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Supplementary Information

for

Highly sensitive and selective detection of Pd^{2+} ions using a triple channel receptor of ferrocene-rhodamine conjugate in aqueous medium and living cells

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Contents

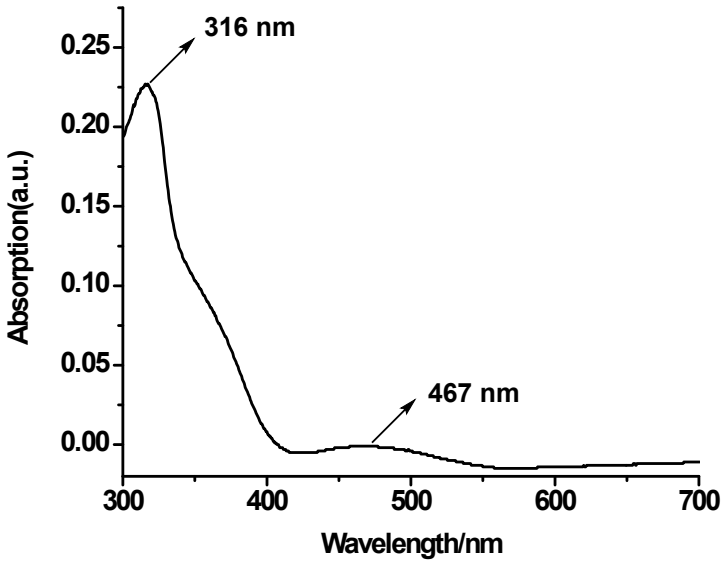


Fig. S1 UV-vis absorbance spectrum of **FR** (10 μM) in H_2O/THF (9:1, v/v) at room temperature.

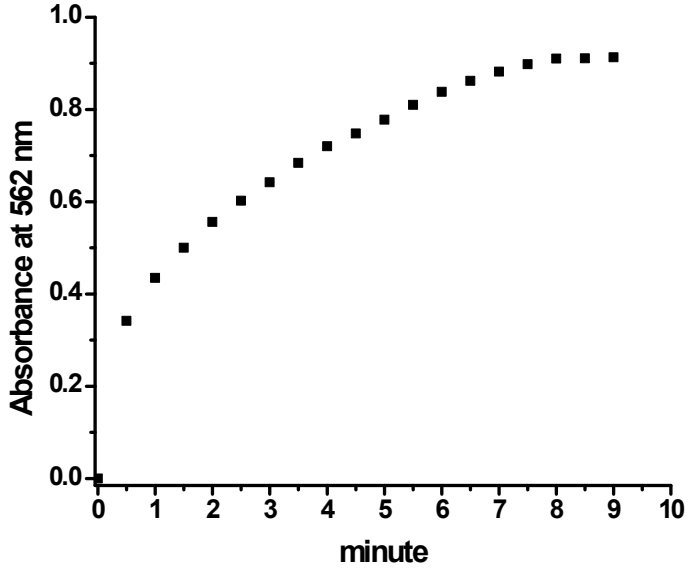
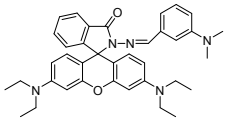
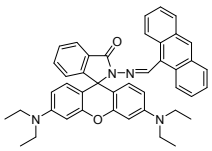
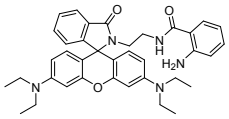
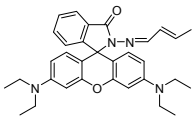
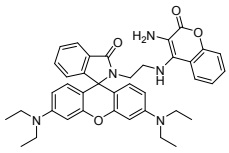
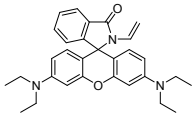
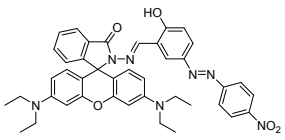
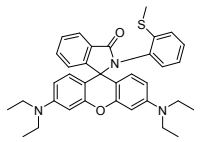
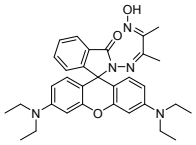
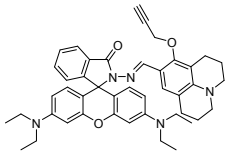
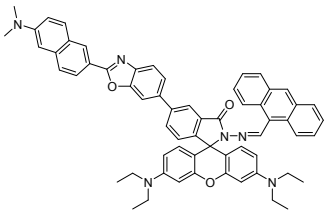
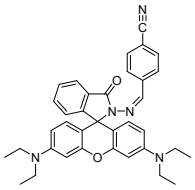
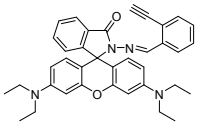
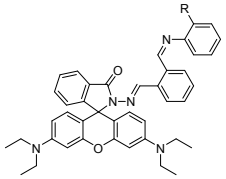
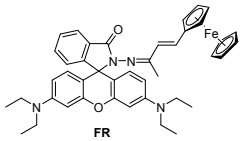


