

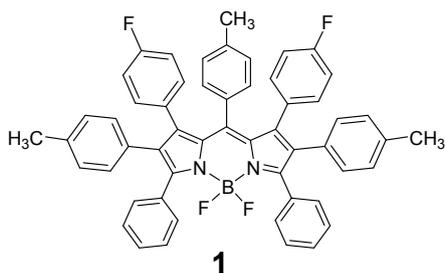
Polyarylated Boron-Dipyrromethenes Containing Three Different Types of Aryl Groups

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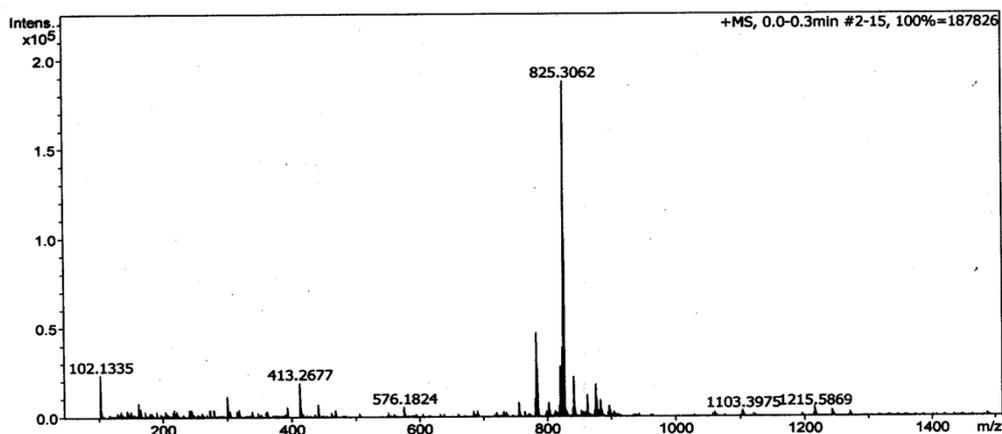
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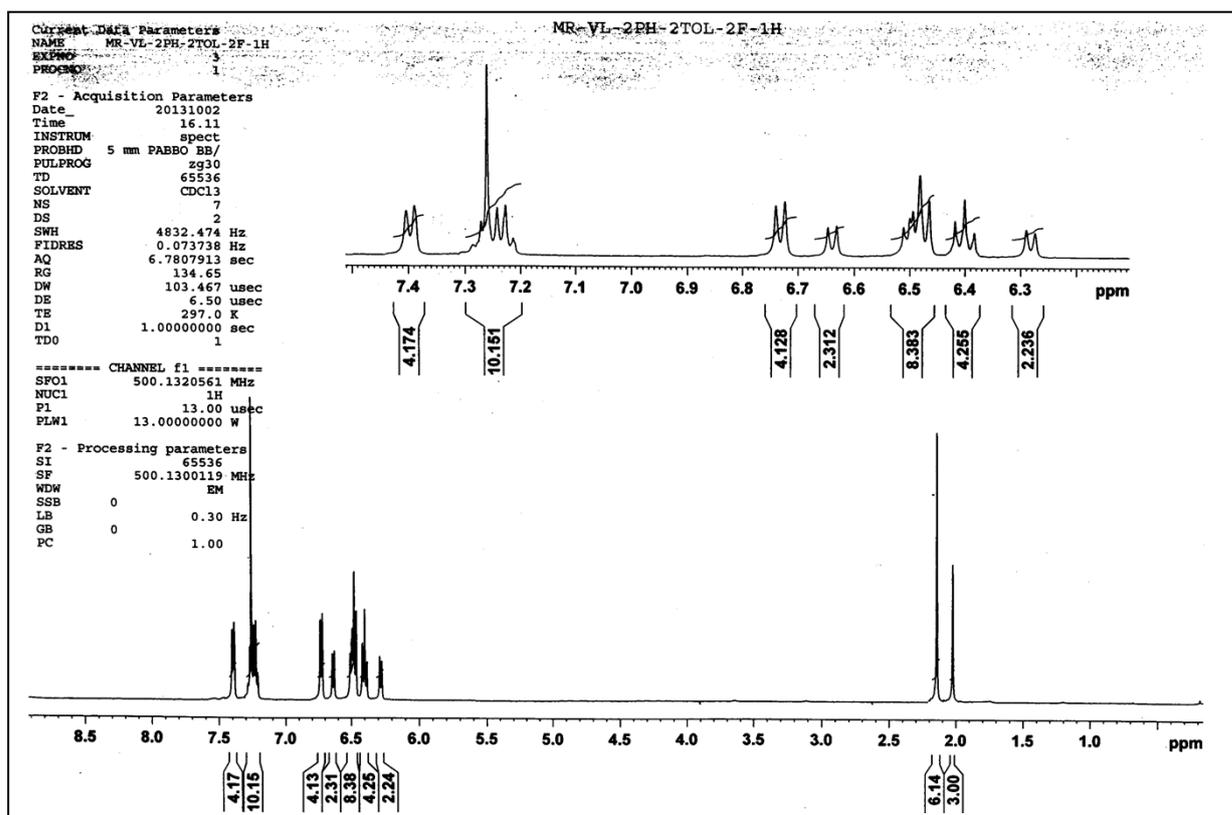
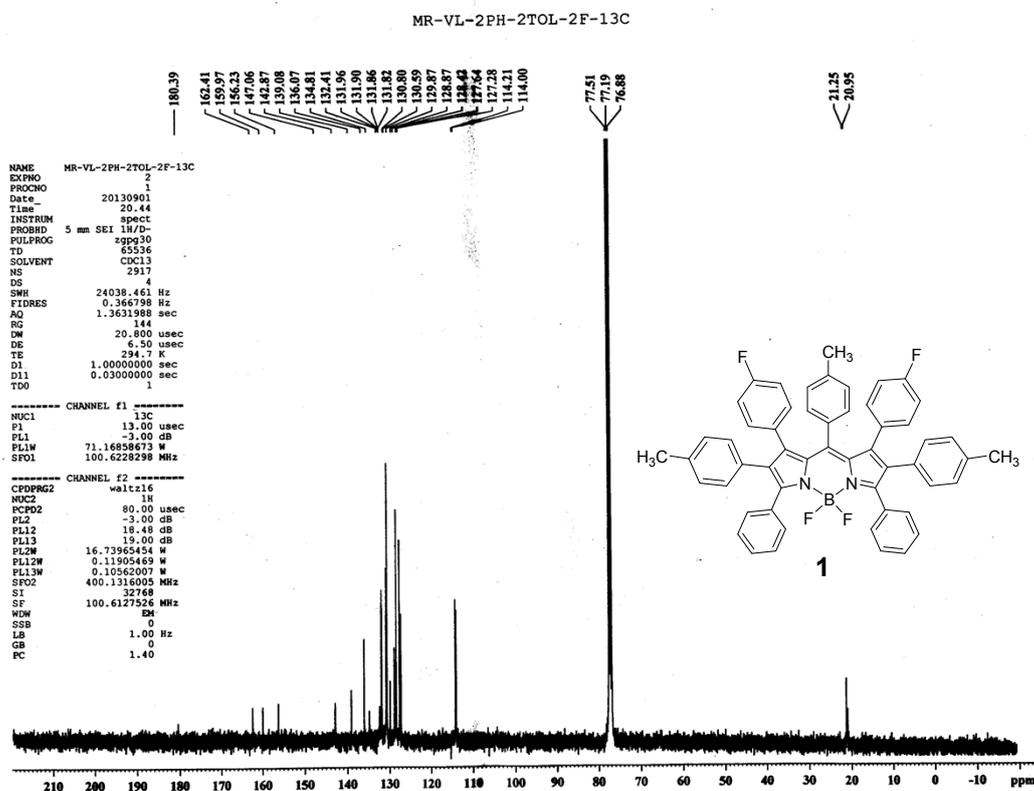
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Sample Name	MR-VL-2PH-2TOL-2F		
Comment	C54H39BF4N2		

Acquisition Parameter					
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Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
825.3062	1	C54H39BF4N2Na	825.3044	2.3	12.9	1	100.00	34.5	even	ok

Figure S1: HRMS of compound 1.

Figure S2: The ^1H NMR spectrum of compound **1** recorded in CDCl_3 Figure S3: The ^{13}C NMR spectrum of compound **1** recorded in CDCl_3

