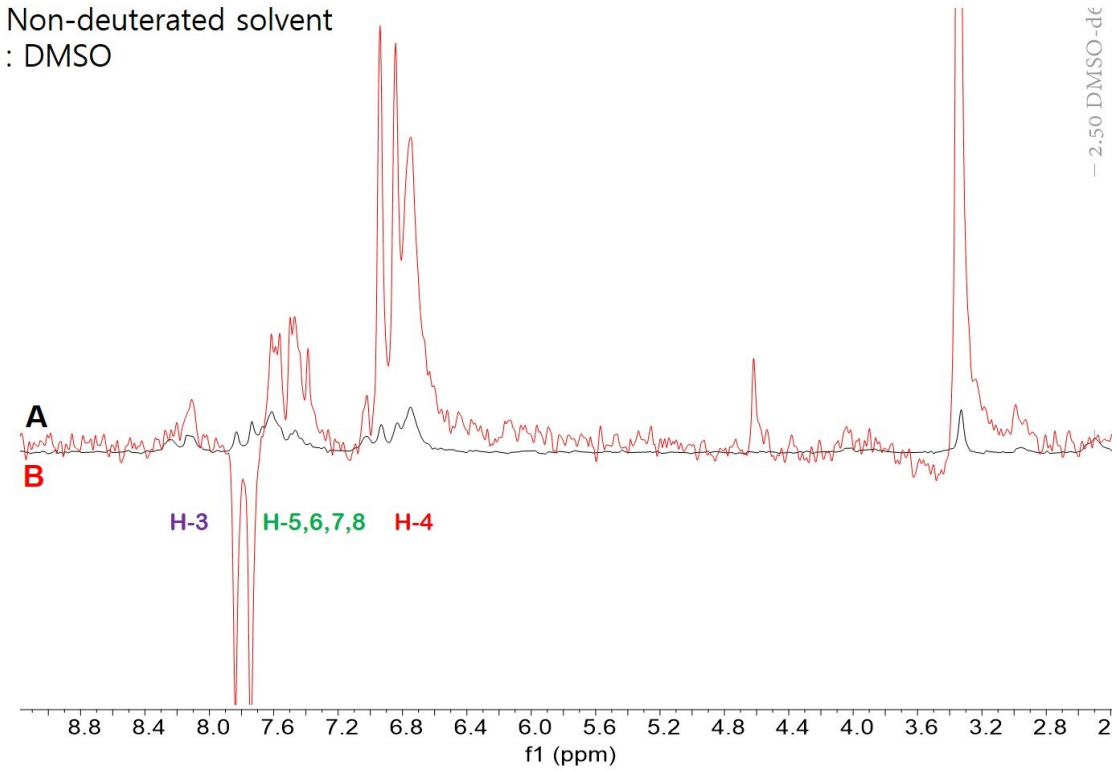

Figure S4 Thermal ^{1}H NMR spectrum of the solution containing catalyst [Ir(IMes)(COD)Cl] (3.5mM) and 1-AIQ (35mM) in dimethyl sulfoxide; (B) Hyperpolarized ^{1}H NMR spectrum of the solution containing catalyst [Ir(IMes)(COD)Cl] (3.5mM), 1-AIQ (35mM) in dimethyl sulfoxide.

Magnetic field G	NMR intensity % H-3	NMR intensity % H-5,6,7,8	NMR intensity % H-4
0.65	0.33	0.51	0.61
30	0.1	0.12	0.05
50	0.19	0.27	0.17
70	0.15	0.21	0.12
90	0.11	0.17	0.15

Figure S5 ^{1}H NMR enhancement levels of 1-AIQ with labeled protons versus the applied magnetic field for hyperpolarization.

Non-deuterated solvent in 0.65G	NMR intensity % H-4	NMR intensity % H-5,6,7,8	NMR intensity % H-3
MeOH	0.002	0.005	0.003
MC	0.002	0.01	0.008
DMSO	0.004	0.017	0.007

Figure S6 ^{1}H NMR enhancement levels of 1-AIQ with labeled protons for non-deuterated solvents, MeOH, MC, and DMSO, after SABRE in the presence of 0.65 G magnetic field.