Fig. S2 Time course of the response of **FR** (10 μM) to 2 equiv of Pd^{2+} in H_2O/THF (9:1, v/v) solution.

Table S1 Comparison of **FR** with some reported Pd^{2+} fluorescent probes.

Probe	Medium	Detection limit	Ref.
	EtOH : H_2O = 1 : 99	1.3 × 10^{-7} M	1
	DMF : H_2O = 1 : 99	3 × 10^{-8} M	2
	EtOH : H_2O = 1 : 1	7.38 × 10^{-8} M	3
	MeOH : PBS = 1 : 1	1.9 × 10^{-7} M	4
	HEPES : CH_3CN =1 : 1	0.1 ppm	5
	EtOH : PBS = 3 : 7	2.13 × 10^{-8} M	6
	EtOH : H_2O = 1 : 1	4.5 × 10^{-7} M	7

	UV : EtOH : H_2O = 4 : 6 Fl: CH_3CN : H_2O = 8 : 2	2.4 × 10^{-9} M	8
	Tris-HCl buffer solution (pH 7.2)	1.5 × 10^{-8} M	9
	EtOH : CH_3CN = 1 : 1	10^{-7} M	10
	EtOH : H_2O = 1 : 1	2.3 × 10^{-7} M	11
	CH_3CN : H_2O = 4 : 1	5.7 × 10^{-8} M	12
	EtOH : H_2O = 1 : 1	1.91 × 10^{-7} M	13
 ROP : R = OH ; ROM : R = OCH_3	EtOH : H_2O = 4 : 6	ROP : 3.49 × 10^{-6} M ROM : 4.64 × 10^{-6} M	14

 FR	THF : H_2O = 1 : 9	8.46×10^{-9} M	Our work

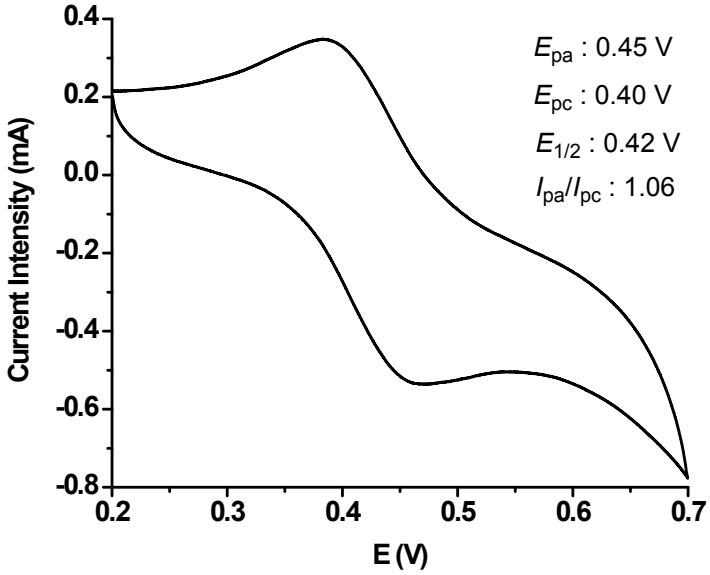


Fig. S3 The CV of **FR** (0.7 mM) in H_2O/THF (1:1, v/v) solution using *n*-Bu_4NClO_4 as supporting electrolyte.