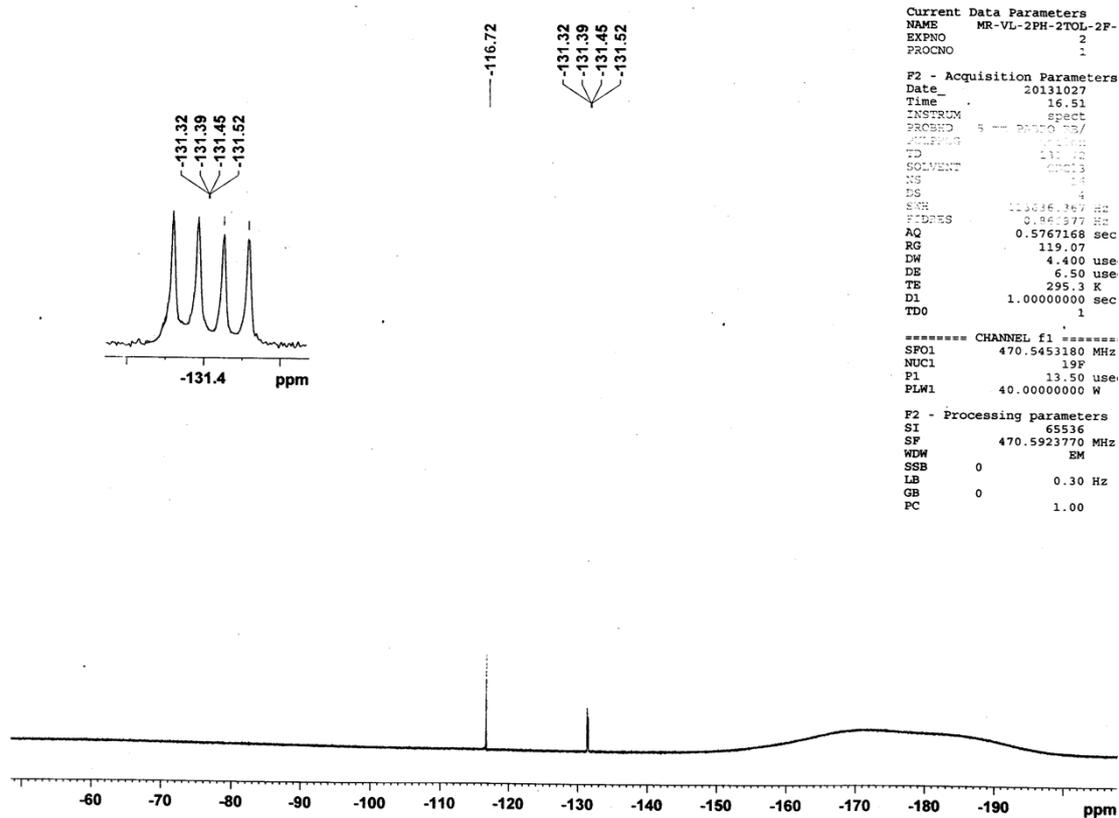


Figure S4: The ^{19}F NMR spectrum of compound **1** recorded in CDCl_3

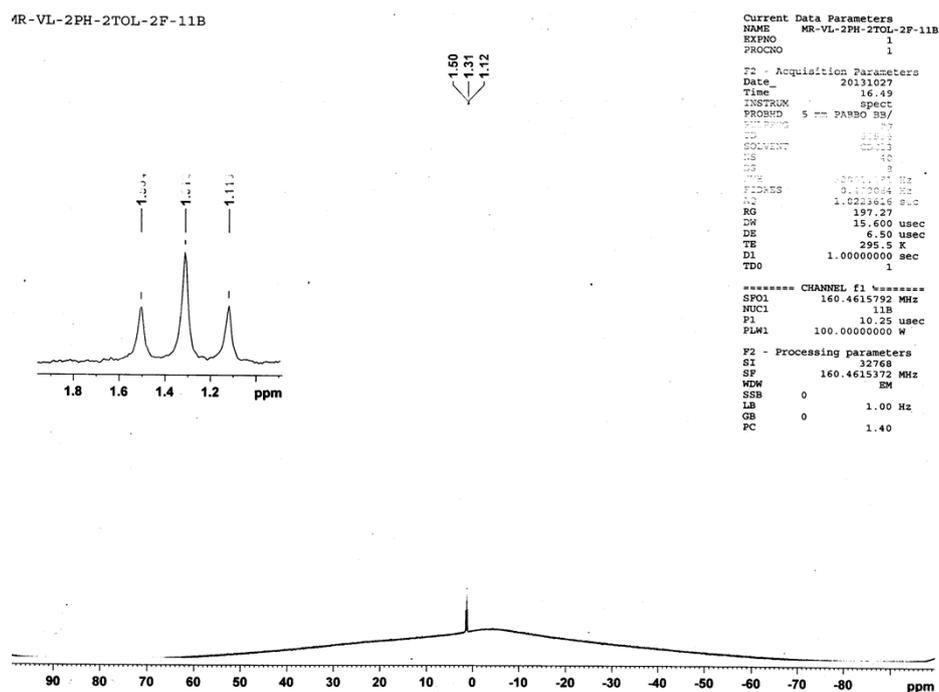
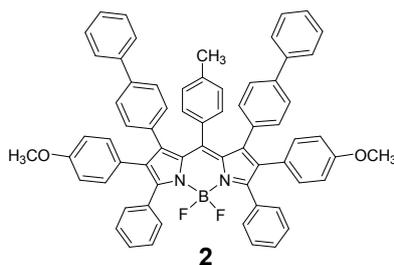


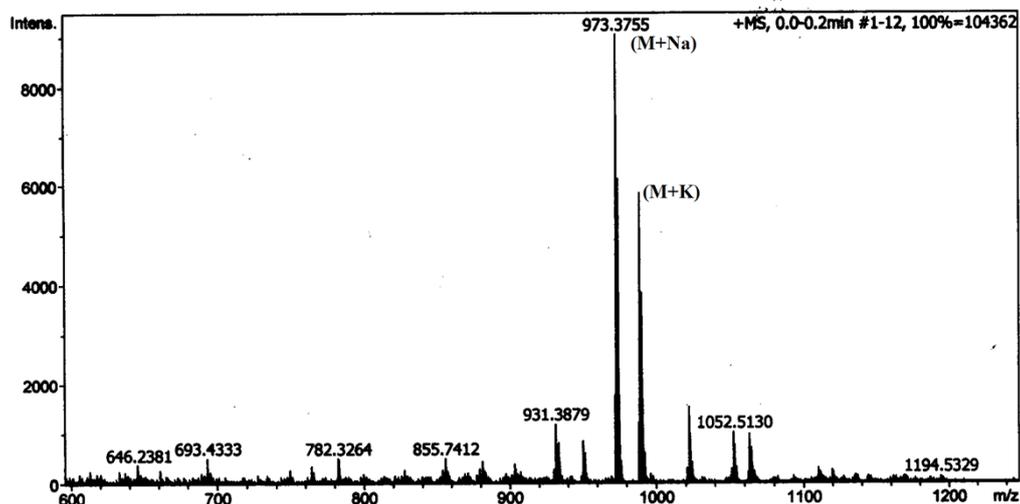
Figure S5: The ^{11}B NMR spectrum of compound **1** recorded in CDCl_3



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Method Tune_pos_Standard_NAI-1500.m	Instrument maXis impact 282001.00081
Sample Name MR-VL-2PH-2OME-2BPH	
Comment C66H49BF2N2O2	

Acquisition Parameter					
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Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
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Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
973.3755	1	C66H49BF2N2NaO2	973.3758	-0.8	10.2	1	100.00	42.5	even	ok

Figure S6: The HRMS spectrum of compound 2.

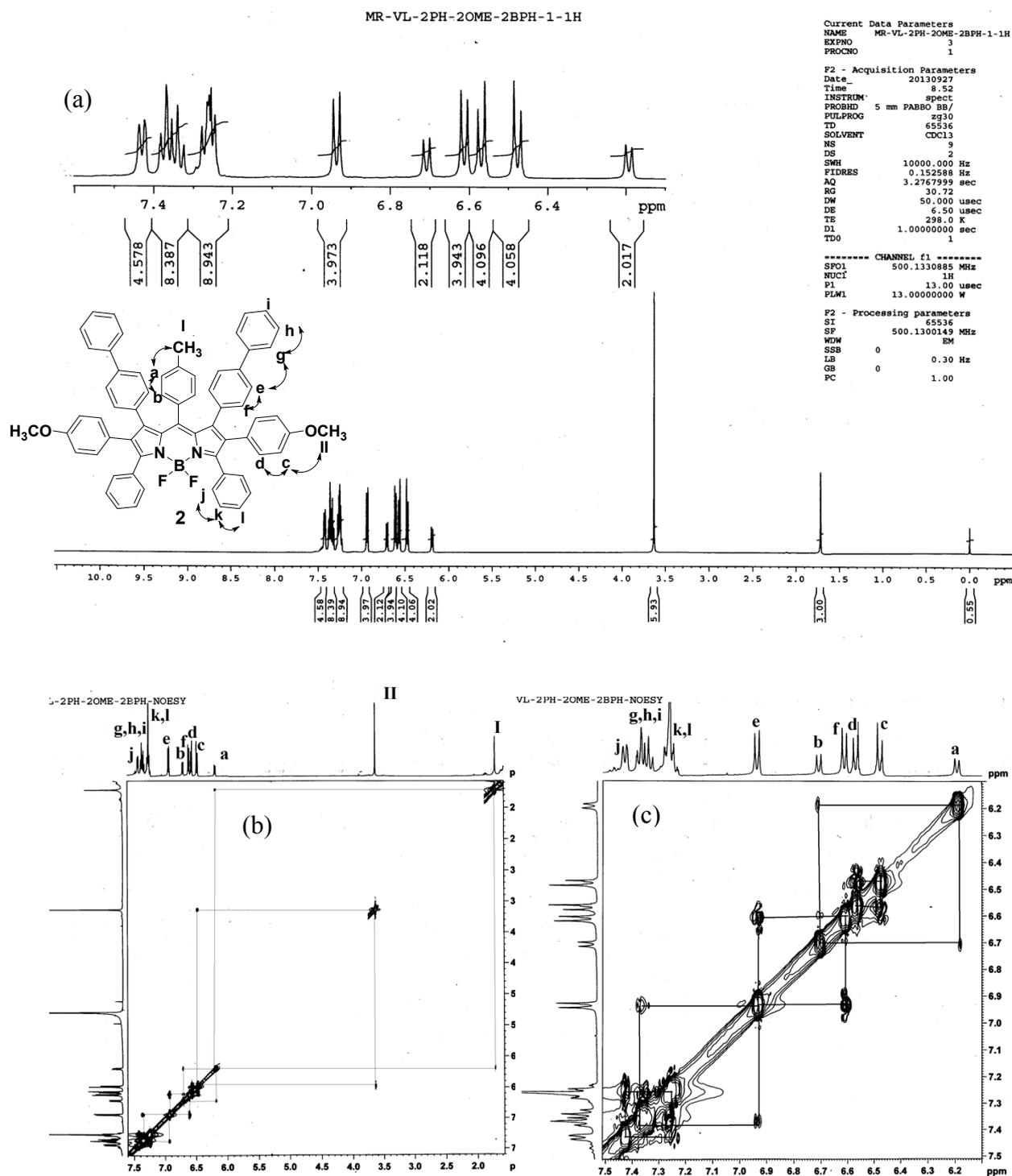
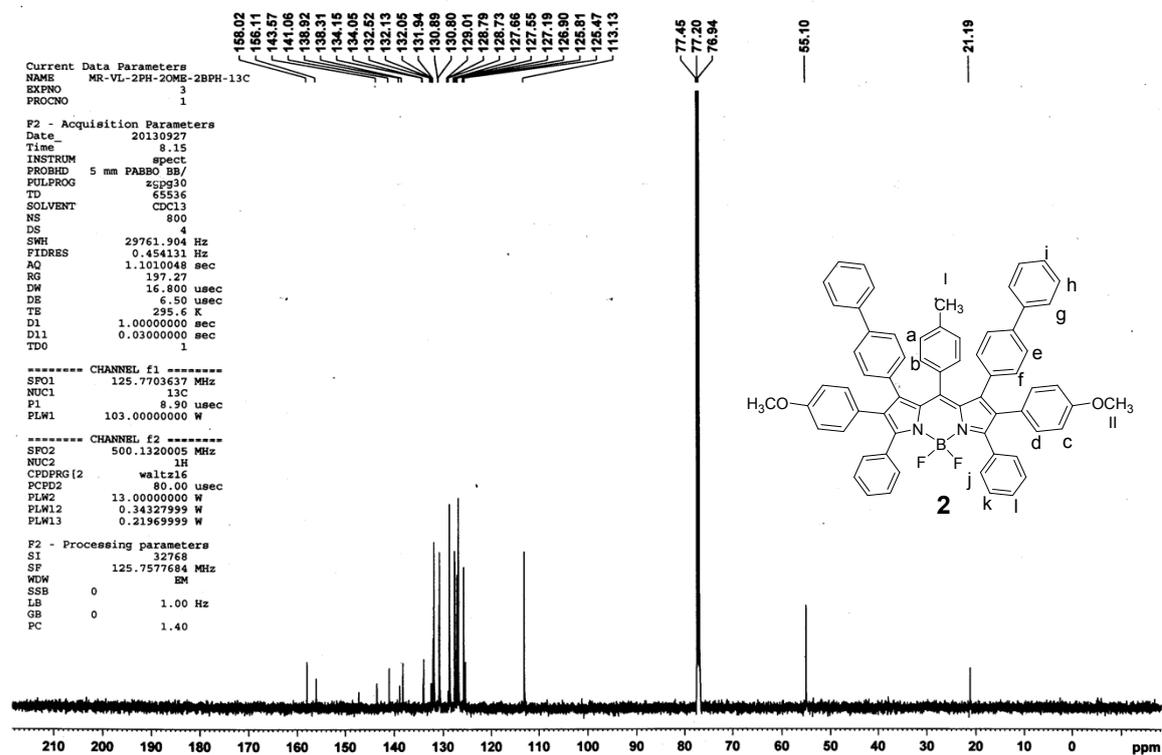
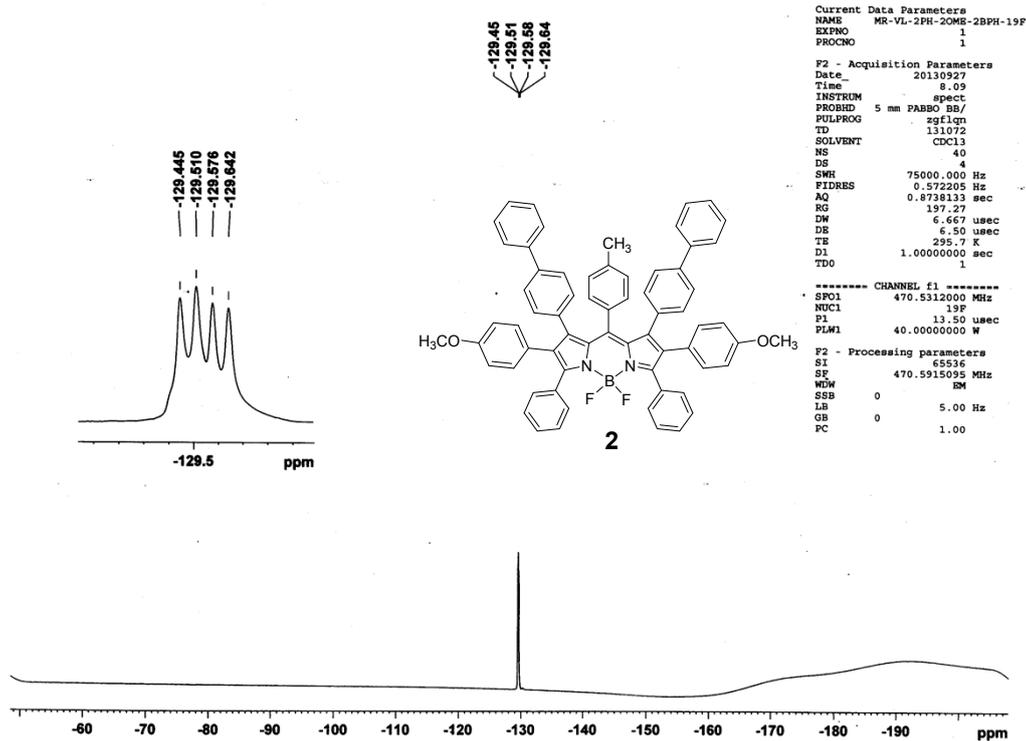