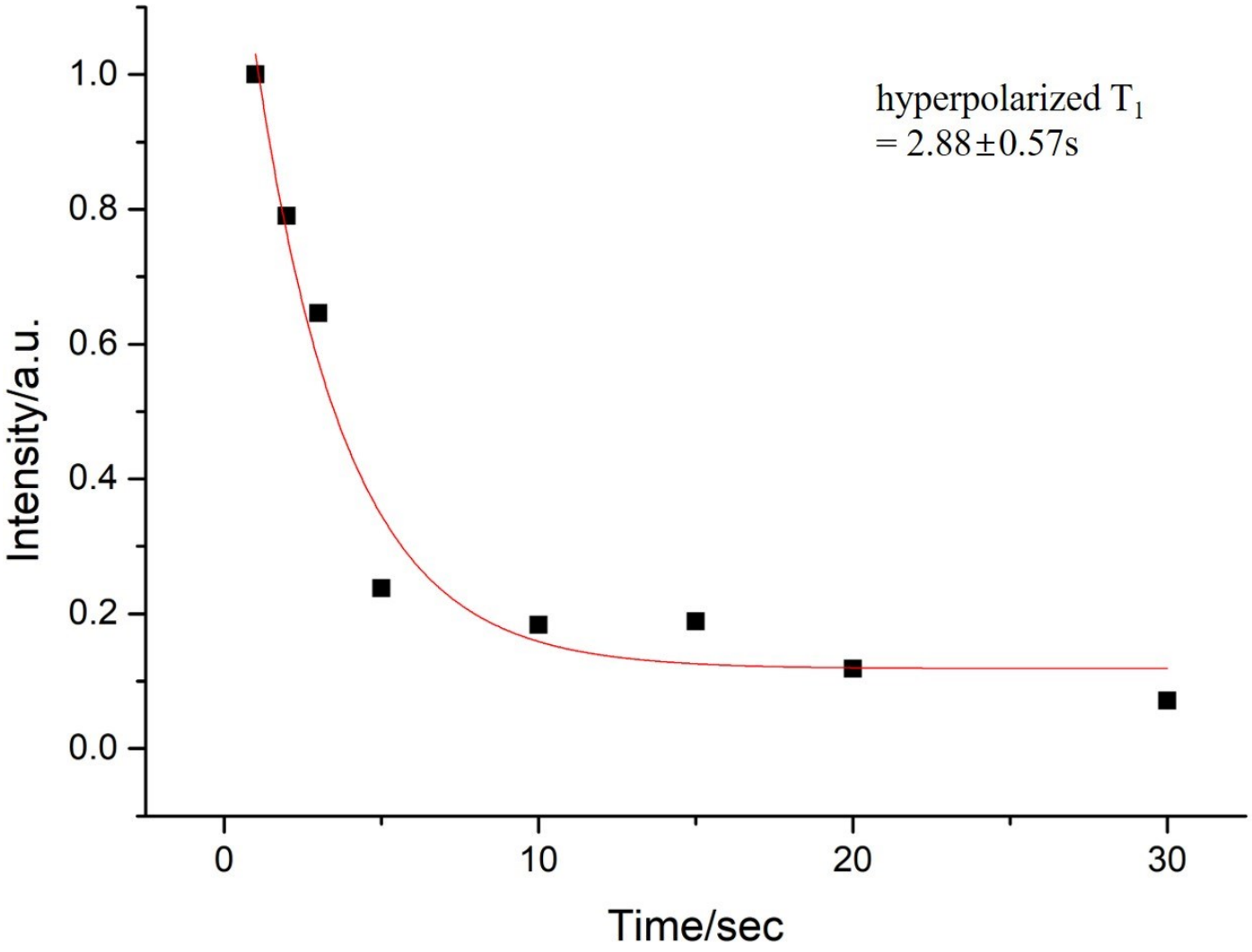

Figure S7 ; T_1 relaxation measurement of hyperpolarized 1-AIQ of 0.65 G magnetic field.