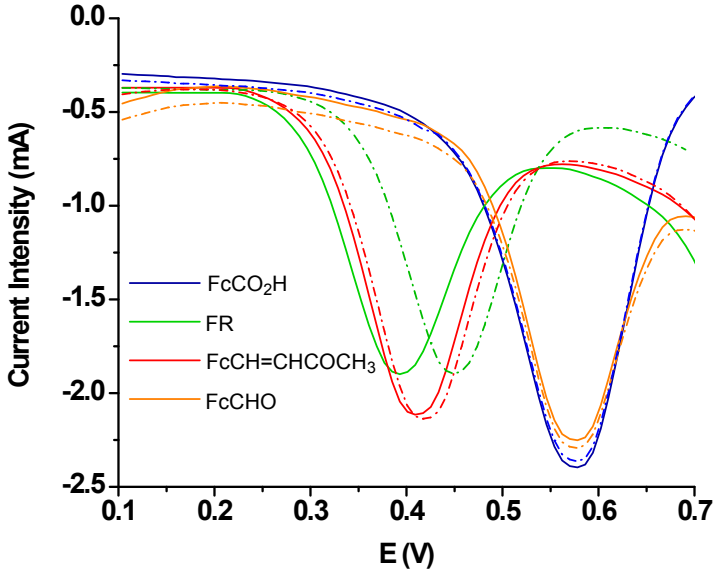


Fig. S4 The DPV assay of $FcCO_2H$, **FR**, $FcCH=CHOCH_3$ and FcCHO (0.7 mM) in H_2O/THF (1:1, v/v) solution containing 0.1 M *n*-Bu_4NClO_4 as supporting electrolyte upon the addition of 0 (solid lines) and 1.0 (dotted lines) equiv $PdCl_2$.

