

Supporting Information

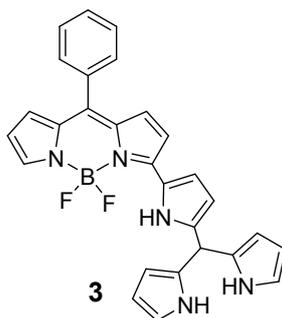
Synthesis, Structure and Spectral and Electrochemical Properties of 3-Pyrrolyl BODIPY-Metal Dipyrin Complexes

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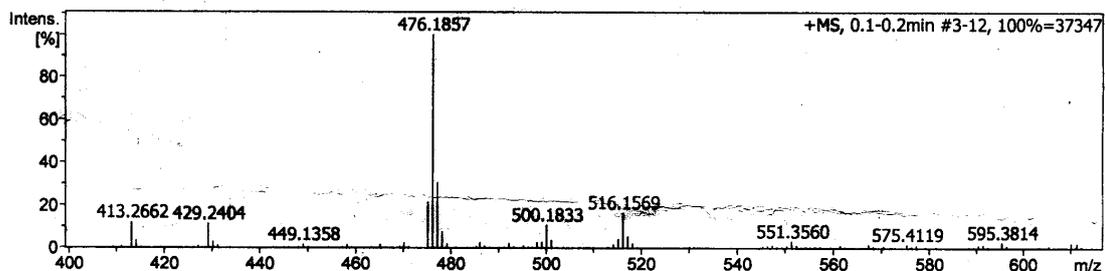
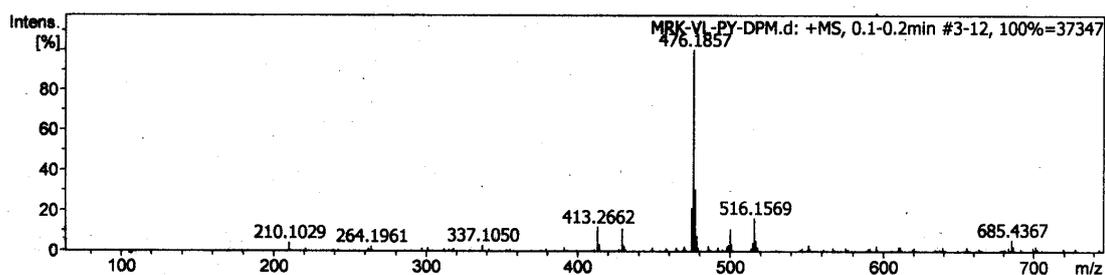
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Analysis Info		Acquisition Date	
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Comment	C28H22BF2N5		

Acquisition Parameter					
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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.

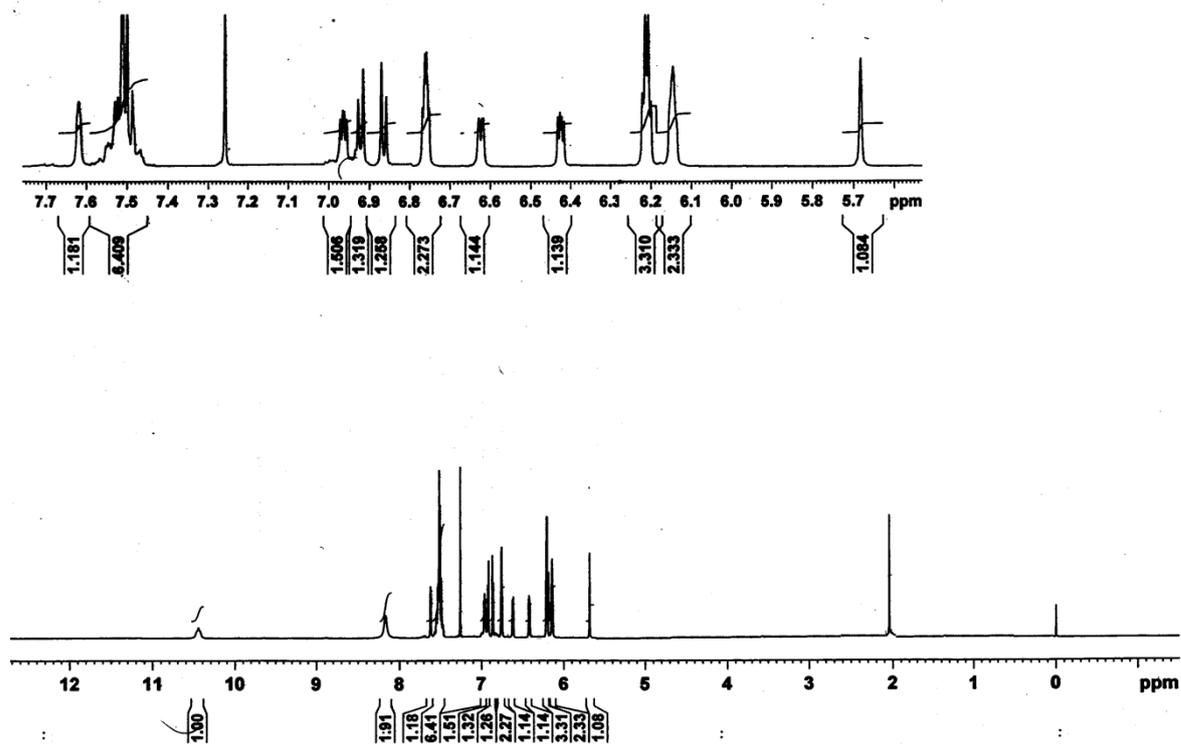


Figure S2a: ^1H NMR spectrum of compound **3** recorded in CDCl_3 .

PH-DPM-NOESY

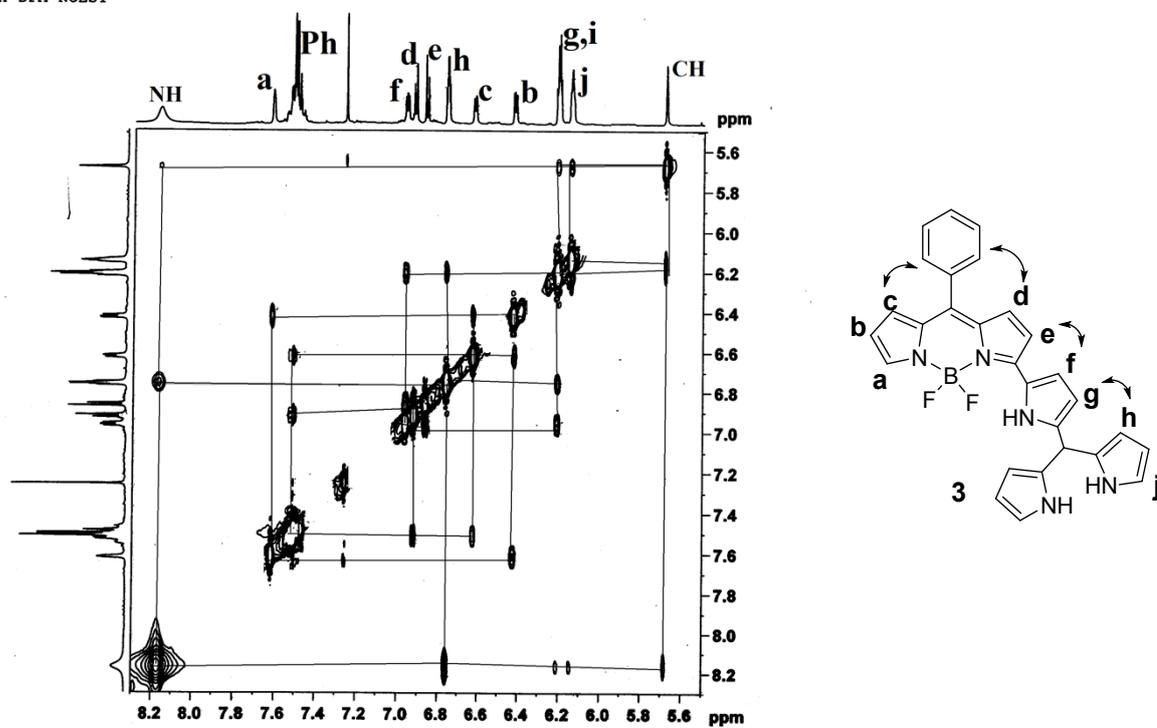


Figure S2b: ^1H - ^1H NOESY NMR spectrum of compound **3** recorded in CDCl_3 .

