

Electronic Supplementary Information for:

# Rhenium(I) tricarbonyl polypyridine complexes showing strong absorption of visible light absorption and long-lived triplet excited states as triplet photosensitizer for triplet-triplet annihilation upconversion

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## 1.0 NMR and HRMS spectra.

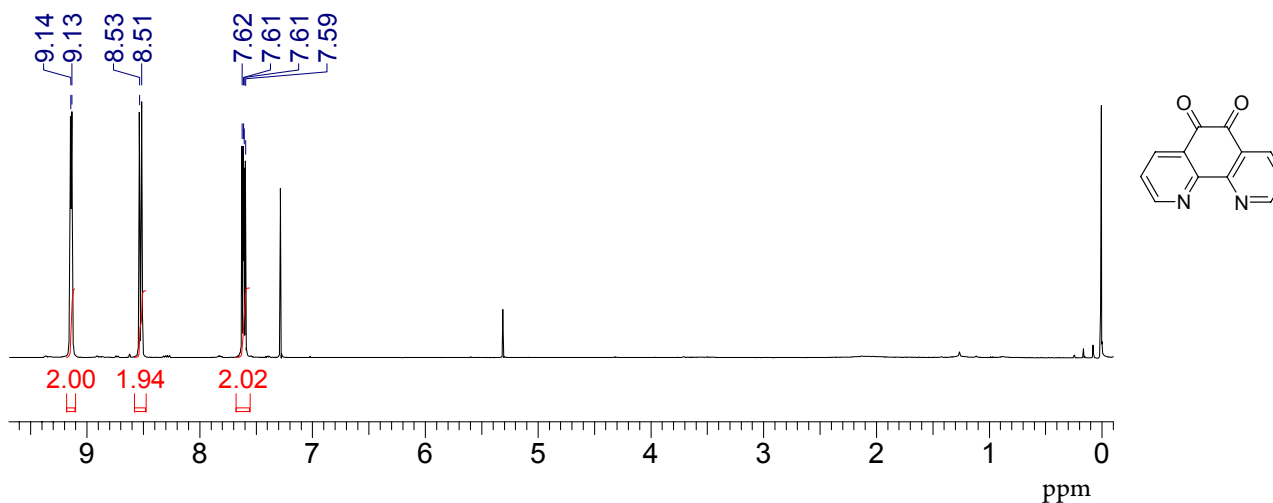


Figure S1.  $^1\text{H}$  NMR of 1,10-phenanthroline-5,6-dione (400 MHz,  $\text{CDCl}_3$ ),  $20^\circ\text{C}$ .

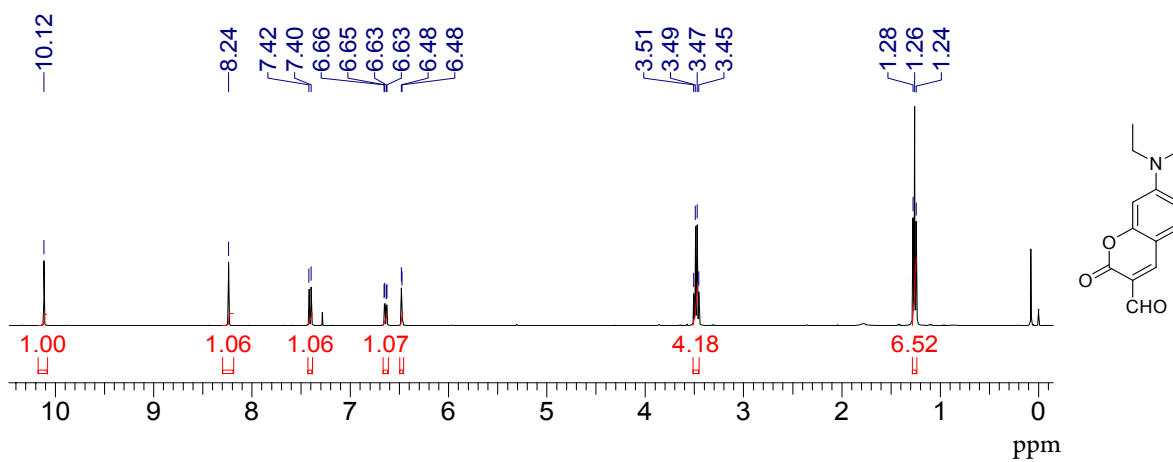


Figure S2.  $^1\text{H}$  NMR of 7-diethylamino-2-oxo-2H-chromene-3-carboxyldehyde (400 MHz,  $\text{CDCl}_3$ ),  $20^\circ\text{C}$ .

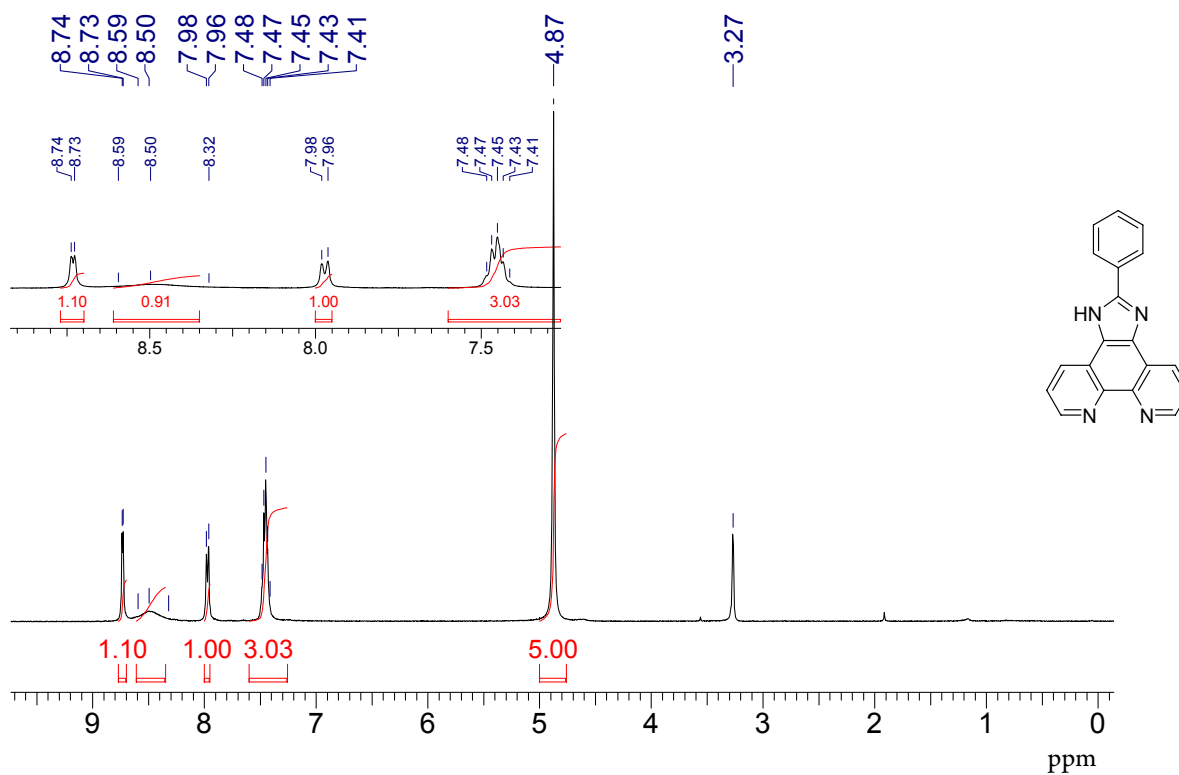


Figure S3. <sup>1</sup>H NMR of L-0 in methanol-d<sub>4</sub> (400 MHz), 20°C.

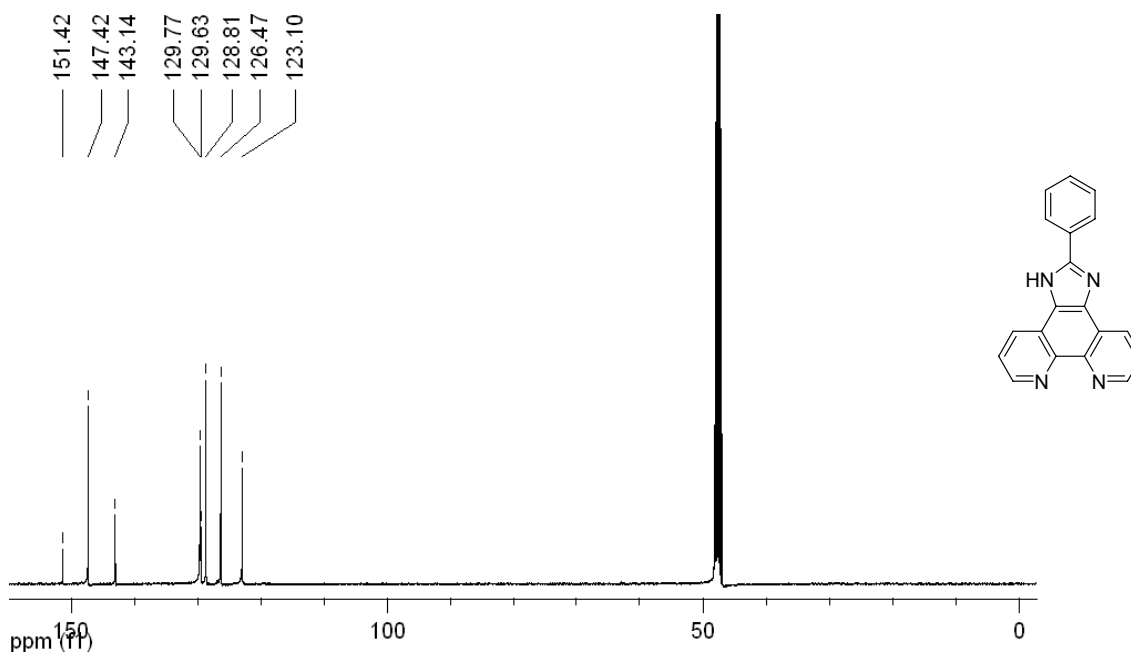


Figure S4. <sup>13</sup>C NMR of L-0 in methanol-d<sub>4</sub> (100 MHz), 20°C.

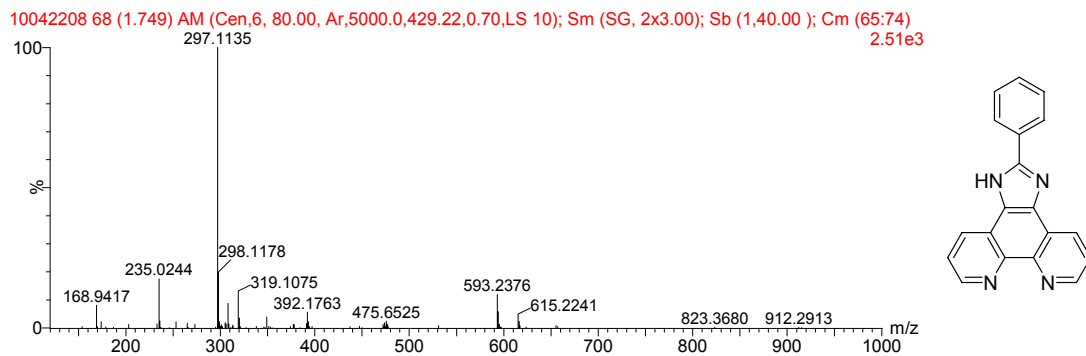


Figure S5. TOF HRMS ESI of L-0, 20°C.

