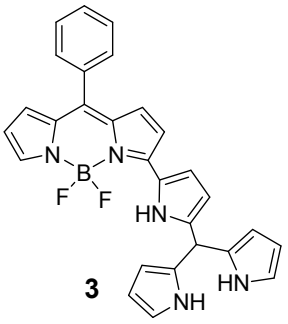
Supporting Information

Synthesis, Structure and Spectral and Electrochemical Properties of 3-Pyrrolyl BODIPY-Metal Dipyrrin Complexes

V. Lakshmi,[a] Way-Zen Lee[b] and M. Ravikanth*[a]

[a]Department of Chemistry, Indian Institute of Technology, Bombay, Powai, Mumbai 400 076, India. E-mail: ravikanth@chem.iitb.ac.in
[b]Instrumentation Center, Department of Chemistry, National Taiwan Normal University, Ting-Chow Road, Taipei, 11677, Taiwan



3

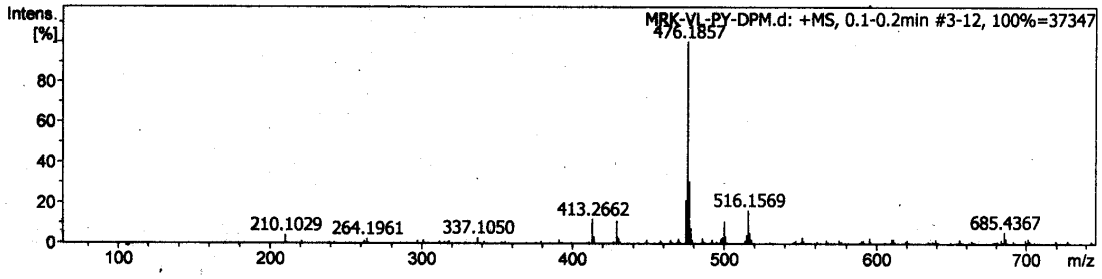
Indian Institute of Technology (B)

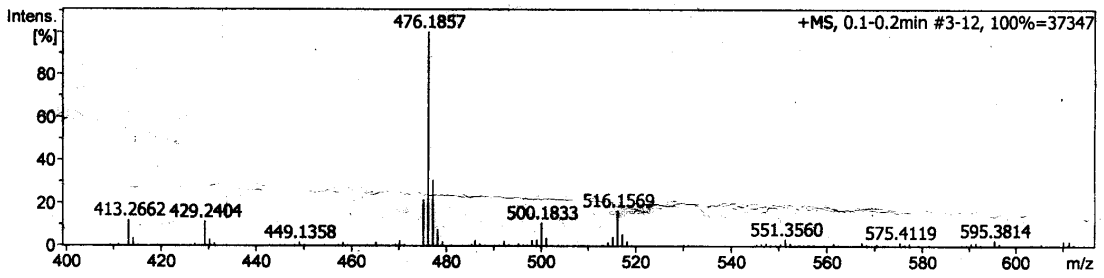
Analysis Info

Analysis Name	D:\Data\MAY 14\MRK-VL-PY-DPM.d	Acquisition Date	5/26/2014 12:57:13 PM
Method	Tune_pos_Standard_NAI-1500.m	Operator	SSK OUT
Sample Name	MRK-VL-PY-DPM	Instrument	maXis impact 282001.00081
Comment	C28H22BF2N5		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1200.0 Vpp	Set Divert Valve	Source





Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
516.1569	1	C28H22BF2KN5	516.1573	-0.8	12.2	1	100.00	19.5	even	ok

Figure S1: HRMS of compound **3**.

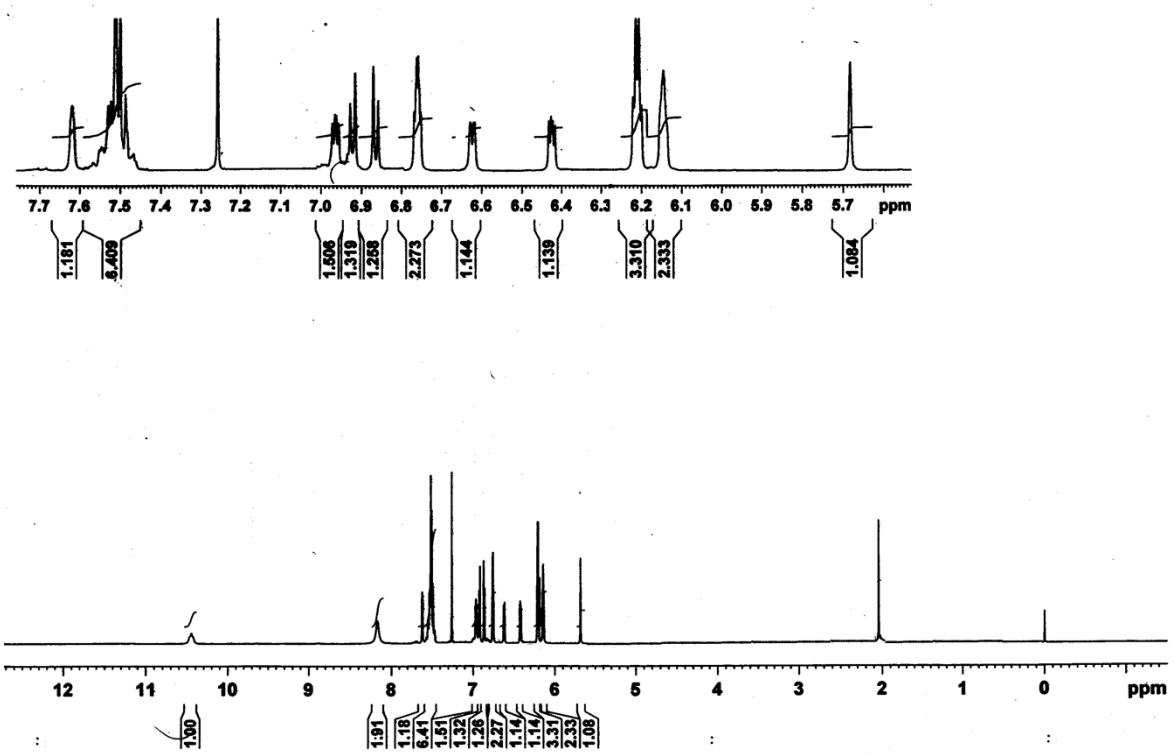


Figure S2a: ^{1}H NMR spectrum of compound **3** recorded in $CDCl_3$.

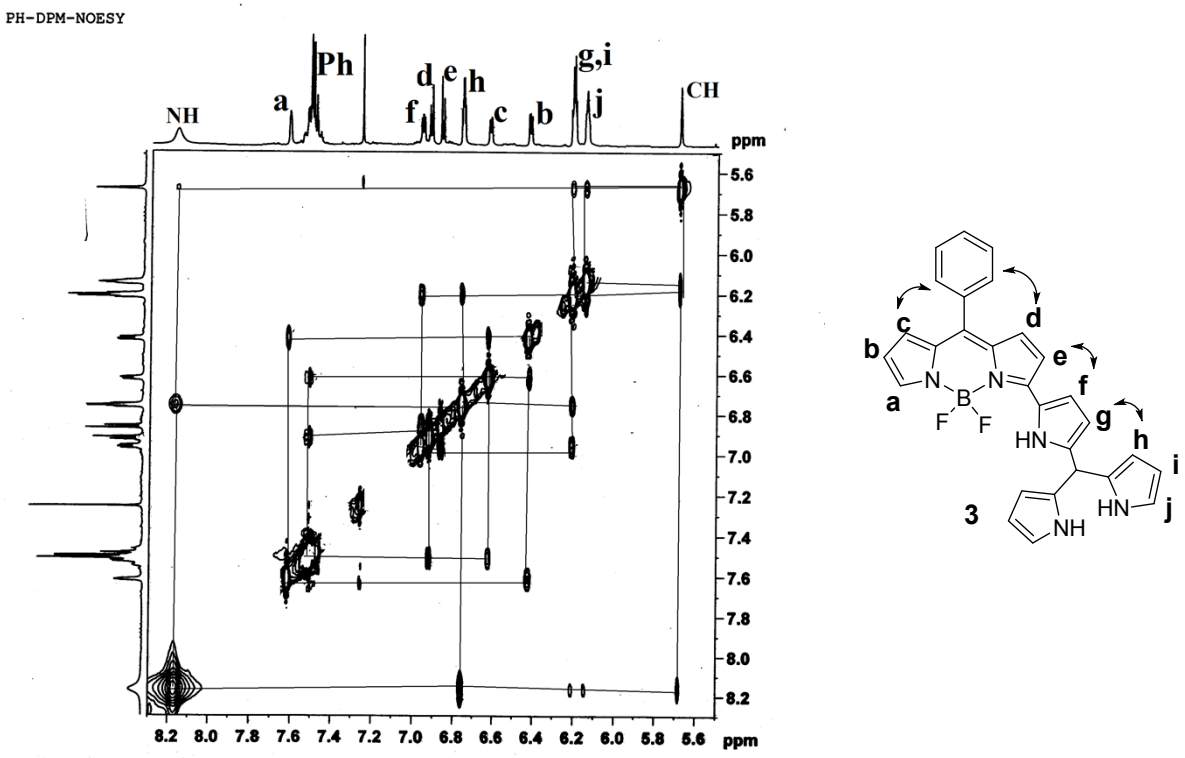


Figure S2b: ^{1}H-^{1}H NOESY NMR spectrum of compound **3** recorded in $CDCl_3$.

