Supporting Information for :

Iron(II) Tetrafluoroborate Complexes of New Tetradentate *C*-Scorpionates as Catalysts for the Oxidative Cleavage of *trans*-Stilbene with H_2O_2

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S1. NMR spectra of intermediate and ligands **L** and **L***

Figure S1. *(a)* ^{1}H-NMR of P1a in $CDCl_3$ at 22 °C

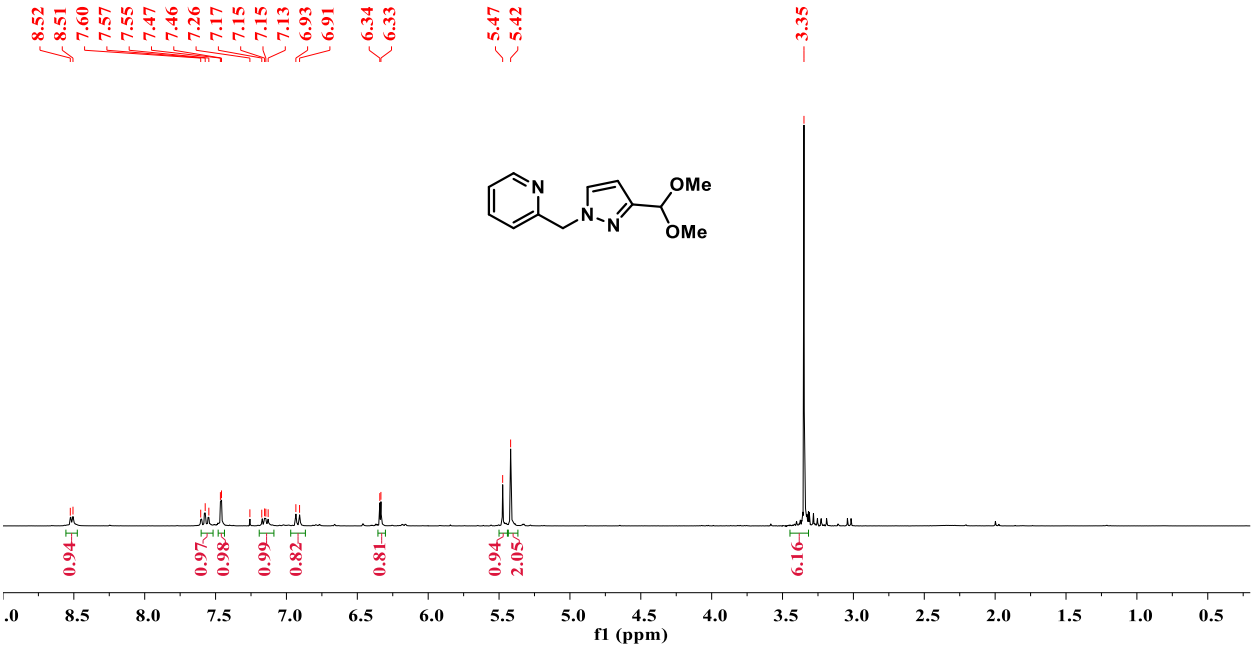


Figure S1. *(b)* ^{13}C-NMR of P1a in $CDCl_3$ at 22 °C

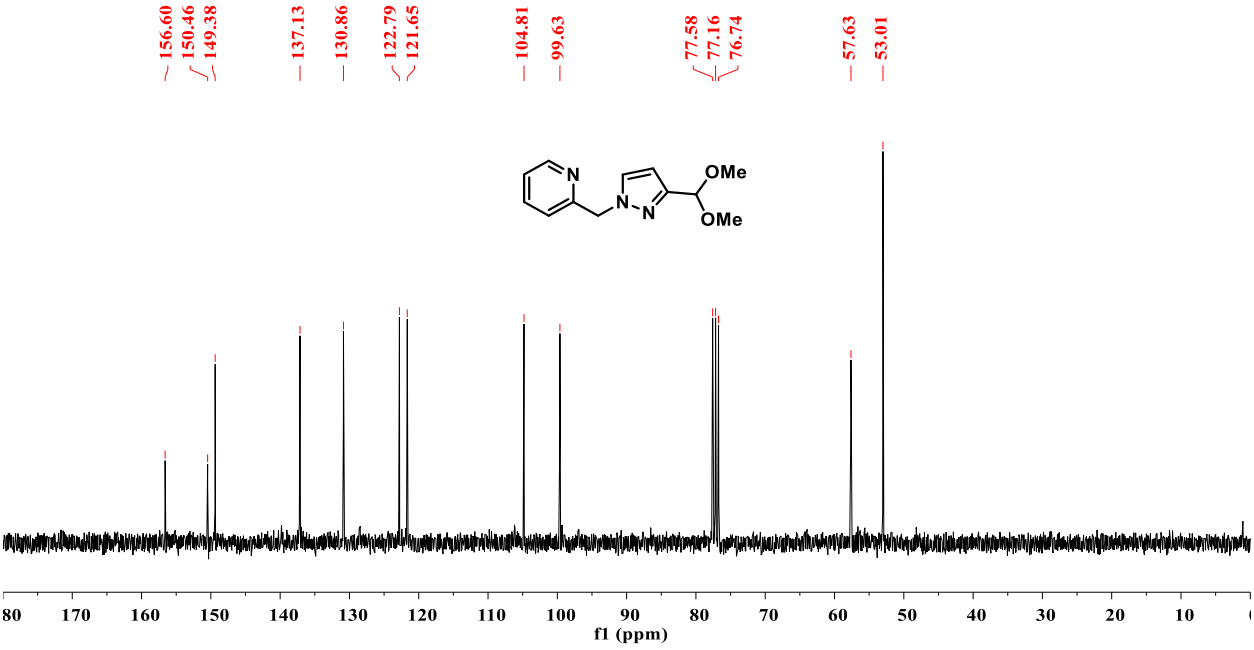
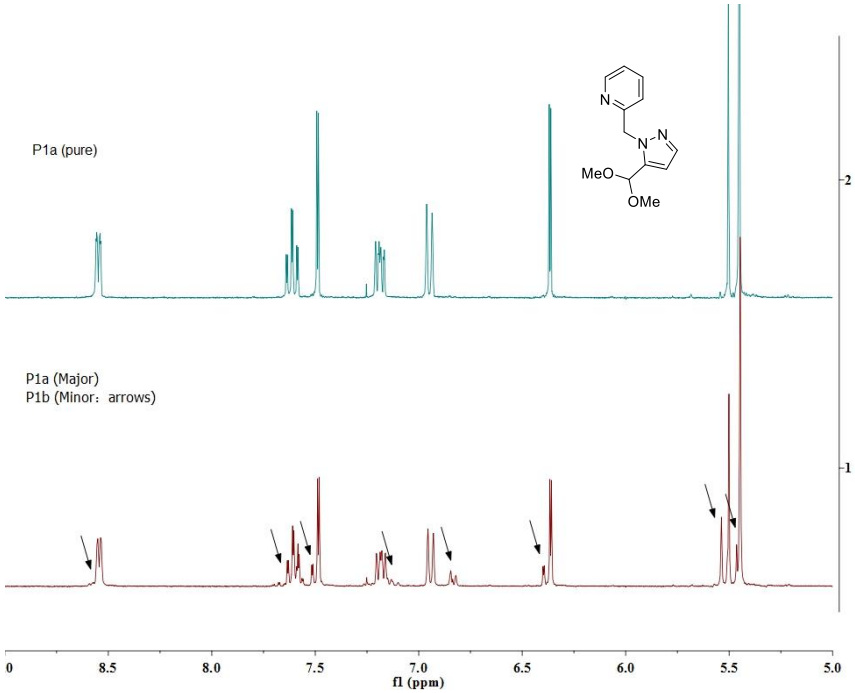