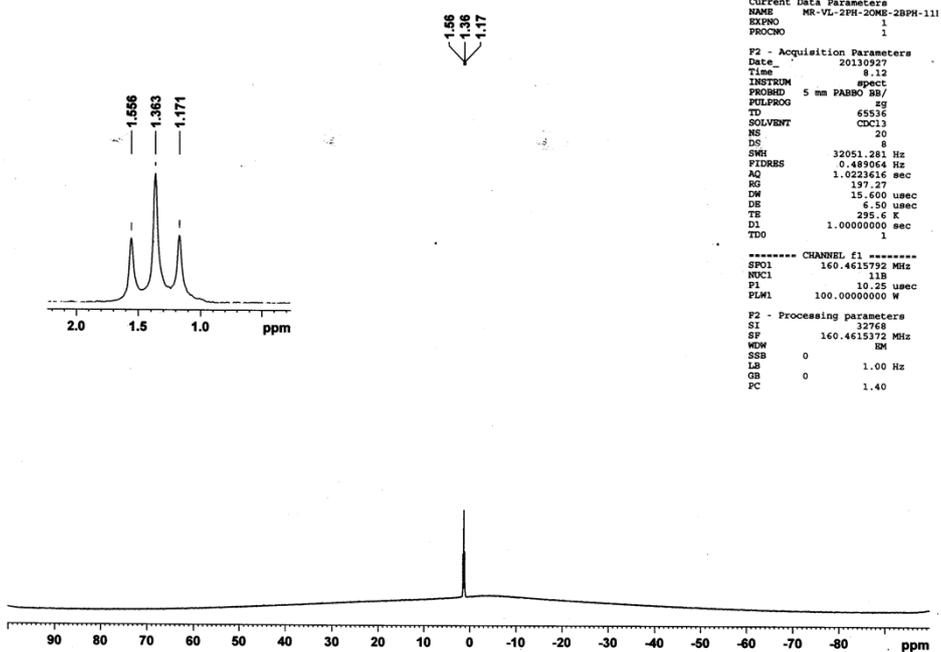
Figure S7: (a) The ^1H NMR spectrum of compound **2** recorded in CDCl_3 . (b) The NOESY NMR spectrum of compound **2** recorded in CDCl_3 . (c) The NOESY NMR spectrum of compound **2** in the selected region.

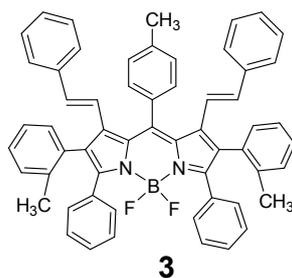
MR-VL-2PH-2OMB-2BPH-13C

Figure S8: The ^{13}C NMR spectrum of compound 2 recorded in CDCl_3 .



MR-VL-2PH-2OMB-2BPH-11B

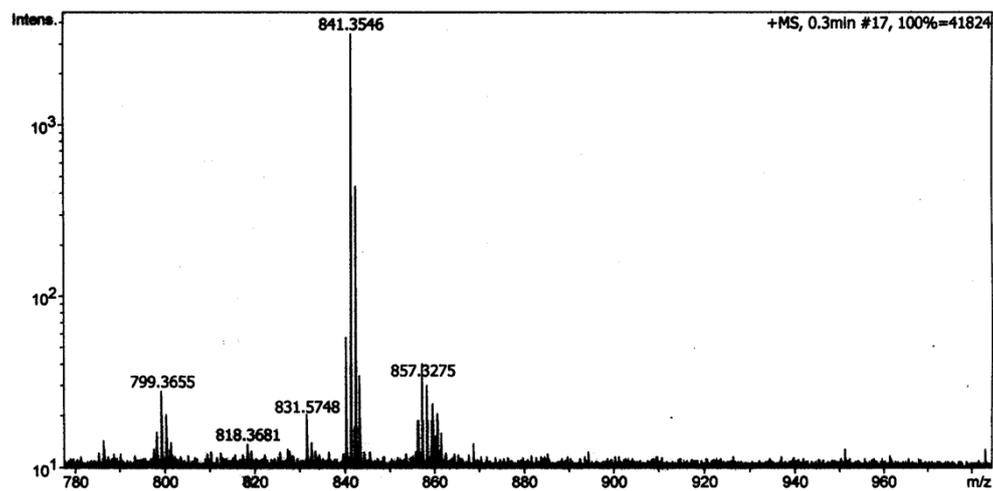




Indian Institute of Technology (B)

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Sample Name	MR-VL-2PH-2-O-TOL-2-VIPH		
Comment	C58H45BF2N2		

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	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
841.3546	1	C58H45BF2N2Na	841.3546	-0.1	41.2	1	100.00	36.5	even	ok

Figure S11: The HRMS spectrum of compound 3.

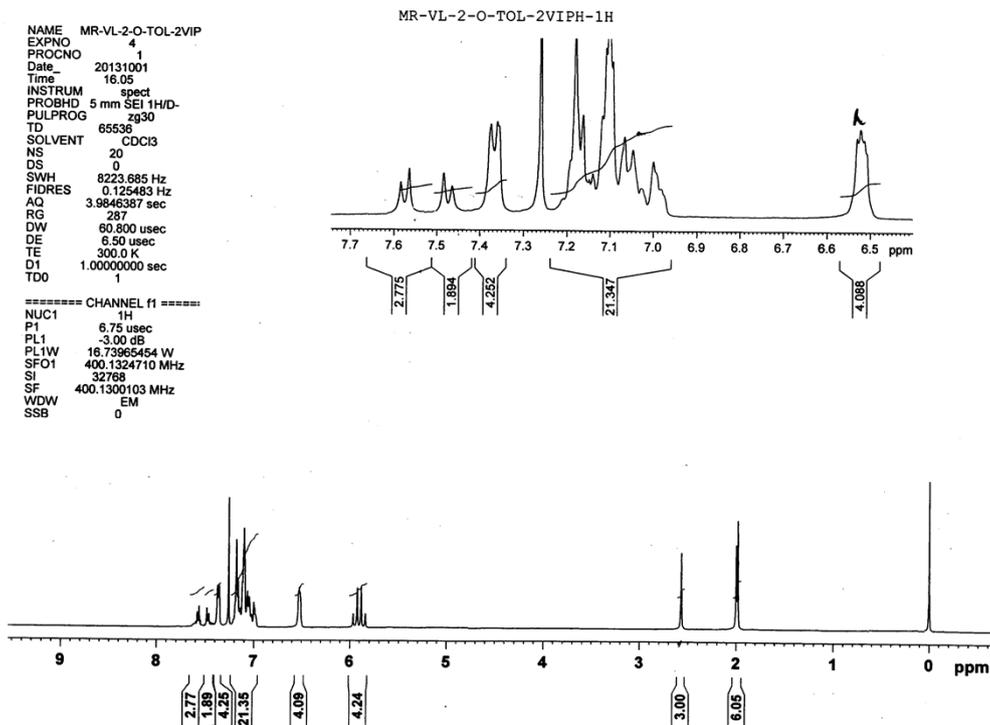


Figure S12: The ^1H NMR spectrum of compound **3** recorded in CDCl_3 .

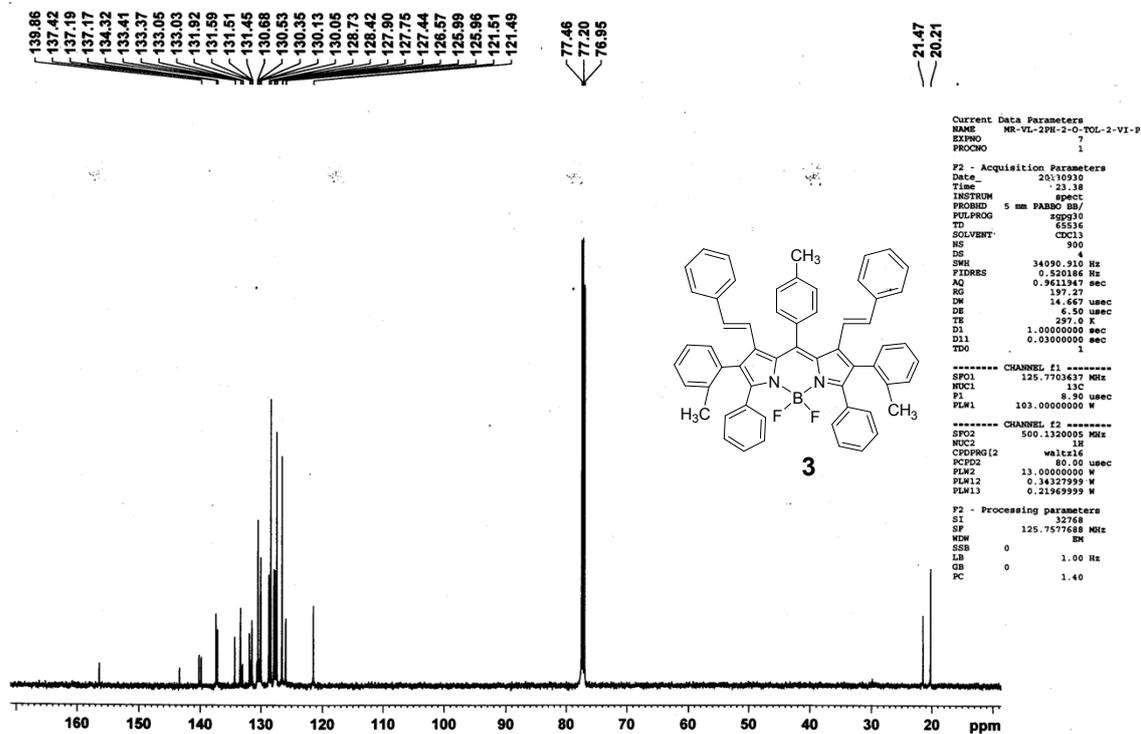


Figure S13: The ^{13}C NMR spectrum of compound **3** recorded in CDCl_3 .