T_1 relaxation, as known as longitudinal relaxation, is the means by which the net magnetization indicates to the equilibrium over time, and can be calculated mathematically,

$y=A_1*exp(-x/T_1)+y_0$[1]

2.SABRE of pyridine

The SABRE experiments were done by the Ir catalyst [Ir(COD)(IMes)(Cl)] (2 mM) in methanol-d6 (0.9 mL for sampling NMR). Approximately 124 mM of pyridine (10 µL in 1mL methanol) was hyperpolarized by the polarization transfer.

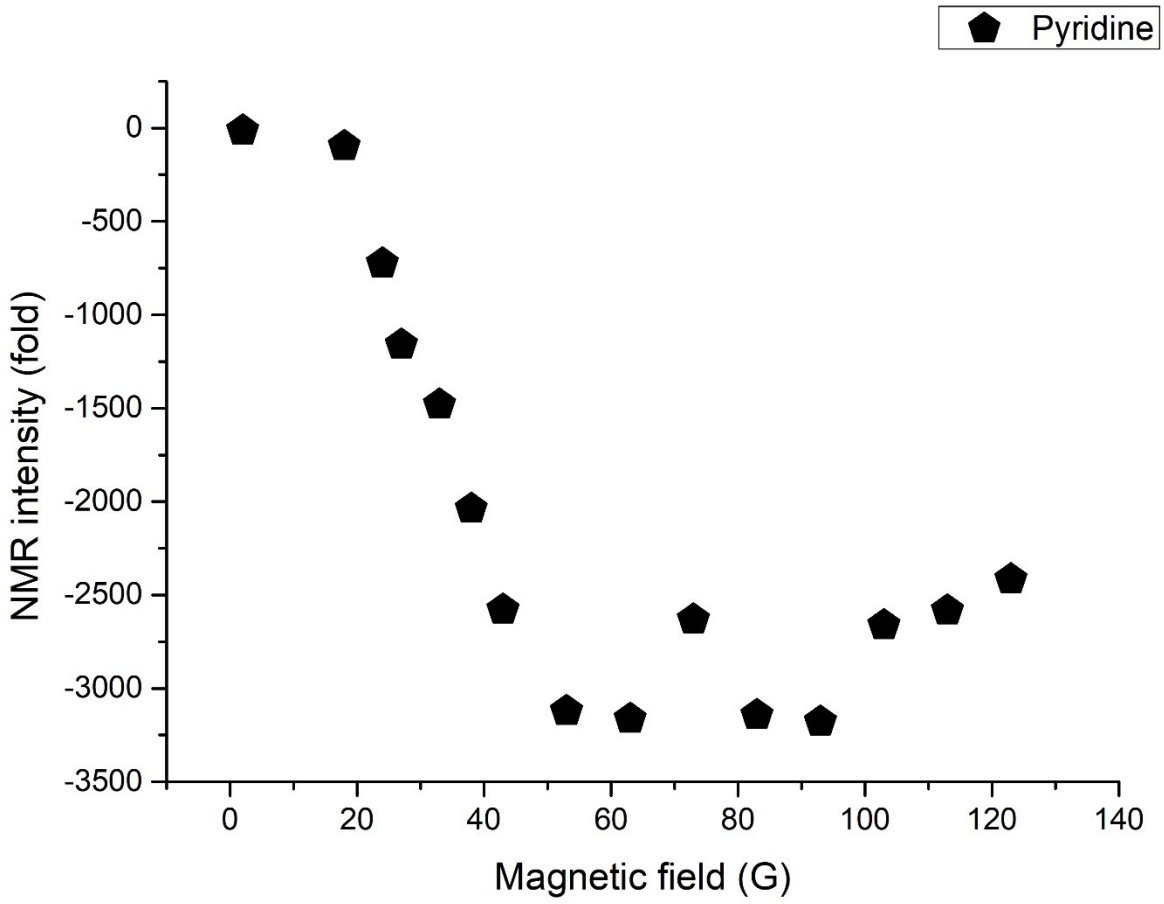

Figure S8 ^{1}H NMR intensity of pyridine in the presence of 0.65G magnetic field.