Figure S1. *(c)* ^{1}H-NMR spectrum of a mixture of P1a and P1b (bottom, maroon spectrum) with resonances for minor component of P1b highlighted by arrows compared to spectrum of pure P1a (top, aqua).



Note: Due to the similarity in solubility (and R_f values) of P1b with both P1a and P2a, it has not yet been possible to isolate pure P1b. As stated in the main text, the mixtures of P1b and P1a are sufficient for either conversion to P2a or for use to make the ligands.

Figure S1. *(d)* ^{13}C-NMR spectrum of a mixture of P1b (major) and P2a (minor) in $CDCl_3$ at 22 °C compared to that of pure P2a, bottom)

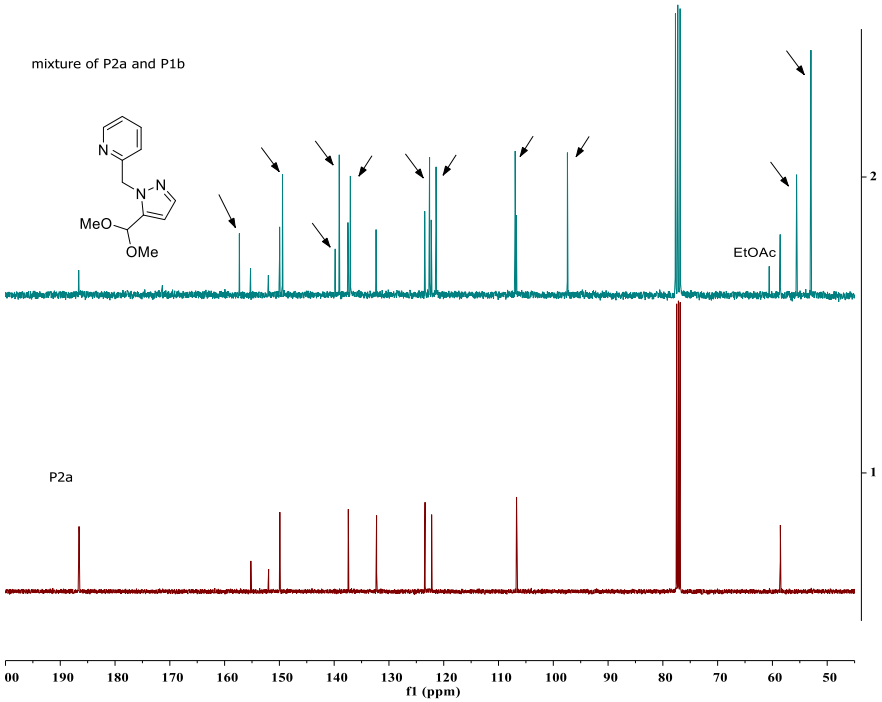


Figure S1. *(e)* ^{1}H-NMR of P2a in $CDCl_3$ at 22 °C

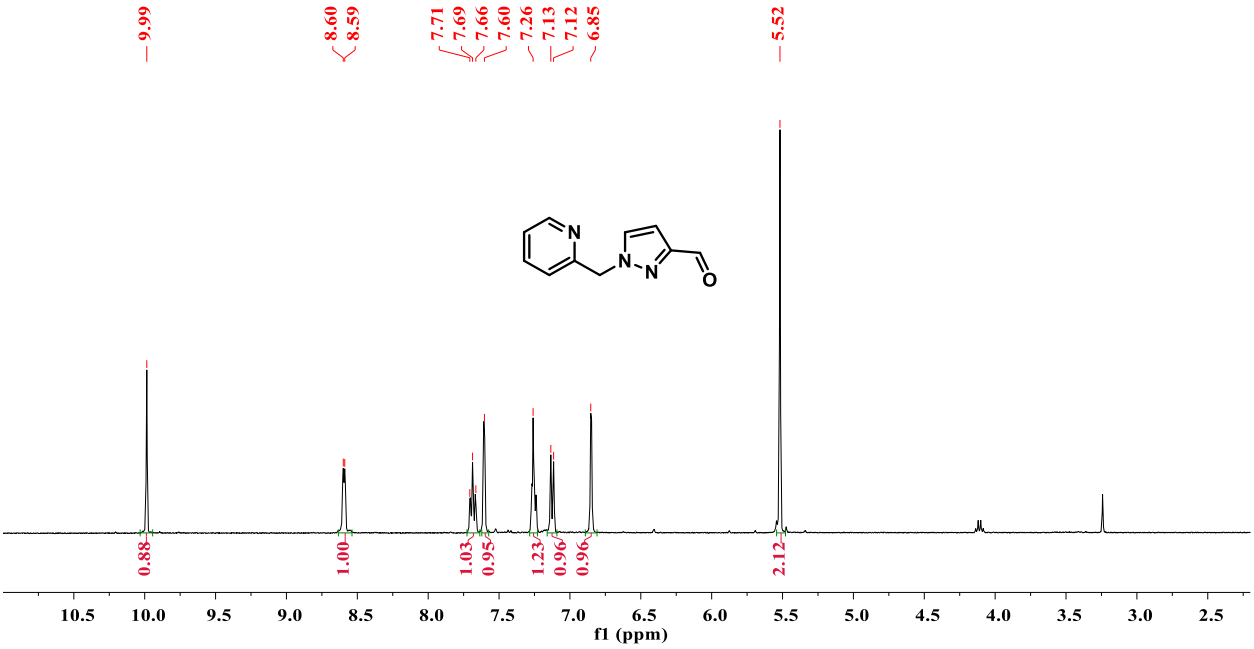