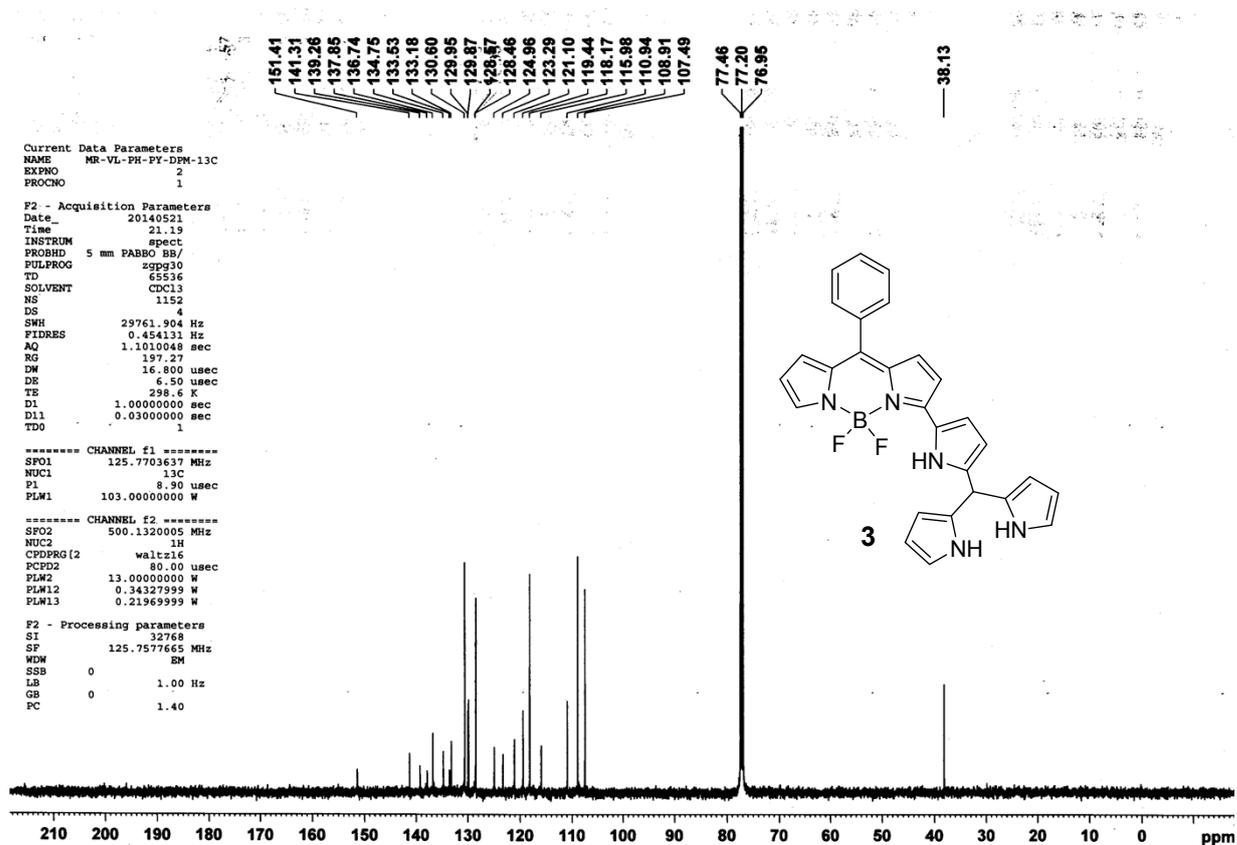


Figure S3: ^{13}C NMR spectrum of compound 3 recorded in CDCl_3 .

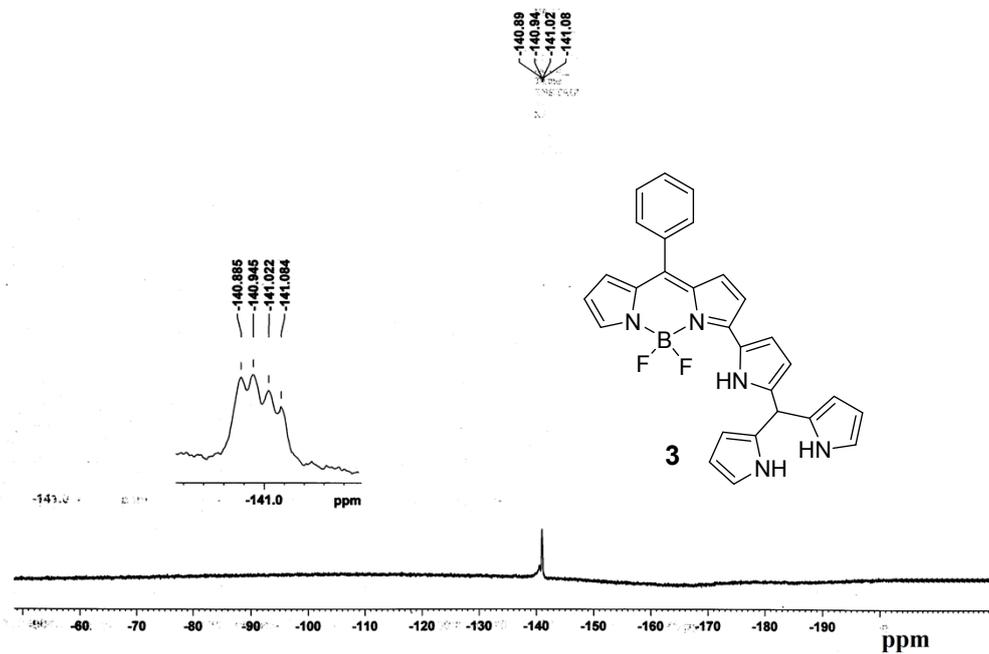


Figure S4: ¹⁹F NMR spectrum of compound 3 recorded in CDCl₃.

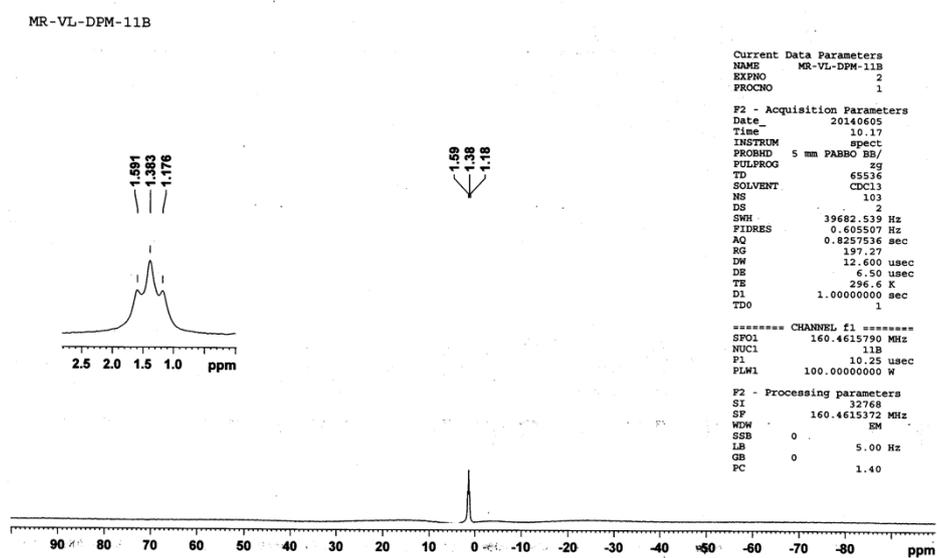
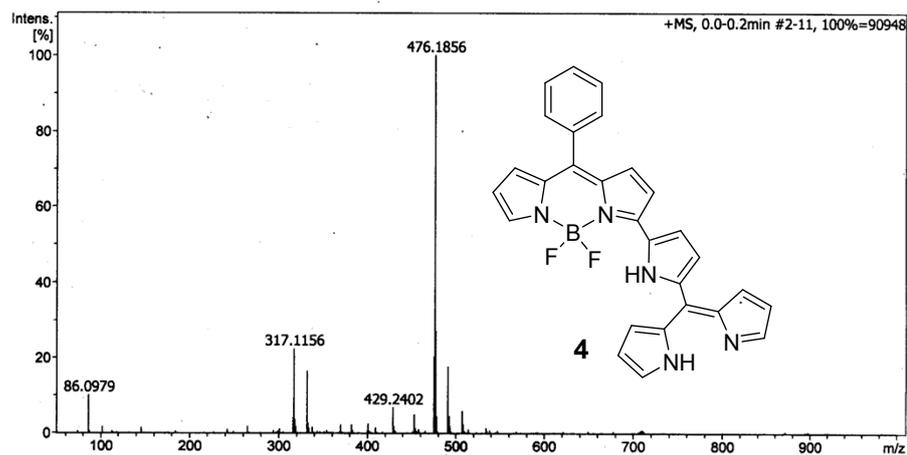


Figure S5: ¹¹B NMR spectrum of compound 3 recorded in CDCl₃.

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Analysis Info
Analysis Name D:\Data\MAY 14\MR-VL-PH-DIPYRRIN.d Acquisition Date 5/12/2014 12:56:19 PM
Method Tune_pos_Standard_NAI-1000.m Operator mr-rs-in
Sample Name MR-VL-PH-DIPYRRIN Instrument maXis impact 282001.00081
Comment C28H20BF2N5

Acquisition Parameter
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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 1000 m/z Set Collision Cell RF 400.0 Vpp Set Divert Valve Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
476.1856	1	C28H21BF2N5	476.1858	0.4	21.1	1	100.00	20.5	even	ok

Figure S6: HRMS of compound 4.