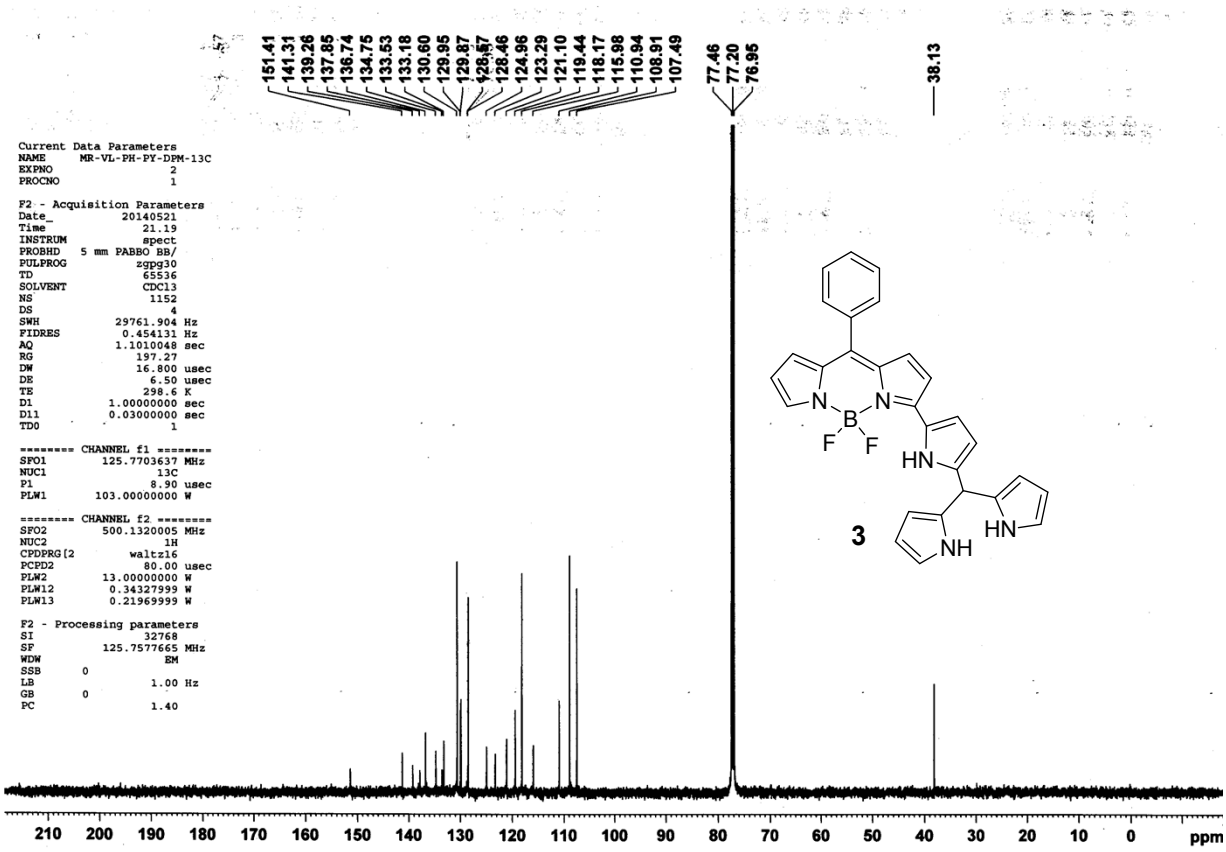


Figure S3: ^{13}C NMR spectrum of compound **3** recorded in $CDCl_3$.

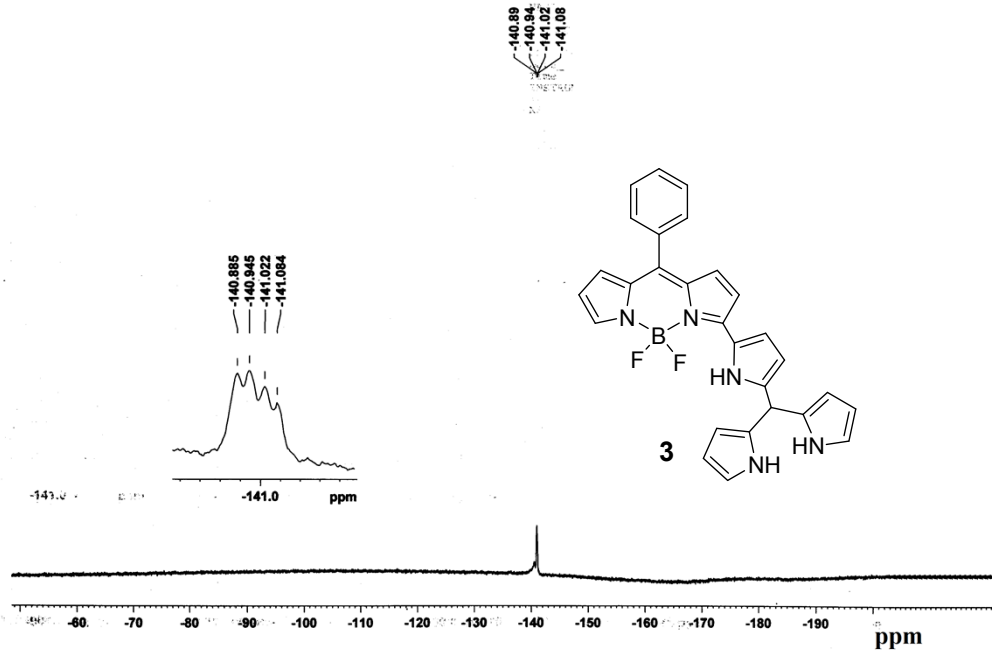


Figure S4: ^{19}F NMR spectrum of compound **3** recorded in $CDCl_3$.

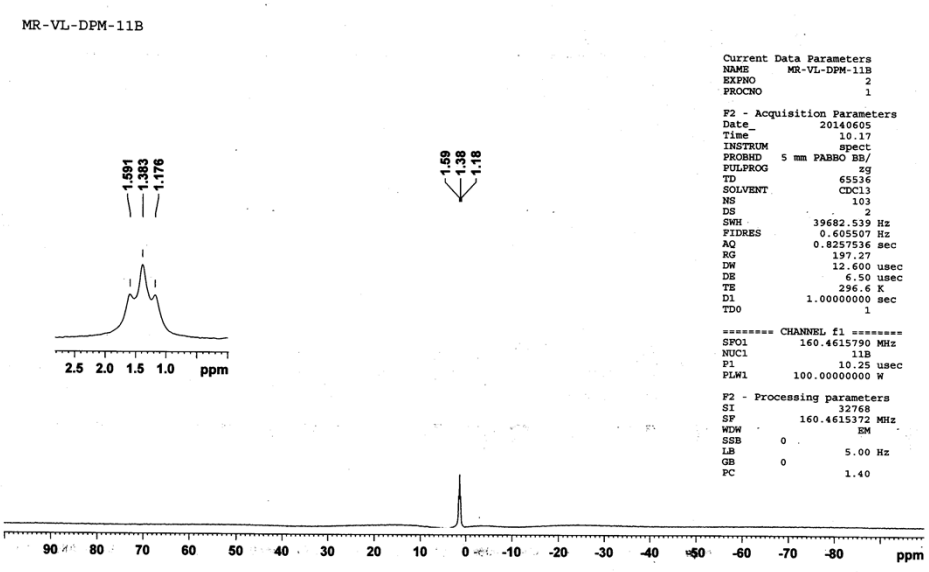


Figure S5: ^{11}B NMR spectrum of compound **3** recorded in $CDCl_3$.

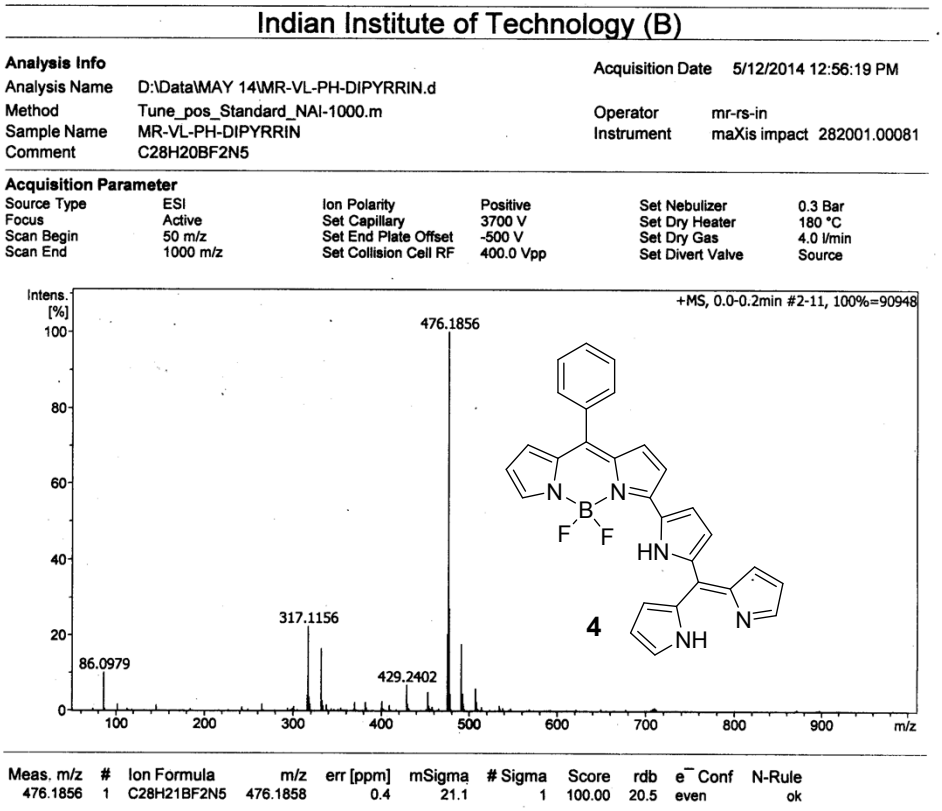


Figure S6: HRMS of compound **4**.