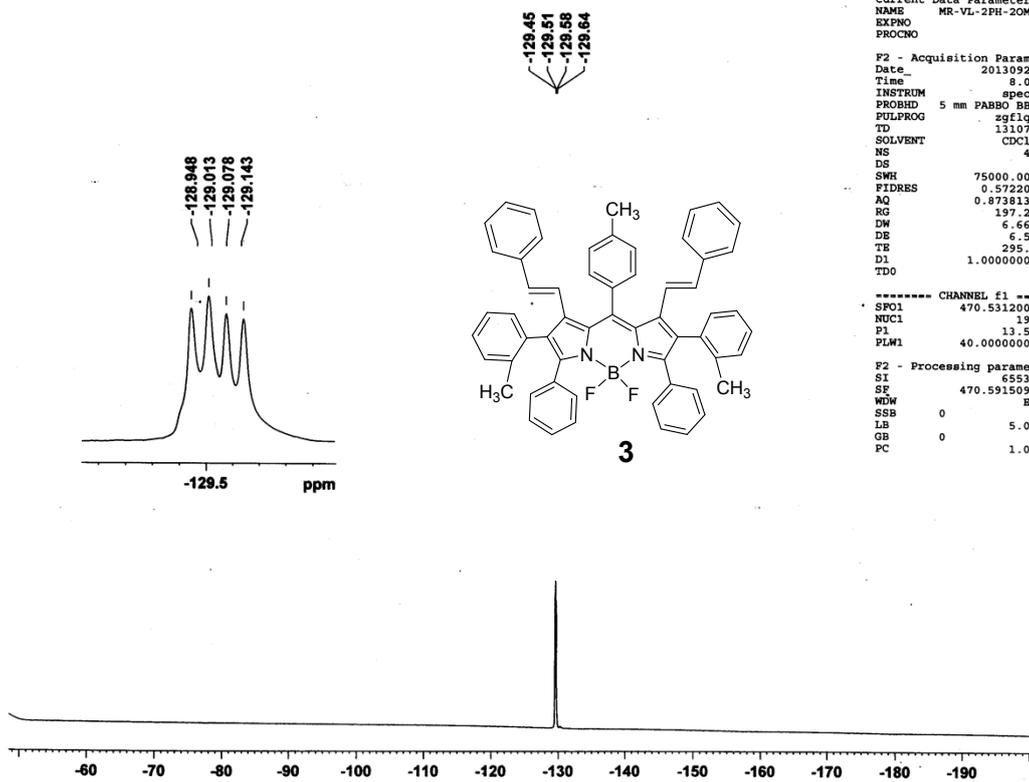


Figure S14: The ^{19}F NMR spectrum of compound **3** recorded in CDCl_3 .

MR-VL-2PH-2-O-TOL-2-ViPH-11B

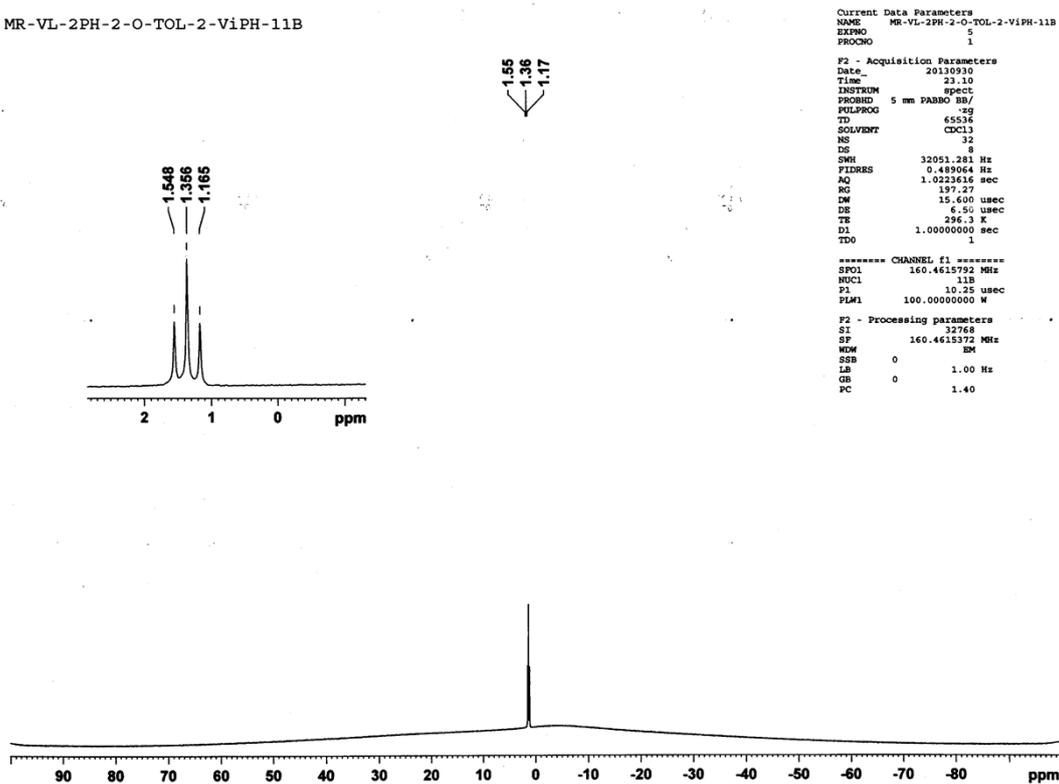
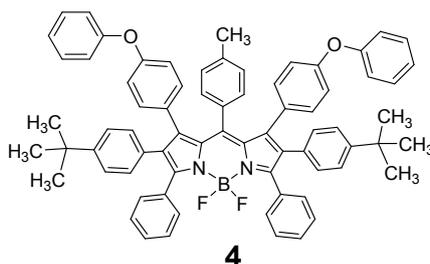


Figure S15: The ^{11}B NMR spectrum of compound **3** recorded in CDCl_3 .

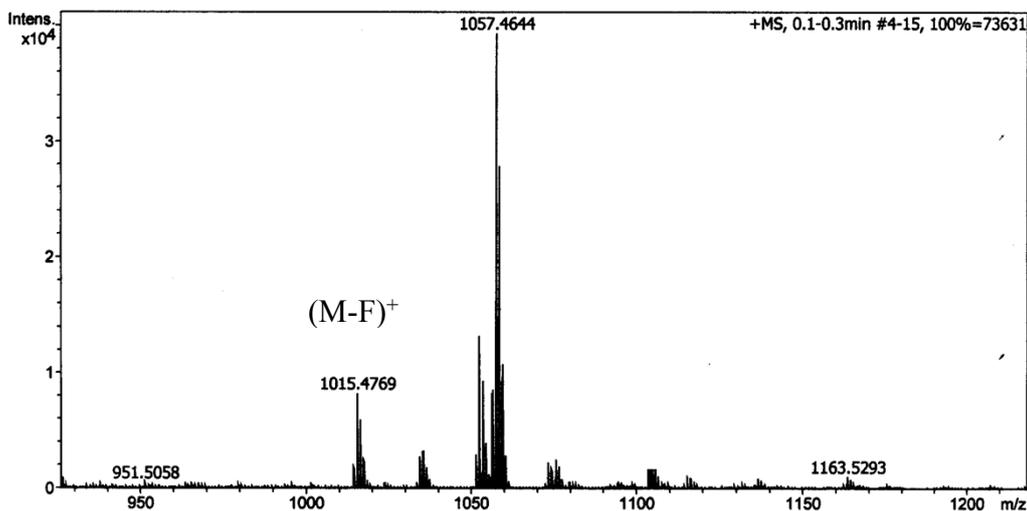


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Comment	C72H61BF2N2O2		

Acquisition Parameter

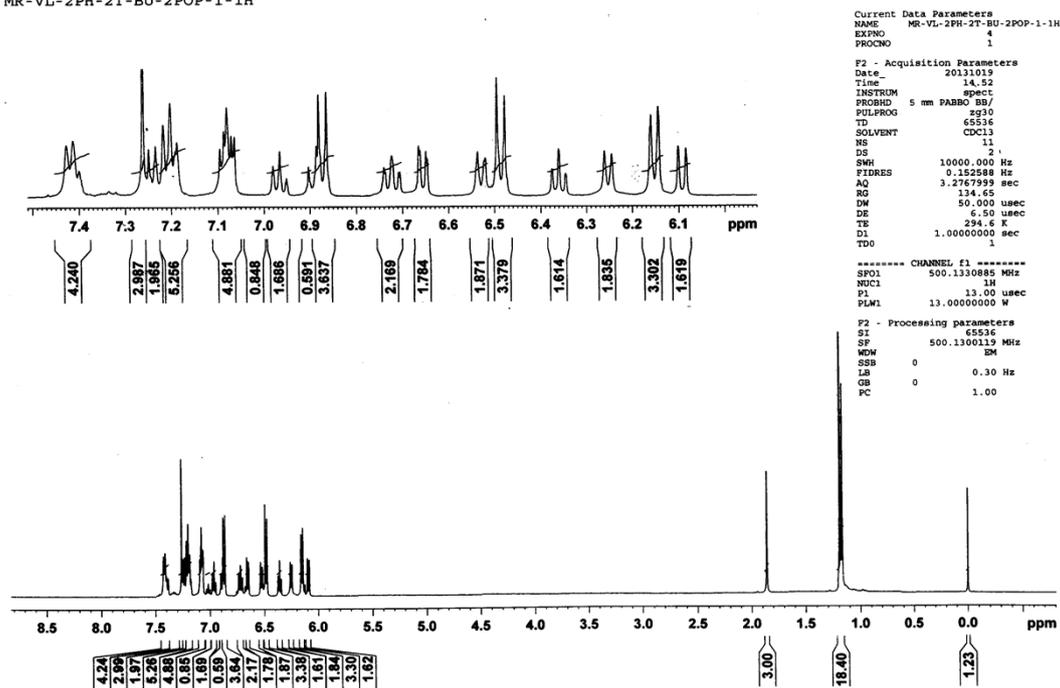
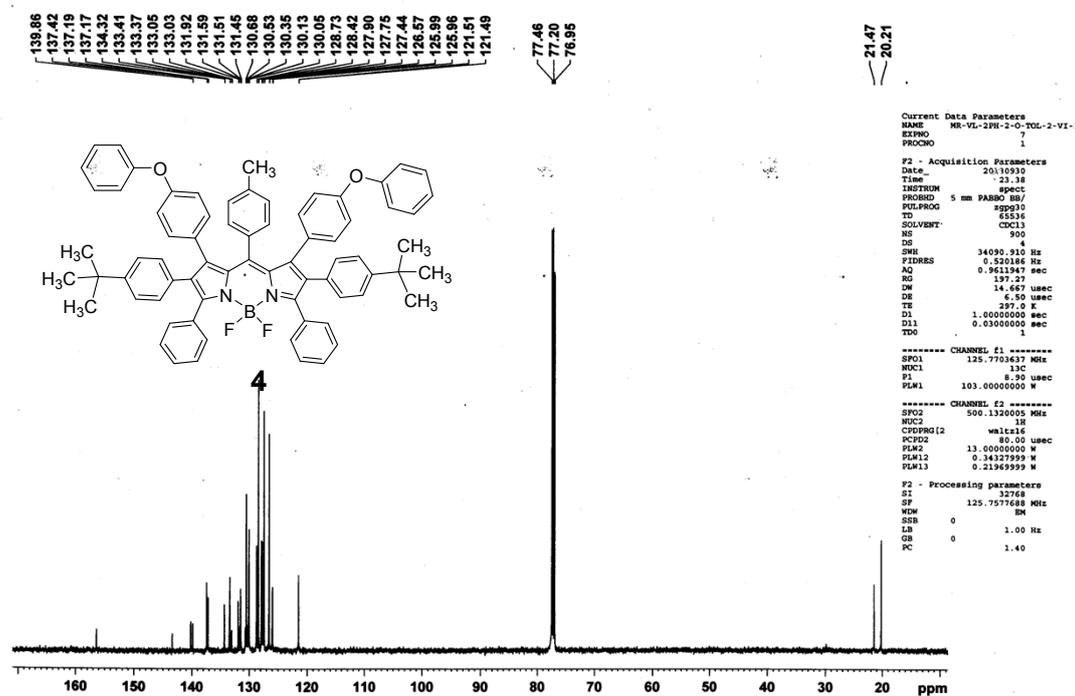
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Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
1057.4644	1	C72H61BF2N2NaO2	1057.4698	4.0	9.5	1	100.00	42.5	even	ok

Figure S16: The HRMS of compound 4.