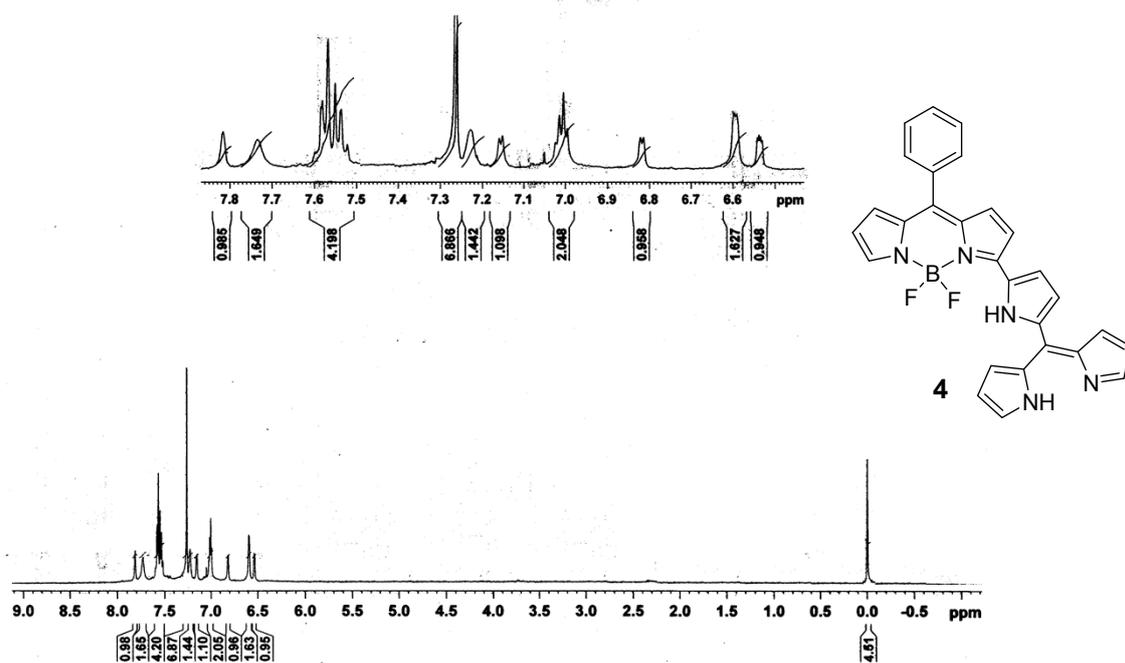


Figure S7: ^1H NMR spectrum of compound **4** recorded in CDCl_3 .

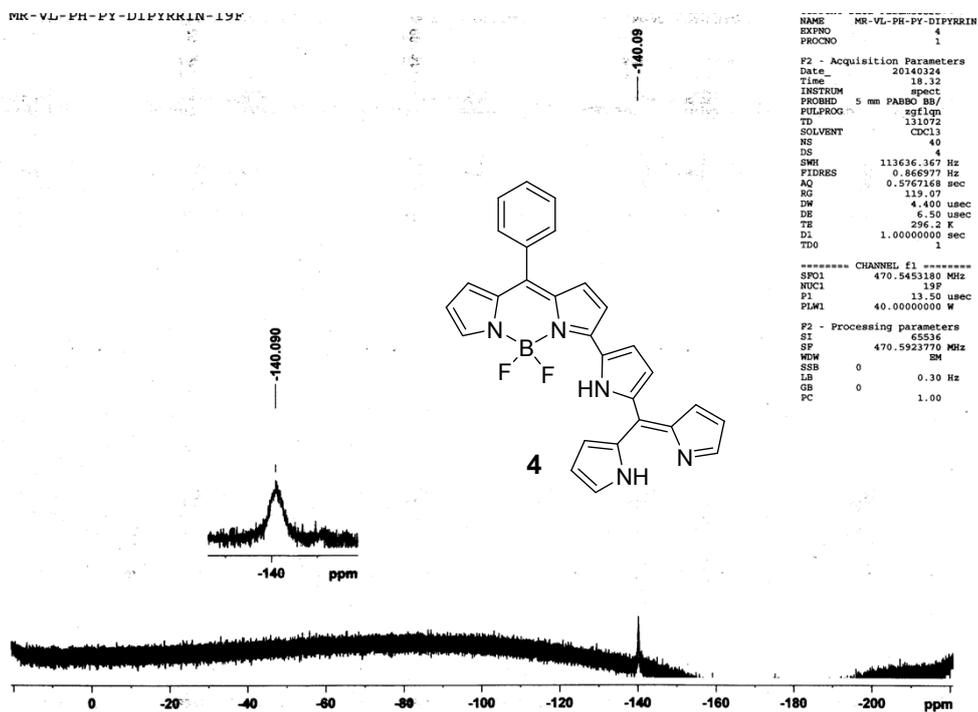


Figure S8: ^{19}F NMR spectrum of compound 4 recorded in CDCl_3 .

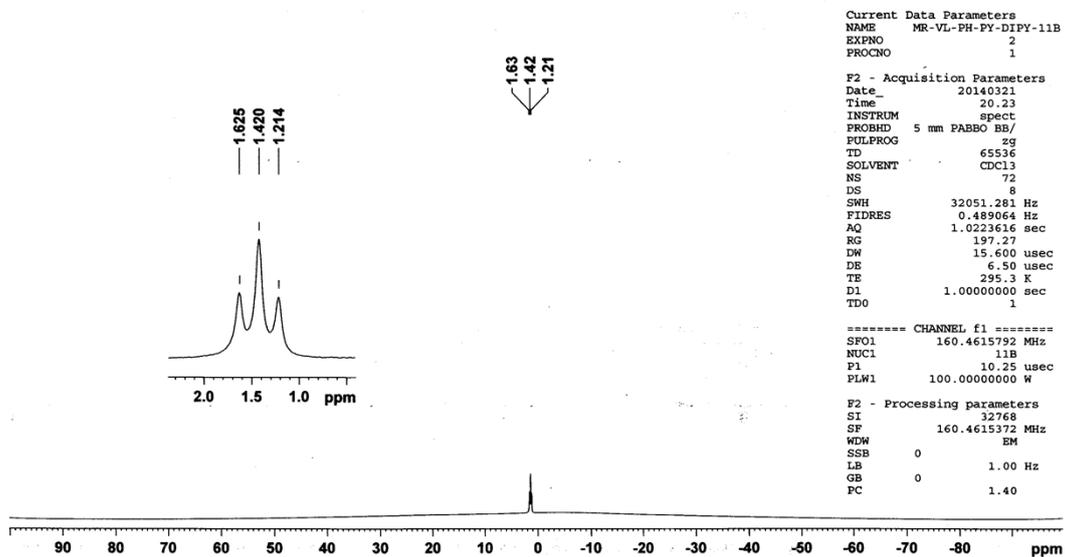


Figure S9: ^{11}B NMR spectrum of compound 4 recorded in CDCl_3 .

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Analysis Info

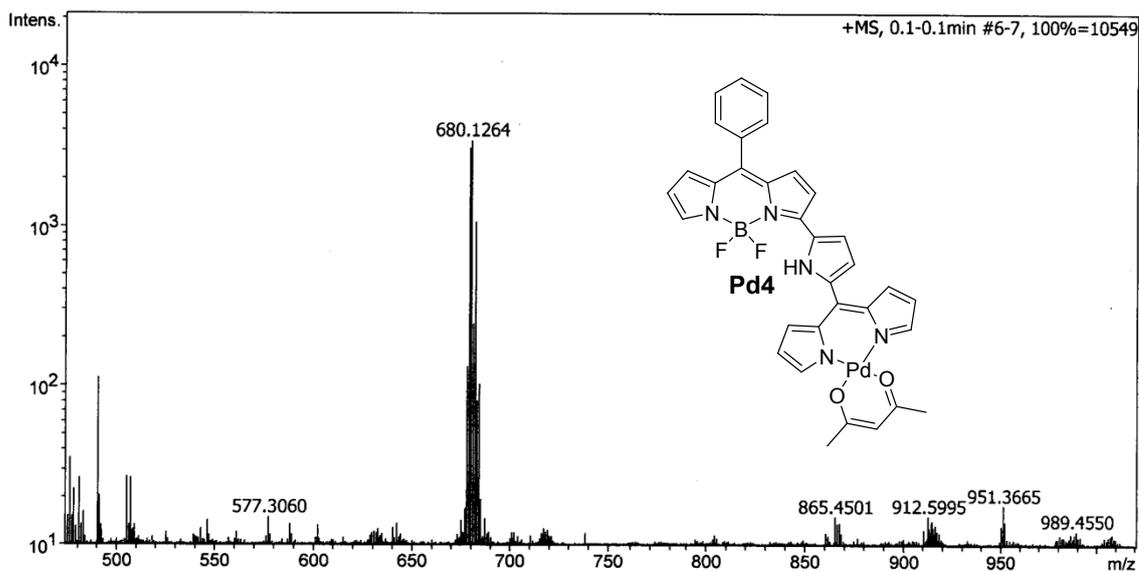
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 Sample Name INN-TK-405-B
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Acquisition Date 2/25/2014 10:07:02 PM