Table S1. J-coupling (Hz) between two hydrides and protons in substrate.

p-H_2	Ir-Py (Py-1), Hz					
	H-3	H-3'	H-4	H-4'	H-5	Aver.
H-1	1.47	-0.45	-0.55	-0.039	-1.6	-0.23
H-2	1.35	0.74	0.197	-0.3	-0.23	0.35

p-H_2	Ir-Py (Py-2), Hz					
	H-3	H-3'	H-4	H-4'	H-5	Aver.
H-1	0.88	0.65	0.19	-0.11	-0.43	0.24
H-2	1.58	-0.51	-0.5	0.033	-0.79	-0.04

p-H_2	Ir-1-AIQ (1-AIQ-1), Hz						
	H-3	H-4	H-5	H-6	H-7	H-8	Aver.
H-1	1.94	0.19	-0.045	-0.24	-0.29	-0.29	0.21
H-2	1.34	0.09	-0.29	-0.29	-0.26	-0.26	0.06

p-H_2	Ir-1-AIQ (1-AIQ-2), Hz						
	H-3	H-4	H-5	H-6	H-7	H-8	Aver.
H-1	0.92	-0.1	-0.31	-0.36	-0.21	-0.24	-0.05
H-2	0.21	-0.28	-0.27	-0.2	-0.25	0.07	-0.12

3.Optimized molecular structure of Ir-Py

Ir	-0.04011900	0.51185000	-0.22155800
C	0.55244200	4.69312500	-2.40652100
C	0.09521000	3.56030300	-3.16606800
C	-0.41932000	2.44514100	-2.52565100
N	-0.35958700	2.33494800	-1.07411700
C	-0.16795100	3.54883700	-0.33396500
C	0.32721600	4.67422500	-0.95932400
H	0.93648000	5.59003900	-2.89910900
H	0.09529500	3.58857100	-4.26104300
H	-0.86193900	1.59048500	-3.04098500
H	-0.38924800	3.50382300	0.73461200
H	0.51153200	5.57347300	-0.36136100
C	-2.96568300	1.61967200	3.70078000
C	-3.31008000	2.01038800	2.36623100
C	-2.48988200	1.65221500	1.29424500
N	-1.30093500	0.93095000	1.46585400

C	-0.99275900	0.51128600	2.76830900
C	-1.78601900	0.83728600	3.87415000
H	-3.58801400	1.90504100	4.55359600
H	-4.21665500	2.59102200	2.16734100
H	-2.73443200	1.92514000	0.26497700
H	-0.10375500	-0.11928700	2.86767500
H	-1.48892000	0.47858000	4.86554400
H	-1.41392600	0.20210100	-0.99936500
H	0.86637900	0.14797800	-1.51688000
C	-0.89421300	-3.67640100	0.03284300
C	0.49368000	-3.72484100	-0.02543500
H	-1.62229000	-4.47949400	0.10388000
H	1.17012700	-4.57482200	0.00081900
C	-0.12457900	-1.49190000	-0.11248600
N	-1.27631500	-2.33653900	-0.05491100
N	0.95859600	-2.41525200	-0.15509300
C	-2.67558000	-1.94012400	-0.14741300
C	-3.48222700	-1.96405800	1.02424400
C	-3.22115900	-1.65620400	-1.43971800
C	-4.84893500	-1.61184400	0.89016800
C	-4.58928000	-1.31066800	-1.51380500
C	-5.42008200	-1.26971900	-0.36108800
H	-5.47990100	-1.60754700	1.78763700
H	-5.02471700	-1.08973000	-2.49665800
C	2.37966200	-2.12331000	-0.31985900
C	2.91909200	-2.10434800	-1.63752800
C	3.19611000	-1.99270600	0.83805900
C	4.31636600	-1.91085600	-1.77287200
C	4.58748100	-1.81374000	0.64637700
C	5.16854600	-1.77061400	-0.64714300
H	4.74966300	-1.88913600	-2.78080400
H	5.23136200	-1.70803500	1.52837100
C	-2.93989000	-2.39055600	2.37929600
H	-1.86042800	-2.19275700	2.48112300
H	-3.45889400	-1.85510600	3.19203400
H	-3.10196700	-3.47449900	2.54436900
C	-2.39752800	-1.80887600	-2.70909700
H	-2.95991700	-1.44348600	-3.58465800
H	-1.44290300	-1.25488500	-2.65654700
H	-2.14958700	-2.87266400	-2.89516300
C	-6.88295300	-0.87601400	-0.47613400
H	-7.43240200	-1.06726900	0.46120100
H	-6.98592900	0.20117800	-0.71185600
H	-7.38712000	-1.43254100	-1.28766500
C	2.60734700	-2.03490000	2.23842000
H	3.40516500	-2.02350500	2.99931500
H	1.95915800	-1.15628000	2.41801100
H	1.99242200	-2.93882600	2.40742300
C	2.04511000	-2.31123300	-2.86440500
H	1.21653400	-1.57954400	-2.90129400