MR-VL-2PH-2T-BU-2POP-1-1H

Figure S17: The ^1H NMR spectrum of compound **4** recorded in CDCl_3 .Figure S18: The ^{13}C NMR spectrum of compound **4** recorded in CDCl_3 .

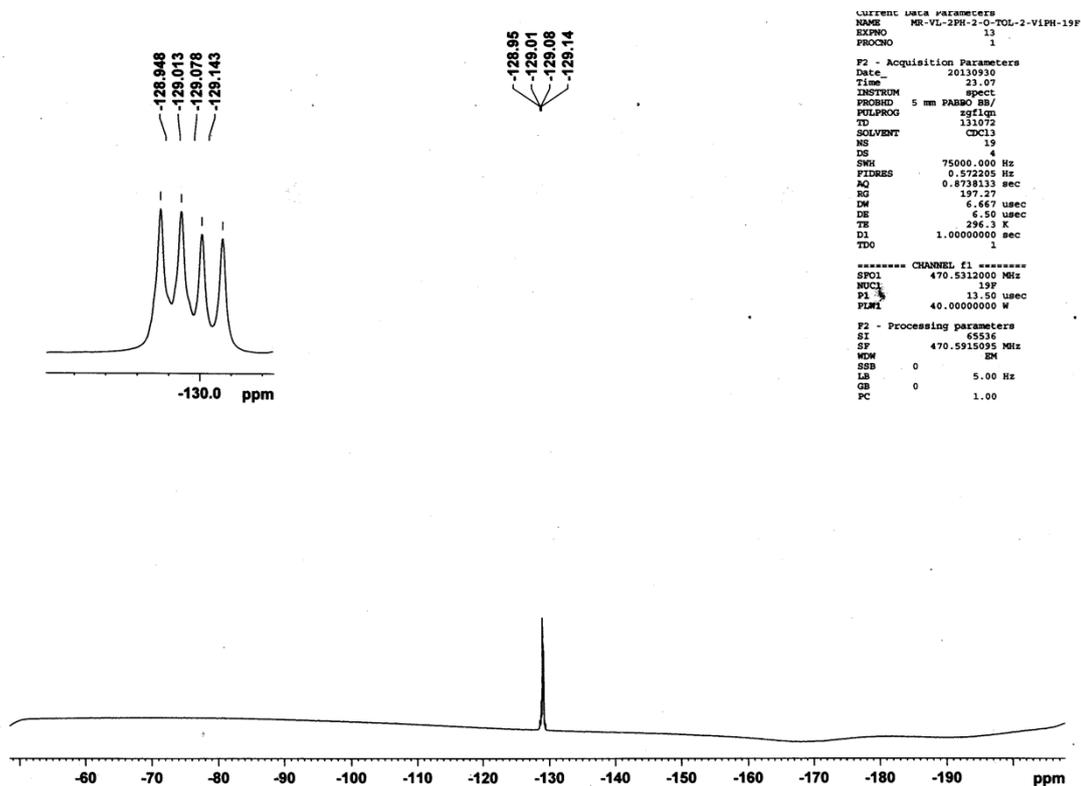


Figure S19: The ^{19}F NMR spectrum of compound **4** recorded in CDCl_3 .

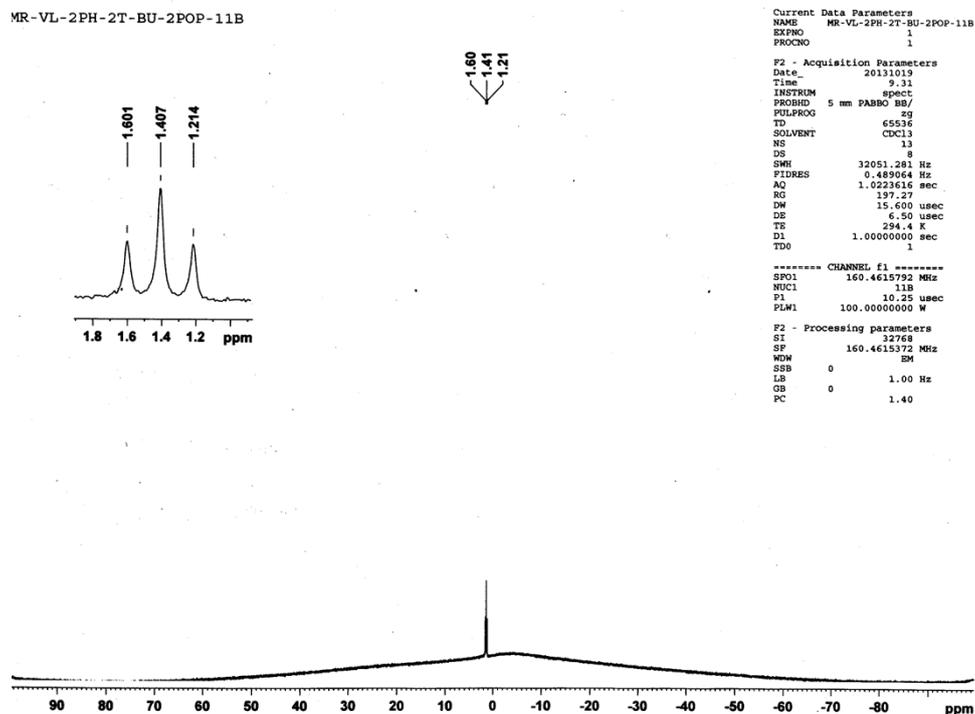
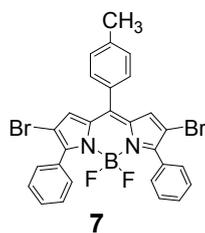


Figure S20: The ^{11}B NMR spectrum of compound **4** recorded in CDCl_3 .



Indian Institute of Technology (B)

Analysis Info

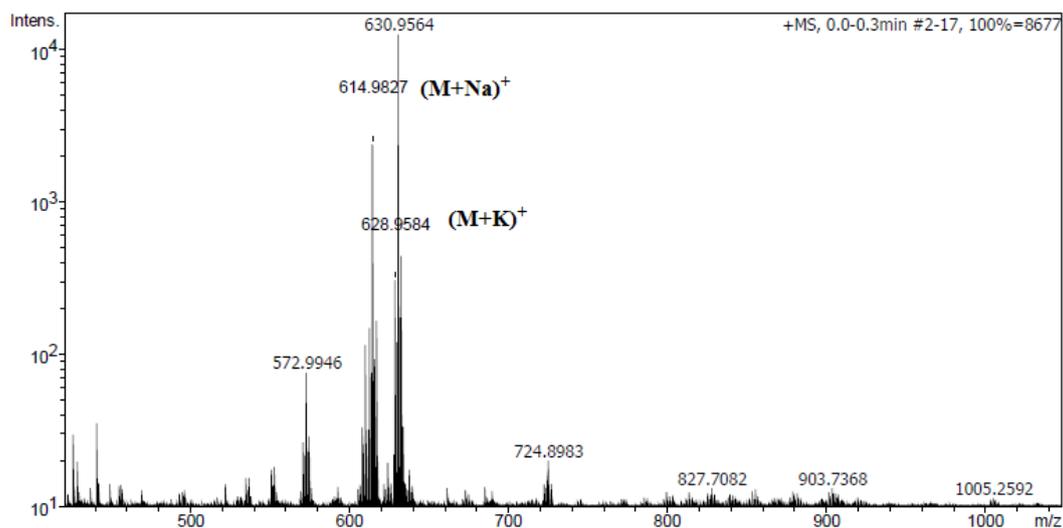
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 Method Tune_pos_Standard_NAI-1500.m
 Sample Name MRK-VL-2PH2BR-1
 Comment C28H19BBR2F2N2

Acquisition Date 9/10/2013 12:15:56 AM

Operator MRK-IN
 Instrument maXis impact 282001.00081

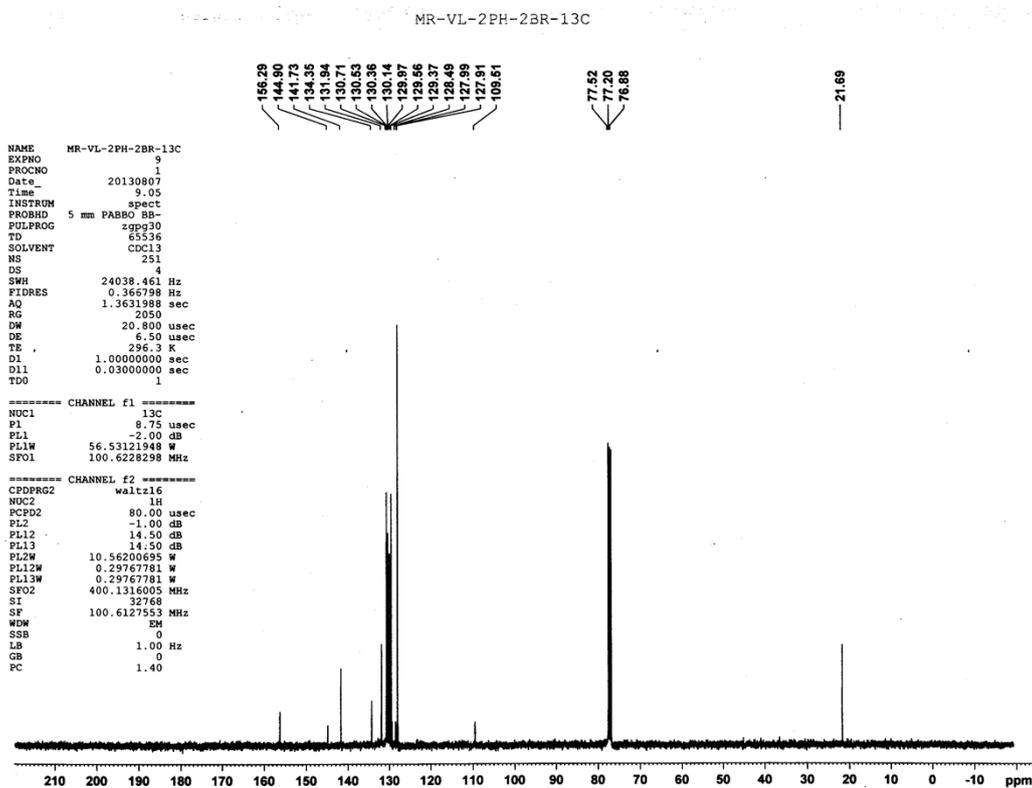
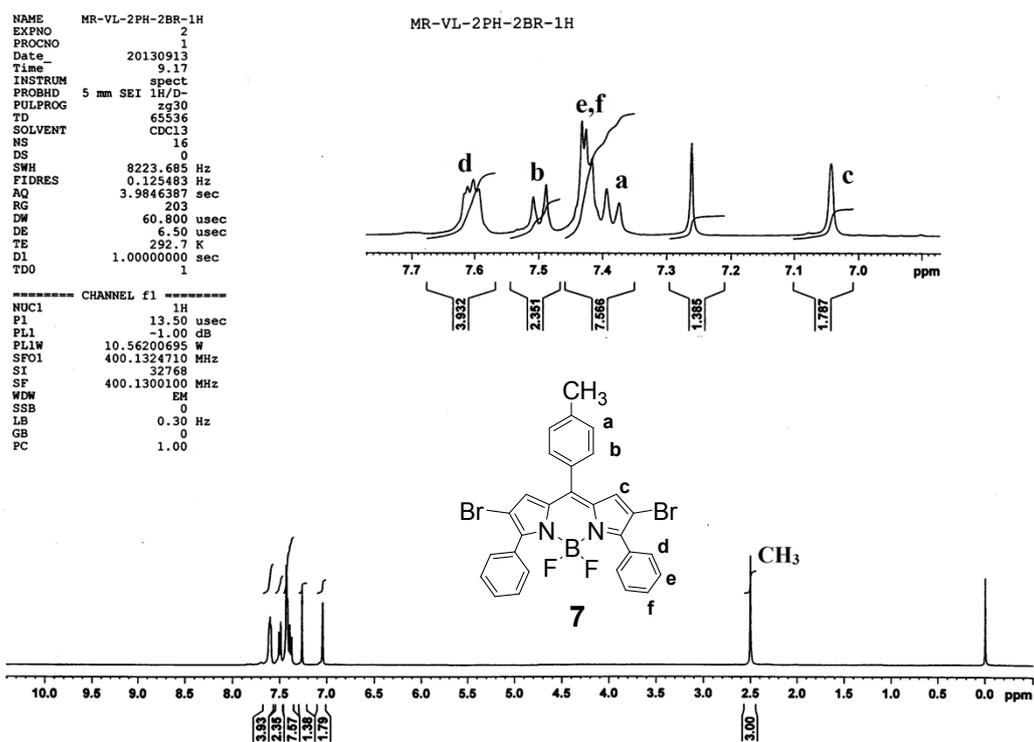
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Scan End	1500 m/z	Set Collision Cell RF	1000.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
628.9584	1	C28H19BBR2F2KN2	628.9613	-4.6	17.1	1	100.00	18.5	even	ok