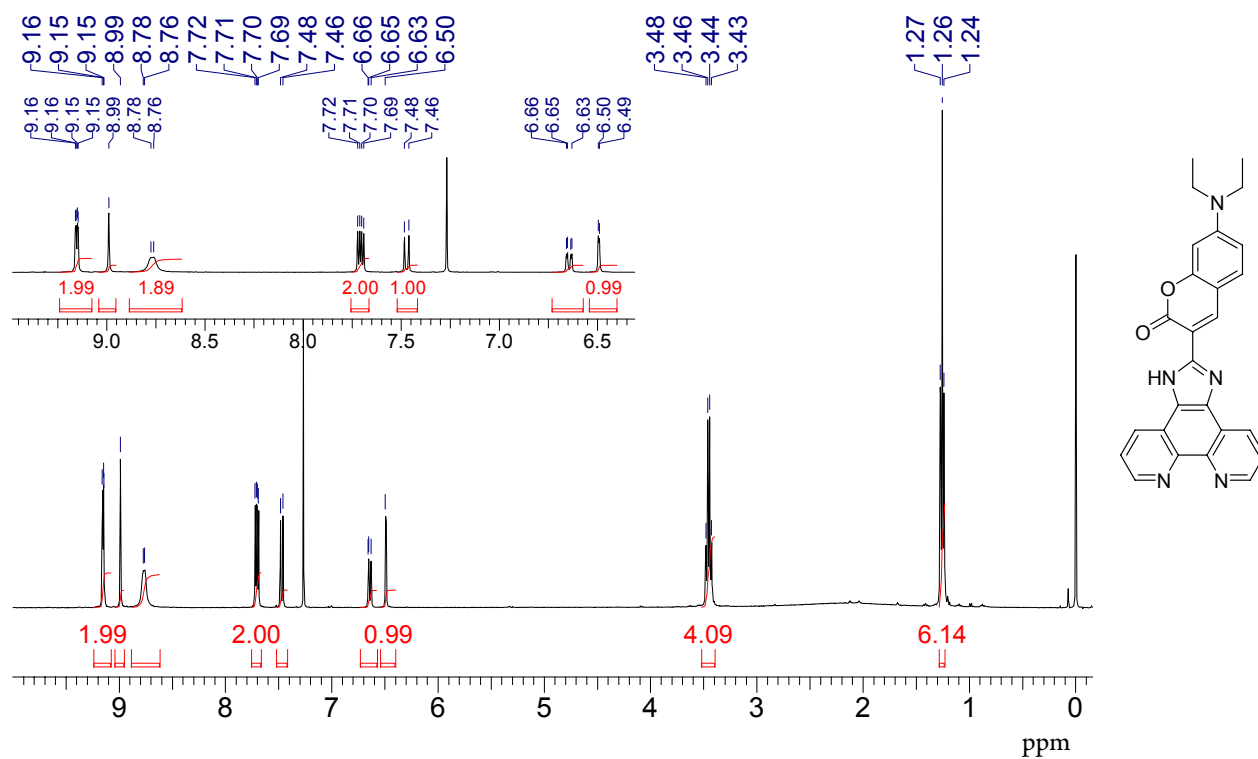


Figure S6. <sup>1</sup>H NMR of L-1 in CDCl<sub>3</sub>(400 MHz), 20°C.

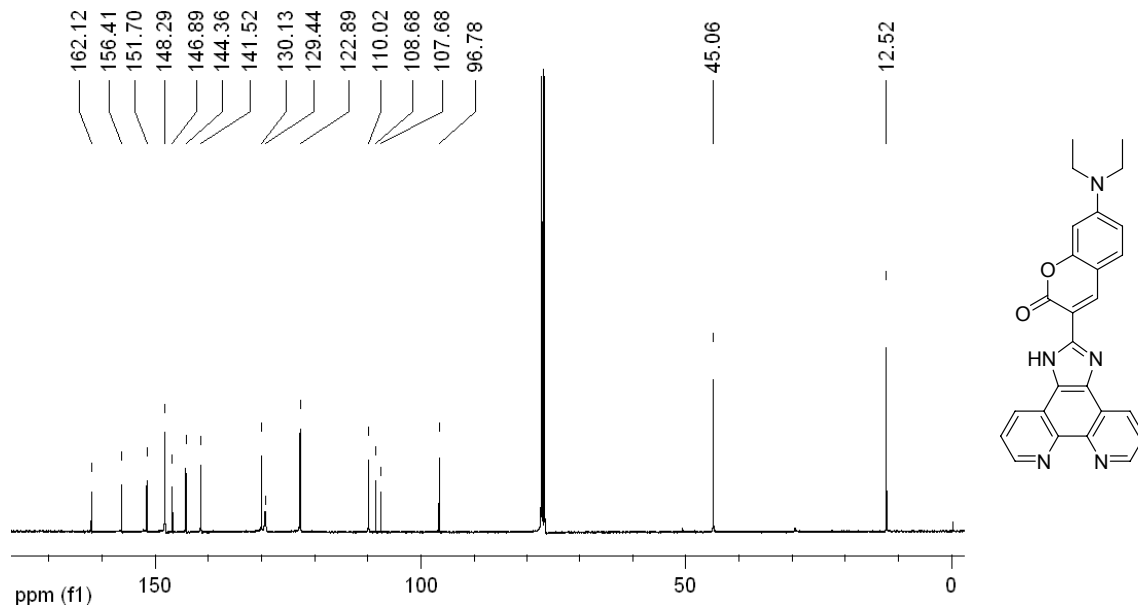


Figure S7.  $^{13}\text{C}$  NMR of L-1 in  $\text{CDCl}_3$  (100 MHz),  $20^\circ\text{C}$ .

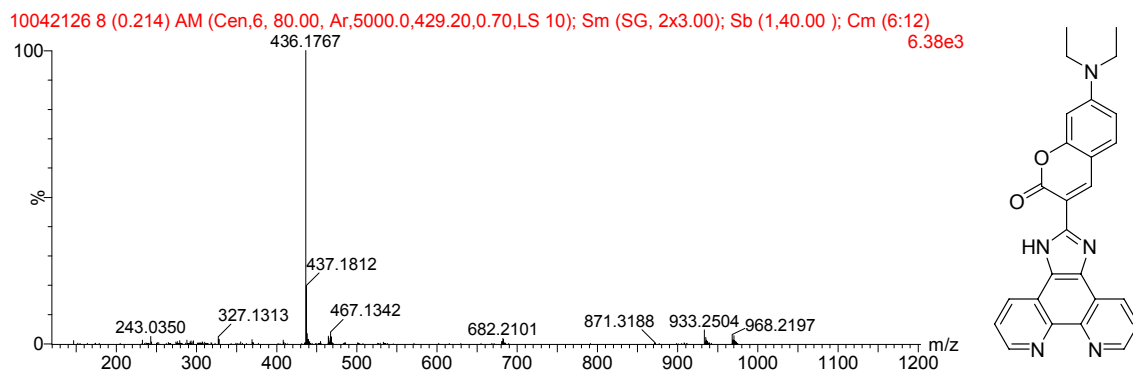


Figure S8. TOF HRMS ESI of L-1,  $20^\circ\text{C}$ .

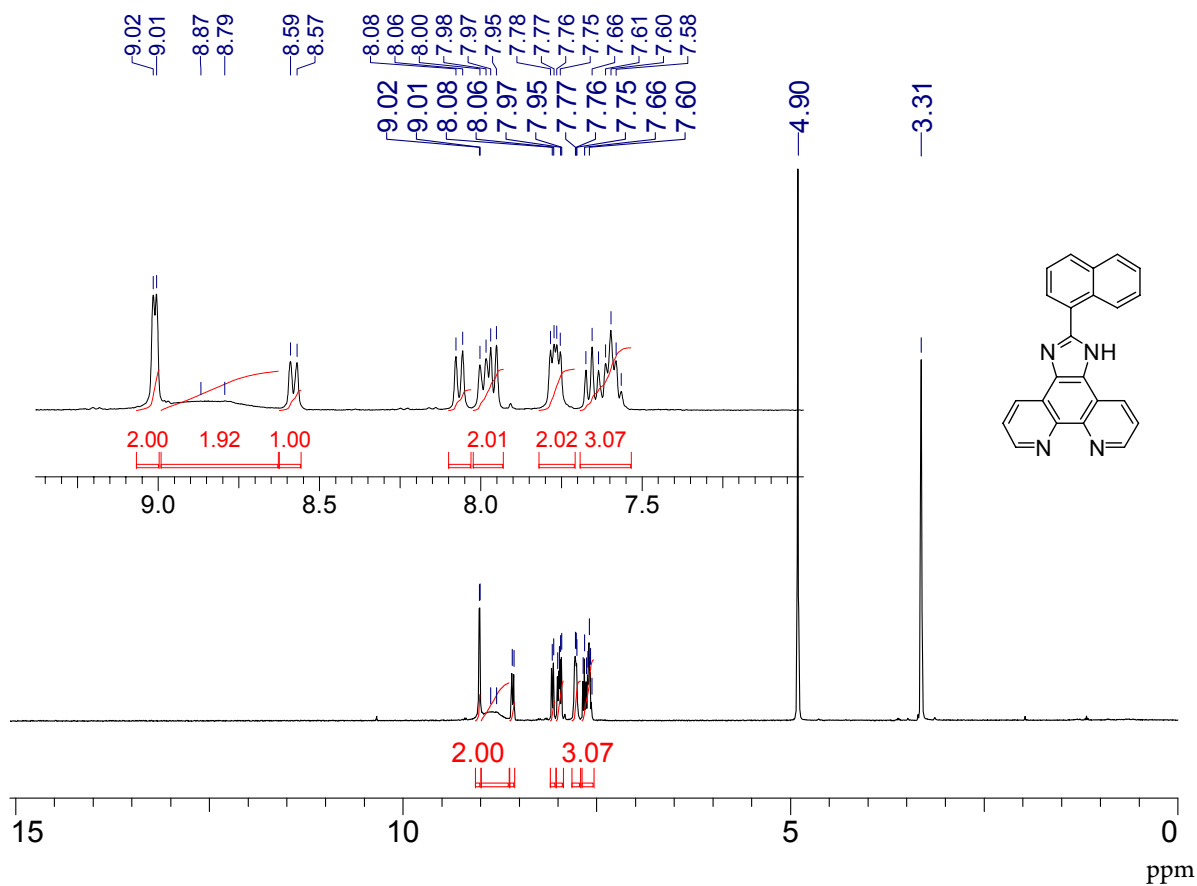


Figure S9. <sup>1</sup>H NMR of L-2 in methanol-d<sub>4</sub> (400 MHz), 20°C.