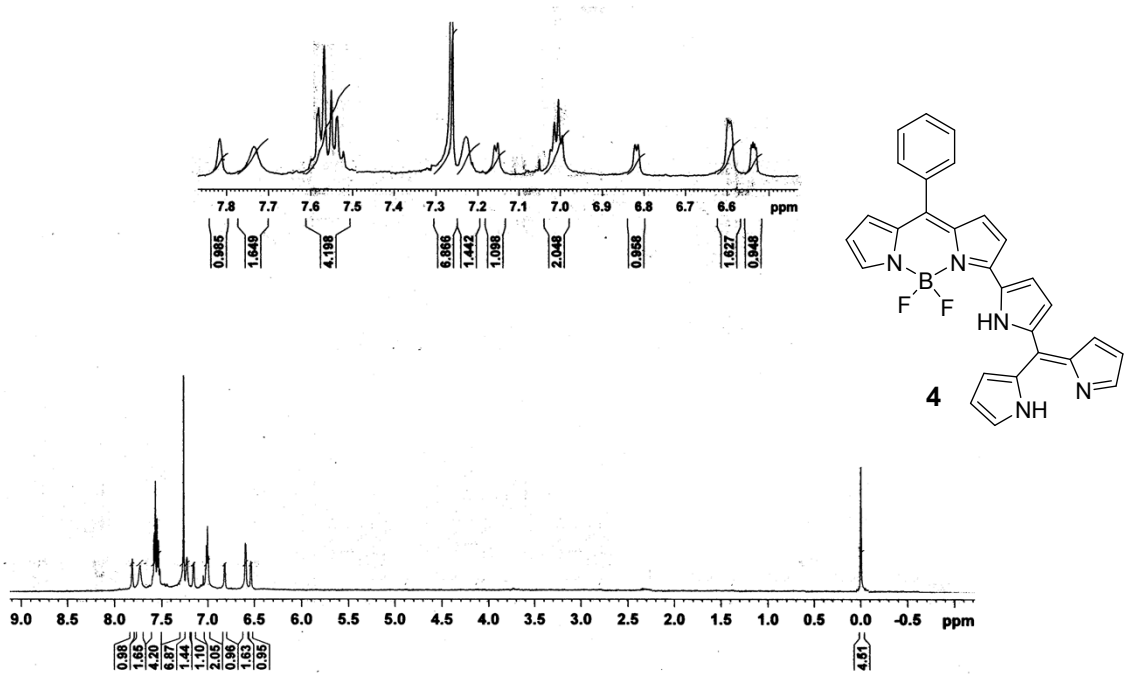


Figure S7: ^{1}H NMR spectrum of compound **4** recorded in $CDCl_3$.

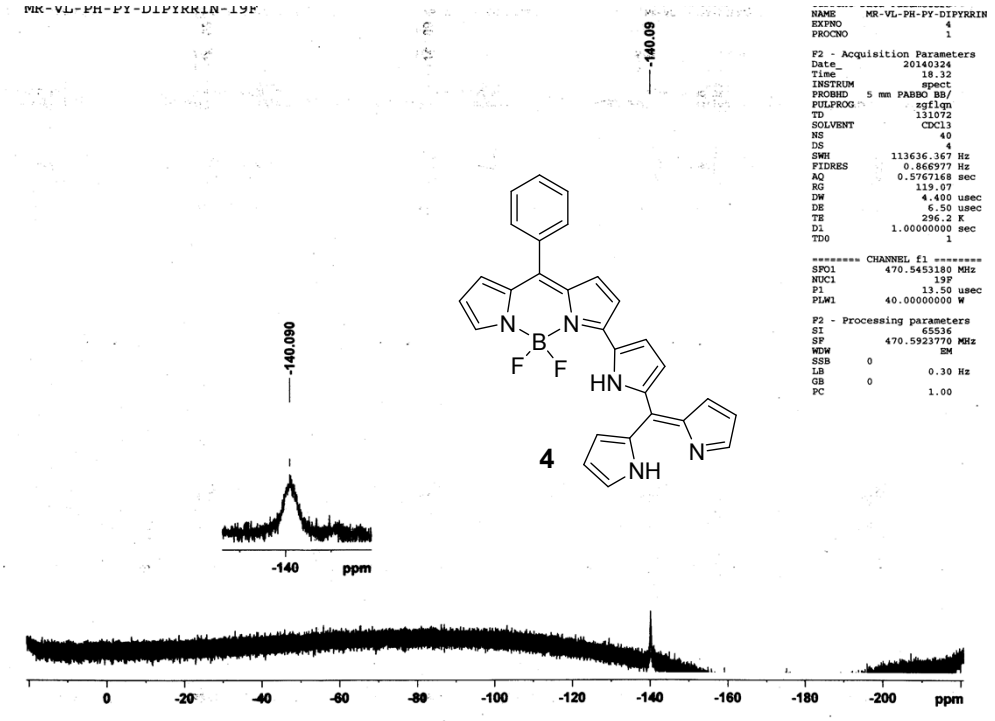


Figure S8: ^{19}F NMR spectrum of compound **4** recorded in $CDCl_3$.

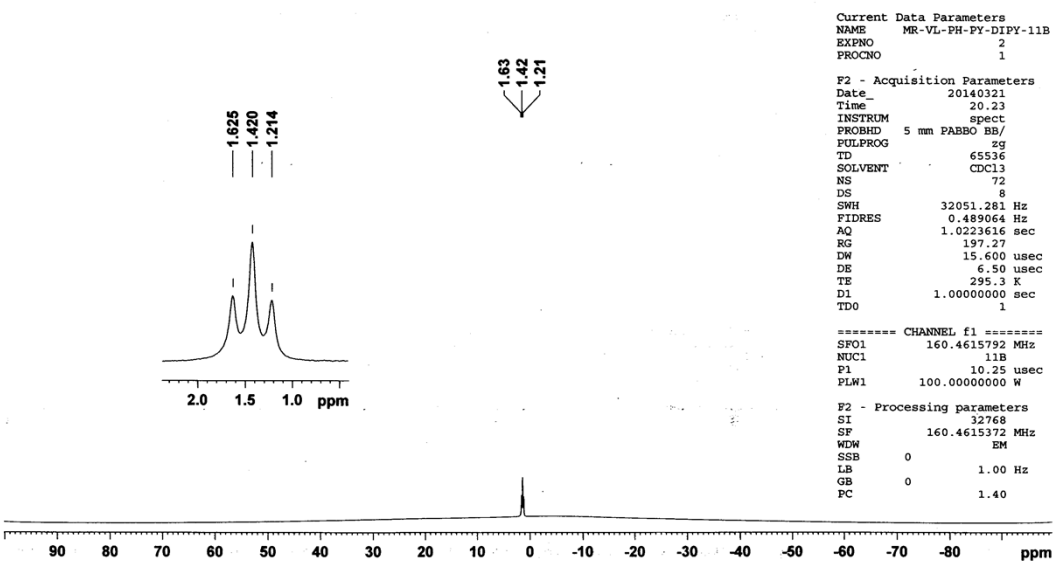


Figure S9: ^{11}B NMR spectrum of compound **4** recorded in $CDCl_3$.

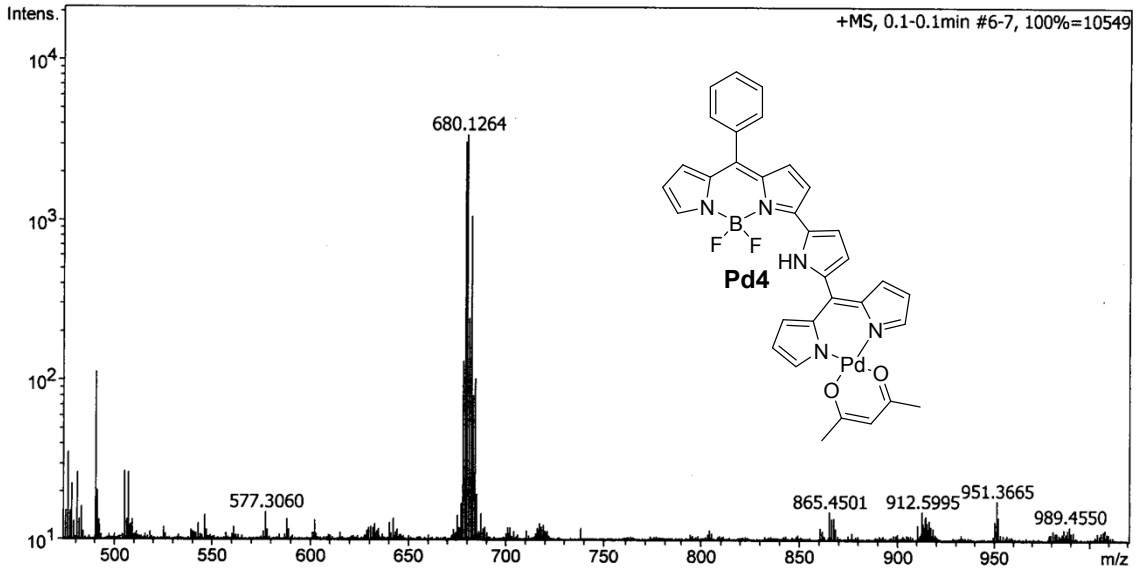
Indian Institute of Technology (B)