Figure S21: The HRMS of compound **7**



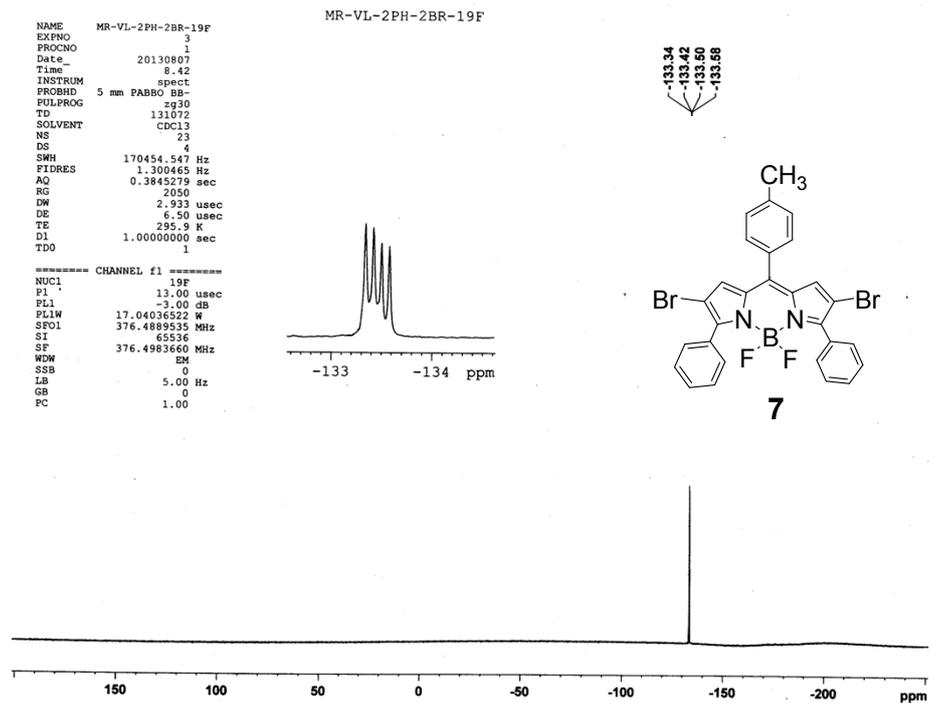


Figure S24: The ^{19}F NMR spectrum of compound 7 recorded in CDCl_3 .

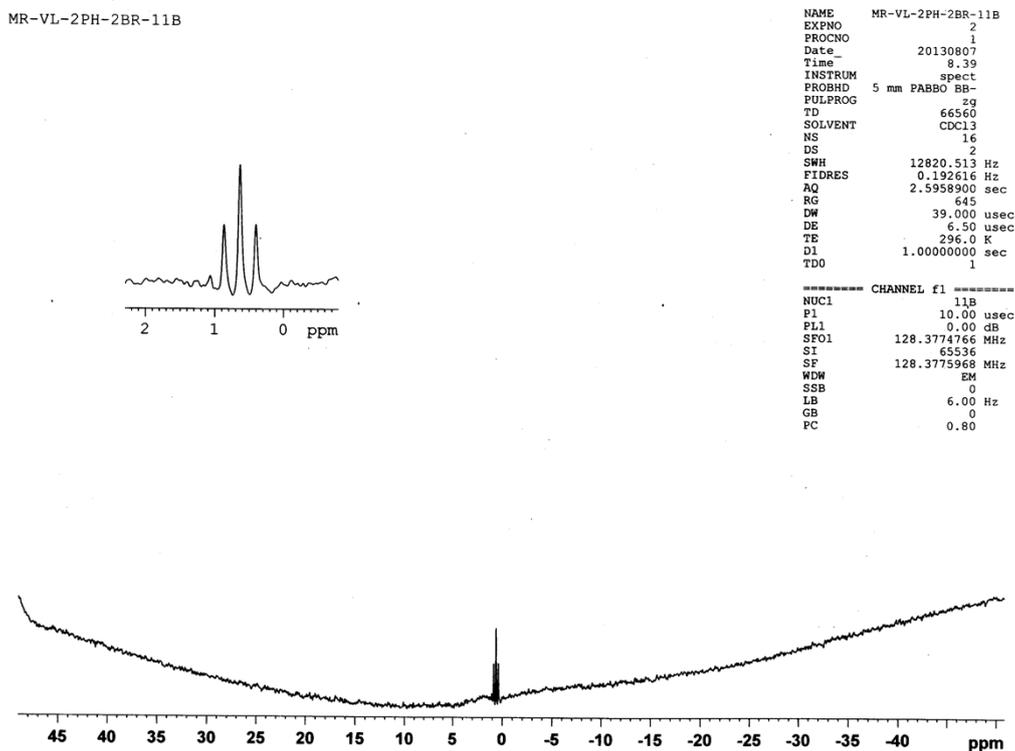
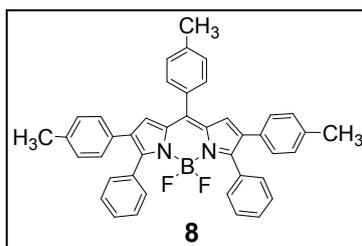


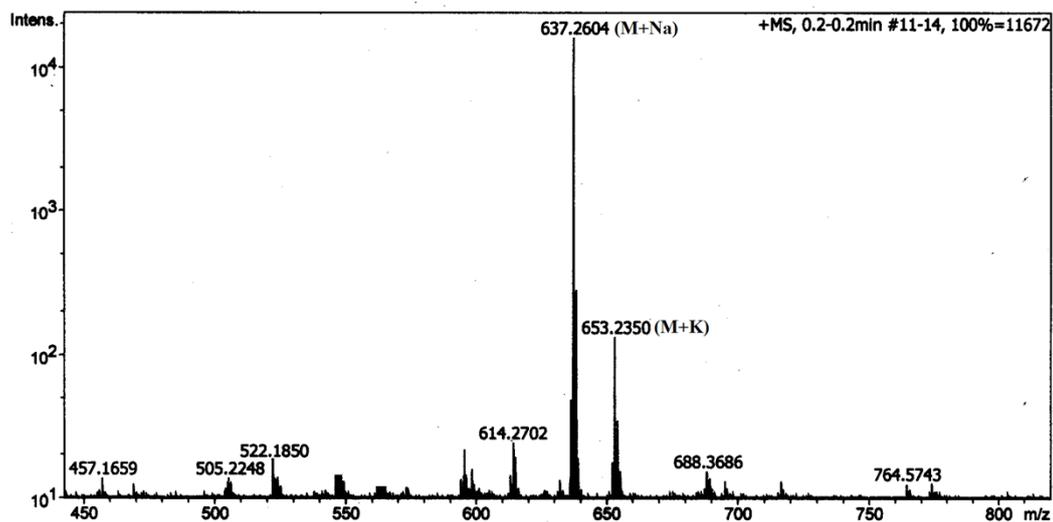
Figure S25: The ^{11}B NMR spectrum of compound 7 recorded in CDCl_3 .



Indian Institute of Technology (B)

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Sample Name	MR-VL-2PH-2TOL		
Comment	C42H33BF2N2		

Acquisition Parameter					
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Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
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Scan End	1000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	Score	m/z	err [mDa]	err [ppm]	mSigma	rdb	e ⁻ Conf	N-Rule	Adduct
637.260431	1	C42H33BF2N2Na	100.00	637.260423	-0.0	-0.0	8.4	26.5	even	ok	M+Na

Figure 26: The HRMS of compound 8.

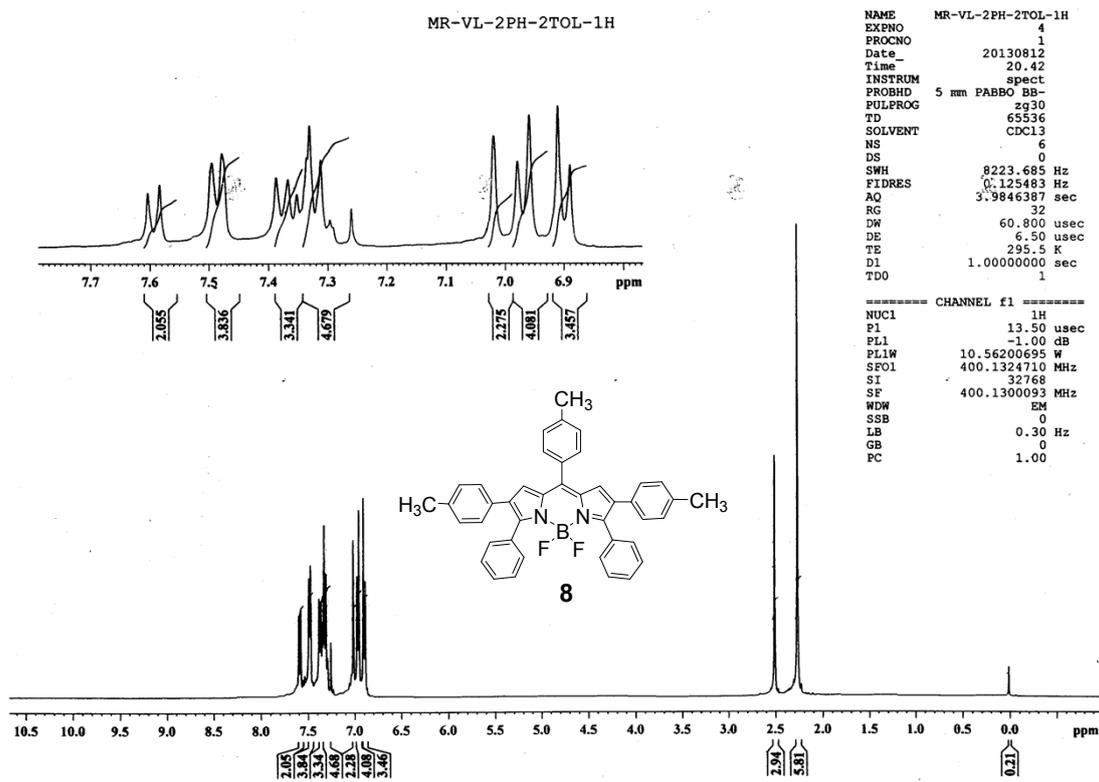


Figure S27: The ^1H NMR spectrum of compound **8** recorded in CDCl_3 .