Figure S1. *(f)* ^{13}C-NMR of P2a in $CDCl_3$ at 22 °C

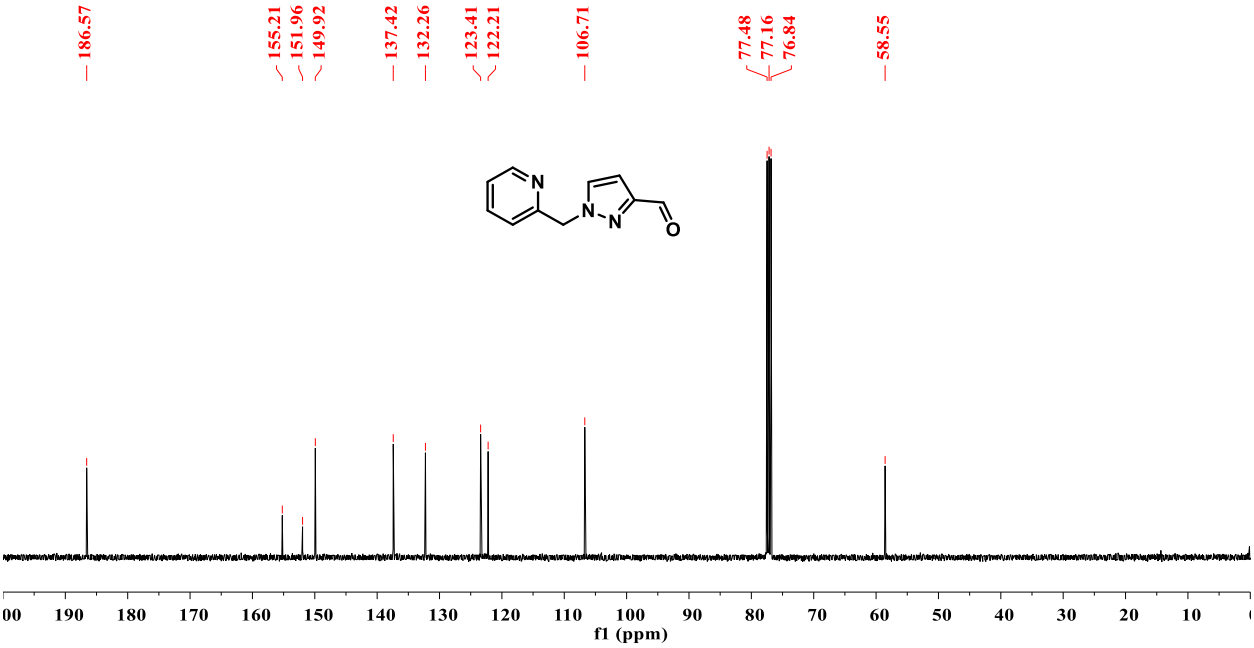


Figure S1. *(g)* ^{1}H-NMR of P2b in $CDCl_3$ at 22 °C

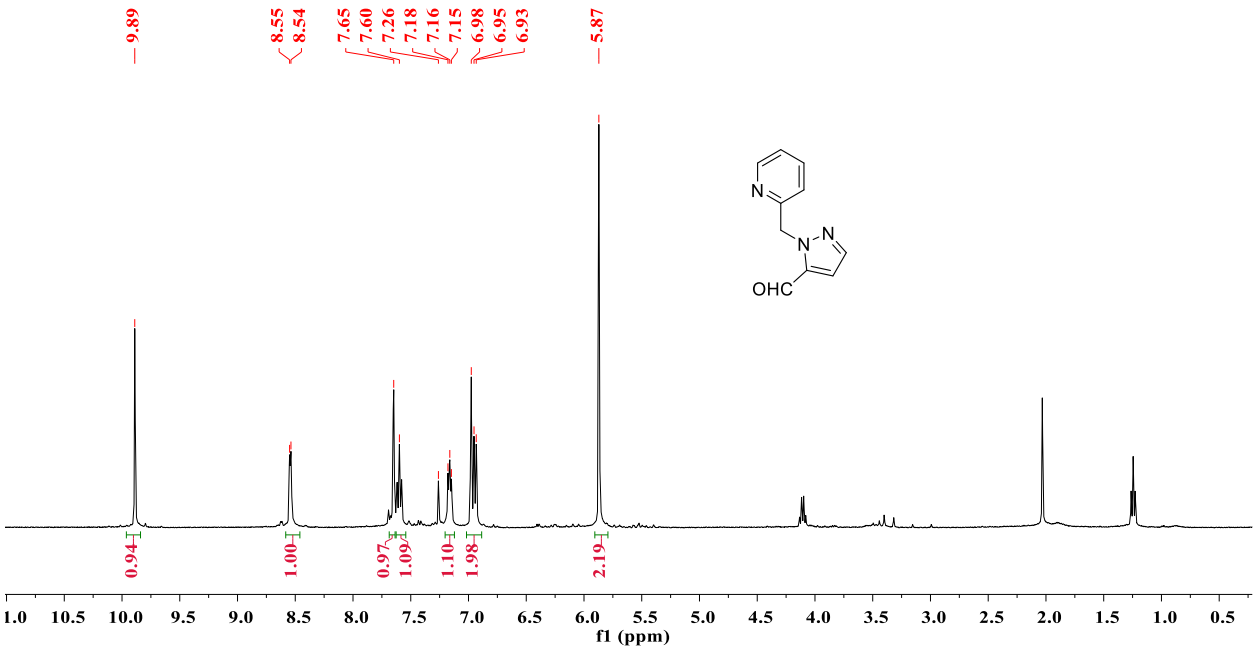


Figure S1. *(h)* ^{13}C-NMR of P2b in $CDCl_3$ at 22 °C

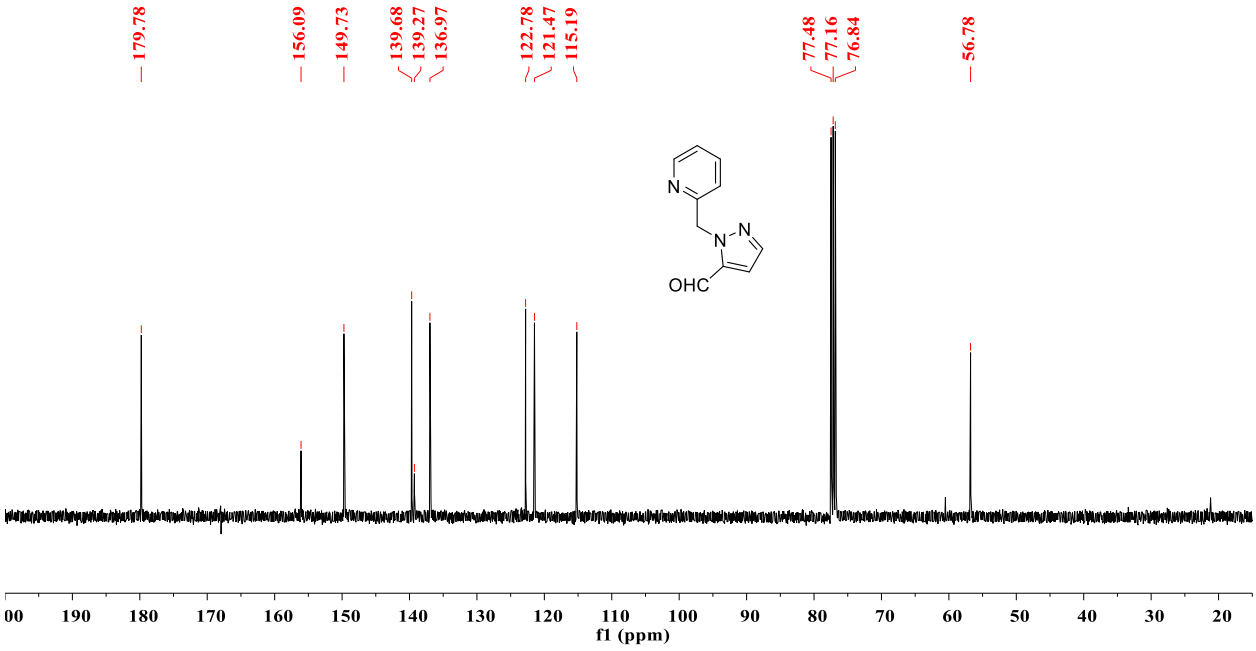


Figure S1. *(i)* ^{1}H-NMR of ligand L in $CDCl_3$ at 22 °C

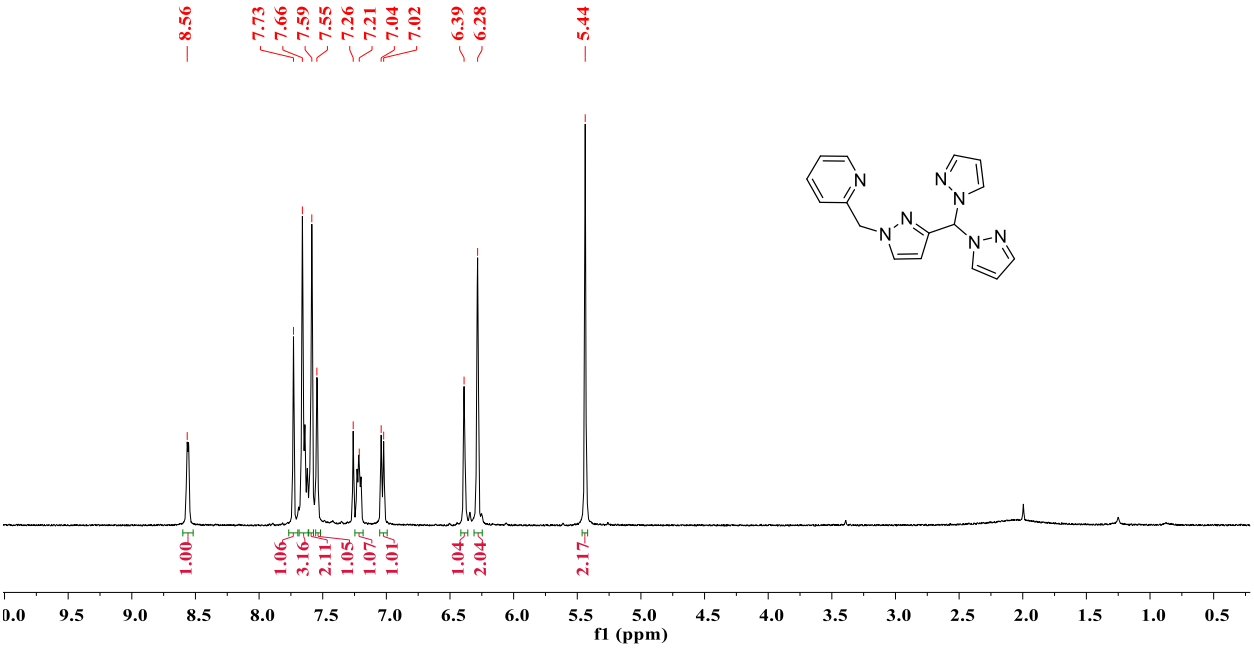