Analysis Info

Analysis Name	D:\Data\FEB-2014\MR-VL-Pd1.d	Acquisition Date	2/25/2014 10:07:02 PM
Method	Tune_pos_Standard_NAI-1000.m	Operator	DM IN
Sample Name	INN-TK-405-B	Instrument	maXis impact 282001.00081
Comment	C33H26BF2N5O2Pd		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
680.1264	1	C33H27BF2N5O2Pd	680.1272	1.2	31.4	1	100.00	22.5	even	ok

Figure S10: The HRMS of compound **Pd4.**

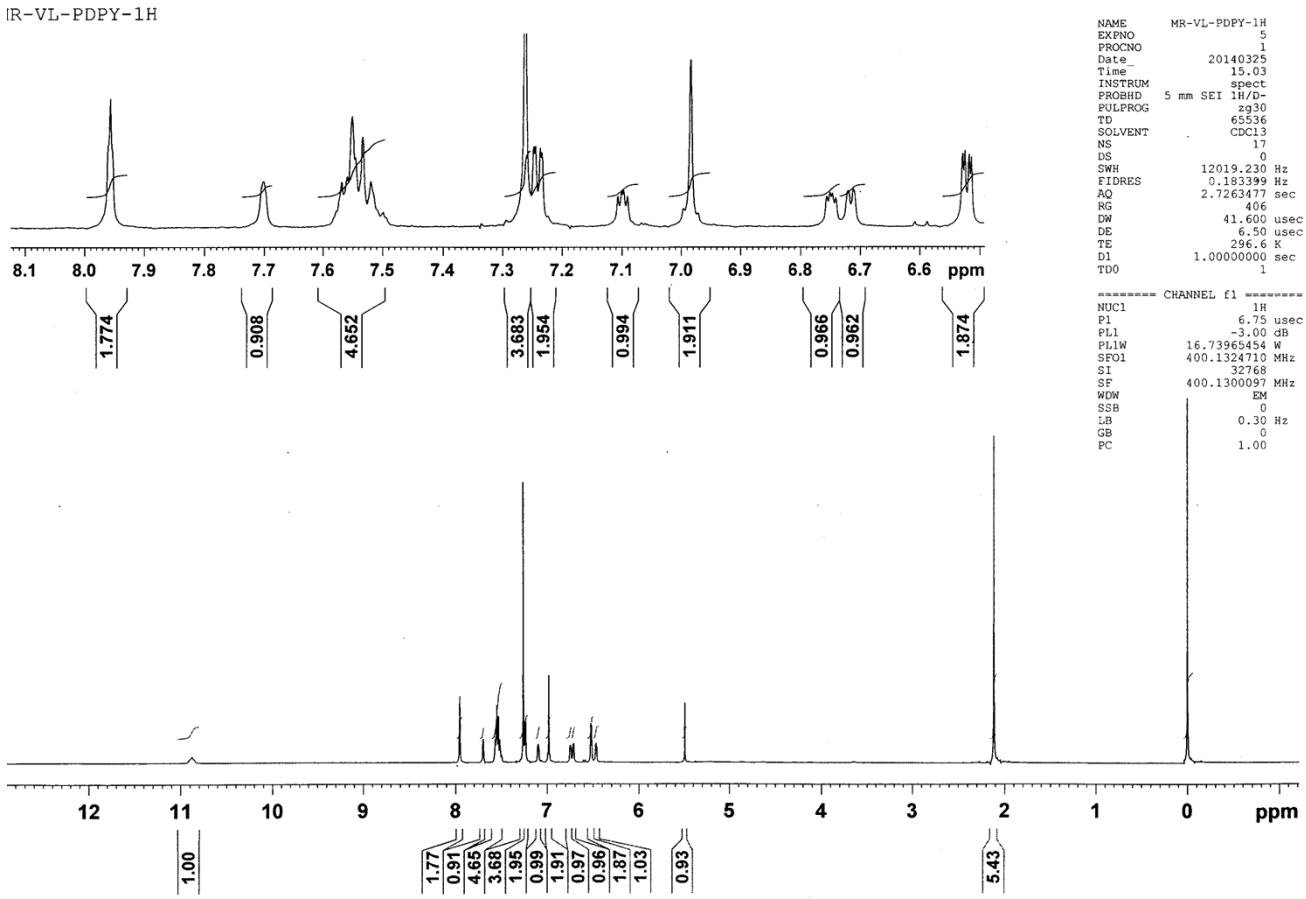


Figure S11a: ^{1}H NMR spectrum of compound **Pd4** recorded in $CDCl_3$.

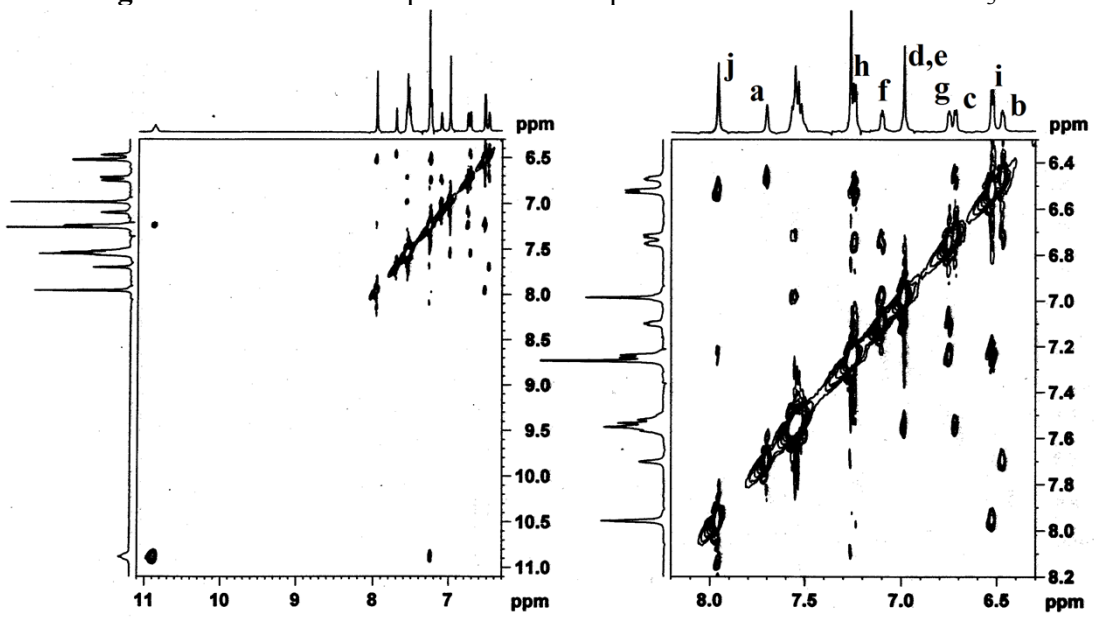


Figure S11b: ^{1}H-^{1}H NOESY NMR spectrum of compound **Pd4** recorded in $CDCl_3$.

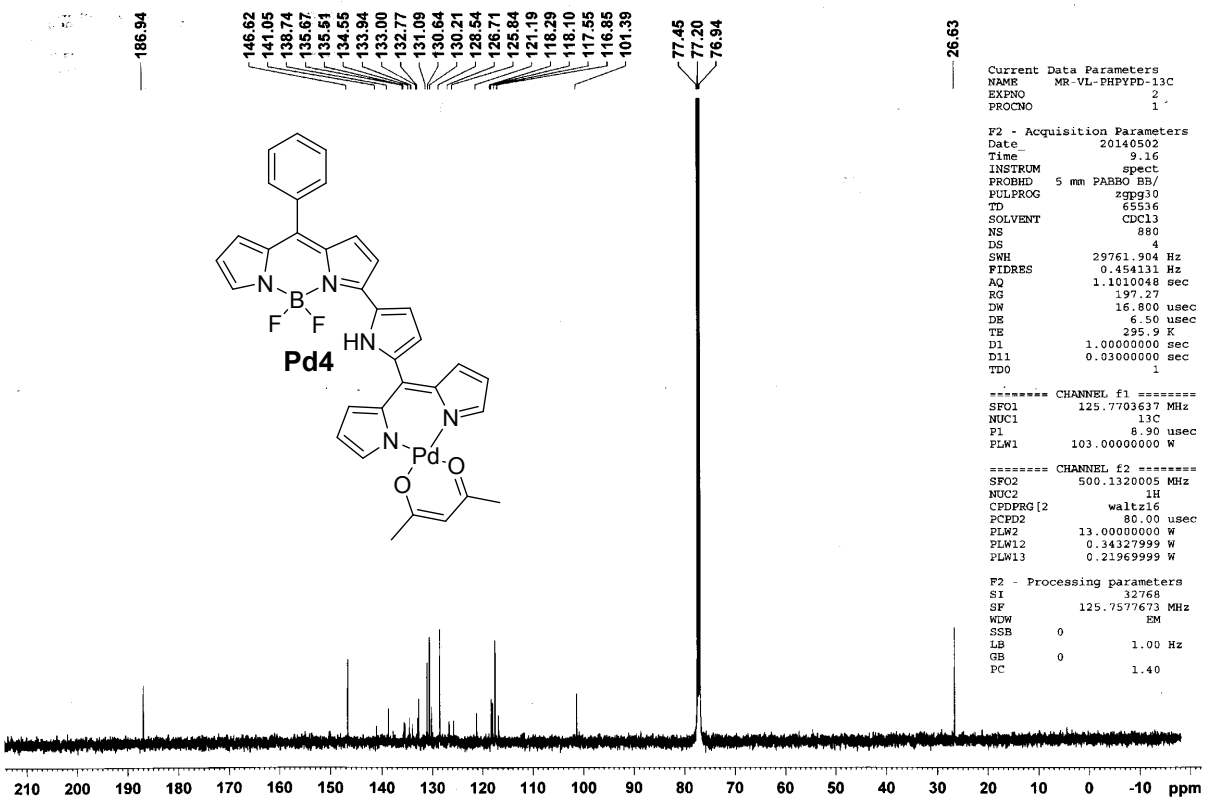


Figure S12: ^{13}C NMR spectrum of compound **Pd4** recorded in $CDCl_3$.