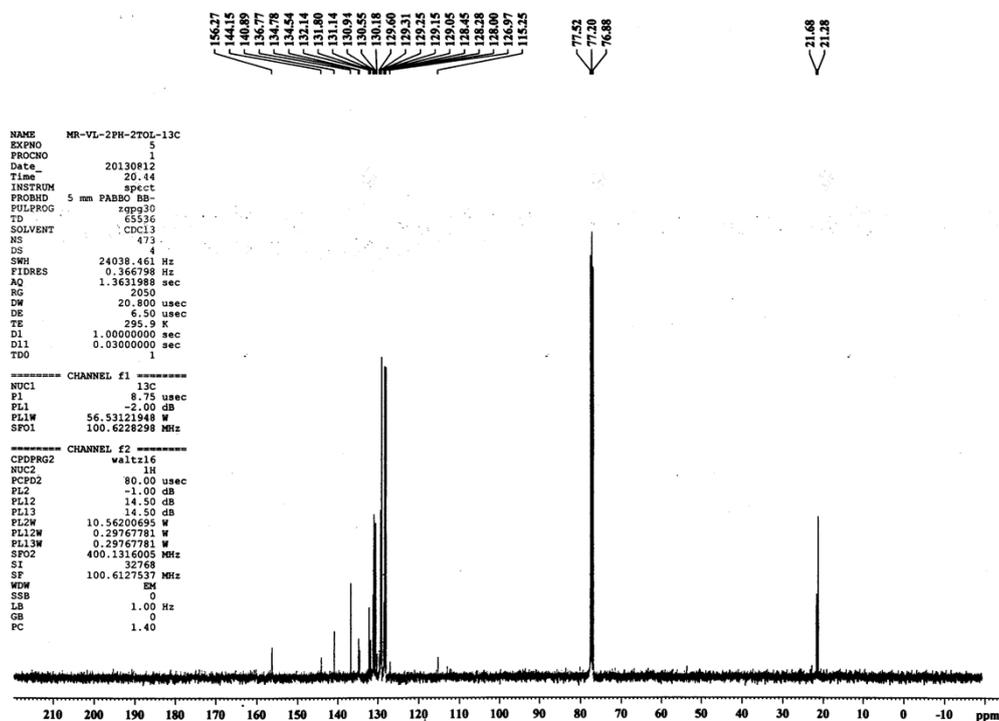
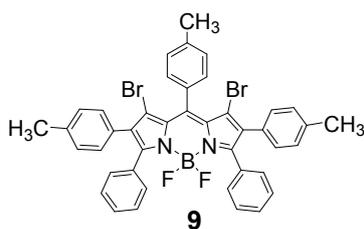


Figure S28: The ^{13}C NMR spectrum of compound **8** recorded in CDCl_3 .



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Analysis Info

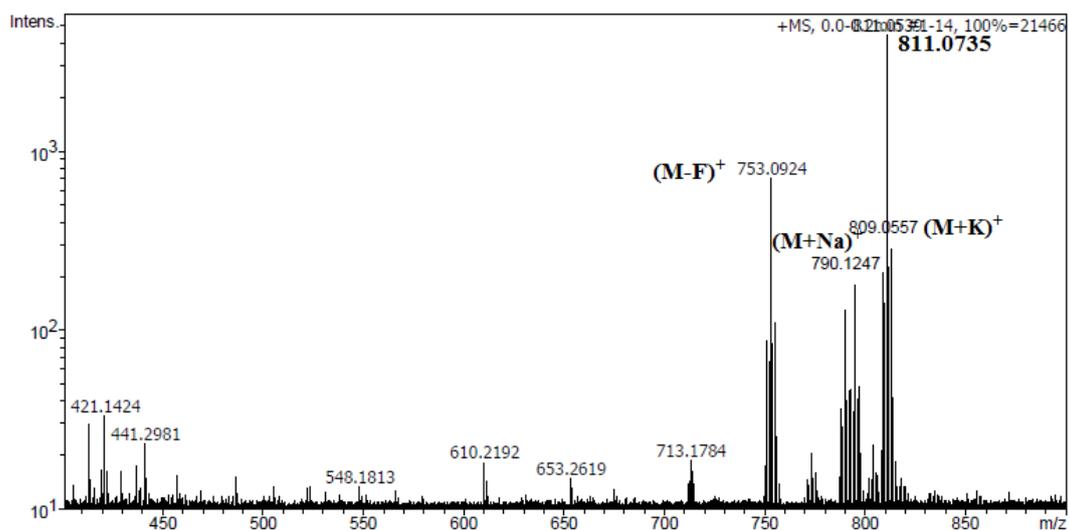
Analysis Name D:\Data\SEPT-13\MR-vl-2-PH-2TOL-2BR.d
 Method Tune_pos_Standard_NAI-1000.m
 Sample Name MR-vl-2-PH-2TOL-2BR
 Comment C42H31BBR2F2N2

Acquisition Date 9/12/2013 8:41:07 PM

Operator MR IN
 Instrument maXis impact 282001.00081

Acquisition Parameter

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Focus	Active	Set Capillary	3500 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	800.0 Vpp	Set Divert Valve	Source

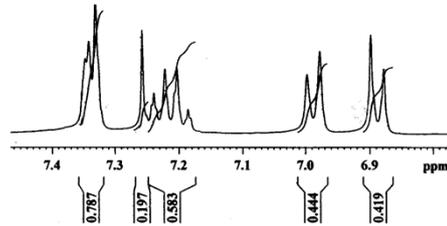


Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
809.0557	1	C42H31BBR2F2KN2	809.0554	0.3	24.6	1	100.00	26.5	even	ok

Figure S31: The HRMS of compound 9.

NAME MR-VL-2PH-2TOL-2BR-1H
 EXPNO 1
 PROCNO 1
 Date_ 20130814
 Time 8.17
 INSTRUM spect
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 PULPROG zg30
 TD 65536
 SOLVENT CDCl3
 NS 44
 DS 0
 SWH 8223.685 Hz
 FIDRES 0.125483 Hz
 AQ 3.9846387 sec
 RG 114
 DW 60.800 usec
 DE 6.50 usec
 TE 294.1 K
 D1 1.00000000 sec
 TDO 1

MR-VL-2PH-2TOL-2BR-1H



----- CHANNEL f1 -----
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 P1 13.50 usec
 PL1 -1.00 dB
 PL1W 10.5620095 W
 SFO1 400.1324710 MHz
 SI 32768
 SF 400.1300106 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

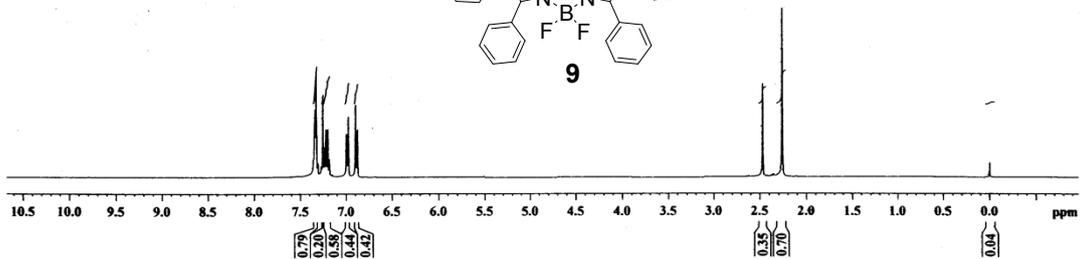
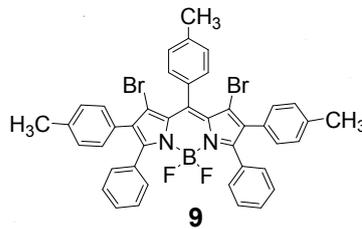


Figure S32: The ^1H NMR spectrum of compound **9** recorded in CDCl_3

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 PROCNO 1
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 Time 8.43
 INSTRUM spect
 PROBHD 5 mm PABBO BB-
 PULPROG zgpg30
 TD 65536
 SOLVENT CDCl3
 NS 1065
 DS 4
 SWH 24038.461 Hz
 FIDRES 0.366798 Hz
 AQ 1.3631988 sec
 RG 2050
 DW 20.800 usec
 DE 6.50 usec
 TE 294.8 K
 D1 1.00000000 sec
 D11 0.03000000 sec
 TDO 1

156.54
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 139.77
 136.18
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21.86
 21.45

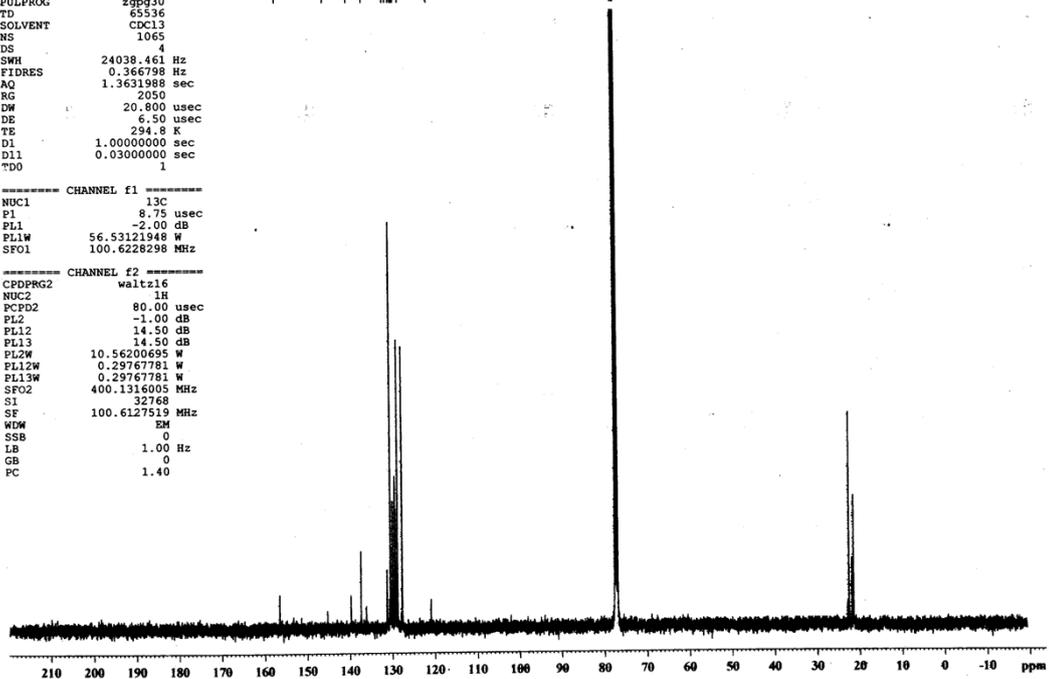


Figure S33: The ^{13}C NMR spectrum of compound **9** recorded in CDCl_3 .