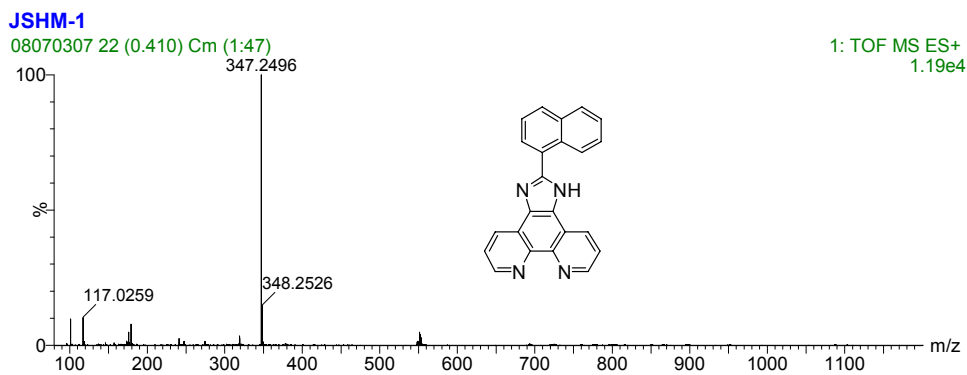
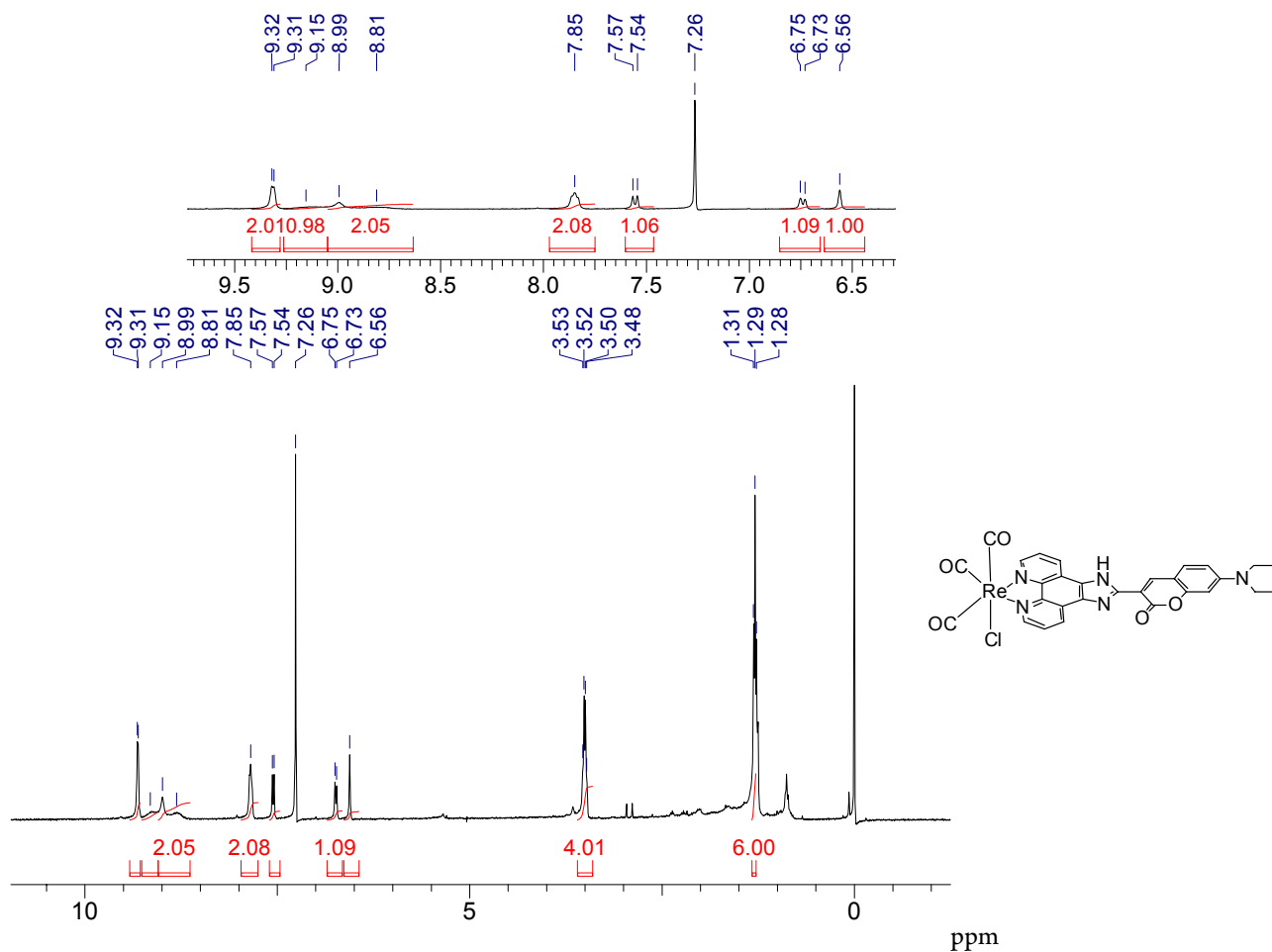
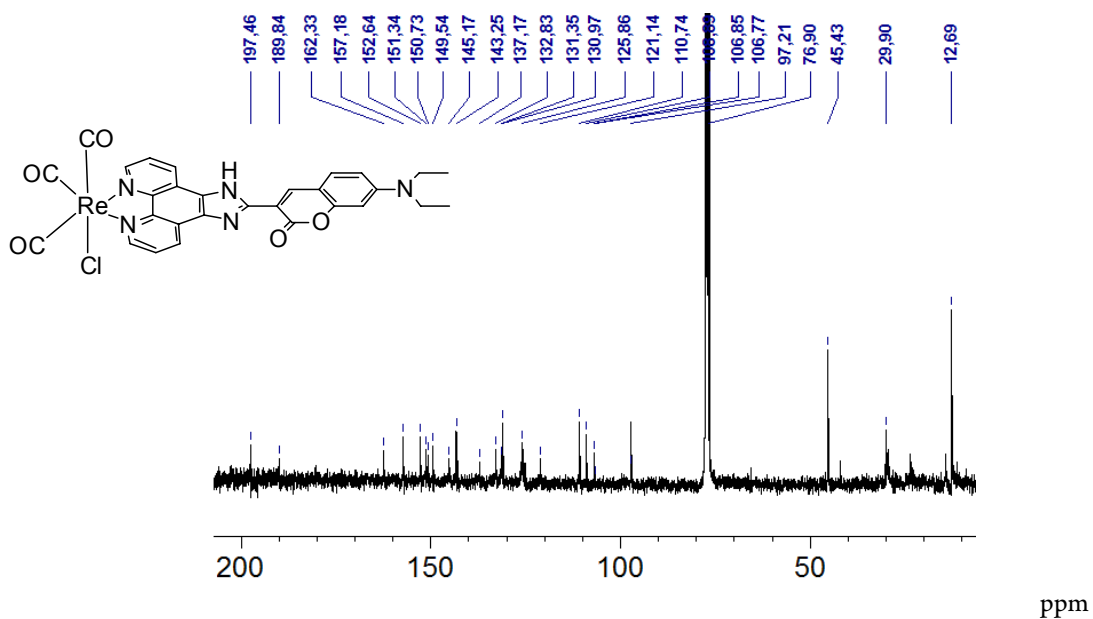


Figure S10. TOF HRMS ESI of L-2, 20°C.



**Figure S11.**  $^1\text{H}$  NMR of **Re-1** in  $\text{CDCl}_3$  (400 MHz),  $20^\circ\text{C}$ .



**Figure S12.**  $^{13}\text{C}$  NMR of **Re-1** in  $\text{CDCl}_3$  (100 MHz),  $20^\circ\text{C}$ .

YXY

15:13:58

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822

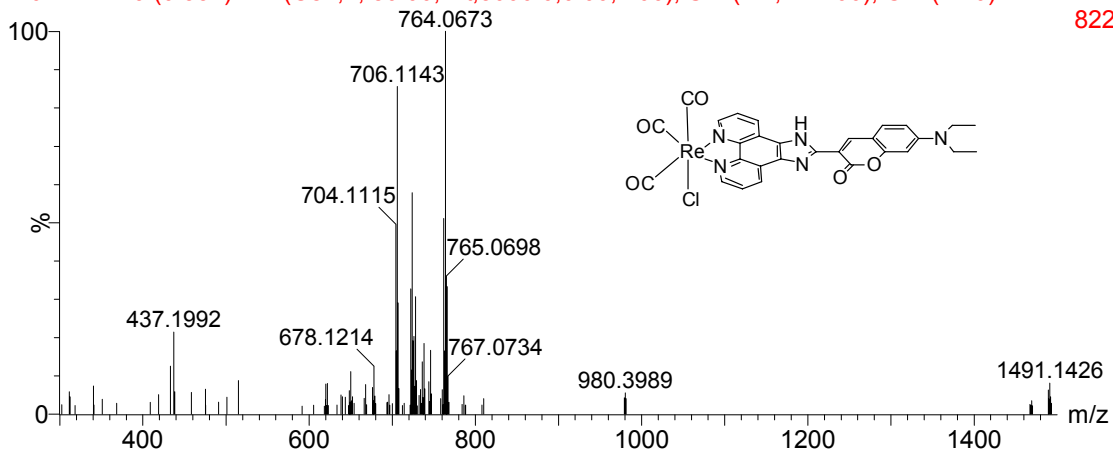


Figure S13. TOF HRMS ESI of **Re-1**, 20°C.

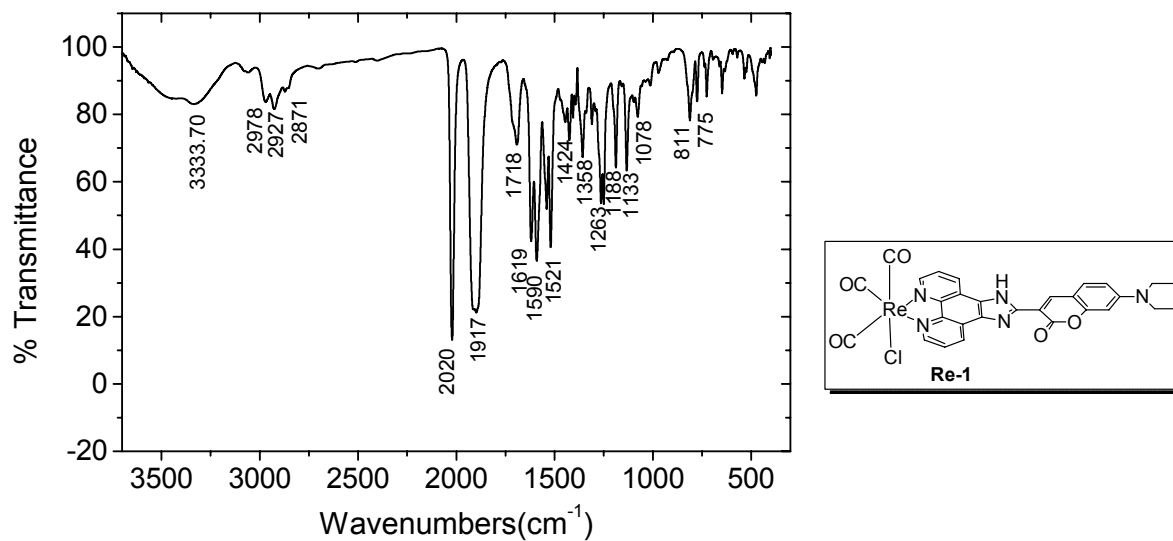


Figure S14. IR spectrum of **Re-1** (KBr disk).