Figure S1. *(j)* ^{13}C-NMR of ligand L in $CDCl_3$ at 22 °C

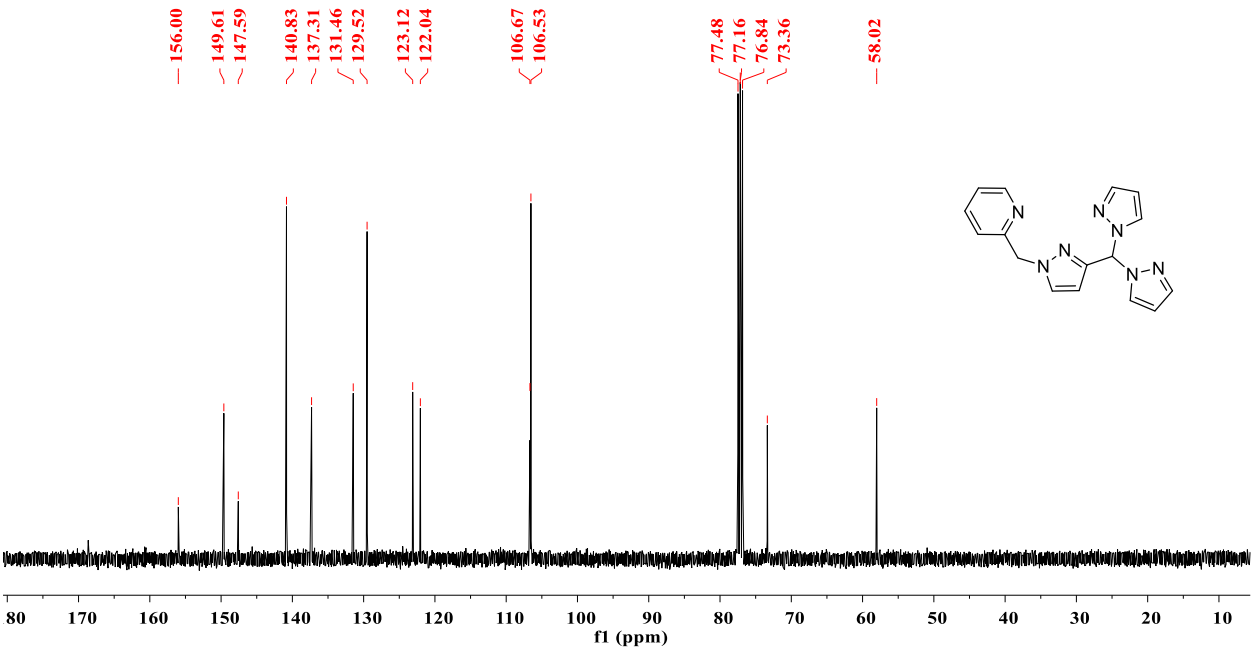


Figure S1. *(k)* ^{1}H-NMR of ligand L* in $CDCl_3$ at 22 °C

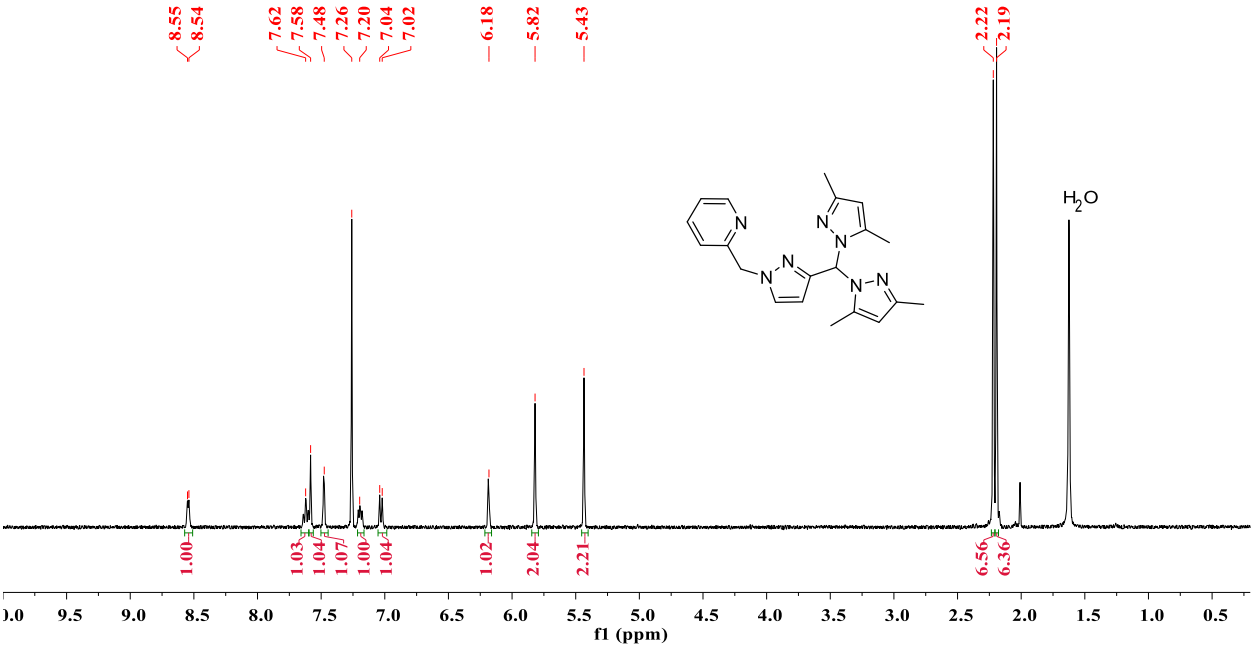
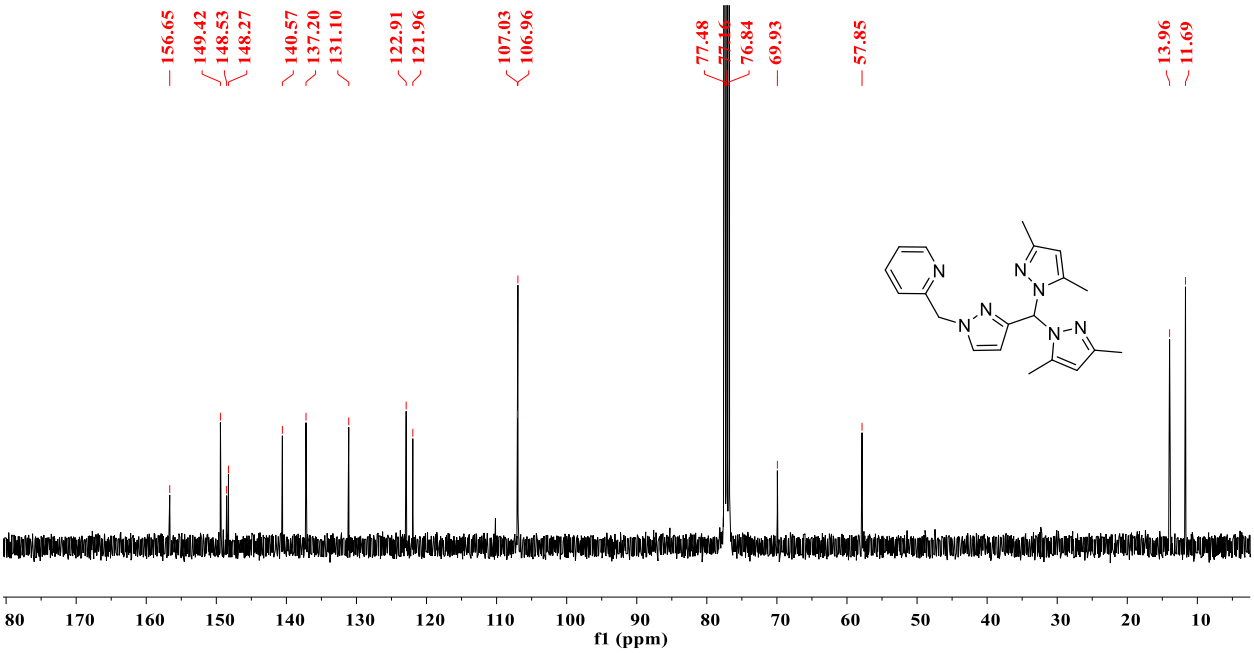


Figure S1. *(l)* ^{13}C-NMR of ligand L* in $CDCl_3$ at 22 °C



S2. NMR spectra of iron complexes **1** and **2**.