Operator DM IN
 Instrument maXis impact 282001.00081

Acquisition Parameter

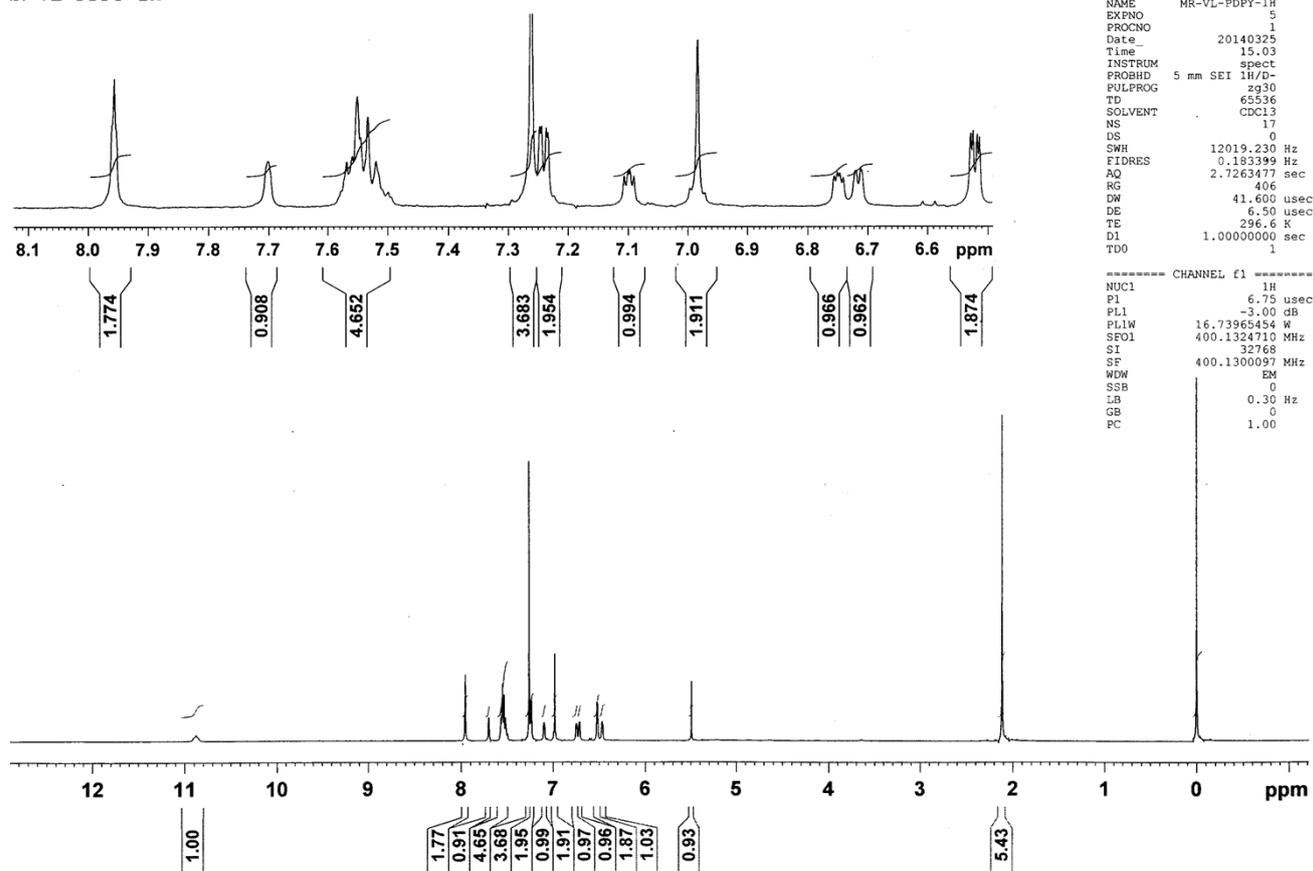
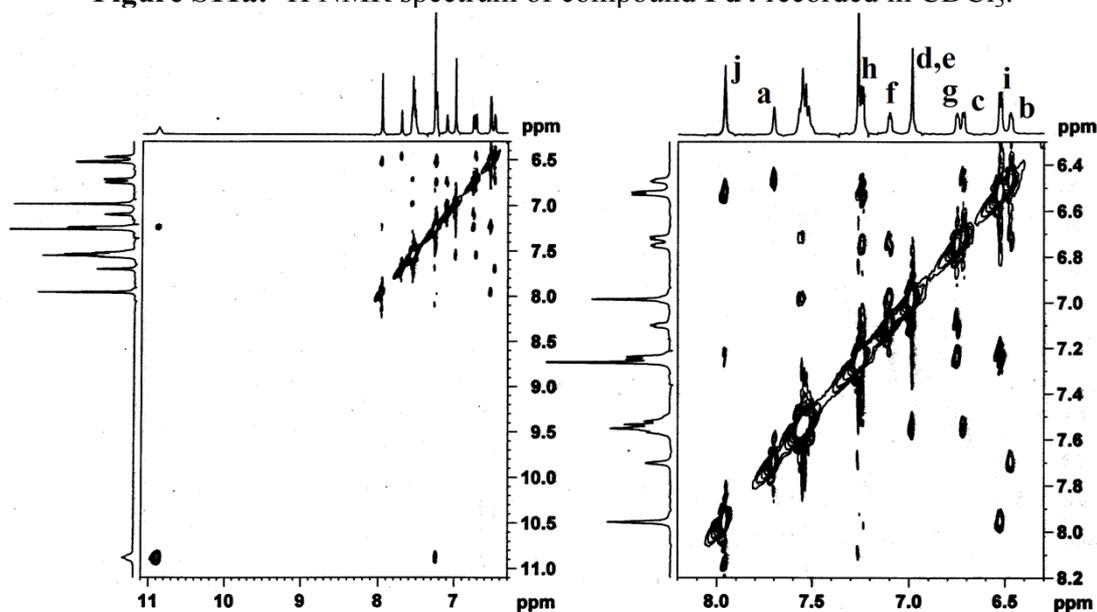
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Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1200 m/z	Set Collision Cell RF	1500.0 Vpp	Set Divert Valve	Source



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.

IR-VL-PDPY-1H

Figure S11a: ^1H NMR spectrum of compound **Pd4** recorded in CDCl_3 .Figure S11b: ^1H - ^1H NOESY NMR spectrum of compound **Pd4** recorded in CDCl_3 .

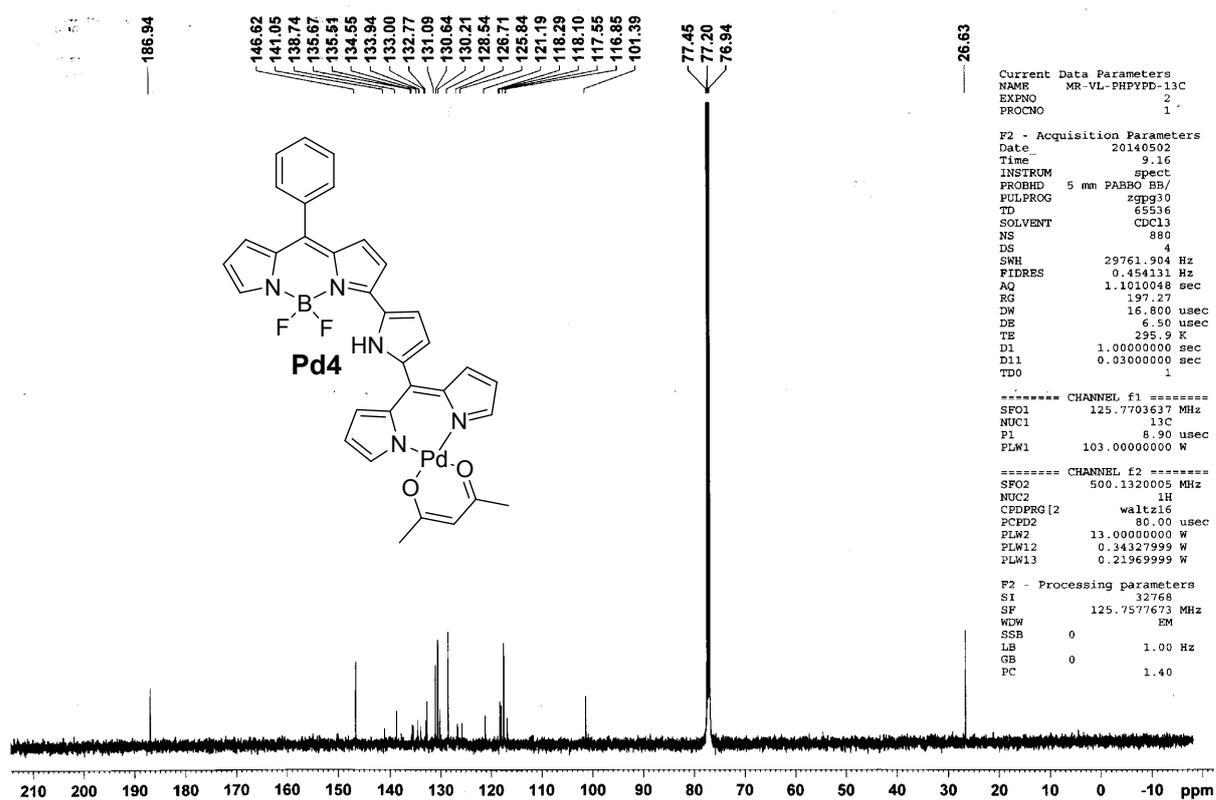


Figure S12: ^{13}C NMR spectrum of compound Pd4 recorded in CDCl_3 .