H	2.63671200	-2.20313200	-3.78866100
H	1.59080800	-3.32092400	-2.87585200
C	6.67102000	-1.61596200	-0.82076500
H	6.92470900	-1.15892000	-1.79328500
H	7.11151500	-0.99459000	-0.02103900
H	7.17350100	-2.60229100	-0.78137600
C	4.14190600	2.64432100	1.60853000
C	4.07615800	2.06812500	0.31112400
C	2.91190600	1.41123300	-0.10893900
N	1.78116900	1.28714800	0.70293600
C	1.84927000	1.87041300	1.96533700
C	2.98667200	2.53537700	2.43811000
H	4.92581600	2.12489600	-0.37655500
H	2.83909300	0.96215300	-1.10047600
H	0.94691600	1.81071100	2.57790500
H	2.96721600	2.97297400	3.44130300
H	5.04054100	3.16357300	1.95453200

4.Optimized molecular structure of Ir-1-AIQ

Ir	0.46888400	-0.06586000	-0.44091900
H	0.26408800	0.04170200	-2.03712600
H	2.00413100	-0.36851900	-0.76176700
C	0.89381300	-4.23867000	-1.32667600
C	-0.44448300	-4.26757000	-1.01438100
H	1.56834300	-5.02516400	-1.65191900
H	-1.16455700	-5.08061300	-1.02490800
C	0.27763700	-2.06316500	-0.73475100
N	1.32752200	-2.90680700	-1.16613300
N	-0.81808100	-2.95174300	-0.65563400
C	2.69038200	-2.53132400	-1.53473200
C	2.94259200	-2.13935000	-2.88083400
C	3.74092200	-2.68080200	-0.58639100
C	4.27850000	-1.83634900	-3.24565900
C	5.05921200	-2.37144600	-1.00269700
C	5.35097300	-1.94327900	-2.32344600
H	4.48725800	-1.53161800	-4.27933400
H	5.87822100	-2.47743900	-0.27972000
C	-2.23017500	-2.64629400	-0.43607000
C	-2.85525700	-2.99995400	0.79064900
C	-2.98548700	-2.16613900	-1.54830800
C	-4.25185300	-2.77280900	0.91363000
C	-4.37085200	-1.95108600	-1.37106900
C	-5.02364300	-2.23284600	-0.14163500
H	-4.74704100	-3.04709600	1.85451300
H	-4.95928500	-1.57652300	-2.21807000
C	1.82461500	-2.05325000	-3.90700600