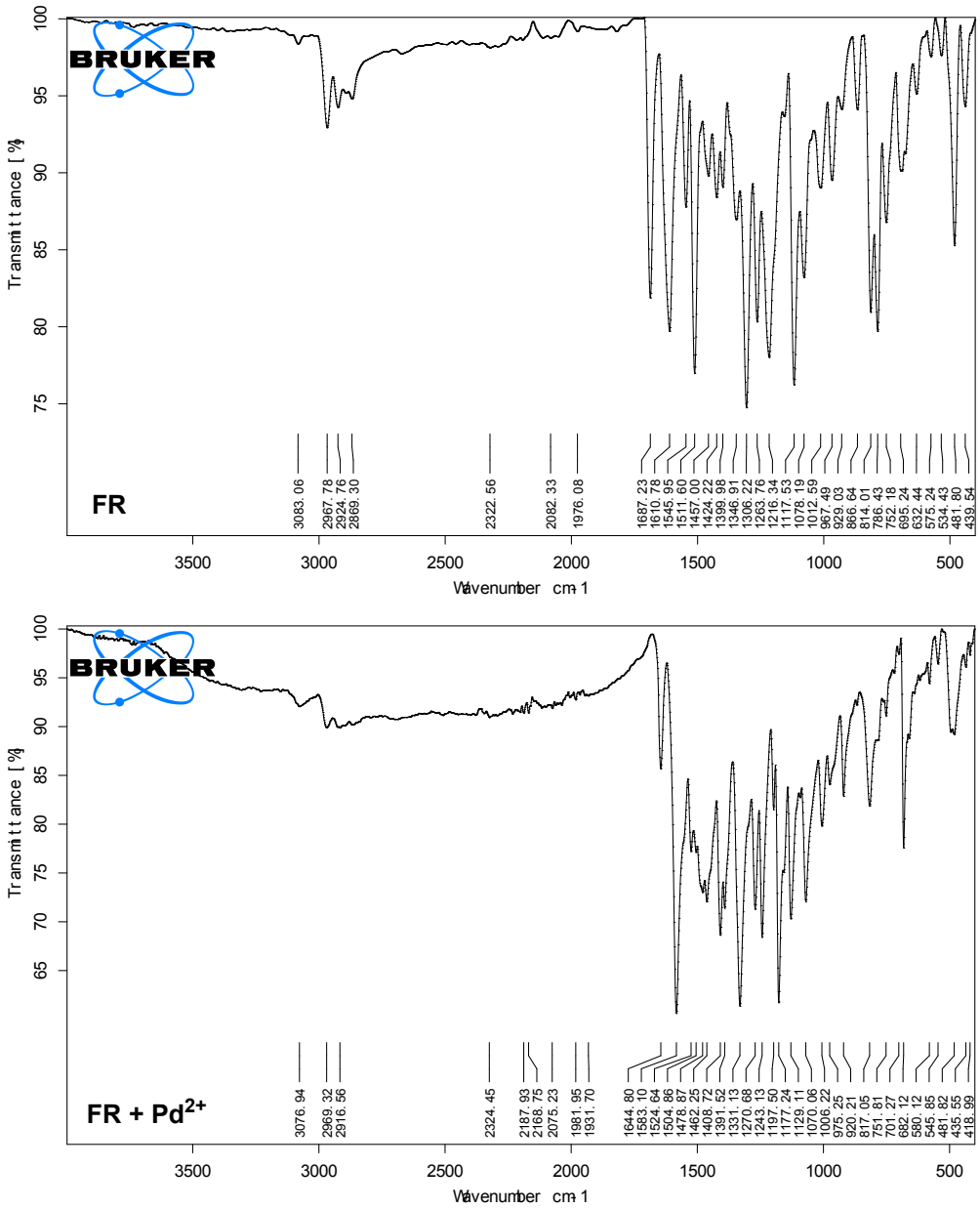


Fig. S5 IR spectra of the probe **FR** and its corresponding Pd^{2+} complex.

Table S2 Cartesian coordinates (in Å) of the structures of **FR** and [**FR**·PdCl]$^+$.

FR

Fe	4.19150932	-4.19022450	-0.58303335
C	2.13506432	-4.13448450	-0.94513335
C	2.81389032	-4.80715750	-2.01492735
H	2.81115232	-4.48383750	-3.04556235
C	3.48915032	-5.93667450	-1.47074135
H	4.11079332	-6.62882150	-2.02222535
C	3.24903732	-5.96633250	-0.06181935
H	3.65121232	-6.68620850	0.63772265
C	2.41930632	-4.85432950	0.26501965
H	2.07341032	-4.58319450	1.25354565
C	5.50951332	-2.86983050	-1.49467235
H	5.43122132	-2.55840950	-2.52715735
C	6.21687332	-4.01392350	-1.01311535
H	6.77257432	-4.71803750	-1.61723535
C	6.02259232	-4.09110250	0.39954065
H	6.40647532	-4.86311050	1.05250565
C	5.19440332	-2.99525750	0.79065765
H	4.84196632	-2.79080450	1.79235465
C	4.87956132	-2.23873250	-0.37988935
H	4.23288132	-1.37277050	-0.42143635
C	0.46644380	-1.60939674	-3.13075396
N	0.14821200	-0.90091000	-2.10515100
N	-0.58944400	0.22910100	-2.23142700

C	-1.19977300	1.06741000	-1.14664100
C	-0.82446700	0.71305100	-3.53255500
C	-1.86602300	2.15511400	-1.99548400
C	-2.23123700	0.29423700	-0.33719000
C	-0.14549000	1.66530800	-0.22508300
O	-0.42878500	0.21587900	-4.56902300
C	-1.64046400	1.93561600	-3.35051800
C	-2.61153100	3.25133900	-1.57194000
C	-3.18757900	-0.52905200	-0.94562700
C	-2.30980500	0.41509200	1.05252100
C	-0.32579900	1.71305000	1.15948500
C	1.03202200	2.24139200	-0.71819400
C	-2.14443800	2.79186500	-4.32808700
H	-2.79358400	3.43194700	-0.51658300
C	-3.12212200	4.11663400	-2.54363100
H	-3.15885200	-0.65099800	-2.02455400
C	-4.16774000	-1.19191700	-0.22467900
O	-1.42492200	1.17307300	1.78670700
C	-3.28420100	-0.23770300	1.80626000
C	0.60189100	2.30696200	2.01513500
C	1.97779000	2.83139200	0.10692900
H	1.21532200	2.21761200	-1.78866400
C	-2.89254800	3.89183600	-3.90985200
H	-1.95015700	2.59195900	-5.37728500
H	-3.70718500	4.97879200	-2.23579500