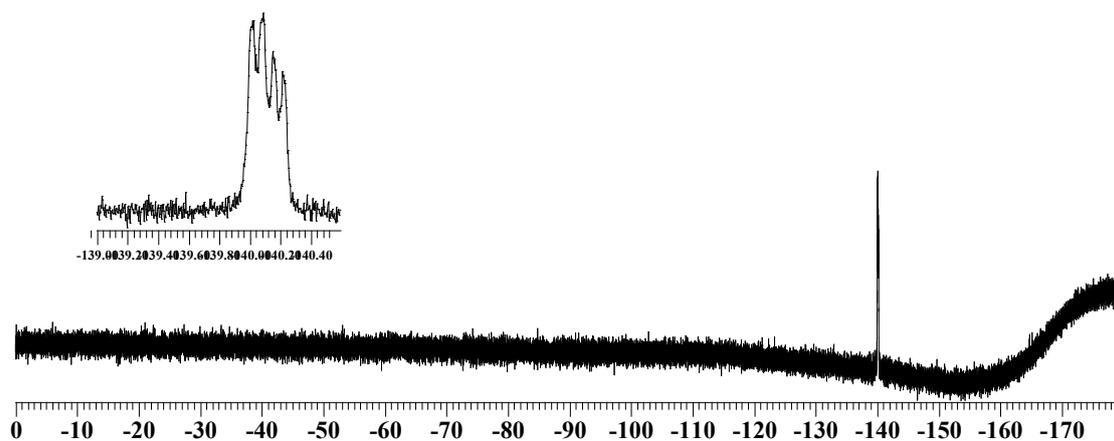


Figure S13: ^{19}F NMR spectrum of compound **Pd4** recorded in CDCl_3 (δ in ppm).

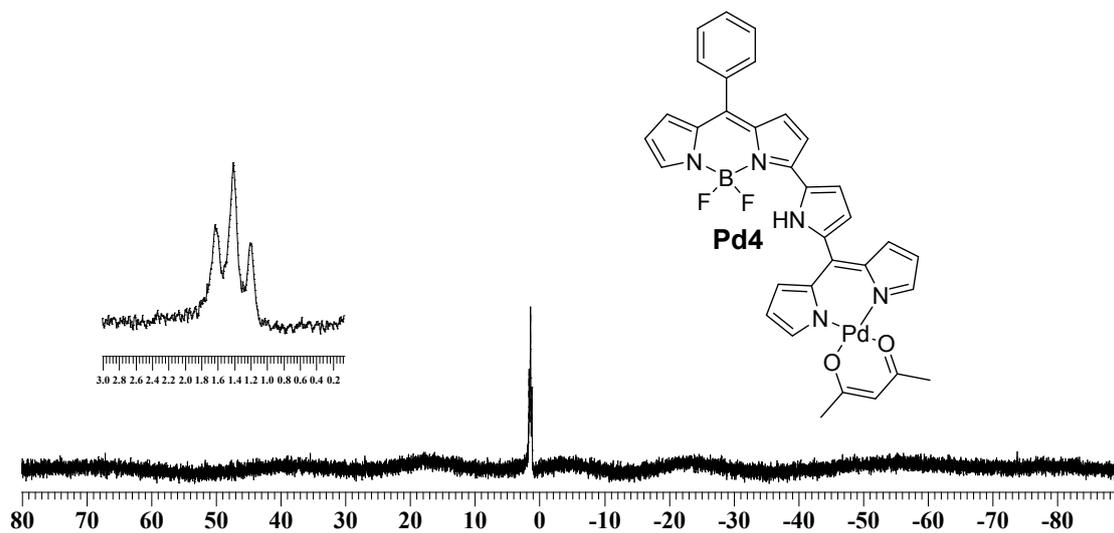
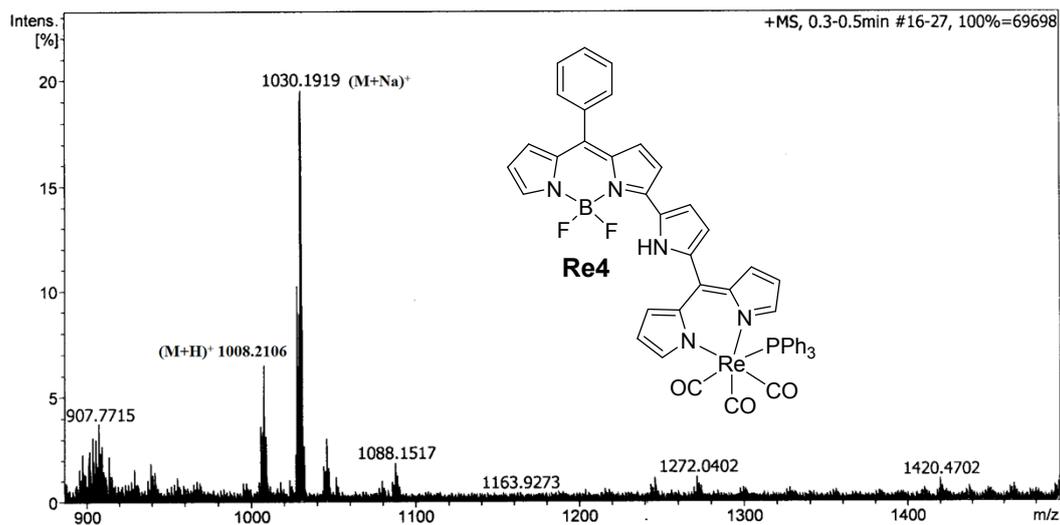


Figure S14: ^{11}B NMR spectrum of compound **Pd4** recorded in CDCl_3 (δ in ppm).

Indian Institute of Technology (B)

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

Acquisition Parameter					
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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
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Figure S15: HRMS of compound Re4.

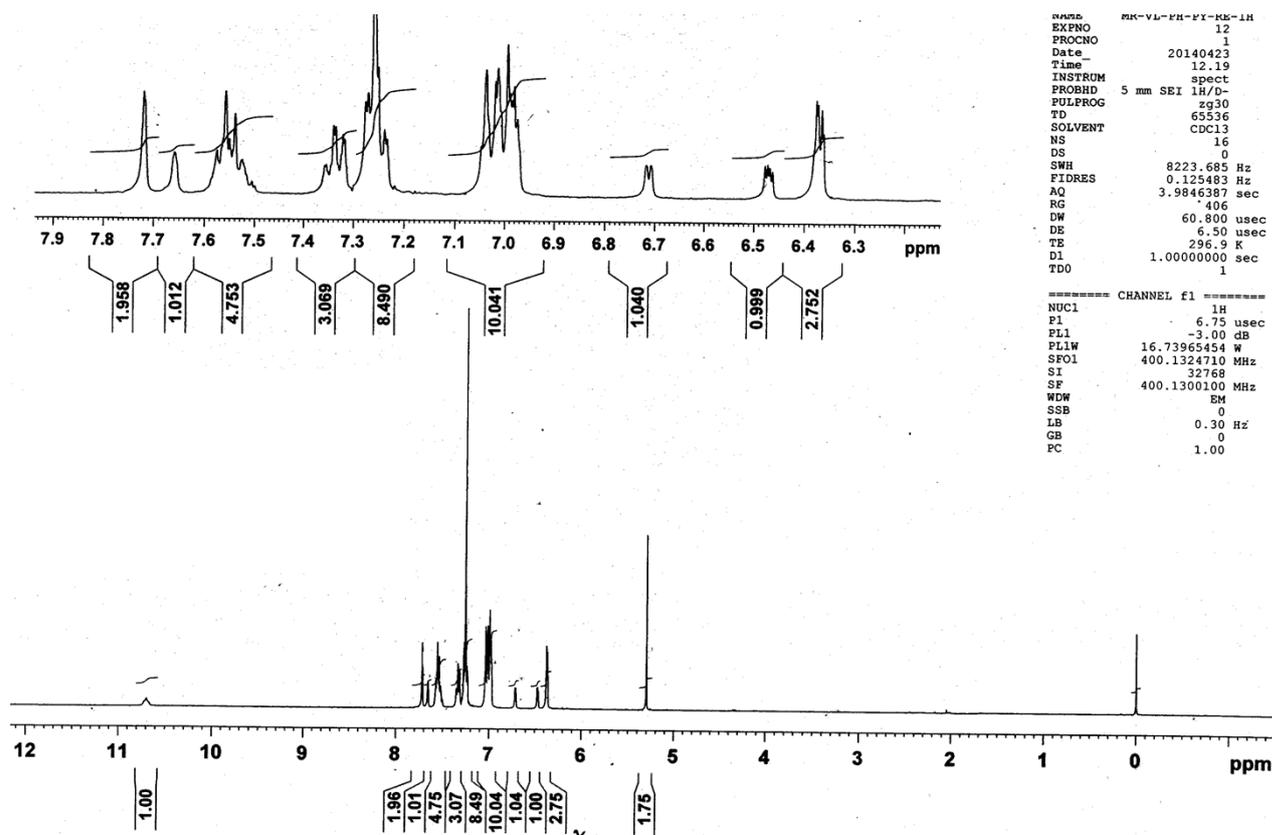


Figure S16a: ^1H NMR spectrum of compound **Re4** recorded in CDCl_3 .