H	1.04735100	-1.32950400	-3.59565600
H	2.21551600	-1.74102400	-4.89023300
H	1.31880600	-3.02851900	-4.04082100
C	3.47410400	-3.15291000	0.83245500
H	2.92773200	-4.11473600	0.85077800
H	4.41892700	-3.29158900	1.38430100
H	2.86010900	-2.42135600	1.38785100
C	6.78192600	-1.65213400	-2.74856400
H	6.81853000	-1.02587000	-3.65700100
H	7.34563300	-1.13502100	-1.95116200
H	7.32446500	-2.59116500	-2.97353400
C	-2.34052400	-1.95376200	-2.90689700
H	-1.96907400	-2.90978500	-3.32554900
H	-3.06475100	-1.53159600	-3.62340100
H	-1.47494700	-1.27023300	-2.84375000
C	-2.11679700	-3.64600200	1.95560000
H	-1.12076300	-4.02639500	1.67310100
H	-1.98901000	-2.93076100	2.79137900
H	-2.69777300	-4.49886900	2.35120400
C	-6.51194100	-1.97501600	0.02518200
H	-6.94029300	-2.57564500	0.84664100
H	-6.70025000	-0.90864800	0.25876700
H	-7.07025200	-2.21085000	-0.89856700
H	-6.67049500	1.97636500	2.58987300
C	-6.01054400	1.93584200	1.71667500
C	-6.44395000	2.49280900	0.47372300
C	-4.74454100	1.34284000	1.82163800
C	-5.60657800	2.44295400	-0.64748000
H	-7.43270800	2.95911400	0.40407900
C	-3.86863700	1.28423800	0.69096200
H	-4.45100100	0.92006600	2.79005300
C	-4.30977500	1.84175700	-0.56337500
H	-5.93238500	2.86886500	-1.60368800
C	-2.53124300	0.69830700	0.75205500
N	-1.71323800	0.61963500	-0.34510900
C	-2.17327600	1.18278600	-1.53895900
H	-1.46684300	1.13297400	-2.36790100
H	3.53800200	2.37486000	6.39559600
C	2.98702700	1.57765100	5.88299200
C	2.44144500	0.51593800	6.62570100
C	2.82740500	1.64743900	4.46160200
C	1.72103600	-0.51869100	5.94055300
H	2.56912800	0.47132100	7.71158400
C	2.11366000	0.62364900	3.76456500
H	3.21676100	2.51980200	3.92334000
C	1.55738500	-0.47627100	4.53537500
H	1.31570700	-1.36891400	6.50302600
C	2.00197000	0.57014100	2.32821800
N	1.06503400	-0.31835100	1.64795100
C	0.65375800	-1.38794200	2.40109300

H	0.05924200	-2.13397000	1.86912600
H	2.85968200	6.85791800	-3.26393600
C	2.32827500	6.33599200	-2.45965800
C	1.71149100	7.06809900	-1.43807300
C	2.27392500	4.89791900	-2.48300600
C	1.00809100	6.36084500	-0.39871800
H	1.75605300	8.16131700	-1.42622200
C	1.59965200	4.17738100	-1.44622200
H	2.73383500	4.37688100	-3.33127500
C	0.94853600	4.94392800	-0.39571300
H	0.51245500	6.91790700	0.40544400
C	1.55016600	2.74089700	-1.37894500
N	0.77454800	2.02419200	-0.38172700
C	0.18084300	2.78465900	0.57471200
H	-0.36944200	2.24288900	1.34740800
C	-3.41244900	1.78138000	-1.68468500
H	-3.69809700	2.21373700	-2.64825300
C	0.25219600	4.19953500	0.62172600
H	-0.25489500	4.72299000	1.43885300
C	0.88924900	-1.52078800	3.78642700
H	0.49941100	-2.40372500	4.30517300
N	2.90668200	1.23594700	1.51531100
H	2.81215400	1.16800200	0.50047700
H	3.76007800	1.62372400	1.91854600
N	-2.02708700	0.24669800	1.94635200
H	-2.57211700	0.28025900	2.80267700
H	-1.06939400	-0.10745200	1.97817000
N	2.28051400	1.94153100	-2.24270900
H	2.94877200	2.35177000	-2.89137900
H	2.11175800	0.93062600	-2.24062300

5.Reference

1 R. v Shchepin, L. Jaigirdar and E. Y. Chekmenev, *Journal of Physical Chemistry C*, 2018, **122**, 4984–4996.