Figure S2. *(a)* ^{1}H-NMR of complex **1** in CD_3CN at 22 °C

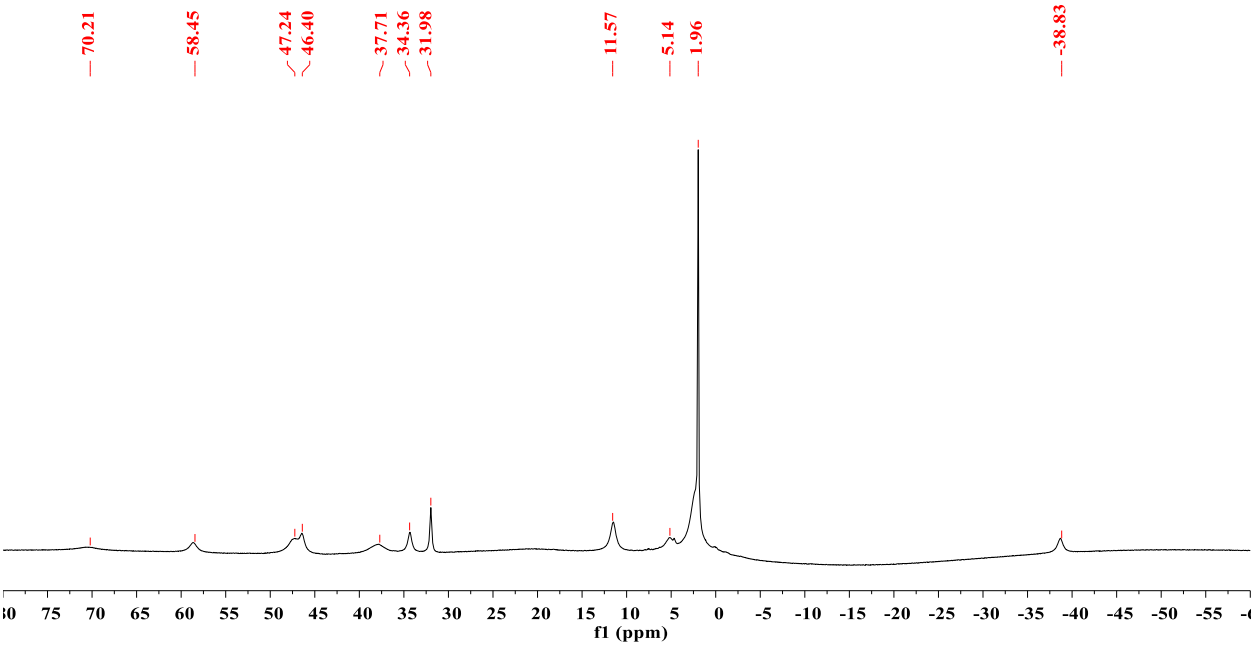
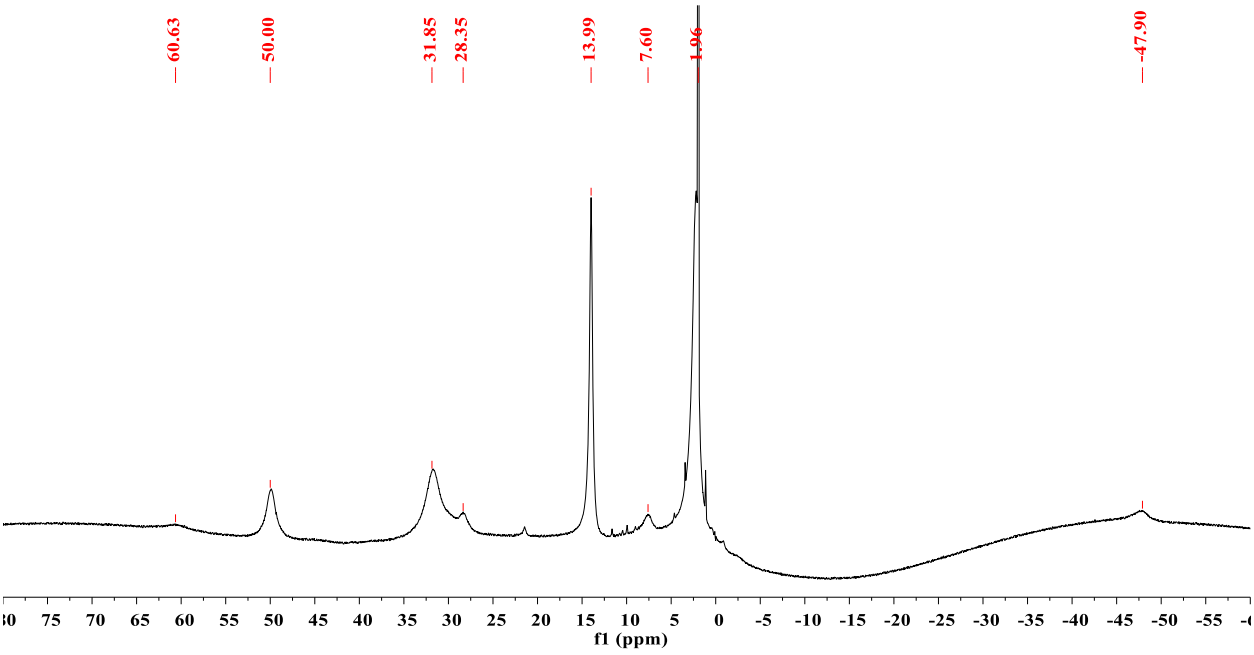
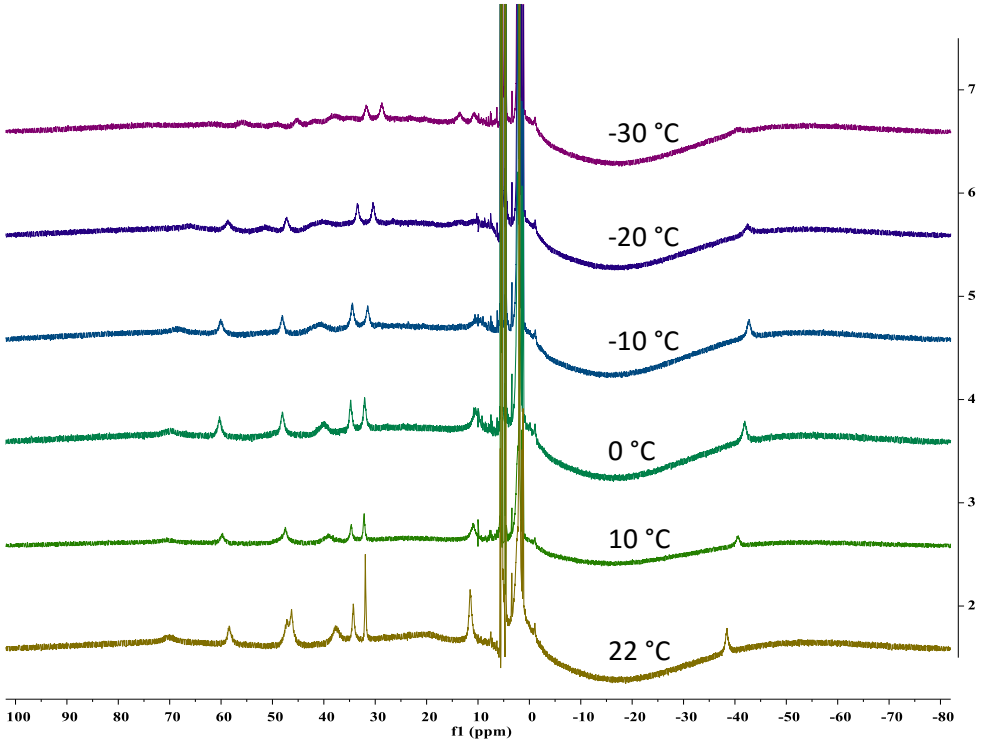