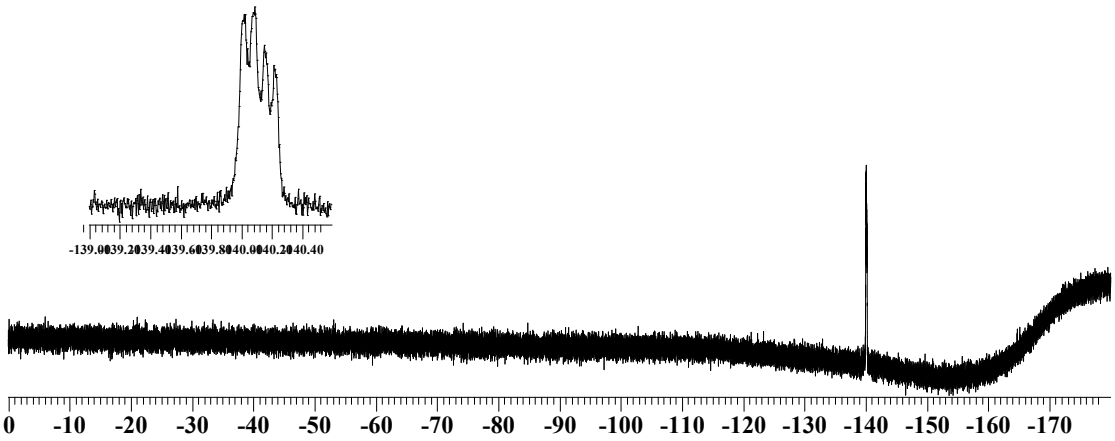


Figure S13: ^{19}F NMR spectrum of compound **Pd4** recorded in $CDCl_3$ (δ in ppm).

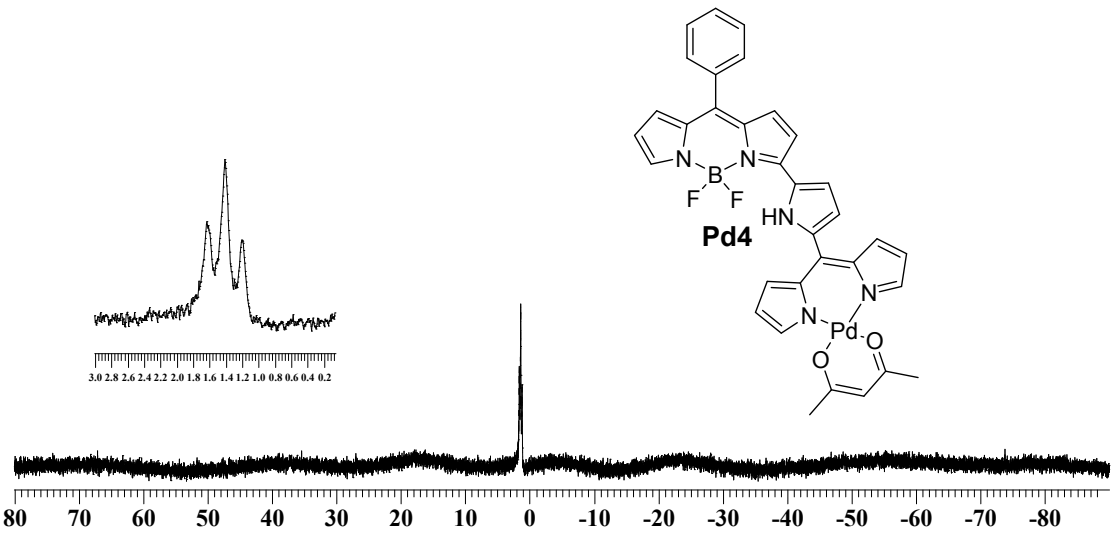


Figure S14: ^{11}B NMR spectrum of compound **Pd4** recorded in $CDCl_3$ (δ in ppm).

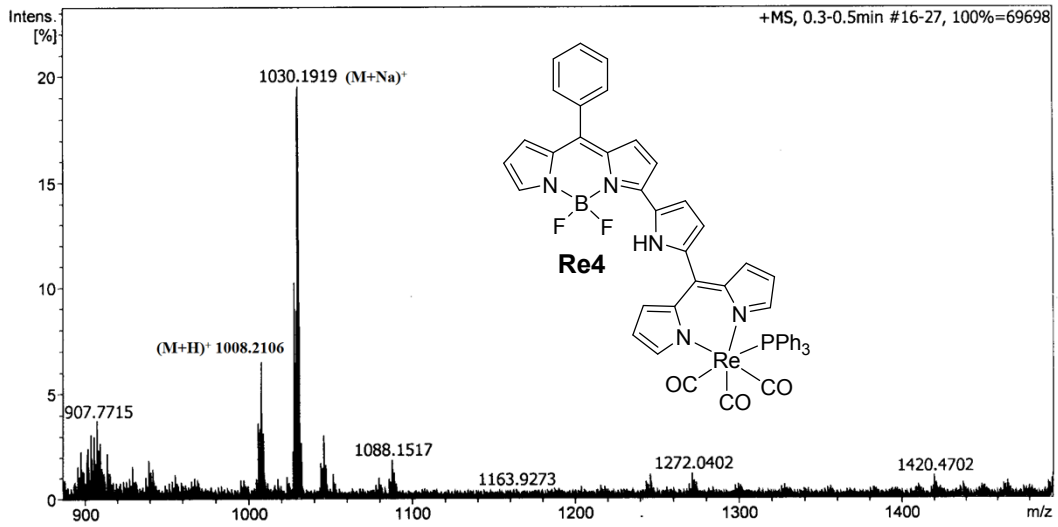
Indian Institute of Technology (B)

Analysis Info

Analysis Name	D:\Data\APR-14\MR-VL-PY-RE.1.d	Acquisition Date	4/23/2014 6:48:17 PM
Method	Tune_pos_Standard_NAI-1500.m	Operator	MR-IN-RS
Sample Name	MR-VL-PY-RE	Instrument	maXis impact 282001.00081
Comment	C49H34BO3F2N5PRe		

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3700 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e⁻ Conf	N-Rule
1008.2106	1	C49H35BF2N5O3PRe	1008.2101	-1.6	18.6	1	100.00	36.0	odd	-

Figure S15: HRMS of compound **Re4.**

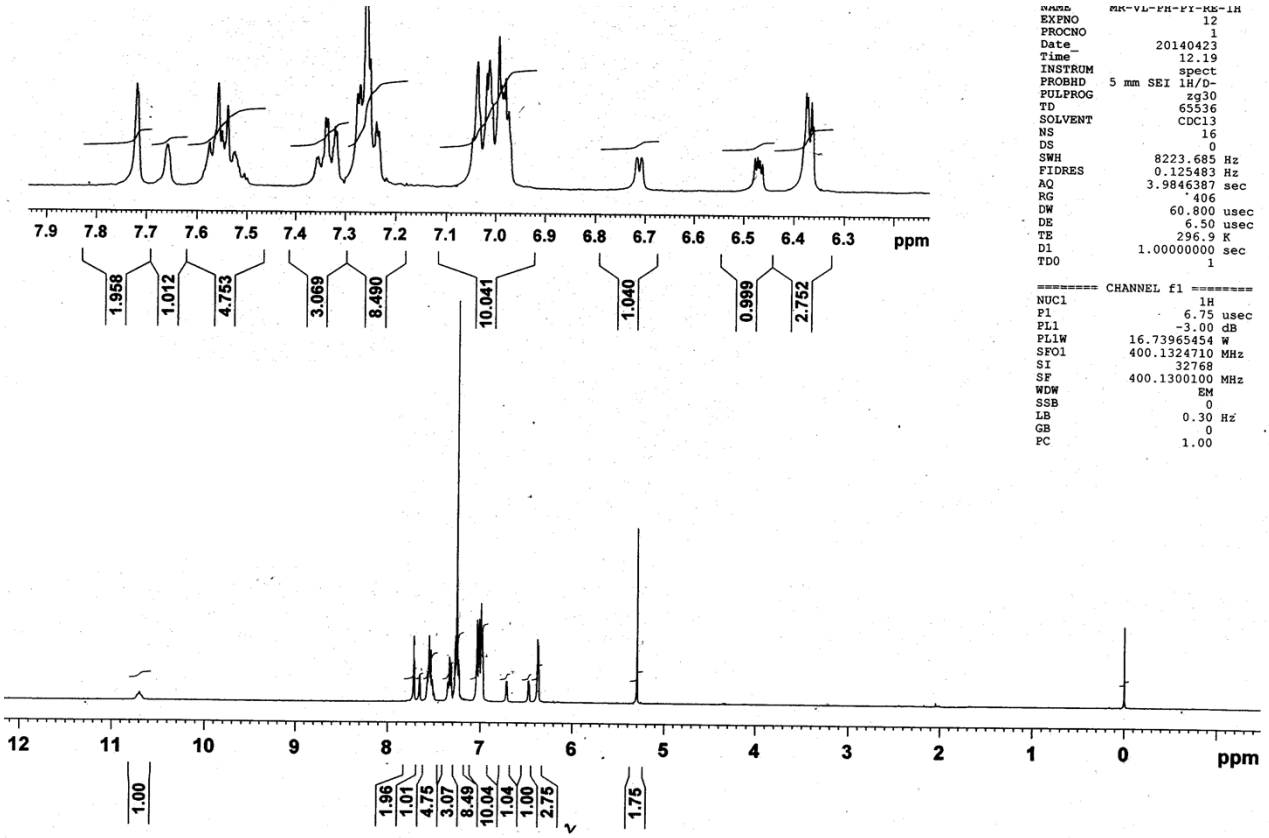


Figure S16a: ^{1}H NMR spectrum of compound **Re4** recorded in $CDCl_3$.