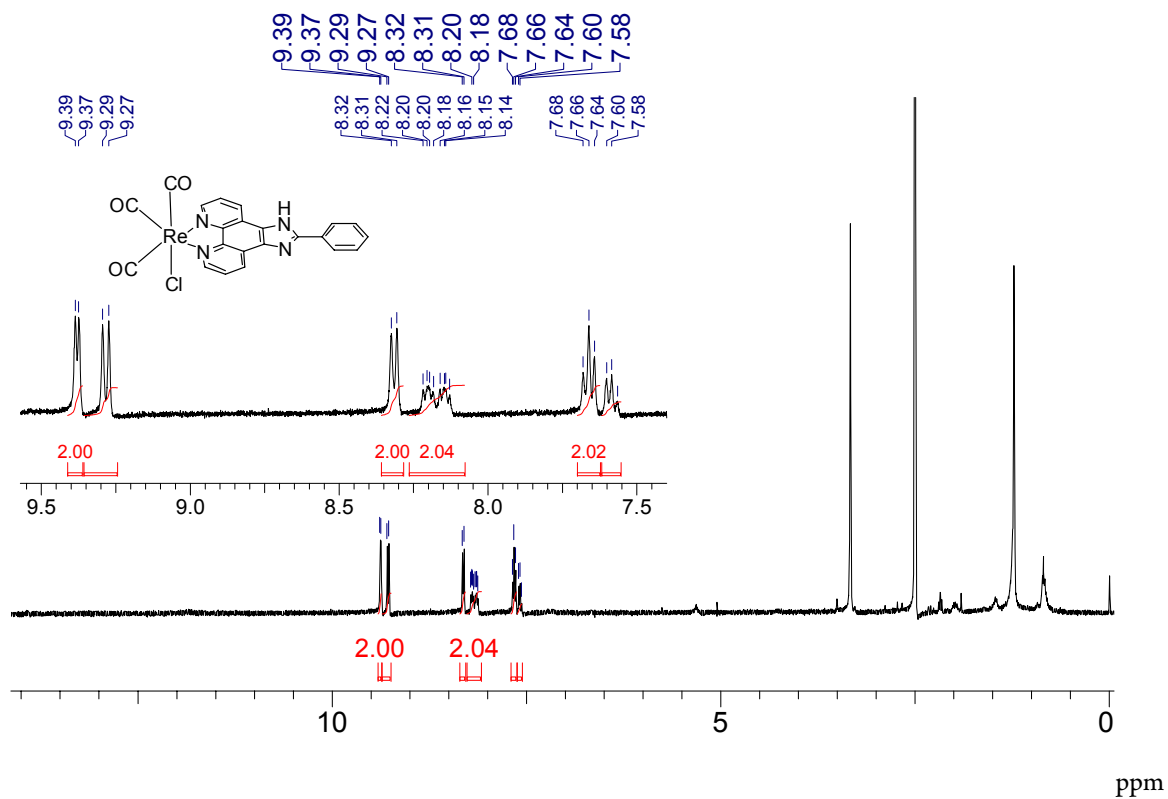


Figure S15. <sup>1</sup>H NMR of Re-0 in DMSO-d<sub>6</sub> (400 MHz), 20°C.

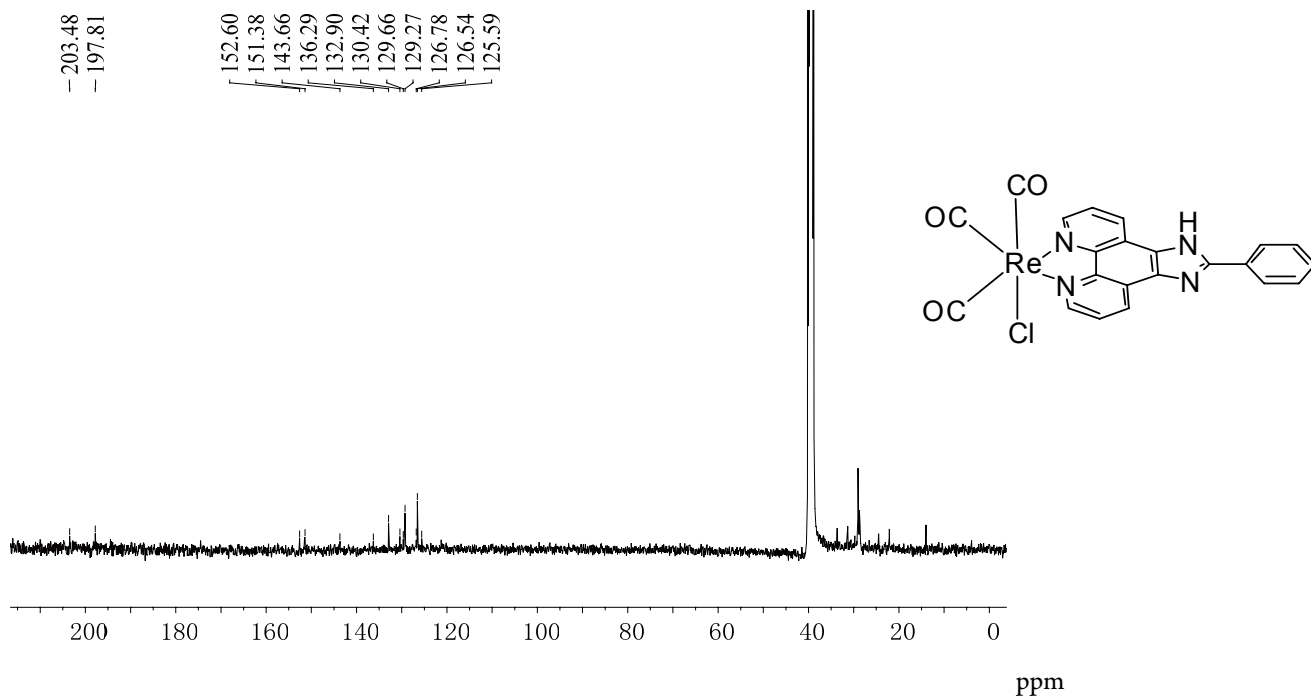


Figure S16. <sup>13</sup>C NMR of Re-0 in DMSO-d<sub>6</sub> (100 MHz), 20°C.

YXY

10:31:17

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1.14e4

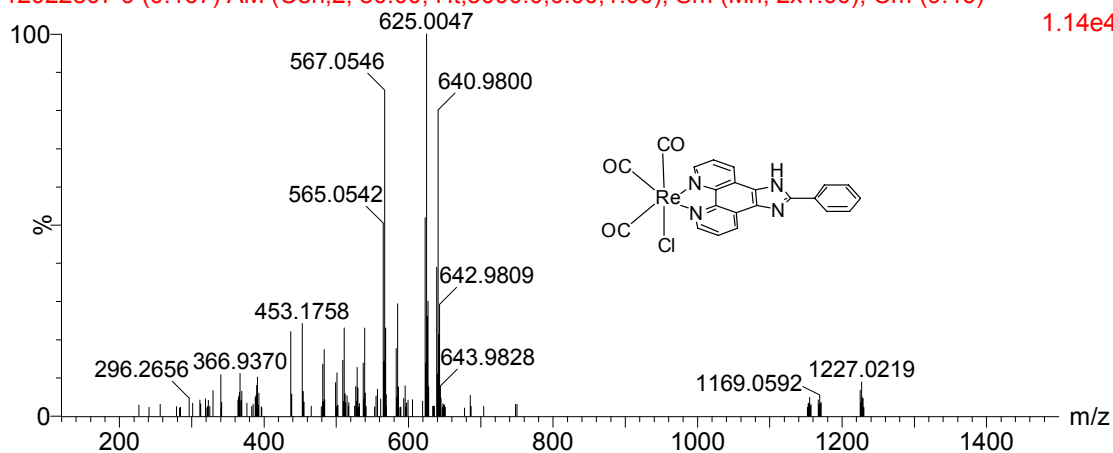


Figure S17. TOF HRMS ESI of **Re-0**, 20°C.

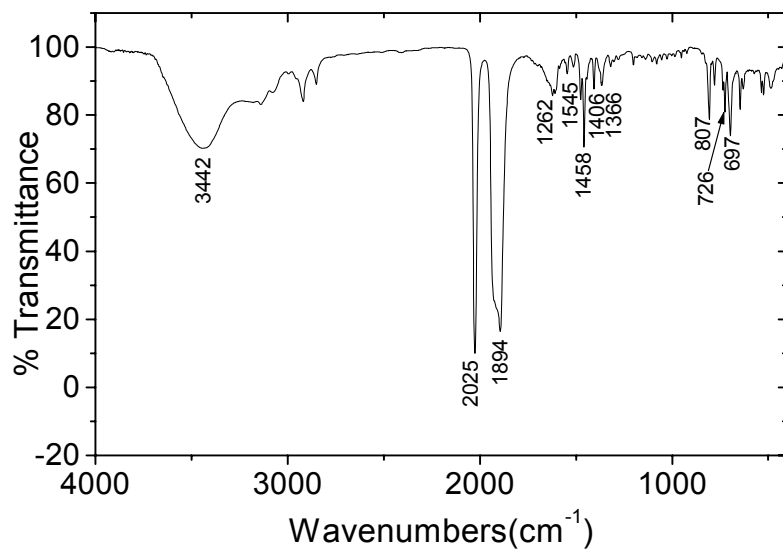
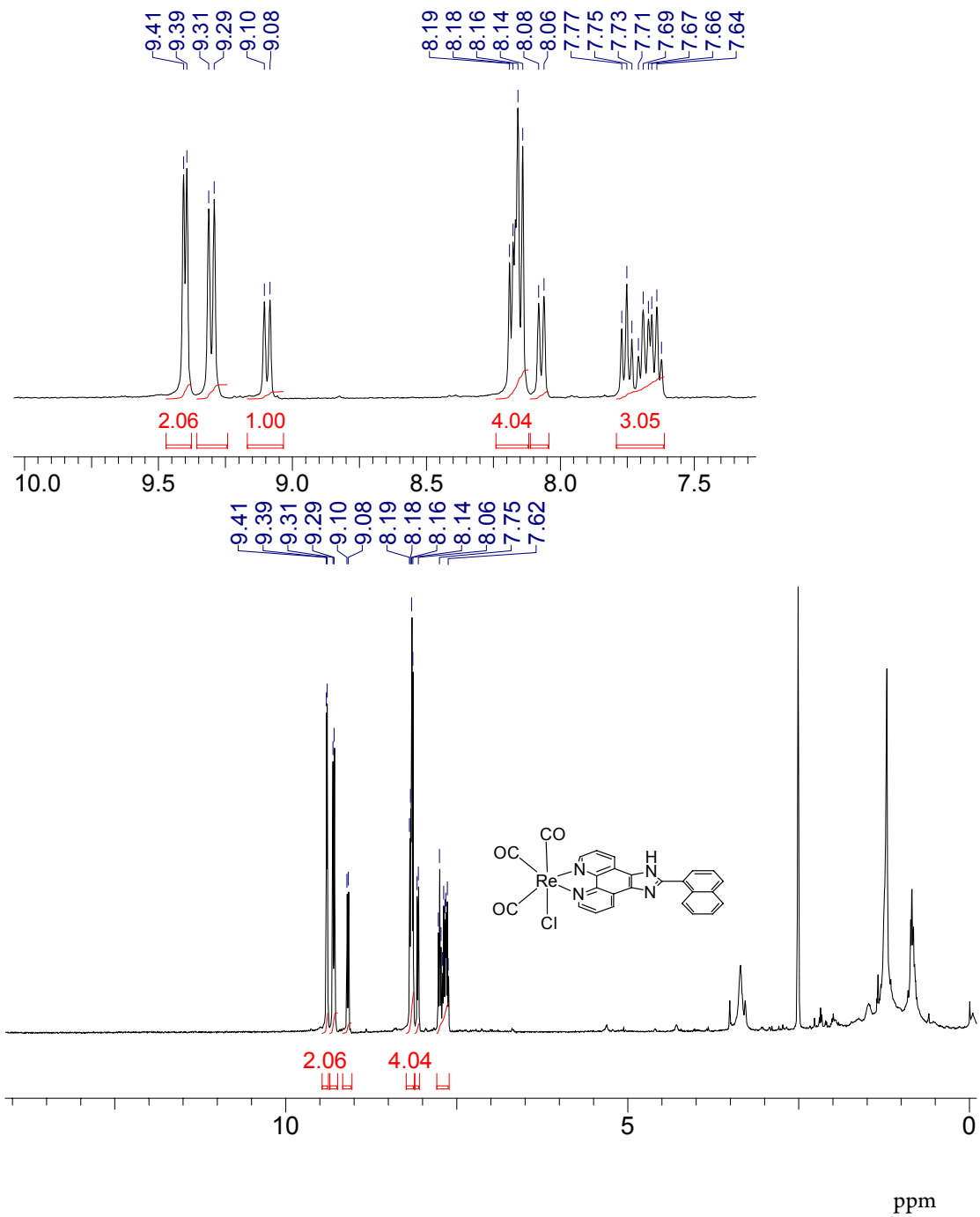


Figure S18. IR spectrum of **Re-0** (KBr disk).