Figure S2. *(b)* ^{1}H-NMR of complex **2** in CD_3CN at 22 °C

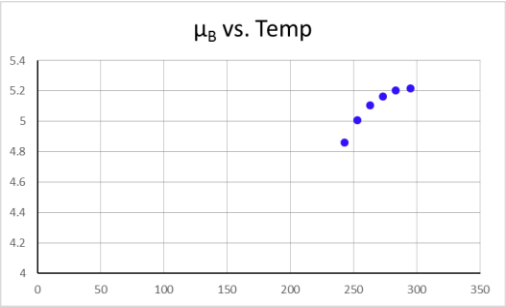


S3. Evans data and plot

Figure S3. (a) Top: Variable temperature ^{1}H-NMR of complex **1** (Evans method) in CD_3CN at range from 22 to -30 °C. (b) bottom: Plot of the relationship between μ_B and temperature.



(a)



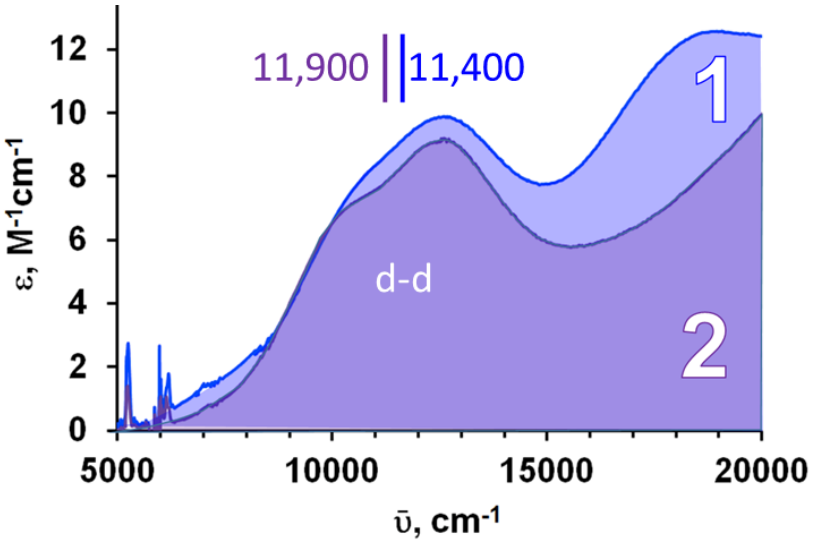
(b)

Table S1. Values of μ_B for **1** in CH_3CN at different temperature

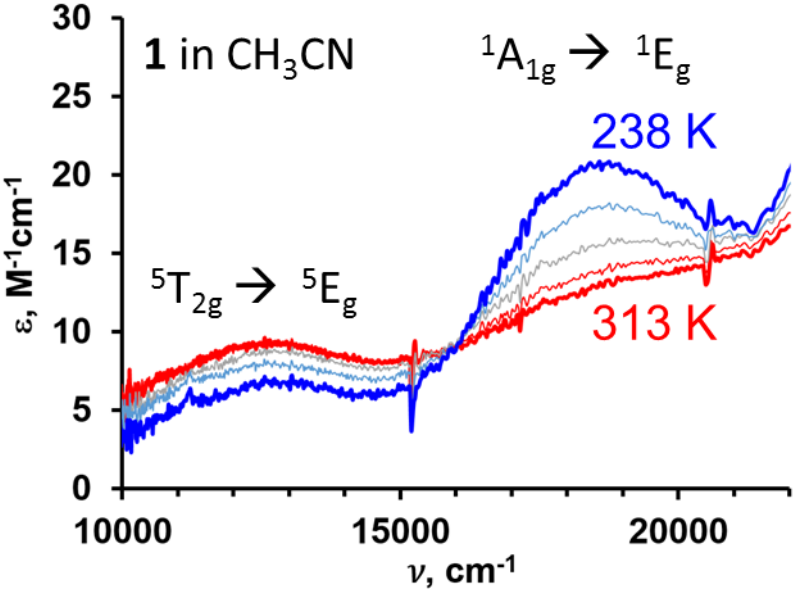
Temp	μ_B
295	5.216
283	5.206
273	5.162
263	5.104
253	5.006
243	4.86

S4. Electronic spectra

Figure S4. Overlay of electronic spectra of **1** and **2** in CH_3CN (a) at room temperature and (b) the spectra of **1** at temperatures between 238 and 313 K.



(a)



(b)

S5. Results of 4 hr photocatalysis experiments

Table S2. Summary of data from photocatalytic experiments[a] performed under same conditions as Table 3 of main text, but for 4h rather than 1.5 hr.

		product[c]						
entry	[Fe] catalyst[b]	a	b	c	d	e	f	%[d]
1	**1**	83	4	5	3	1	2	98
2	**2**	76	4	6	5	1	5	97
3	$[Fe(tpa)(CH_3CN)_2](BF_4)_2$	77	10	4	5	1	2	99
4	$[Fe(H_2O)_6](BF_4)_2$	38	30	1	1	1	9	80
5	none	26	1	0	0	0	0	27

[a.] 0.04 mmol *trans*- stilbene, 0.0032 mmol, 8 mol% RFT, 3 mL 9:1 CH_3CN:H_2O, 30°C, 440-450 nm 12W, 4h. [b.] 0.0040 mmol 10 mol%. [c.] labelling as per Figure 5, GC yield, errors in a ± 3%, in b-f ± 1% [d.] % conversion.