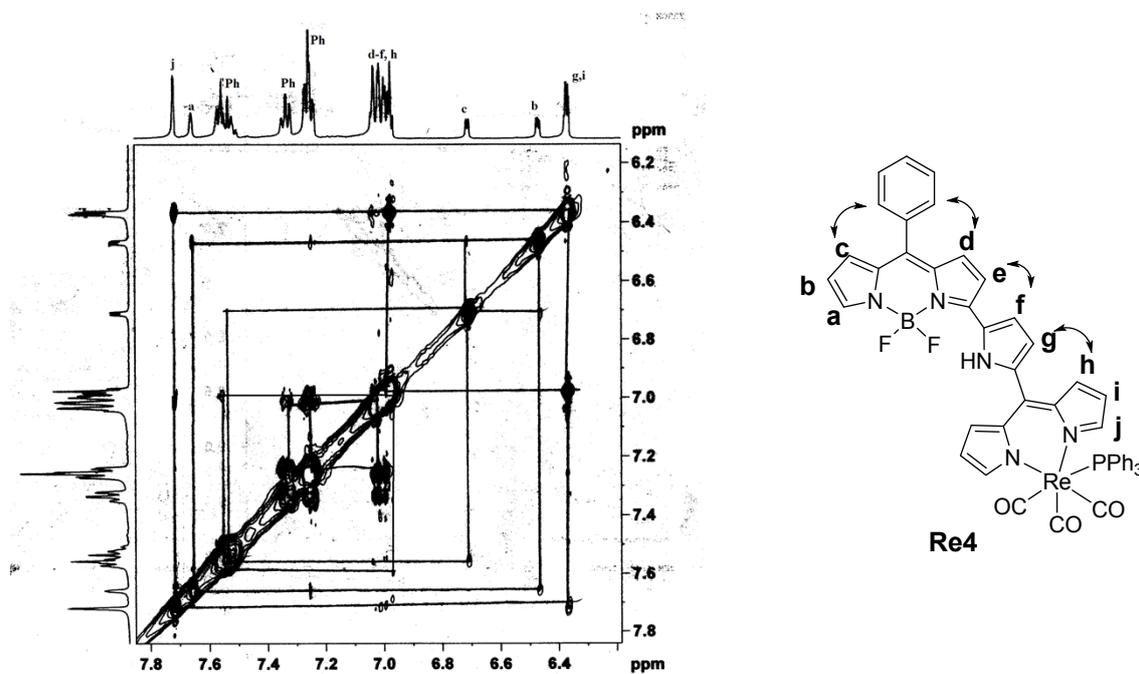


Figure S16b: ^1H - ^1H NOESY NMR spectrum of compound **Re4** recorded in CDCl_3 .

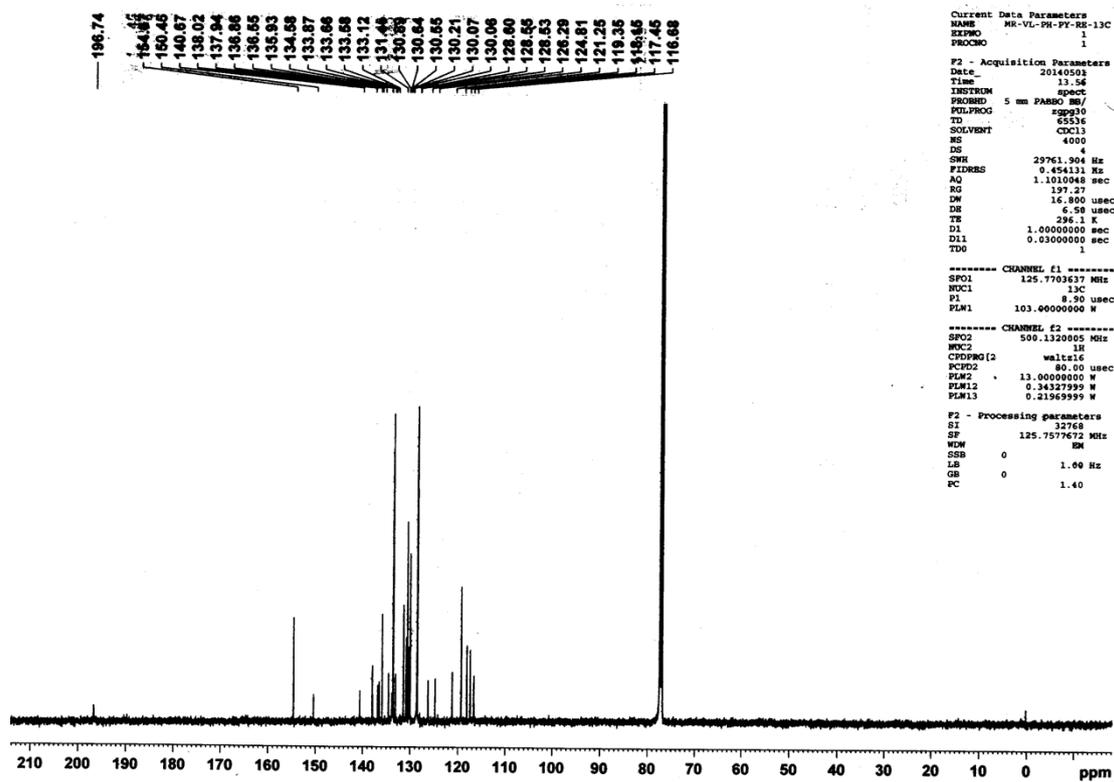


Figure S17: ^{13}C NMR spectrum of compound **Re4** recorded in CDCl_3 .

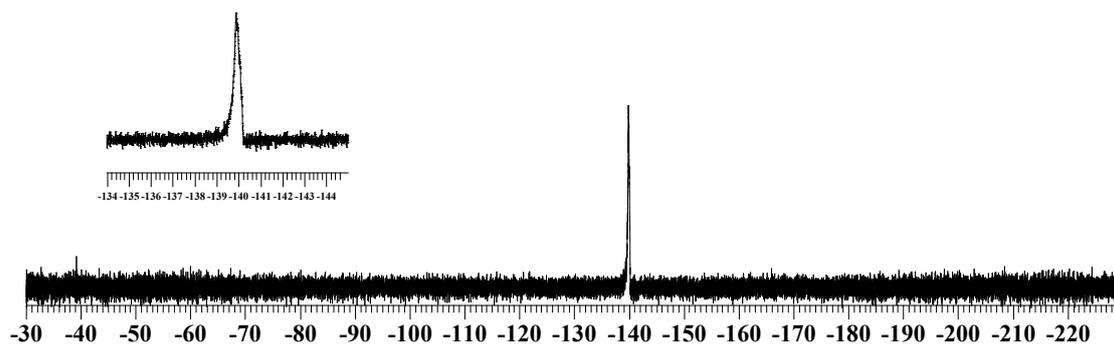


Figure S18: ^{19}F NMR spectrum of compound **Re4** recorded in CDCl_3 (δ in ppm).

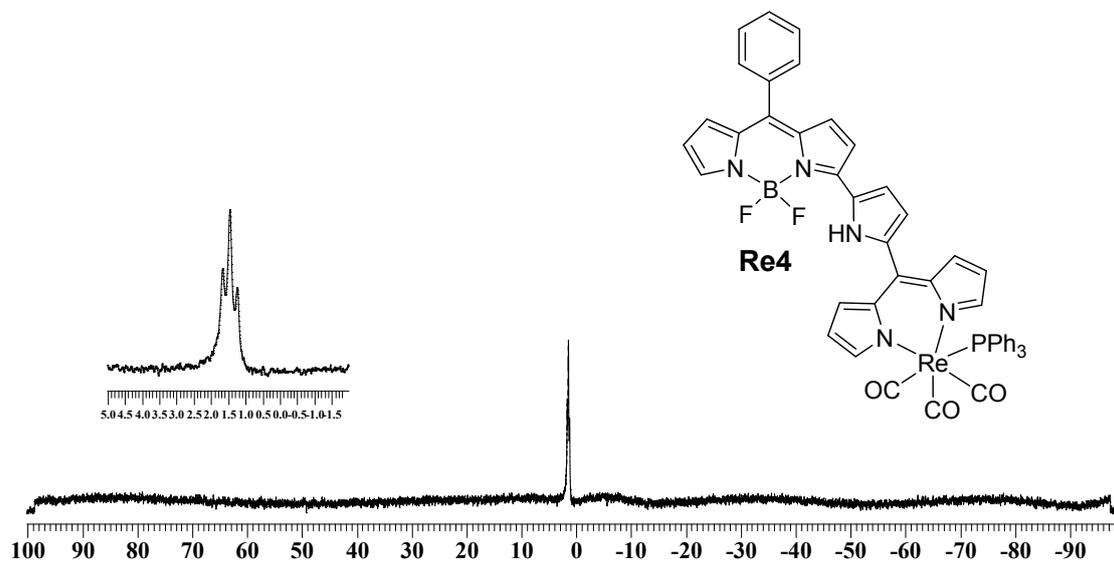


Figure S19: ^{11}B NMR spectrum of compound **Re4** recorded in CDCl_3 (δ in ppm).