**Figure S19.**  $^1\text{H}$  NMR of **Re-2** in  $\text{DMSO-d}_6$  (400 MHz), 20°C.

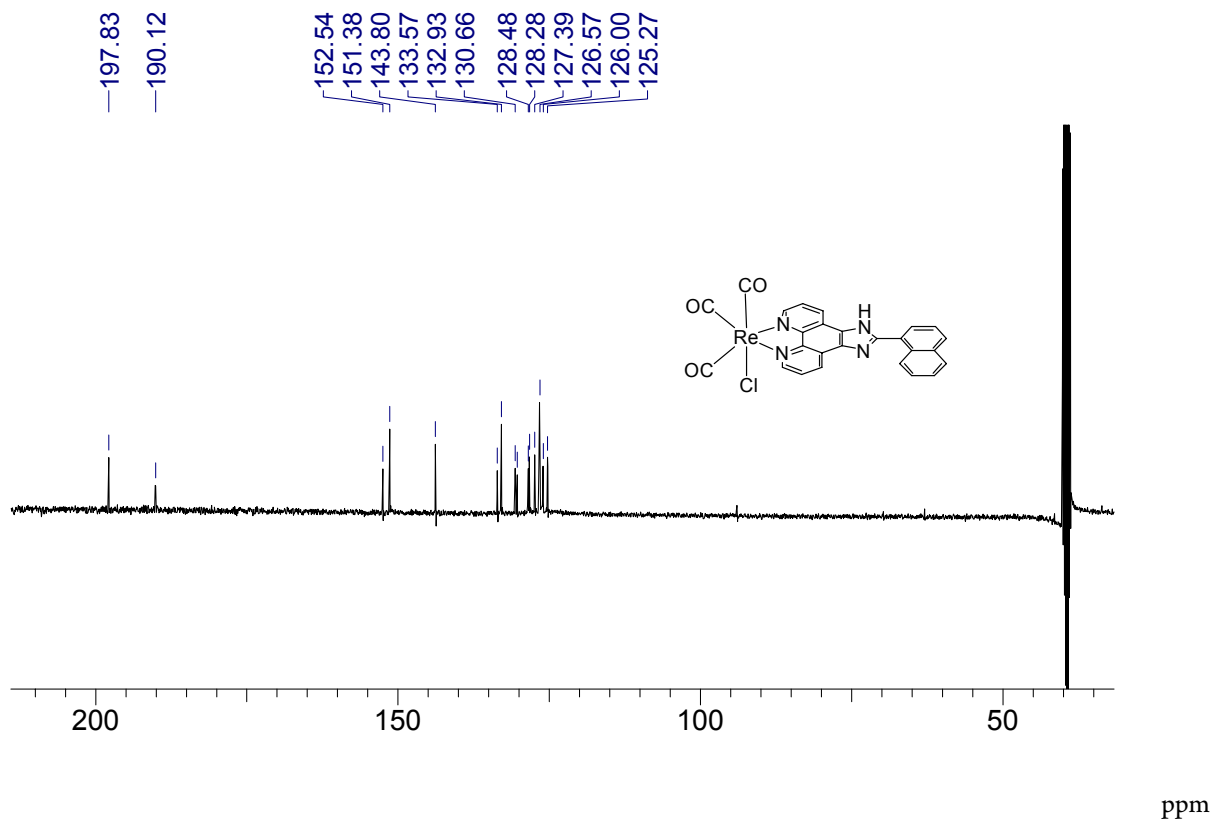


Figure S20.  $^{13}\text{C}$  NMR of **Re-2** in  $\text{DMSO-d}_6$  (100 MHz),  $20^\circ\text{C}$ .

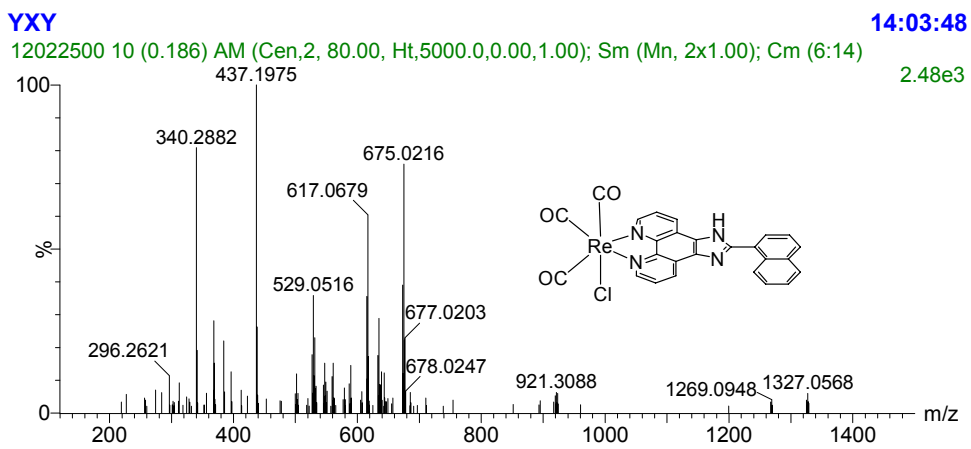
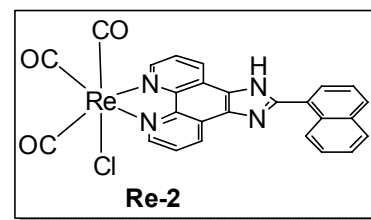
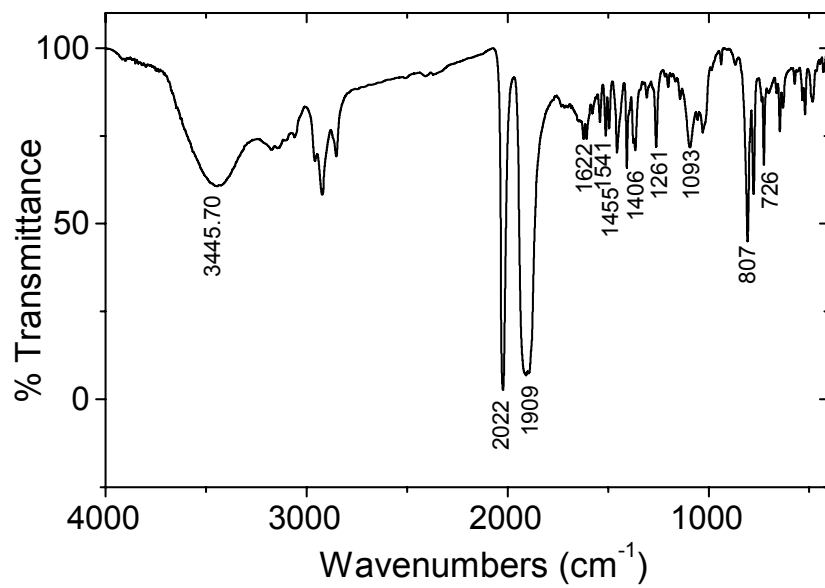
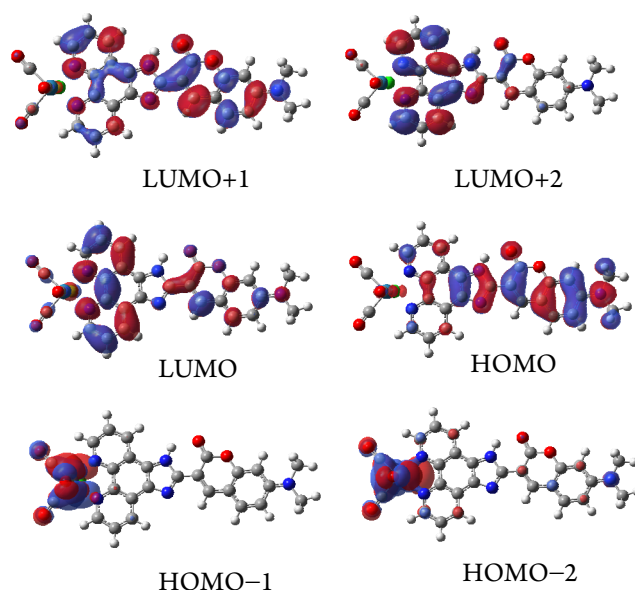


Figure S21. TOF HRMS ESI of **Re-2**,  $20^\circ\text{C}$ .



**Figure S22.** IR spectrum of **Re-2** (KBr disk).

## 2.0 DFT calculations.

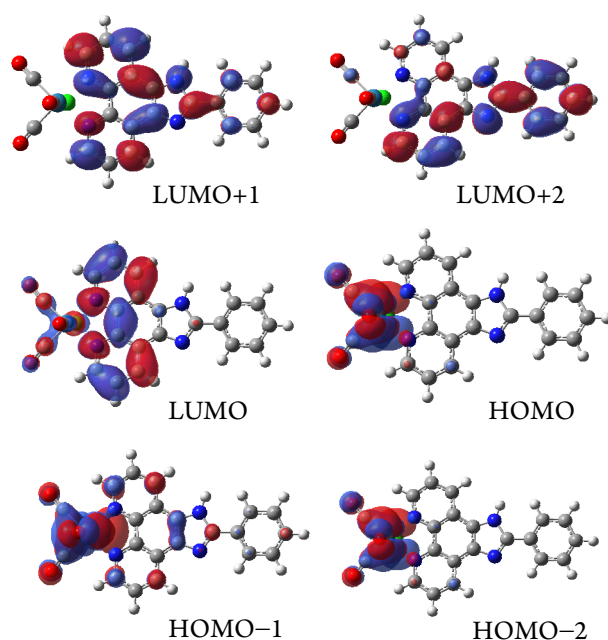


**Figure S23.** Electron density maps of the frontier molecular orbitals of complex **Re-1** based on the optimized ground-state geometry. Toluene was used as solvent in the calculations (PCM model). Calculated at the B3LYP/6-31G/LANL2DZ level with Gaussian 09W.

**Table S1.** Electronic excitation energies (eV) and corresponding oscillator strengths ( $f$ ), main configurations and CI coefficients of the low-lying electronically excited states of complex **Re-1**, Calculated by TDDFT//B3LYP/6-31G/LanL2DZ, based on the DFT//B3LYP/6-31G/LanL2DZ Optimized Ground State Geometries.

	Electronic transition	TDDFT//B3LYP/6-31G				
		Energy (eV) <sup>a</sup>	$f^b$	Composition <sup>c</sup>	CI <sup>d</sup>	character
Singlet	S <sub>0</sub> →S <sub>1</sub>	2.63 eV 471 nm	0.0025	H-1 →L	0.6407	MLCT
	S <sub>0</sub> →S <sub>2</sub>	2.69 eV 460 nm	0.4306	H →L	0.5738	ILCT
				H-2→L	0.3637	MLCT
	S <sub>0</sub> →S <sub>3</sub>	2.84 eV 437 nm	0.0269	H-2→L	0.5342	MLCT
Triplet	S <sub>0</sub> →S <sub>4</sub>	2.92 eV 425 nm	1.0011	H→L+1	0.6938	ILCT
	S <sub>0</sub> →T <sub>1</sub>	2.08 eV 597 nm	0.0000 <sup>e</sup>	H→L	0.3954	ILCT
				H→L+1	0.5560	ILCT
	S <sub>0</sub> →T <sub>2</sub>	2.48 eV 500 nm	0.0000	H→L	0.4425	ILCT
				H-2→L	0.3253	MLCT
				H→L+1	0.3126	ILCT
	S <sub>0</sub> →T <sub>3</sub>	2.52 eV 493 nm	0.0000	H-1→L	0.5649	MLCT
				H-1→L+1	0.2712	MLCT

<sup>a</sup> Only the selected low-lying excited states are presented. <sup>b</sup> oscillator strength. <sup>c</sup> H stands for HOMO and L stands for LUMO. Only the main configurations are presented. <sup>d</sup> The CI coefficients are in absolute values. <sup>e</sup> No spin-orbital coupling effect was considered, thus the  $f$  values are zero.