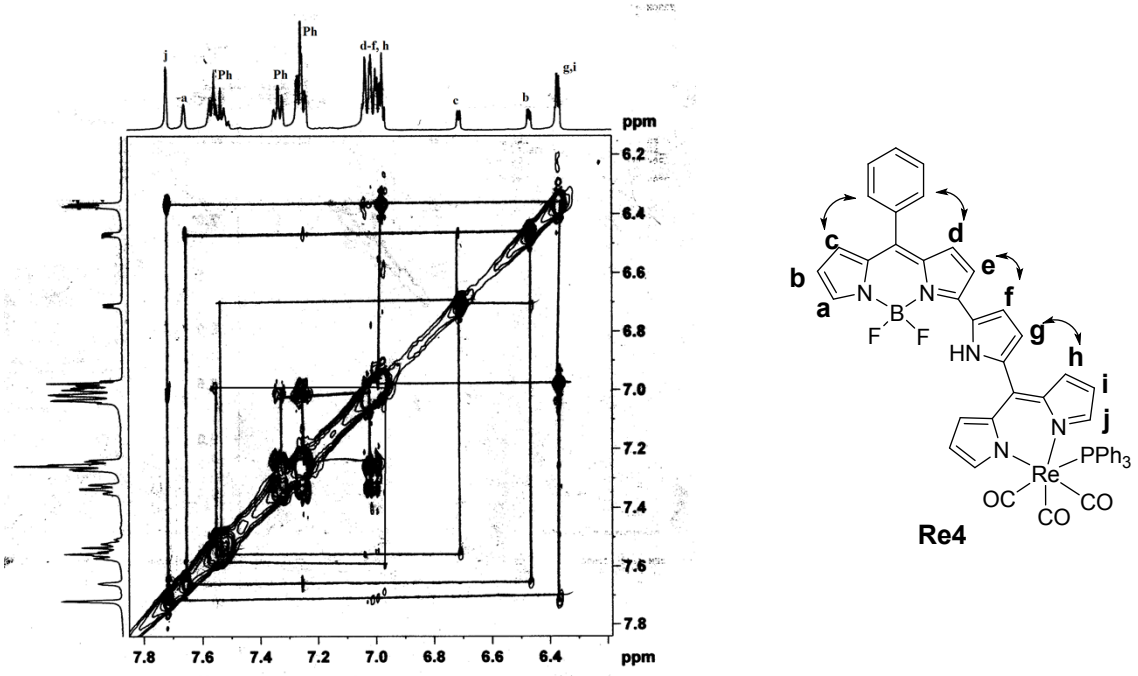


Figure S16b: ^{1}H-^{1}H NOESY NMR spectrum of compound **Re4** recorded in $CDCl_3$.

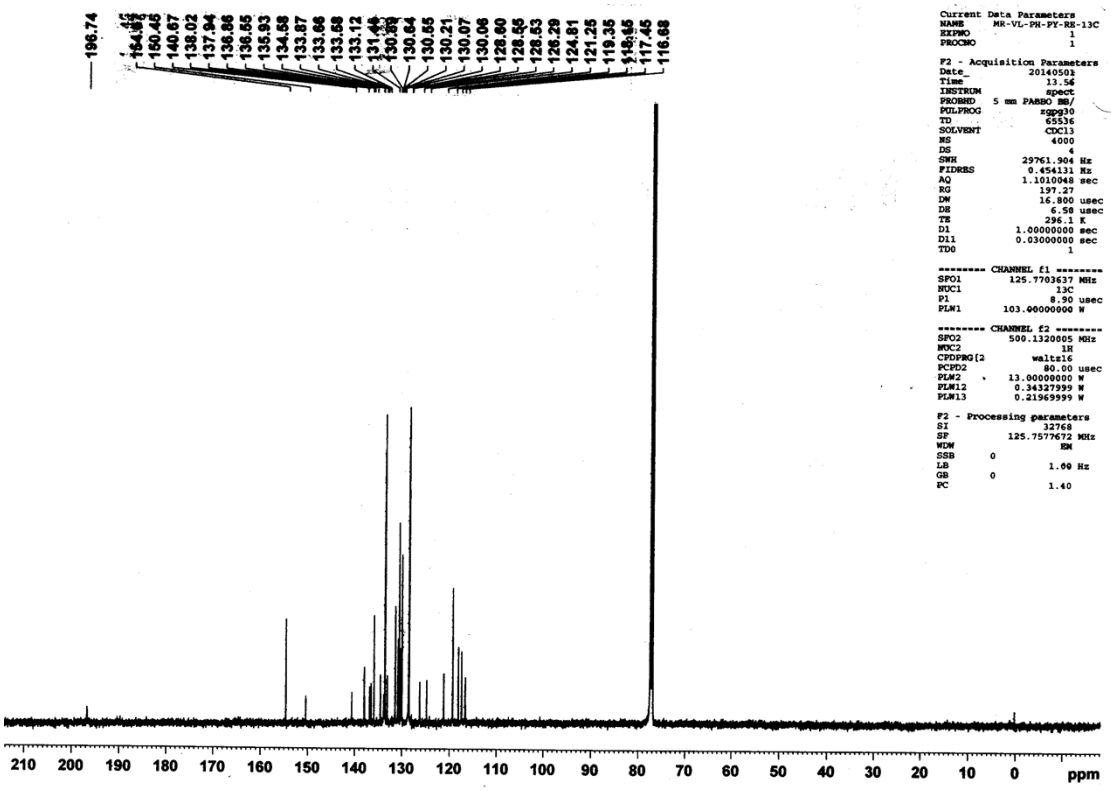


Figure S17: ^{13}C NMR spectrum of compound **Re4** recorded in $CDCl_3$.

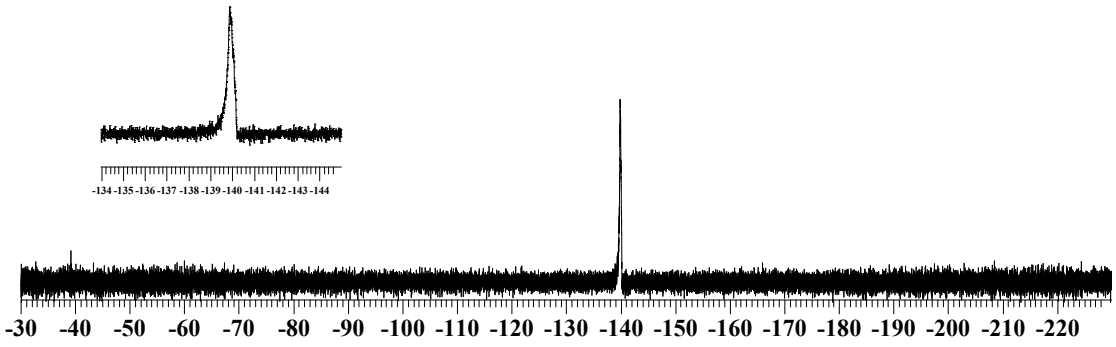


Figure S18: ^{19}F NMR spectrum of compound **Re4** recorded in $CDCl_3$ (δ in ppm).

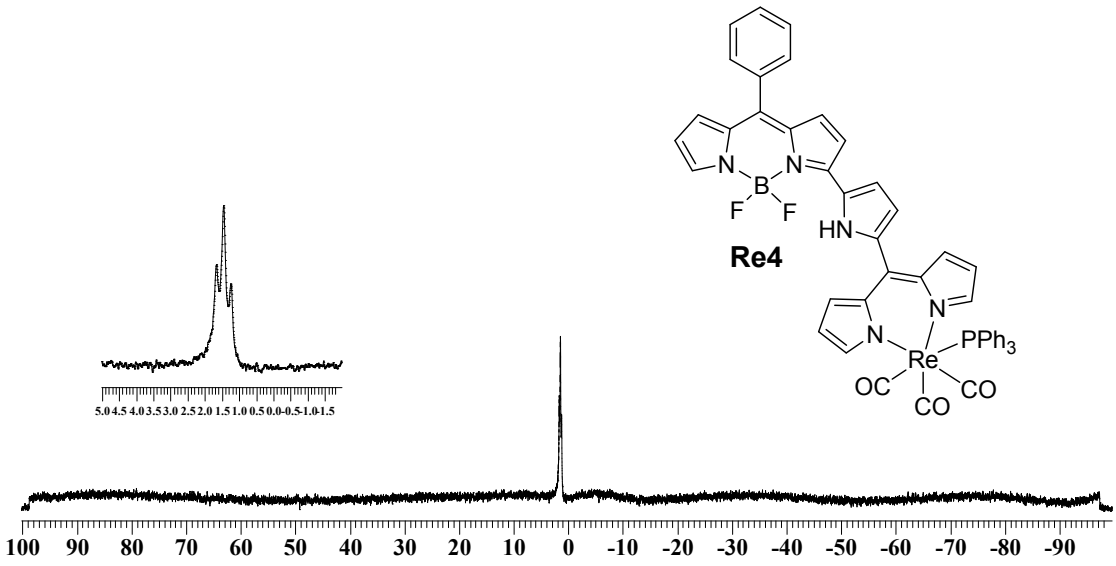


Figure S19: ^{11}B NMR spectrum of compound **Re4** recorded in $CDCl_3$ (δ in ppm).