H	-4.88385200	-1.79845200	-0.76372000
C	-4.24777200	-1.05842600	1.18653800
H	-3.24459300	-0.10404300	2.87907700
H	0.37552900	2.27913900	3.07223200
C	1.77731200	2.90046400	1.51190600
H	2.86927900	3.24365300	-0.34631300
H	-3.30172000	4.58119100	-4.64260800
N	-5.22594500	-1.70713000	1.92221500
N	2.68563300	3.53449700	2.34693700
C	-6.12587600	-2.68221400	1.31249700
C	-5.39492500	-1.46603200	3.35130000
C	3.92854600	4.09547800	1.82046500
C	2.47665600	3.56803700	3.79189400
H	-6.39452600	-3.41165400	2.08512700
H	-5.58384100	-3.24796700	0.54797700
C	-7.40215700	-2.06922500	0.72024900
H	-6.45308800	-1.62245700	3.59035000
H	-5.19561300	-0.41077200	3.56469300
C	-4.52987800	-2.36548300	4.24516000
H	4.26711200	4.85468000	2.53299000
H	3.71276300	4.63548800	0.89153500
C	5.05586500	3.07915800	1.58544600
H	1.42463000	3.80151600	3.99362800
H	3.05066200	4.41411100	4.18352800
C	2.88036500	2.28955200	4.54214100

H	-7.97813900	-1.54558600	1.49030600
H	-8.04088500	-2.84955300	0.29212500
H	-7.16527500	-1.34866000	-0.06754100
H	-4.75822700	-3.42231000	4.07277100
H	-4.71397300	-2.14795700	5.30299500
H	-3.46522500	-2.21724100	4.04411100
H	5.36349800	2.60708800	2.52320700
H	5.93142500	3.57806300	1.15540000
H	4.74513000	2.28683200	0.89894300
H	2.34726800	1.41662300	4.15527700
H	2.64639700	2.38647600	5.60819500
H	3.95319400	2.09782500	4.44794000
C	0.07135742	-1.25129180	-4.57549186
H	-0.97250189	-1.01918297	-4.61268357
H	0.63712146	-0.40311504	-4.90015667
H	0.27494477	-2.08276437	-5.21744635
C	1.29029620	-2.88993287	-2.90033166
C	1.49598558	-3.07179611	-1.52751789
H	1.64987993	-3.54008220	-3.67033516
H	1.12015205	-2.31229276	-0.87421565

[**FR**·PdCl]$^{+}$

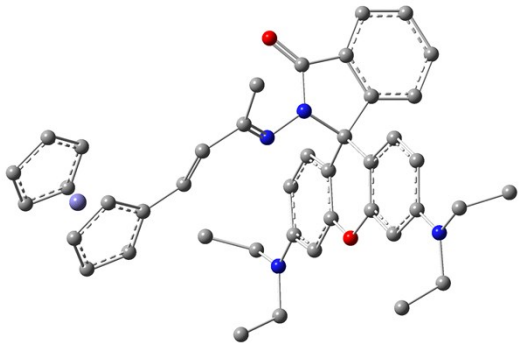
Fe	-4.49899947	4.50528631	-0.24669633
C	-4.39276594	2.98992433	-1.66228265
C	-5.76602011	3.23772937	-1.32036964
H	-6.42513632	2.53190875	-0.83667677