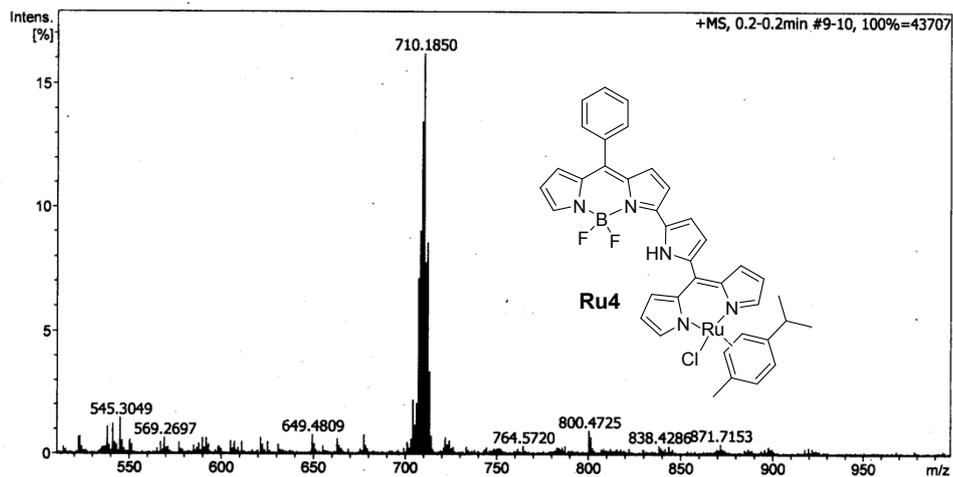
Indian Institute of Technology (B)

Analysis Info
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 Method Tune_pos_Standard_NAI-1000.m
 Sample Name MR-VL-RU
 Comment C38H33BCIF2N6Ru

Acquisition Date 5/12/2014 12:50:46 PM
 Operator mr-rs-in
 Instrument maXis impact 282001.00081

Acquisition Parameter

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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	1000 m/z	Set Collision Cell RF	400.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
710.1850	1	C38H33BF2N5Ru	710.1851	-2.1	21.2	1	100.00	25.0	odd	

Figure S20: HRMS of compound Ru4.

S17

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 PROCNO 1

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 Date 20140509
 Time 17.25
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 20
 DS 2
 SWH 12500.000
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 DE 6.50
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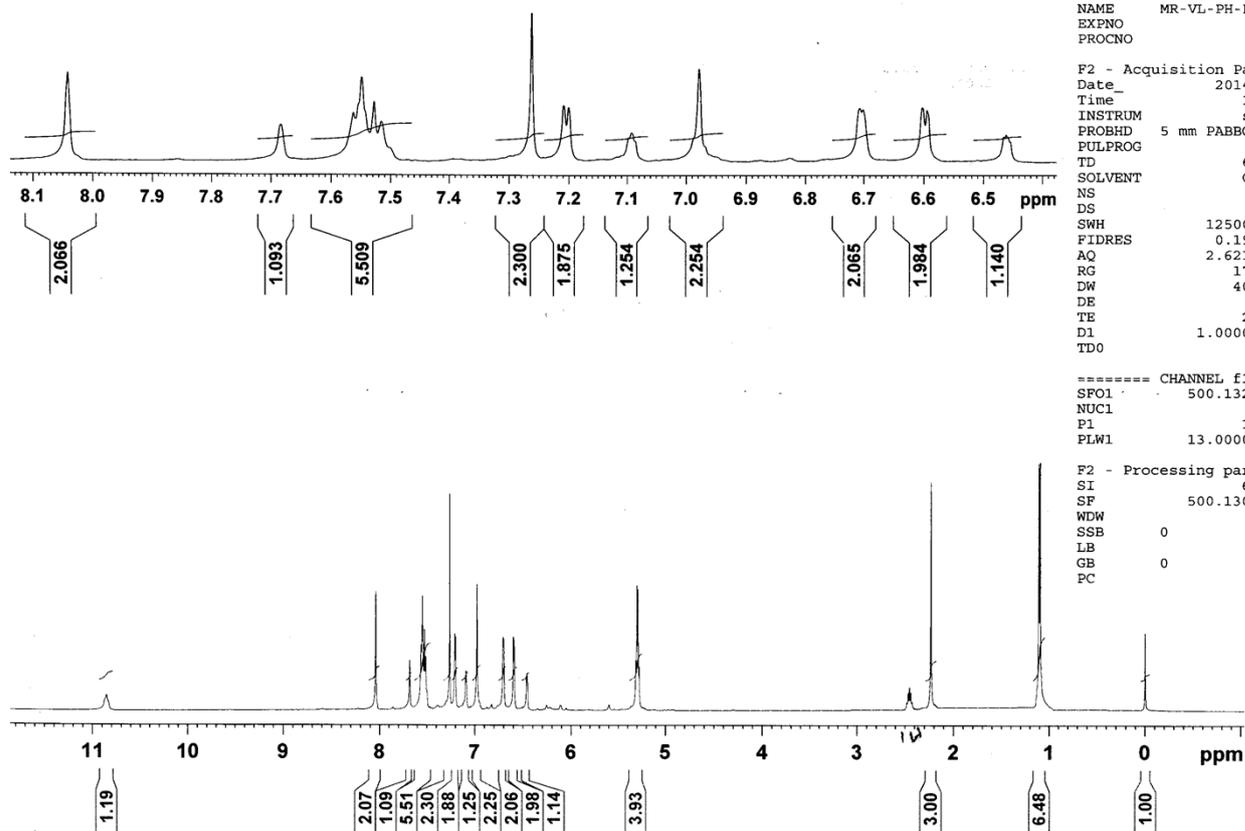


Figure S21a: ^1H NMR spectrum of compound **Ru4** recorded in CDCl_3 .

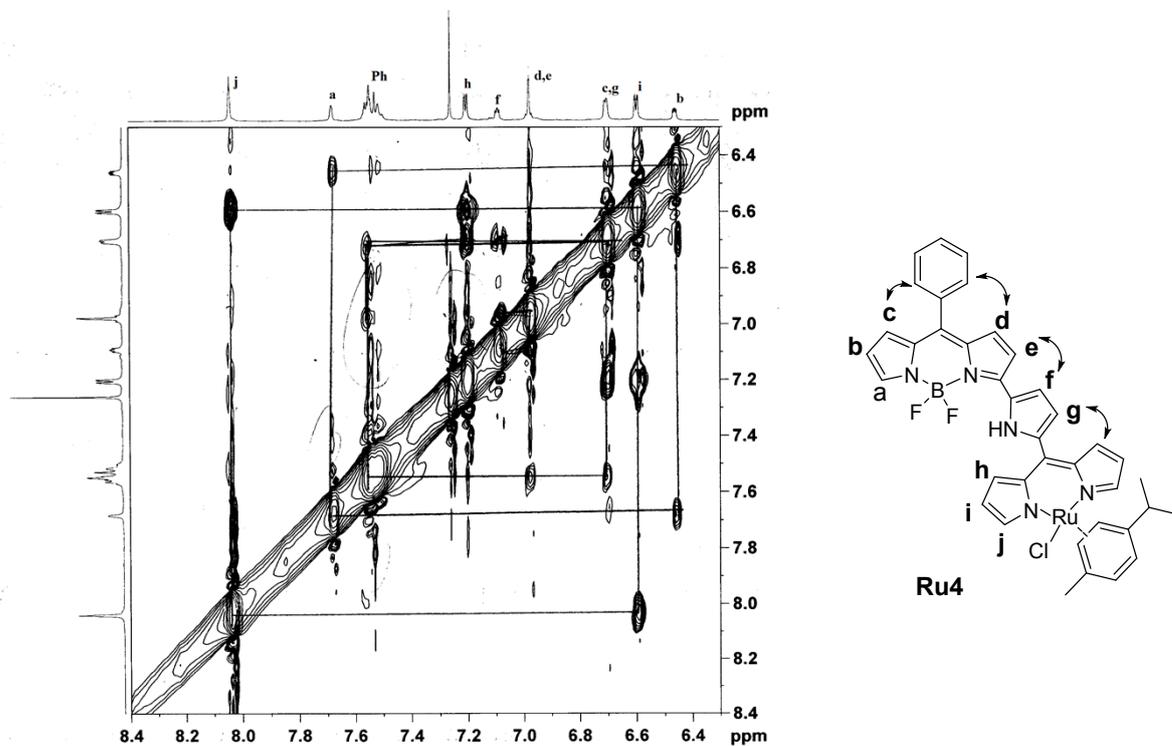


Figure S21b: ^1H - ^1H NOESY NMR spectrum of compound **Ru4** recorded in CDCl_3 .