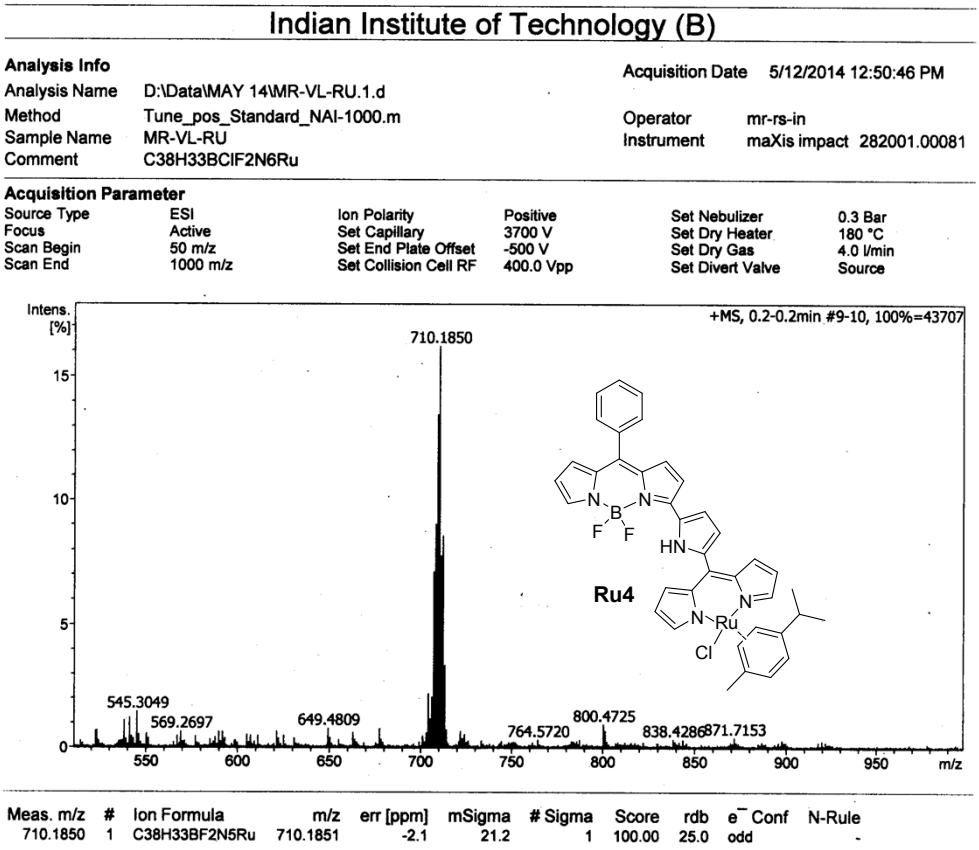


Figure S20: HRMS of compound **Ru4**.

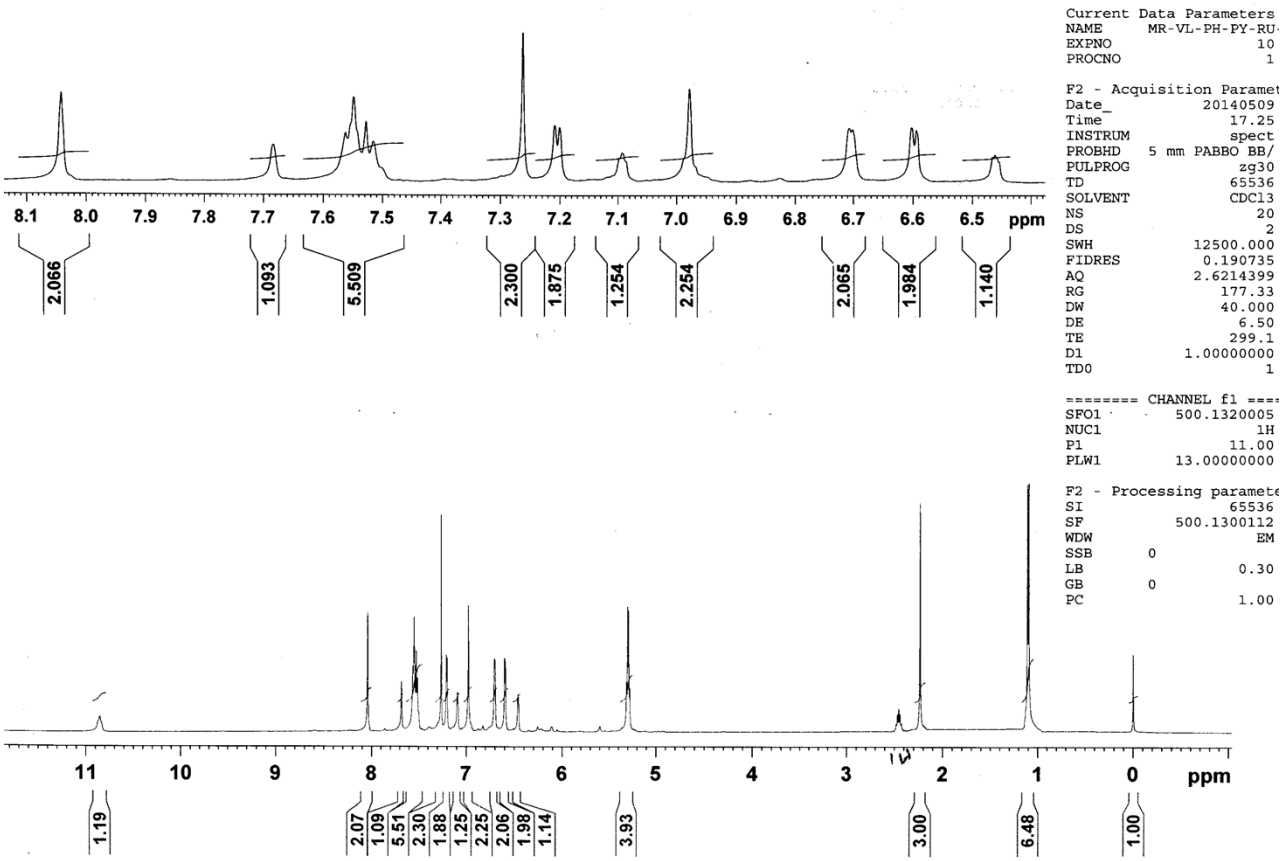


Figure S21a: ^{1}H NMR spectrum of compound **Ru4** recorded in $CDCl_3$.

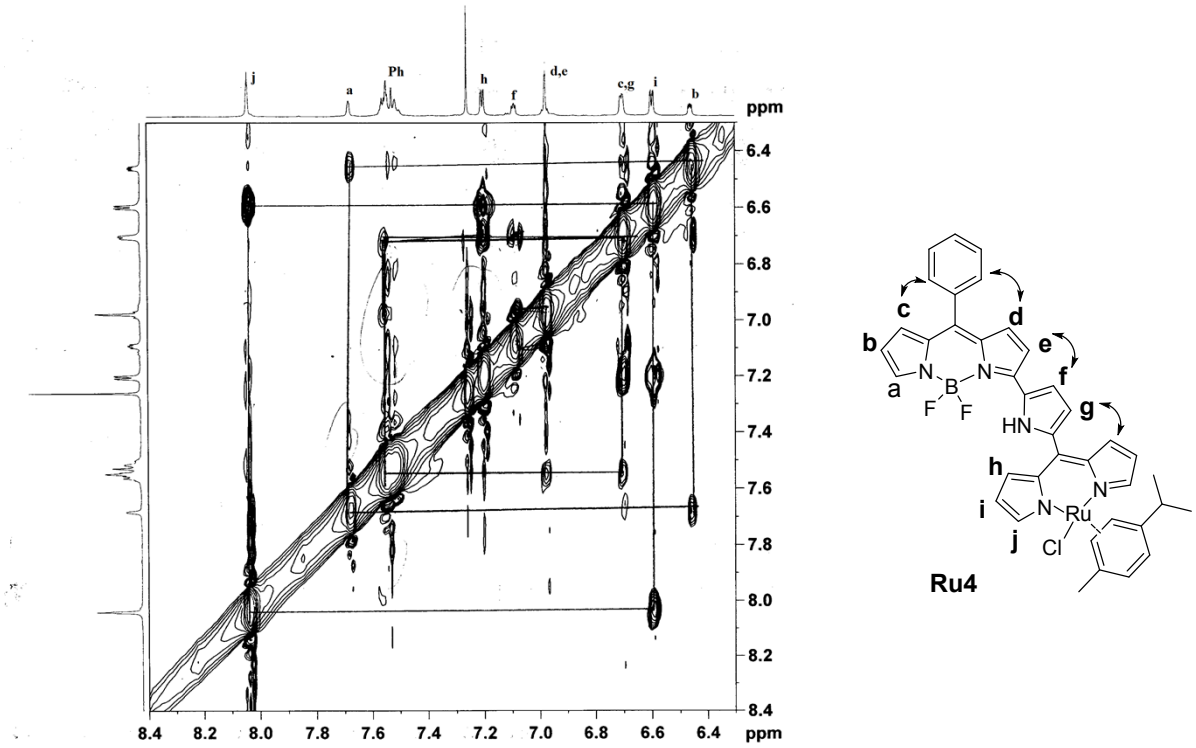


Figure S21b: ^{1}H-^{1}H NOESY NMR spectrum of compound **Ru4** recorded in $CDCl_3$.