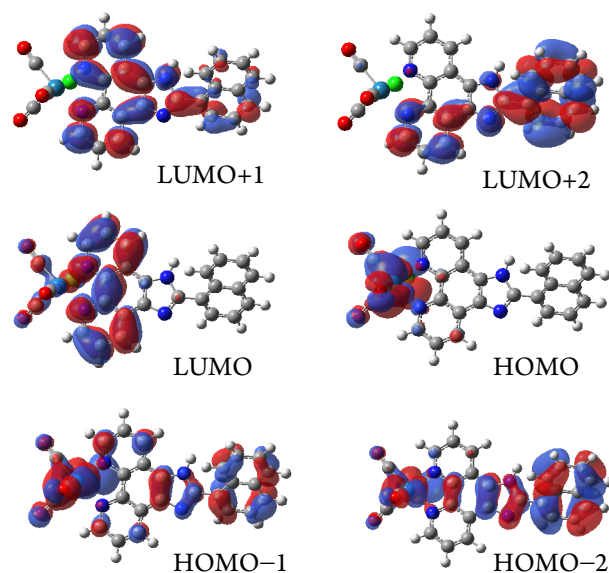


**Figure S24.** Electron density maps of the frontier molecular orbitals of complex **Re-0** based on the optimized ground-state geometry. Toluene was used as solvent in the calculations (PCM model). Calculated at the B3LYP/6-31G/LANL2DZ level with Gaussian 09W.

**Table S2.** Electronic excitation energies (eV) and corresponding oscillator strengths ( $f$ ), main configurations and CI coefficients of the low-lying electronically excited states of complex **Re-0**. Calculated by TDDFT//B3LYP/6-31G/LanL2DZ, based on the DFT//B3LYP/6-31G/LanL2DZ Optimized Ground State Geometries.

	Electronic transition	TDDFT//B3LYP/6-31G				
		Energy (eV) <sup>a</sup>	$f^b$	Composition <sup>c</sup>	CI <sup>d</sup>	character
Singlet	$S_0 \rightarrow S_1$	2.59 eV 479 nm	0.0021	H→L	0.7038	MLCT
	$S_0 \rightarrow S_2$	2.72 eV 456 nm	0.1107	H-1→L	0.6980	MLCT
	$S_0 \rightarrow S_3$	3.08 eV 402 nm	0.0188	H-2→L	0.1339	MLCT
Triplet	$S_0 \rightarrow T_1$	2.48 eV 501 nm	0.0000 <sup>e</sup>	H→L+1	0.6808	MLCT
				H-2→L+1	0.1770	MLCT
				H-1→L+1	0.1542	MLCT
	$S_0 \rightarrow T_2$	2.52 eV 493 nm	0.0000	H-1→L	0.6677	MLCT
				H→L	0.1367	MLCT

<sup>a</sup> Only the selected low-lying excited states are presented. <sup>b</sup> oscillator strength. <sup>c</sup> H stands for HOMO and L stands for LUMO. Only the main configurations are presented. <sup>d</sup> The CI coefficients are in absolute values. <sup>e</sup> No spin-orbital coupling effect was considered, thus the  $f$  values are zero.



**Figure S25.** Electron density maps of the frontier molecular orbitals of complex **Re-2** based on the optimized ground-state geometry. The solvent toluene was considered in the calculations (PCM model). Calculated at the B3LYP/6-31G/LANL2DZ level with Gaussian 09W.

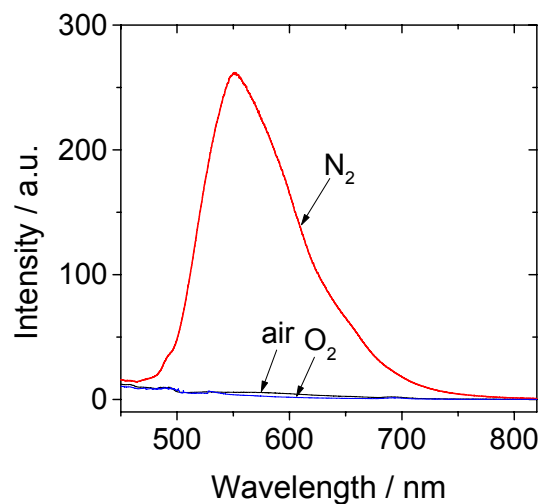
**Table S3.** Electronic Excitation Energies (eV) and corresponding oscillator Strengths ( $f$ ), main configurations and CI coefficients of the low-lying electronically excited states of complex **Re-2**. Calculated by TDDFT//B3LYP/6-31G/LanL2DZ based on the DFT//B3LYP/6-31G/LanL2DZ Optimized Ground State Geometries.

	Electronic transition	TDDFT//B3LYP/6-31G				
		Energy (eV) <sup>a</sup>	$f^b$	Composition <sup>c</sup>	CI <sup>d</sup>	character
Singlet	$S_0 \rightarrow S_1$	2.60 eV 476 nm	0.0020	H $\rightarrow$ L	0.6977	MLCT
	$S_0 \rightarrow S_2$	2.73 eV 455 nm	0.1158	H-1 $\rightarrow$ L	0.6545	ILCT
				H-2 $\rightarrow$ L	0.2362	ILCT
				H-2 $\rightarrow$ L	0.6505	MLCT
	$S_0 \rightarrow S_3$	3.03 eV 409 nm	0.0216	H-2 $\rightarrow$ L	0.6505	ILCT
	Triplet	$S_0 \rightarrow T_1$	2.45 eV 505 nm	0.0000 <sup>e</sup>	H-1 $\rightarrow$ L	0.2194
H-1 $\rightarrow$ L					0.3521	MLCT
H-2 $\rightarrow$ L					0.6505	ILCT
$S_0 \rightarrow T_2$		2.51 eV 494 nm	0.0000	H-1 $\rightarrow$ L+1	0.2743	MLCT
				H-1 $\rightarrow$ L	0.4100	ILCT
				H $\rightarrow$ L	0.4376	MLCT

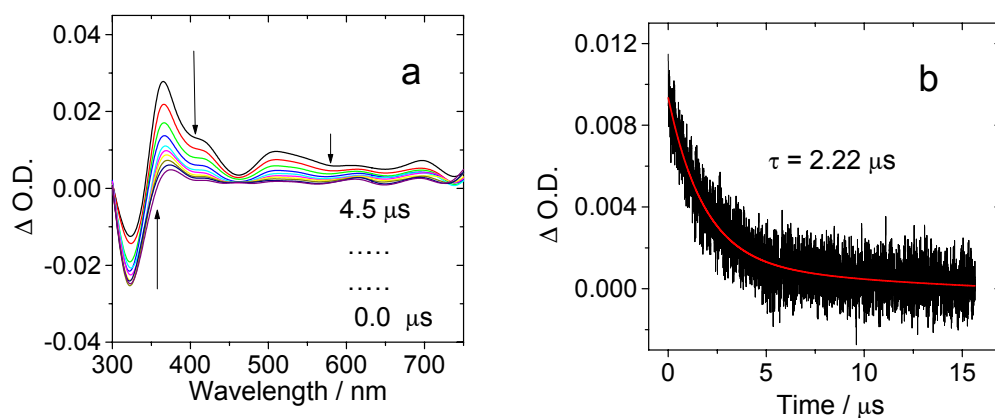
<sup>a</sup> Only the selected low-lying excited states are presented. <sup>b</sup> oscillator strength. <sup>c</sup> H stands for HOMO and L stands for LUMO. Only the main configurations are presented. <sup>d</sup> The CI coefficients are in absolute values. <sup>e</sup> No spin-orbital coupling effect was considered, thus the  $f$  values are zero.



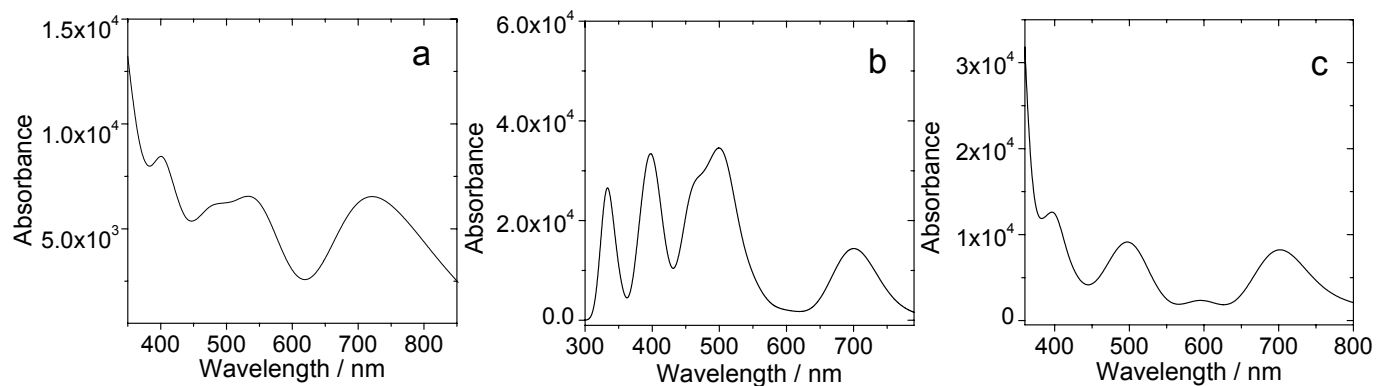
### 3.0 Transient absorption details



**Figure S26.** The emission spectra of **Re-2** ( $\lambda_{\text{ex}} = 428 \text{ nm}$ ) under different atmosphere.  $c = 1.0 \times 10^{-5} \text{ mol/dm}^3$  in toluene, 25 °C.

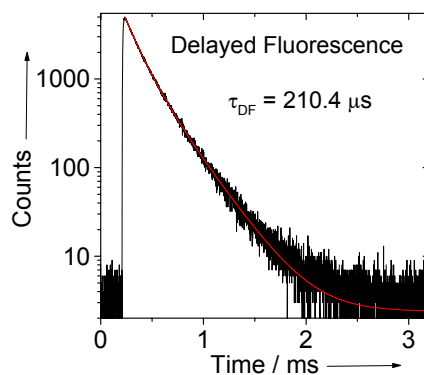


**Figure S27.** Nanosecond time-resolved transient absorption difference spectra of **Re-0** in deaerated toluene at room temperature after pulsed excitation ( $\lambda_{\text{ex}} = 355 \text{ nm}$ ). Decay traces of **Re-0** (b) at 470nm, In deaerated toluene,  $c = 1.0 \times 10^{-5} \text{ M}$ . 25 °C.