C	-6.05693661	4.59188678	-1.63815764
H	-7.00240490	5.08588811	-1.46052265
C	-4.88116077	5.20345467	-2.17495725
H	-4.78245038	6.23476874	-2.48463269
C	-3.85162436	4.22570684	-2.18674805
H	-2.83422168	4.36799942	-2.52607525
C	-4.78103744	4.05748281	1.75806347
H	-5.42745638	3.24522891	2.06108696
C	-5.17376106	5.40557323	1.49652153
H	-6.17038599	5.80854450	1.61406772
C	-4.03901789	6.11141962	0.99128732
H	-4.02303318	7.14402625	0.66967748
C	-2.94022164	5.19933427	0.94105934
H	-1.94604594	5.42178475	0.57765977
C	-3.40042211	3.93299653	1.41696317
H	-2.82335401	3.01923524	1.45727588
C	-0.89537221	1.37100760	-2.07908571
N	-0.93068300	0.10188400	-1.81694900
N	0.16684000	-0.77567000	-1.97176800
C	1.92854800	-2.25064700	-0.10143100
C	-0.23140100	-2.01453800	-2.11316700
C	1.87036600	-3.15073200	-1.28742000
C	3.04455600	-1.38471600	0.08314900
C	0.92723900	-2.27076400	0.88682200
O	-1.44555000	-2.45577300	-2.11454800

C	0.83624600	-3.05461700	-2.24188500
C	2.84140900	-4.15732800	-1.42723900
C	4.10258900	-1.21825600	-0.84946900
C	3.11942400	-0.57876700	1.24798600
C	1.02908600	-1.39337900	2.00979800
C	-0.25896300	-3.06837200	0.83879900
C	0.77276200	-3.98582800	-3.28483600
H	3.62997400	-4.24248000	-0.68505600
C	2.77988800	-5.06405300	-2.48321800
H	4.07453700	-1.78765600	-1.77075600
C	5.15031000	-0.36120700	-0.62089600
O	2.13207900	-0.60693300	2.18090000
C	4.16749400	0.29166200	1.50212800
C	0.05410000	-1.28248300	2.97533100
C	-1.24994000	-2.95731800	1.77101200
H	-0.41347400	-3.73417000	-0.00022900
C	1.74112800	-4.97862800	-3.41323300
H	-0.04901800	-3.91850100	-3.98989900
H	3.53242800	-5.84211100	-2.57045000
H	5.93205600	-0.29371600	-1.36552800
C	5.22413700	0.42585800	0.57399800
H	4.11554200	0.87832600	2.40868300
H	0.22564900	-0.58178300	3.77957300
C	-1.13868800	-2.05003700	2.88192400
H	-2.16797600	-3.50081800	1.59662300

H	1.68314600	-5.68821200	-4.23323100
N	6.27228100	1.27748500	0.79995900
N	-2.12141100	-1.93625600	3.80887900
C	7.30686000	1.52829700	-0.20876900
C	6.40773700	2.01639800	2.05889000
C	-3.31762900	-2.80062800	3.82267800
C	-2.08274600	-0.87595500	4.82833000
H	7.67023300	2.54875100	-0.05032500
H	6.85309600	1.52645900	-1.20360700
C	8.48024000	0.54397200	-0.14400500
H	7.47774400	2.17913100	2.22449000
H	6.07053600	1.38256200	2.88416400
C	5.66981800	3.36021600	2.06754500
H	-3.48984800	-3.06895500	4.87217800
H	-3.08096400	-3.73146000	3.30761400
C	-4.57104200	-2.15975700	3.22266800
H	-1.10966800	-0.89871500	5.33377800
H	-2.82309500	-1.14530100	5.58565000
C	-2.38245800	0.52871000	4.29002200
H	8.96403400	0.57472000	0.83730400
H	9.23087200	0.79806100	-0.89938100
H	8.14806100	-0.48274400	-0.32206900
H	6.03875400	4.01501700	1.27186400
H	5.82360100	3.87108700	3.02349300
H	4.59475800	3.22600000	1.91985100