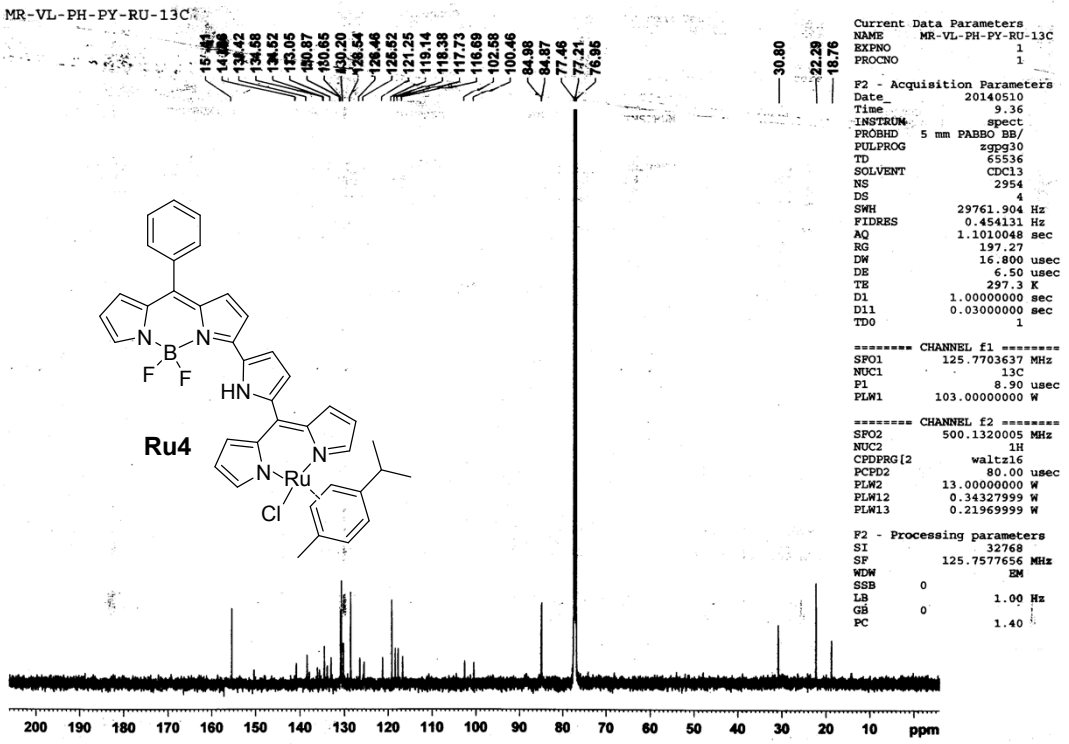


Figure S22: ^{13}C NMR spectrum of compound **Ru4** recorded in $CDCl_3$.

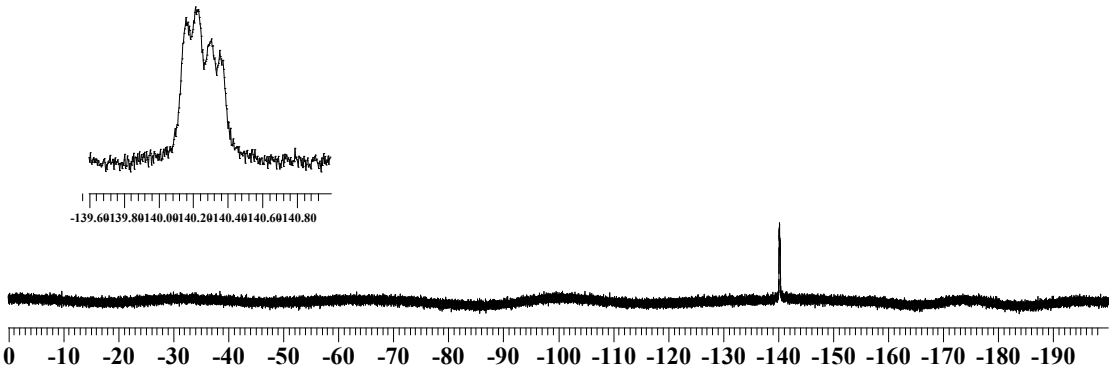


Figure S23: ^{19}F NMR spectrum of compound **Ru4** recorded in $CDCl_3$ (δ in ppm).

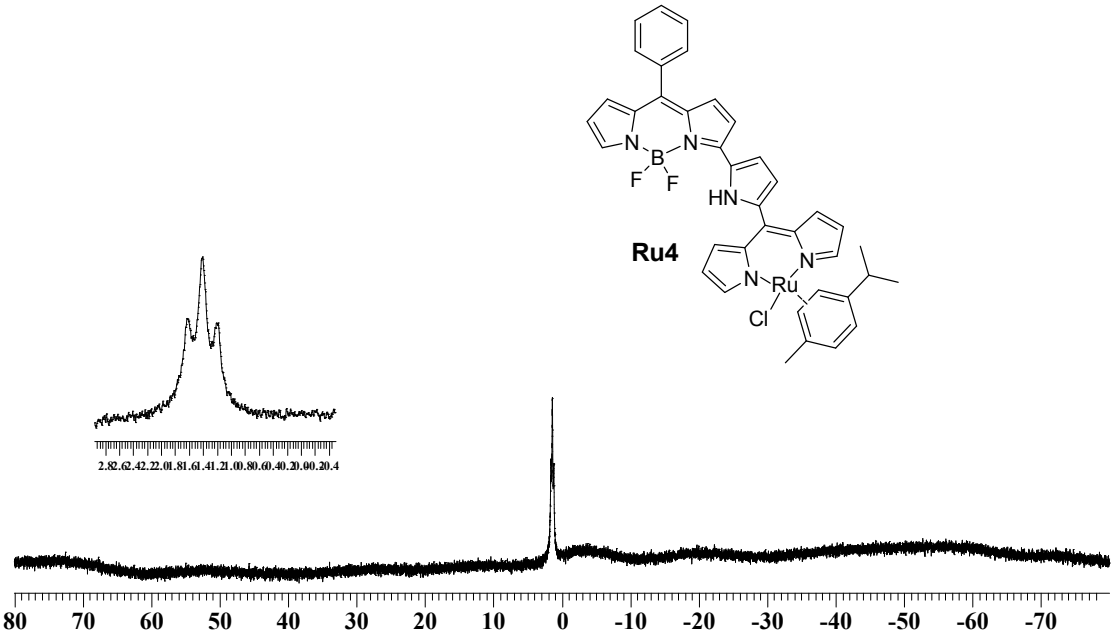


Figure S24: ^{11}B NMR spectrum of compound **Ru4** recorded in $CDCl_3$ (δ in ppm).

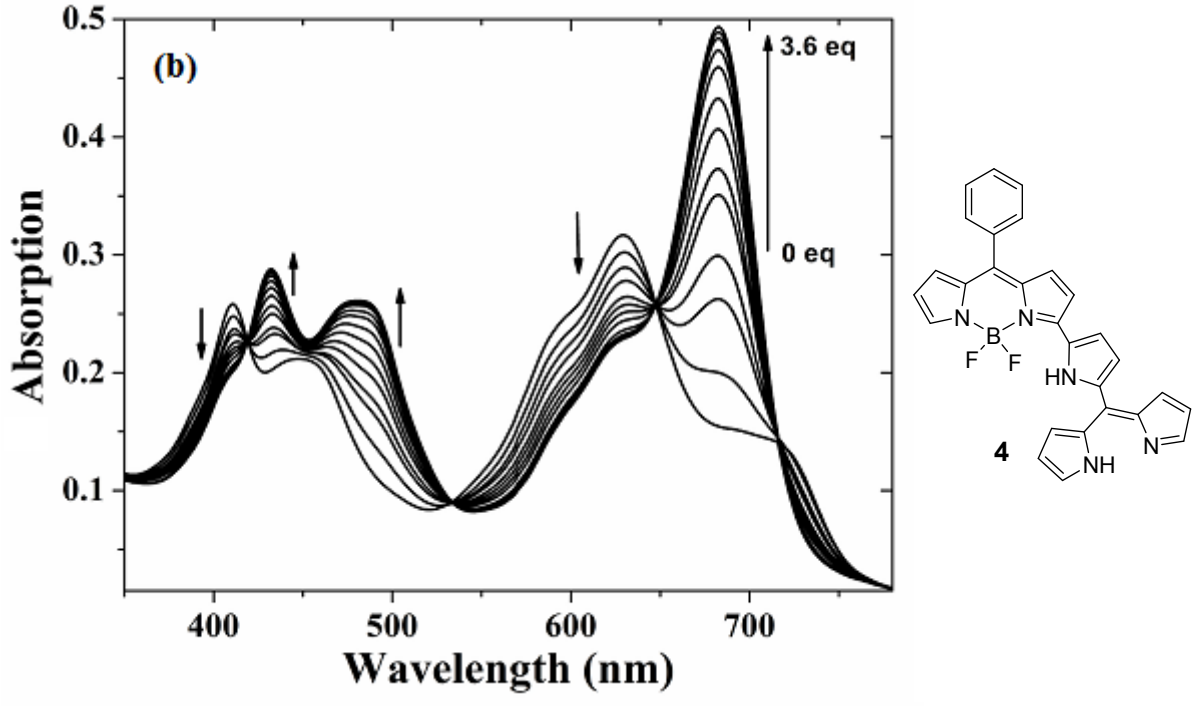


Figure S25: The protonated absorption spectra of compound **4** in CH_2Cl_2.