S6. Time course of photocatalytic experiments catalyzed by RFT and **1** (purple) or **2** (green).

Figure S5. Overlay plot of relative GC yield versus time

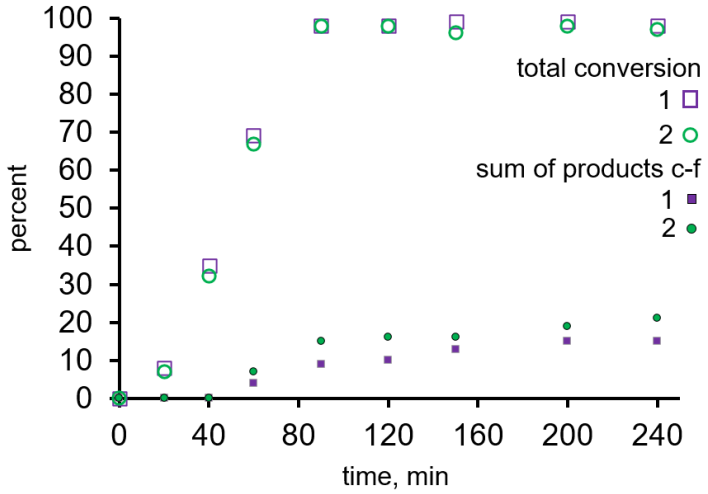
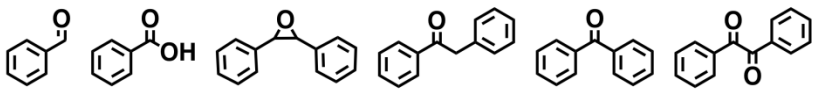


Table S3. GC yields for photocatalysed reactions using RFT and either 1 or 2 as catalysts

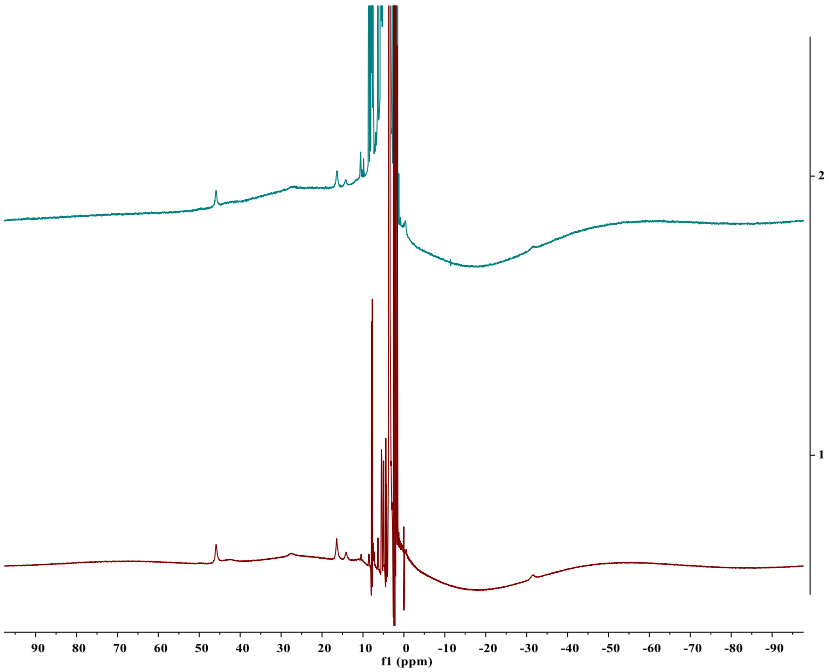
	Catalyst 1							Catalyst 2						
Time (min)	a	b	c	d	e	f	Total conversion	a	b	c	d	e	f	Total conversion
0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
20	8	0	0	0	0	0	8	7	0	0	0	0	0	7
40	35	0	0	0	0	0	35	32	0	0	0	0	0	32
60	65	1	1	1	0	1	69	60	2	3	1	0	1	67
90	89	2	2	2	1	2	98	83	4	5	3	1	2	98
120	88	3	2	2	1	2	98	82	5	5	3	1	2	98
150	86	4	4	2	1	2	99	80	4	5	4	1	2	96
200	84	4	5	3	1	2	99	79	4	6	4	1	4	98
240	83	4	5	3	1	2	98	76	4	6	5	1	5	97



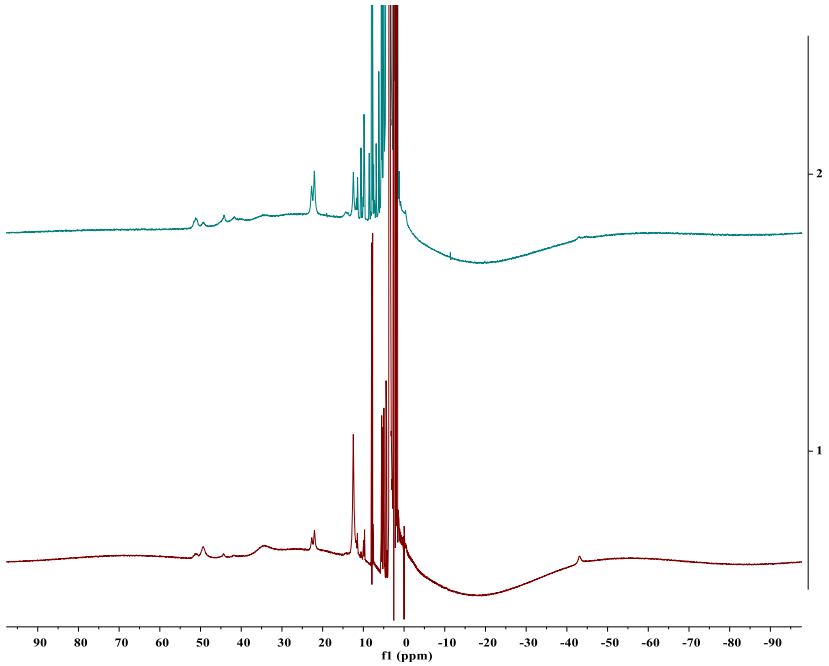
a **b** **c** **d** **e** **f**

S7. Stability test for **1** and **2** under conditions of photocatalysis.

Figure S6. ^{1}H NMR spectra for solutions of RFT and either (a) **1** or (b) **2** in 1 mL 10 vol% D_2O in CD_3CN before (bottom maroon spectrum) and after (top aqua spectrum) irradiation at 450 nm 90 min.



(a)



(b)