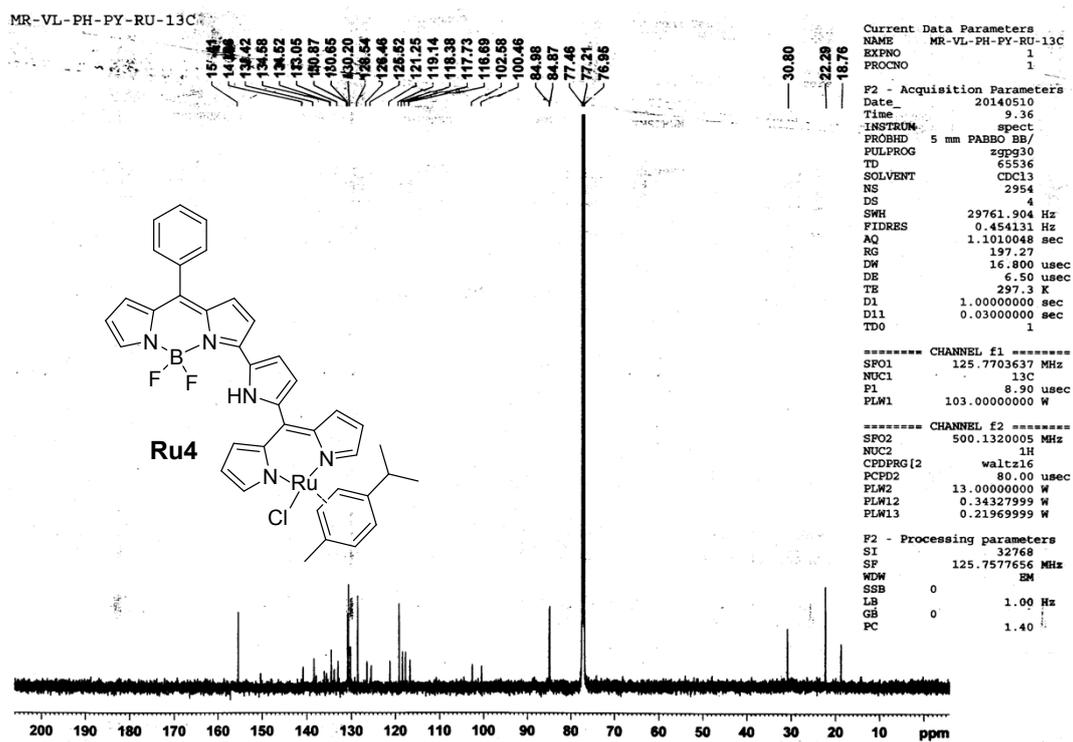


Figure S22: ^{13}C NMR spectrum of compound **Ru4** recorded in CDCl_3 .

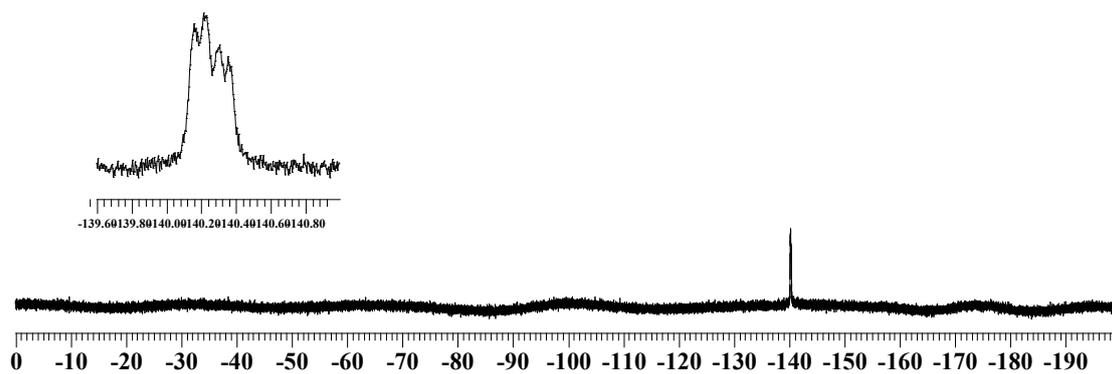


Figure S23: ^{19}F NMR spectrum of compound **Ru4** recorded in CDCl_3 (δ in ppm).

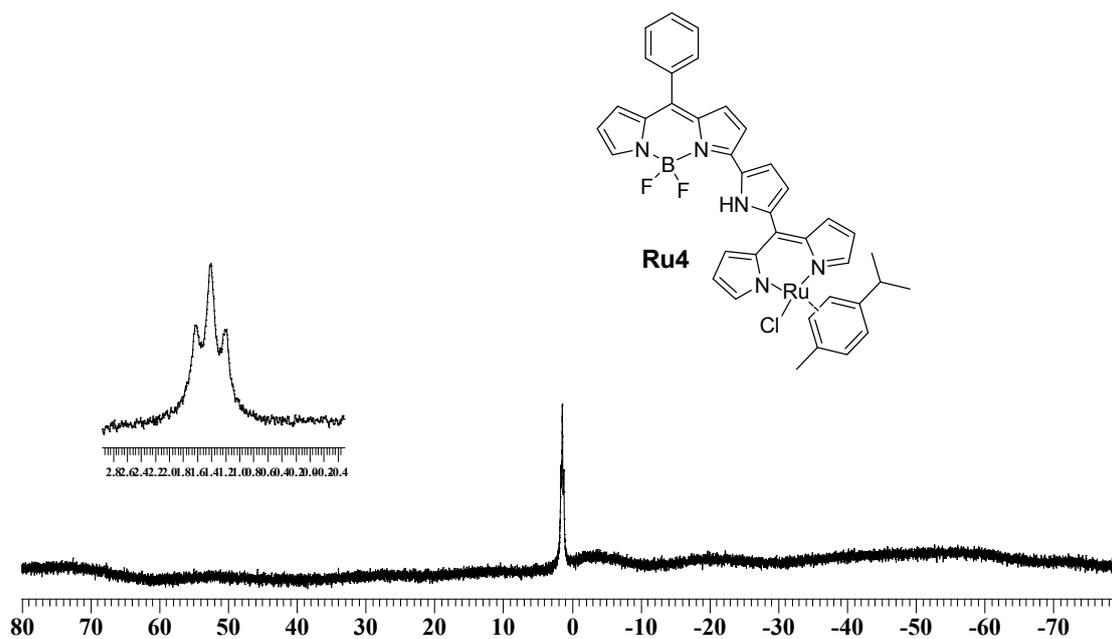


Figure S24: ^{11}B NMR spectrum of compound **Ru4** recorded in CDCl_3 (δ in ppm).

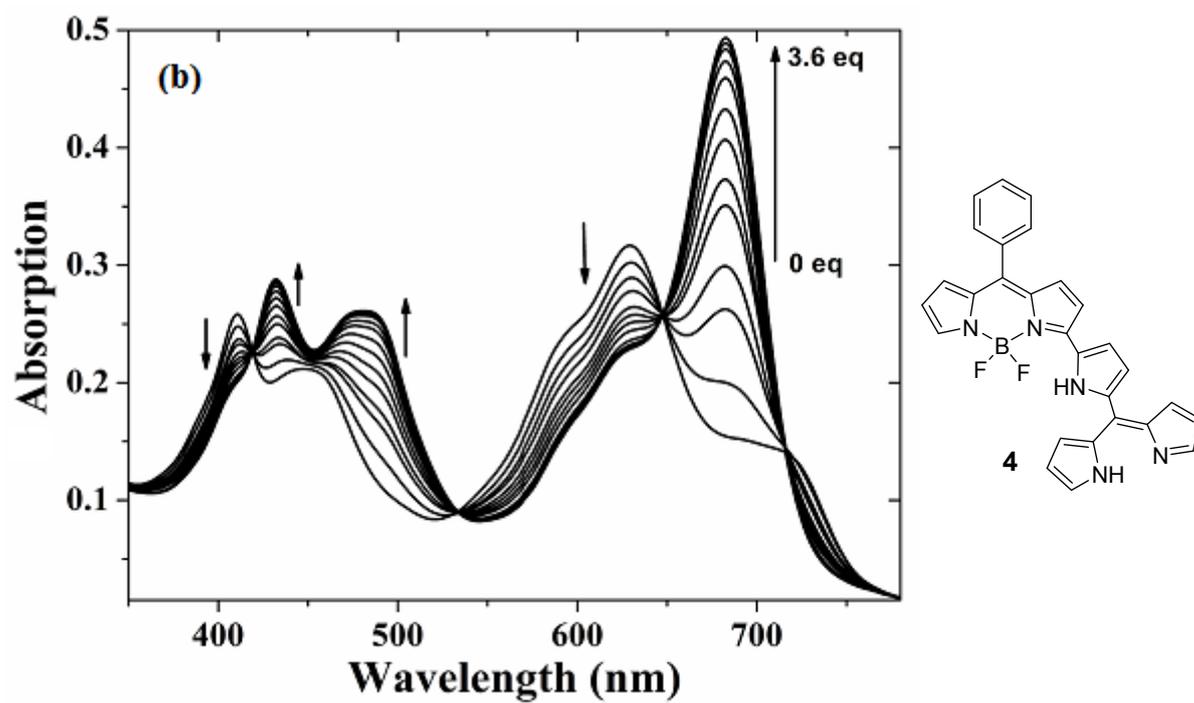


Figure S25: The protonated absorption spectra of compound **4** in CH_2Cl_2 .