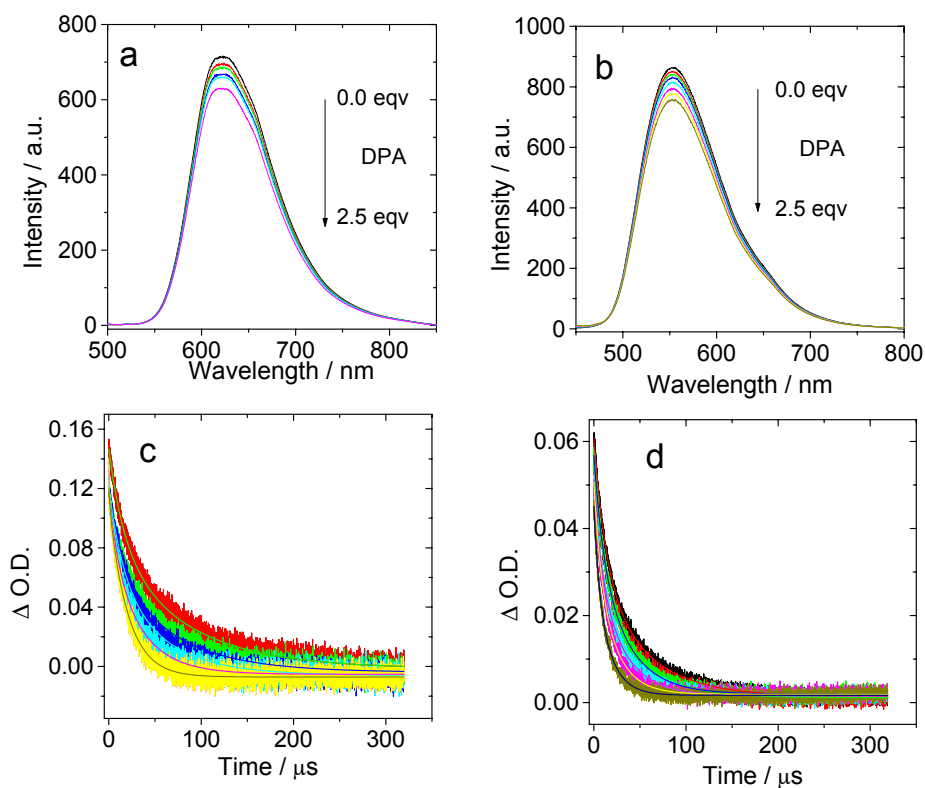


**Figure S28.** The calculated transient absorption spectra were presented (a) **Re-0**, (b) **Re-1** and (c) **Re-2**. Toluene was used as solvent in the calculations. Calculated by DFT at the B3LYP/6-31G level using Gaussian 09W.

### 3.0 TTA upconversion details



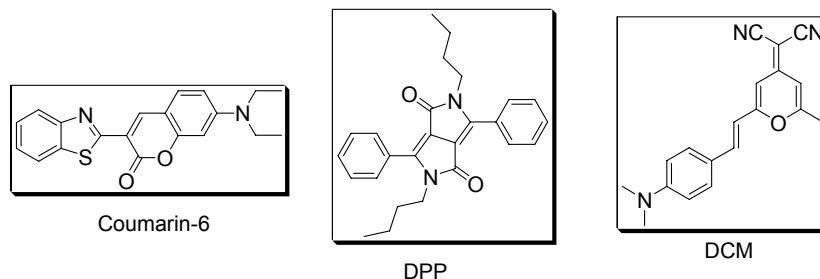
**Figure S29.** Delayed fluorescence observed in the TTA upconversion with **Re-2** as triplet photosensitizer and DPA as the triplet acceptor. Excited at 473 nm (nanosecond pulsed OPO laser synchronized with spectrofluorometer) and monitored at 410 nm. Under this circumstance the **Re-2** is selectively excited and the emission is due to the upconverted emission of DPA.

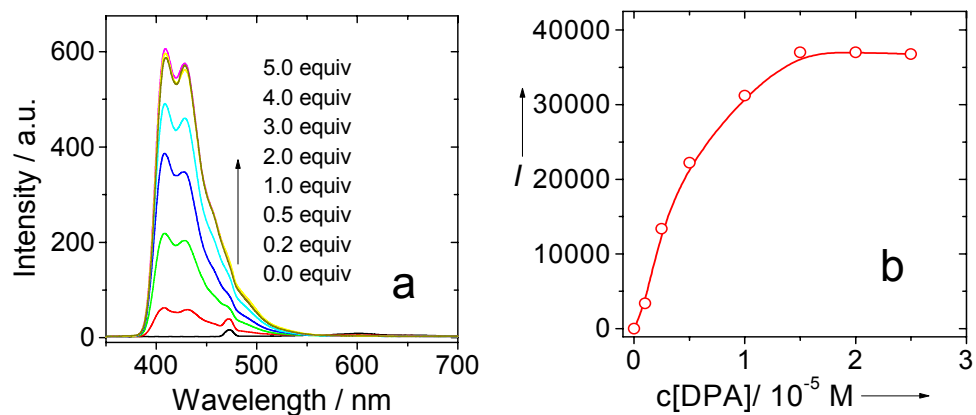


**Figure S30.** Quenching of the phosphorescence of the triplet photosensitizers with increasing the concentration of DPA, (a)  $\text{Ru}(\text{dmb})_3^{2+}$  ( $\lambda_{\text{ex}} = 450 \text{ nm}$ ), (b) **Re-0** ( $\lambda_{\text{ex}} = 439 \text{ nm}$ ). Quenching of the lifetime of the triplet photosensitizers with increasing the concentration of DPA, (c) **Re-1**, (d) **Re-2**.

**Table S4.** The TTA upconversion quantum yields were measured with different quantum yields standards, similar results were observed. The followings are the results with diketopyrrolopyrrole (DPP,  $\Phi_{\text{F}} = 69\%$  in DMSO) and 4-dicyanomethylene-2-methyl-6-(*p*-(dimethylamino)styryl)-4H-pyran (DCM,  $\Phi_{\text{F}} = 10\%$  in dichloromethane)

Standard	Coumarin	DPP	DCM
$\Phi_{\text{UC}}$	17.0%	19.4%	16.7%





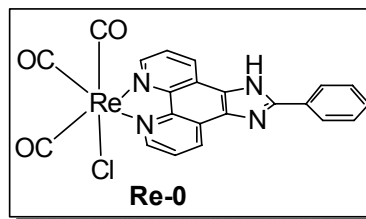
**Figure S31.** Upconverted emission of DPA with increasing DPA concentration. (a) **Re-1** as the triplet sensitizer; (b) integrated upconversion intensity with **Re-1** as triplet sensitizer with increasing DPA concentration; Excited with 473 nm laser (5 mW).  $c[\text{sensitizer}] = 5.0 \times 10^{-6}$  M. In deaerated toluene at 20 °C.

## 4.0 DFT calculation details

### Re-0. Ground state geometry.

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1



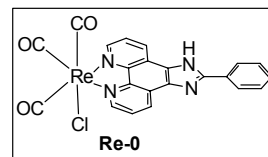
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C	1.18028300	2.92135800	0.09460200
H	-2.21464500	3.11997200	0.14654000
C	1.29047800	1.51408000	0.10066900
H	2.06896500	3.54312900	0.07070900
C	0.08876100	0.74892800	0.12854100
C	0.11219100	-0.69206800	0.13085800
C	1.33426400	-1.41040300	0.11015000
C	-1.12381800	-2.67972000	0.14436200
C	1.28808400	-2.81877700	0.10815700
C	0.05212300	-3.44837800	0.12538600
H	-2.09876700	-3.14607200	0.14668800
H	2.21569000	-3.37789500	0.08896200
H	-0.02484300	-4.52862200	0.11878600
N	-1.09991200	-1.33445000	0.15076700
C	-0.07793800	3.50457300	0.11506200
H	-0.19364700	4.58121600	0.10553800
C	2.53899400	-0.63757500	0.08515800
C	2.50367800	0.76098400	0.07795400
C	4.61733500	0.00056900	0.03413400
H	4.17561800	2.09858700	0.01808800
N	3.84499900	-1.09358000	0.05914700
N	3.83304600	1.15289500	0.04575900
N	-1.14333300	1.34904800	0.15186800
C	6.07666700	-0.00218500	-0.00262600
C	6.74782500	-1.24052500	-0.04200300
C	8.14106000	-1.28447800	-0.07972100
C	8.88689900	-0.09825600	-0.07894700
C	8.22790800	1.13599400	-0.03918400
C	6.83283500	1.18543000	-0.00074800
H	6.15810700	-2.14936000	-0.04337100
H	8.64692800	-2.24371300	-0.11072900
H	9.97075200	-0.13511200	-0.10901400
H	8.79869200	2.05861300	-0.03753600
H	6.34683400	2.15657100	0.03300700
Re	-2.84635000	-0.02094900	0.04793100
C	-4.19579500	1.32703300	-0.20896100
O	-4.98148700	2.19160500	-0.38142000
C	-3.11753100	-0.03172800	1.94084800
O	-3.27310000	-0.03702000	3.11729100
Cl	-2.31028300	-0.00033100	-2.44731000
C	-4.15198200	-1.41048900	-0.21738100
O	-4.91066700	-2.29699300	-0.39578200

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29 30 1.5 34 1.0  
30 35 1.0  
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36 37 1.0 39 1.0 42 1.0  
37 38 2.0  
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39 40 2.0  
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42 43 2.0  
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### Re-0. Triplet state geometry.

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3



C	-1.22198900	2.71900700	0.07353500
C	1.19974500	2.90086200	0.02059600
H	-2.21210100	3.15128800	0.09242900
C	1.29367000	1.49576800	0.04517100
H	2.08611400	3.52311400	-0.00241700
C	0.10165100	0.71515400	0.07903300
C	0.12863800	-0.69290700	0.12298200
C	1.35189400	-1.44441300	0.12846300
C	-1.12659300	-2.68801300	0.19792300
C	1.28712700	-2.84199500	0.16857700
C	0.03680300	-3.46690500	0.20386200
H	-2.10195100	-3.15499000	0.22138100
H	2.20458700	-3.41845300	0.17043400
H	-0.04868300	-4.54545600	0.23214800
N	-1.10242500	-1.33928600	0.15987200
C	-0.09657600	3.49909000	0.04191300
H	-0.19729300	4.57738200	0.03591900
C	2.54996500	-0.67122600	0.08586200
C	2.50278000	0.73653700	0.04428200
C	4.62228400	-0.00464300	0.02045200
H	4.15468200	2.08836800	-0.03844400
N	3.86184500	-1.10992200	0.07143500
N	3.82654400	1.13738900	0.00326700
N	-1.17143100	1.31990600	0.06806200
C	6.08026800	0.00539600	-0.01495600
C	6.76592000	-1.22718100	-0.01003400
C	8.15963400	-1.25845700	-0.04520900
C	8.89298900	-0.06433400	-0.08552600
C	8.22019900	1.16401300	-0.09016000
C	6.82451700	1.20145400	-0.05505200
H	6.18812700	-2.14309400	0.02051400
H	8.67545100	-2.21282500	-0.04175600
H	9.97718000	-0.09070200	-0.11319700
H	8.78106700	2.09205700	-0.12109400
H	6.32875600	2.16719600	-0.05875700
Re	-2.79745300	0.01774900	0.03628500
C	-4.13926500	1.37272300	-0.28802000
O	-4.93481800	2.21299900	-0.50966700
C	-3.03412500	0.17421000	1.95311400
O	-3.18798500	0.26778200	3.11676800
Cl	-2.61967900	-0.37852600	-2.45192700
C	-4.17553300	-1.40435000	0.00737100
O	-4.96946600	-2.26896800	-0.00451000