H	-4.87086600	-1.27036800	3.78523500
H	-5.39621000	-2.87800200	3.27122900
H	-4.42038900	-1.88088300	2.17666200
H	-1.65223900	0.84205300	3.54067100
H	-2.35972200	1.24840300	5.11530300
H	-3.36573400	0.56627600	3.81691000
Pd	-2.70765329	-0.54714884	-1.05130720
Cl	-4.24925929	-2.21593784	-0.44012920
C	0.48094288	1.88049915	-2.54574956
H	1.11448093	2.02568152	-1.69577802
H	0.92393834	1.16078900	-3.20200584
H	0.36067981	2.80902421	-3.06370517
C	-2.44924175	2.05486267	-1.80298487
C	-3.68849563	1.80363398	-1.42412611
H	-3.87196012	1.25575016	-0.52353514
H	-2.40330066	3.10088332	-2.02350750



FR

Fig. S6 A DFT-optimized structure of **FR**, calculated using the B3LYP/LANL2DZ basis set.

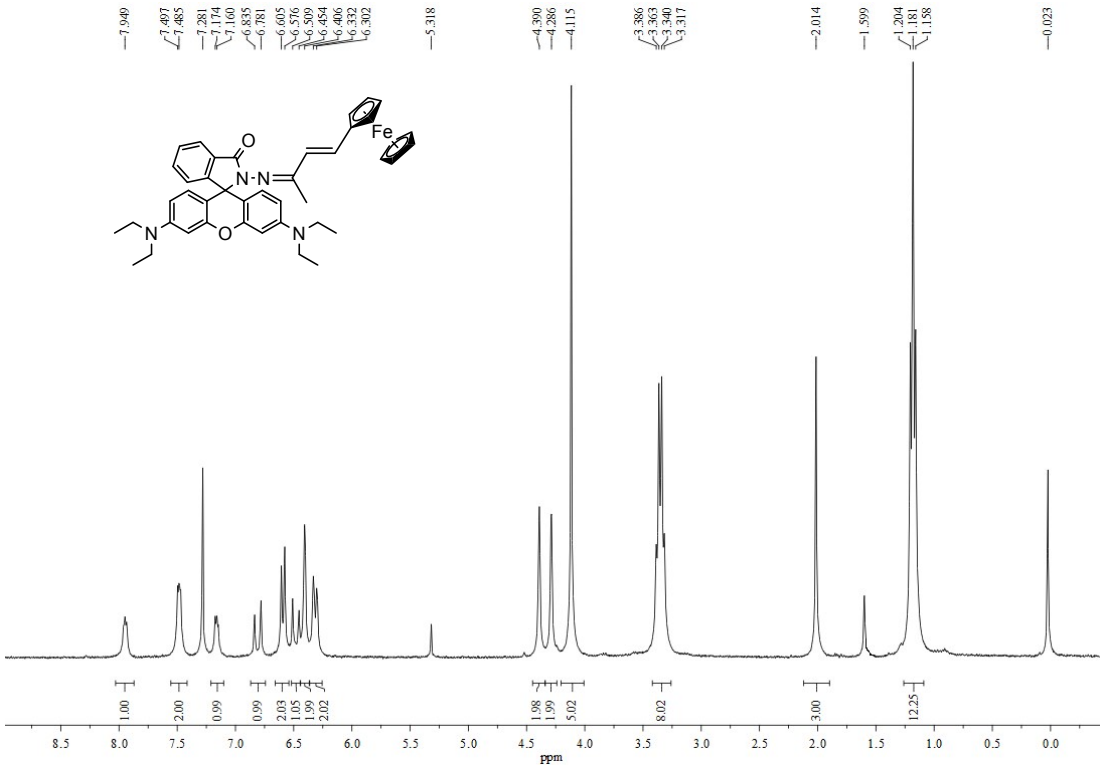


Fig. S7 ^{1}H NMR spectrum of **FR.**

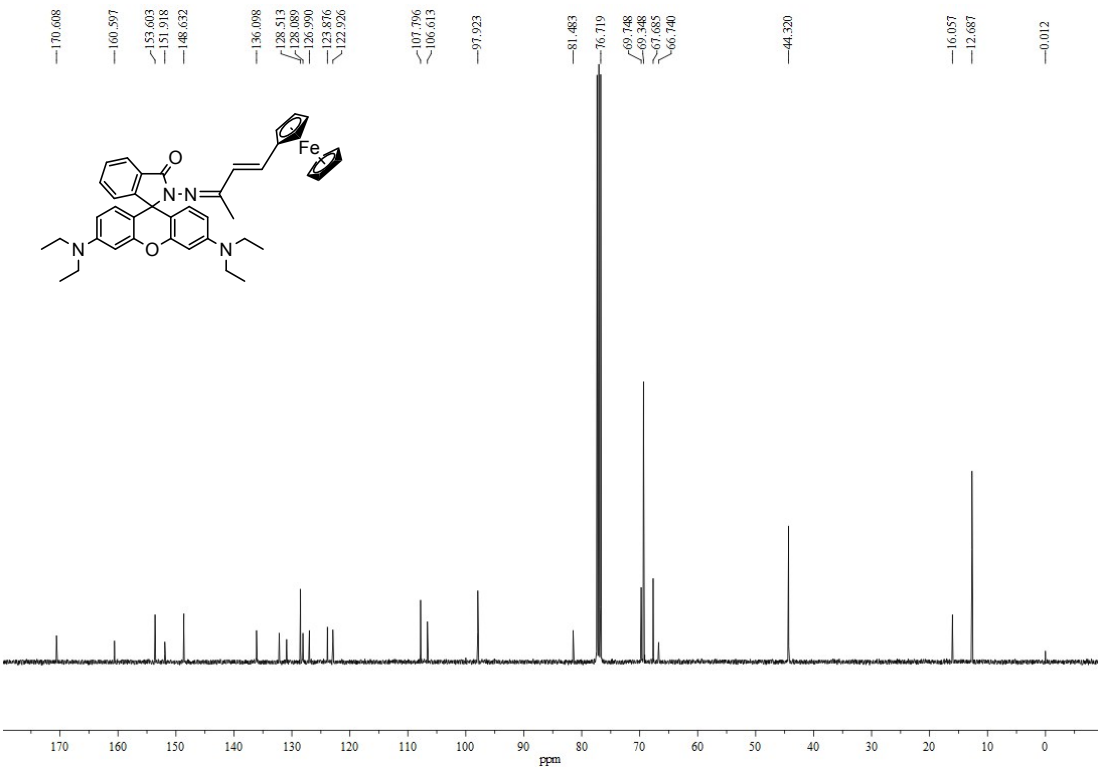


Fig. S8 ^{13}C NMR spectrum of **FR.**

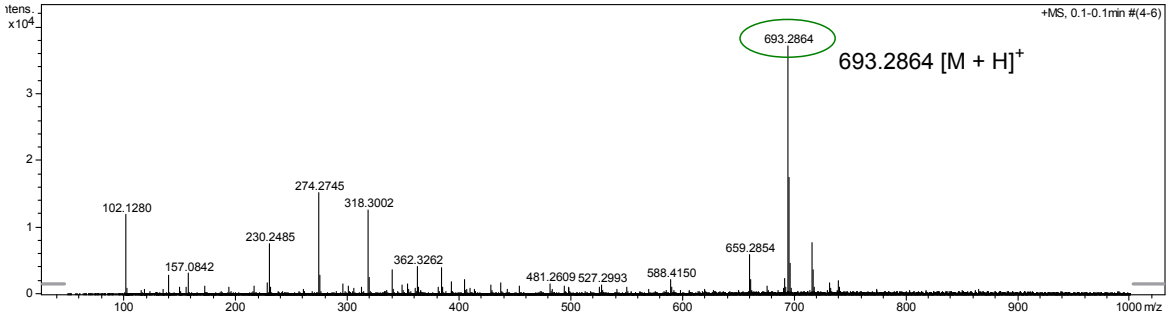


Fig. S9 HR-MS spectrum of **FR.**

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