1 3 1.0 16 2.0 24 1.0

2 4 1.5 5 1.0 16 1.5

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4 6 1.5 19 1.5

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C	-2.84036100	-2.70878900	0.14417500
C	-0.42506000	-2.74860100	0.12641900
C	-1.63411400	-3.42863900	0.13571600
H	-3.79575500	-3.21402900	0.14088200
H	0.52452800	-3.26985100	0.11609500
H	-1.66672600	-4.51122100	0.13137600
N	-2.87044700	-1.36365700	0.14742600
C	-2.04697700	3.51334400	0.09530100
H	-2.20604200	4.58437500	0.07801900
C	0.73868600	-0.51895800	0.10863400
C	0.64461000	0.88112300	0.09774900
C	2.77561300	0.21839100	0.07729400
H	2.33054400	2.27269100	0.06259500
N	2.06227600	-0.91991100	0.09667500
N	1.94926400	1.33181000	0.07847100
C	4.22414700	0.30353100	0.05410600
C	5.00194500	-0.83412000	0.04695300
H	4.50148500	-1.79724500	0.06053800
O	4.25906800	2.71370300	0.04119400
C	4.84726600	1.61747900	0.03594100
O	6.25244800	1.65152400	0.01010300
C	7.03925700	0.50246100	0.00076000
C	8.41229500	0.67744900	-0.02866200
H	8.79714600	1.68628200	-0.04298200
C	6.41992700	-0.77013000	0.02069600
C	7.27921800	-1.89663900	0.01045400
H	6.84041300	-2.88934300	0.02496700
C	8.65180400	-1.75539600	-0.01843200
H	9.27033200	-2.64212300	-0.02595100
C	9.25967600	-0.45837900	-0.03957500
N	10.62908500	-0.31920300	-0.07022300
C	11.23168700	1.01781600	-0.09675400
H	12.31689300	0.92056500	-0.12258700
H	10.91740100	1.58224000	-0.98400300
H	10.96118200	1.59827500	0.79461700
C	11.49919200	-1.50019000	-0.08048800
H	11.32039100	-2.12641500	-0.96378200
H	12.53907500	-1.17456800	-0.10233200
H	11.35459500	-2.11588300	0.81628100
N	-3.02496100	1.31657000	0.13575400
Re	-4.67041000	-0.12417800	0.03674100
C	-6.07558900	1.16401100	-0.22667400
O	-6.89871500	1.99245900	-0.40342700
C	-4.93834900	-0.13542400	1.92966900
O	-5.09299200	-0.14194600	3.10652300
Cl	-4.13833600	-0.09892100	-2.45966100
C	-5.91589900	-1.56879700	-0.21708100
O	-6.63665800	-2.48869000	-0.38745500

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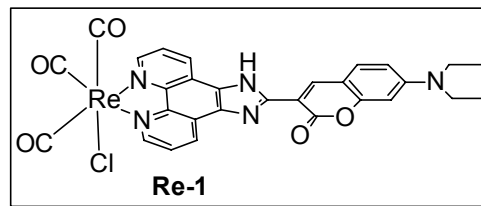
S6

### Re-1. Triplet state geometry.

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	-3.15709200	2.65978300	0.11250300
C	-0.76645100	2.99477000	0.09222800
H	-4.16606200	3.04559600	0.11183700
C	-0.59693000	1.59171600	0.10050800
H	0.09646900	3.65058600	0.07948600
C	-1.76394600	0.77309400	0.11372400
C	-1.67705700	-0.66693200	0.12100200
C	-0.42514100	-1.33257900	0.11802200
C	-2.82595900	-2.70926100	0.13756800
C	-0.41174300	-2.74081500	0.12528000
C	-1.61892200	-3.42605200	0.13589500
H	-3.77871800	-3.21898600	0.13980100
H	0.53744800	-3.26251800	0.12104700
H	-1.64775100	-4.50819200	0.13970000
N	-2.85927900	-1.36258400	0.13139500
C	-2.04864000	3.52197700	0.09901300
H	-2.21136500	4.59202100	0.09091200
C	0.75158500	-0.51115000	0.10412100
C	0.65063600	0.90270000	0.09443600
C	2.79315100	0.24649800	0.07920100
H	2.31881300	2.30210800	0.06608400
N	2.05723800	-0.90992800	0.09575300
N	1.94366500	1.35877800	0.07971900
C	4.20246900	0.31509700	0.06022400
C	5.00014800	-0.89386400	0.05799100
H	4.49397800	-1.84881000	0.07521700
O	4.25281300	2.72258900	0.04187400
C	4.83552800	1.61273200	0.03989800
O	6.23886900	1.65820600	0.01393700
C	7.02505600	0.48621500	0.00395200
C	8.38490400	0.66501200	-0.02979400
H	8.76597900	1.67619400	-0.04711500
C	6.39371500	-0.80149400	0.02873900
C	7.28813000	-1.92379200	0.01913100
H	6.85980400	-2.92007200	0.03774600
C	8.65871200	-1.76842700	-0.01417000
H	9.28304400	-2.65194300	-0.02085900
C	9.25512400	-0.47010600	-0.04090800
N	10.62520700	-0.30708500	-0.07706900
C	11.21736200	1.03712300	-0.11137600



H	12.30226100	0.94788500	-0.14157100
H	10.89157000	1.59131300	-0.99938000
H	10.94302100	1.61461000	0.77923700
C	11.51314600	-1.47716200	-0.08595400
H	11.33245600	-2.10519100	-0.96627600
H	12.54796900	-1.13916500	-0.11151900
H	11.37105700	-2.08860700	0.81280200
N	-3.01997700	1.31943000	0.12079200
Re	-4.66433000	-0.12713500	0.03593100
C	-6.08165400	1.15209500	-0.19995000
O	-6.92345400	1.96612700	-0.36216500
C	-4.90315300	-0.13772200	1.92794200
O	-5.04365600	-0.14437700	3.10689500
Cl	-4.17873300	-0.10200100	-2.49077700
C	-5.91332000	-1.57200500	-0.19058900
O	-6.64740300	-2.48537700	-0.34612900

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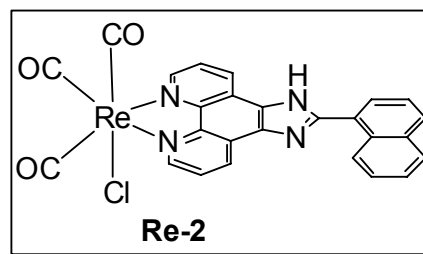
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49 50 1.0 52 1.0 55 1.0  
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55 56 2.0  
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### Re-2. Ground state geometry.

Symbolic Z-matrix:

Charge = 0 Multiplicity = 1

C	1.62982500	-2.61051600	-0.48055500
C	-0.78064100	-2.58186100	-0.60682100
H	2.57421700	-3.13044100	-0.54916500
C	-0.75589900	-1.20335800	-0.30061900
H	-1.72323600	-3.09100400	-0.77237300
C	0.51072200	-0.58575100	-0.09359300
C	0.62374000	0.81553200	0.22434700
C	-0.52422000	1.63878200	0.34714900
C	2.04022600	2.61984300	0.69985900
C	-0.34449000	3.00149100	0.66152500
C	0.94281200	3.48644100	0.83754100
H	3.05238800	2.97646000	0.82590900
H	-1.21196200	3.64280200	0.75810700
H	1.12021300	4.52708900	1.07751400
N	1.88944400	1.31591700	0.40192400
C	0.41437100	-3.27962800	-0.69459300
H	0.42689500	-4.33624400	-0.92944000
C	-1.79423300	1.01498300	0.13209200



C	-1.89163800	-0.34580700	-0.17751800
C	-3.92157300	0.61142900	-0.08516800
H	-3.68120900	-1.44867900	-0.60638700
N	-3.05060600	1.59545800	0.18545800
N	-3.24843800	-0.58776300	-0.31036700
N	1.67885800	-1.29798900	-0.18665600
Re	3.50886400	-0.11921900	0.06688100
C	4.74460900	-1.51187500	-0.41611500
O	5.47128100	-2.38815200	-0.73539500
C	3.66174300	-0.54281300	1.91994300
O	3.74823100	-0.80617900	3.07447200
Cl	3.13396400	0.46175300	-2.41165500
C	4.95588900	1.14362400	0.17412400
O	5.81668300	1.95175900	0.22853000
C	-5.36951800	0.79226500	-0.22594900
C	-6.33325200	-0.21181800	0.14900600
C	-5.80296800	1.99789200	-0.76928800
C	-6.00119400	-1.42196400	0.82824100
C	-7.72340300	0.04009600	-0.13551300
C	-7.17170500	2.24528600	-1.01249700
H	-5.06290700	2.74559200	-1.02896200
C	-6.97122300	-2.35234600	1.15126800
H	-4.97955500	-1.60163200	1.14130400
C	-8.69463300	-0.94638200	0.20062900
C	-8.11110400	1.27708500	-0.72262700
H	-7.47303300	3.19201100	-1.44700500
C	-8.33009200	-2.12390900	0.82014800
H	-6.69237400	-3.25990400	1.67665700
H	-9.73626100	-0.74577800	-0.03168400
H	-9.16315100	1.44833900	-0.92928400
H	-9.07953300	-2.86606800	1.07342400

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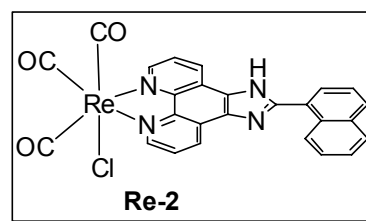
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## Re-2. Triplet state geometry.

Symbolic Z-matrix:

Charge = 0 Multiplicity = 3

C	1.62393500	-2.63454100	-0.46719600
C	-0.80142700	-2.55660900	-0.57624000
H	2.56577900	-3.16109700	-0.52411300
C	-0.75741100	-1.18021900	-0.28118300
H	-1.74436600	-3.06824900	-0.72620900
C	0.50368900	-0.54589000	-0.08493500
C	0.61278500	0.82271600	0.23208100
C	-0.53099700	1.67889400	0.37331800
C	2.05392000	2.62925500	0.70118200
C	-0.33161600	3.02868400	0.68527000
C	0.97245200	3.50586600	0.84961500
H	3.06934500	2.98256800	0.81943100



H	-1.18837800	3.68322800	0.79315500
H	1.16207900	4.54466700	1.08694900
N	1.89938600	1.32192900	0.40378300
C	0.42905900	-3.27603900	-0.65973700
H	0.42440900	-4.33757500	-0.87426000
C	-1.79673000	1.05482500	0.16543700
C	-1.88585100	-0.31584000	-0.14757300
C	-3.92283100	0.63001800	-0.05211000
H	-3.66245900	-1.42796300	-0.58345100
N	-3.05829100	1.62169400	0.21822200
N	-3.24082000	-0.56482900	-0.27895600
N	1.71107500	-1.26284000	-0.20070100
Re	3.45805600	-0.15083800	0.03928600
C	4.67163400	-1.54750300	-0.52313000
O	5.38906300	-2.40629800	-0.89226500
C	3.62480400	-0.68972000	1.89200200
O	3.73727900	-1.01642000	3.01802500
Cl	3.38987800	0.72547200	-2.33131800
C	4.96589900	1.10557000	0.29562700
O	5.83846400	1.87446000	0.45688800
C	-5.36901400	0.80539600	-0.18870000
C	-6.33076200	-0.22132000	0.12919400
C	-5.80779500	2.03436400	-0.67743700
C	-6.00021400	-1.45582900	0.76280700
C	-7.71885100	0.03246700	-0.16399900
C	-7.17417400	2.28197400	-0.92646500
H	-5.06958300	2.79806600	-0.89129800
C	-6.96744500	-2.40782100	1.02838100
H	-4.98387400	-1.63932200	1.08990700
C	-8.68682200	-0.97544400	0.11182900
C	-8.10925800	1.29238300	-0.69769400
H	-7.47828200	3.24598600	-1.31900900
C	-8.32209700	-2.17695300	0.68396900
H	-6.68886400	-3.33446100	1.51939400
H	-9.72637700	-0.77243300	-0.12759900
H	-9.15971800	1.46442200	-0.91165200
H	-9.06902300	-2.93573900	0.89119700

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