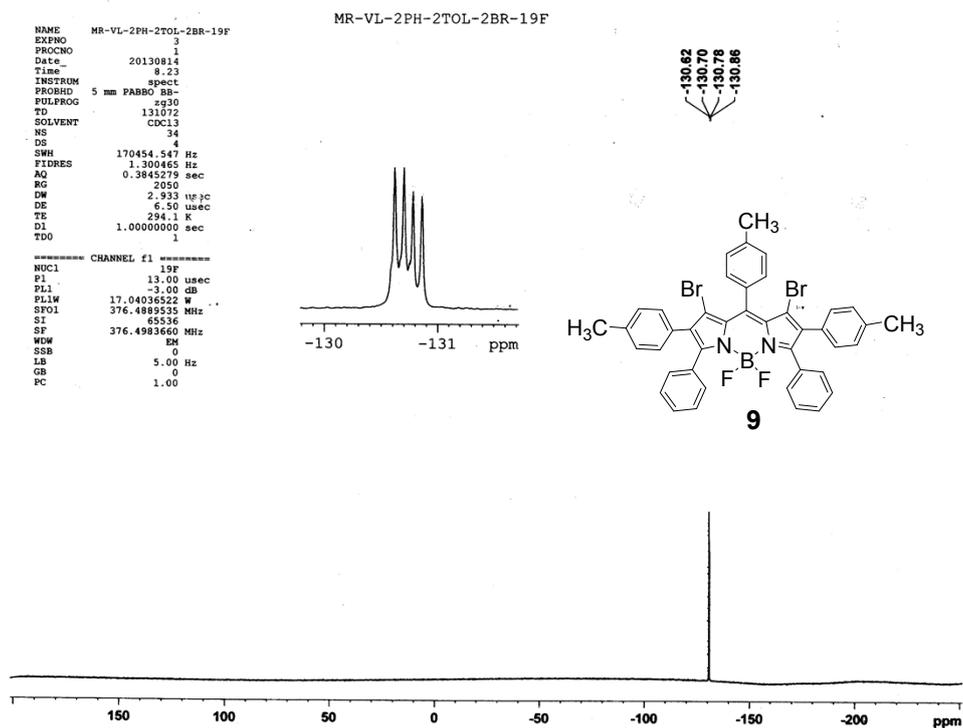


Figure S34: The ^{19}F NMR spectrum of compound **9** recorded in CDCl_3 .

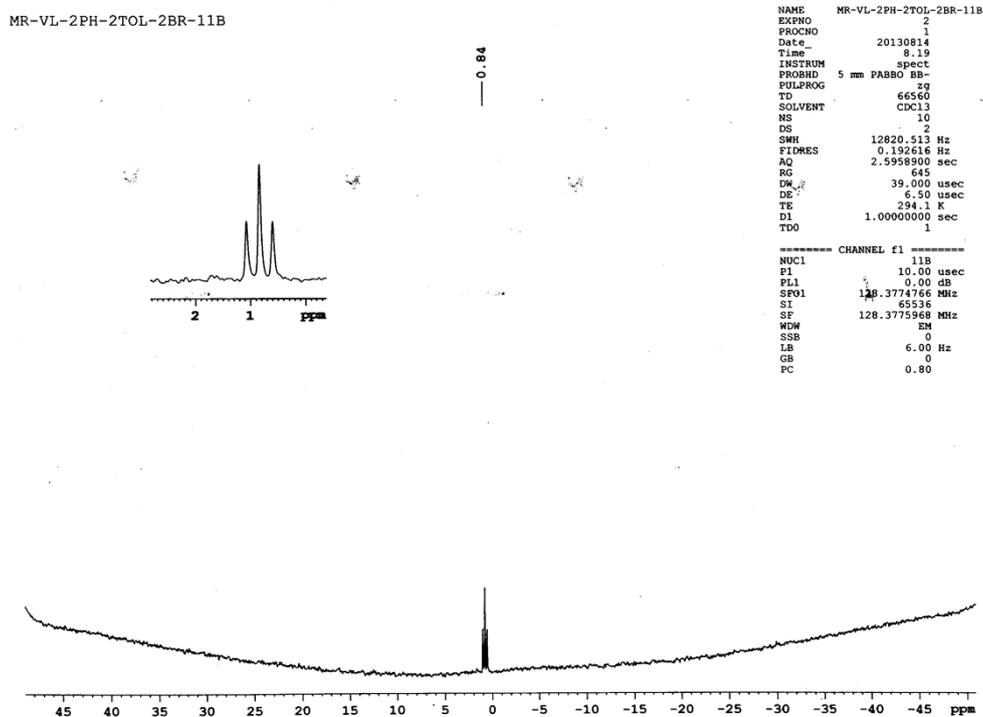
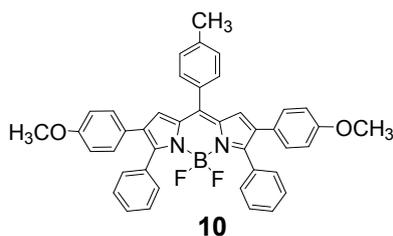


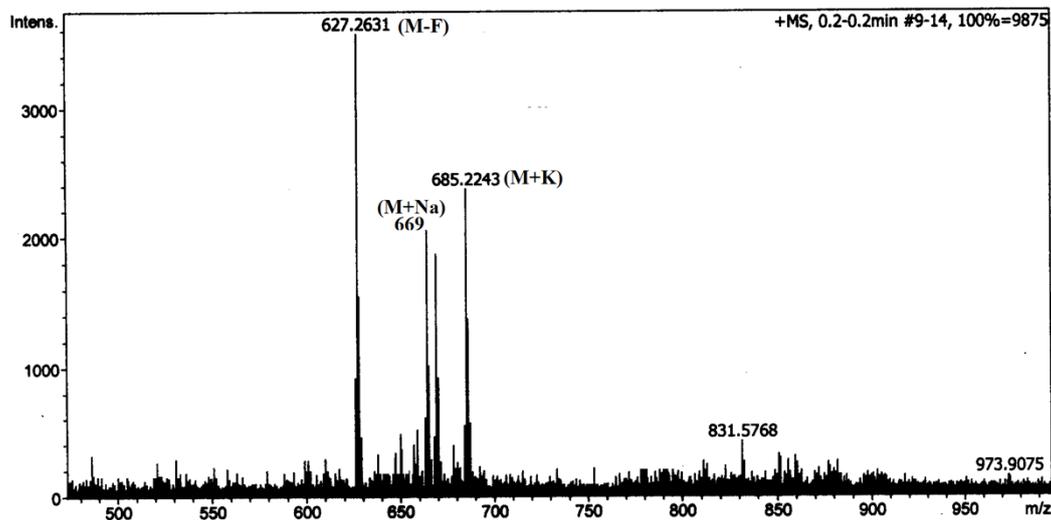
Figure S35: The ^{11}B NMR spectrum of compound **9** recorded in CDCl_3 .



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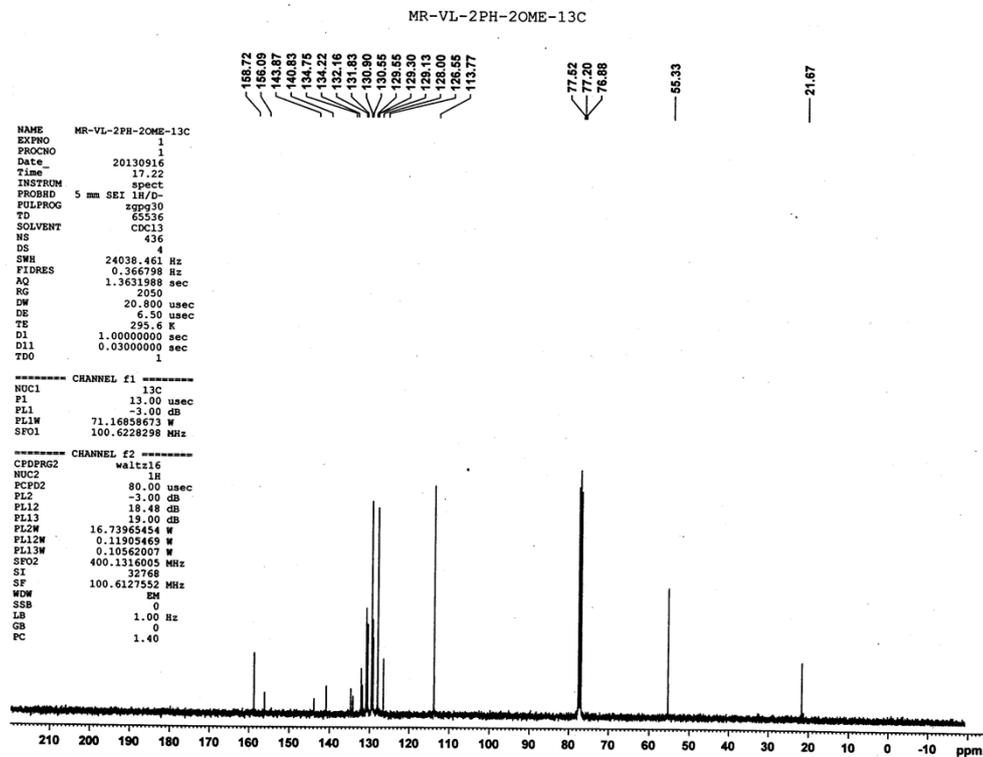
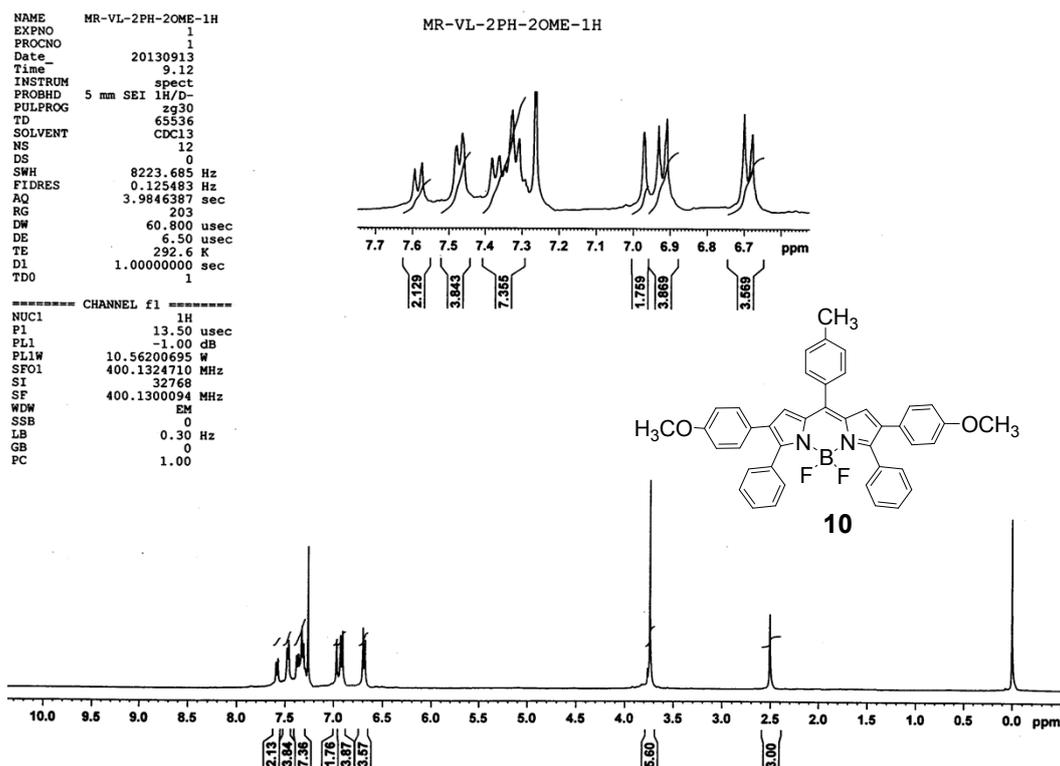
Analysis Info		Acquisition Date	9/12/2013 8:49:58 PM
Analysis Name	D:\Data\SEPT-13\MR-vi-2PH-2OME-2.d	Operator	MR IN
Method	Tune_pos_Standard_NAI-1000.m	Instrument	maXis impact 282001.00081
Sample Name	MR-vi-2PH-2OME-2		
Comment	C42H33BF2N2O2		

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 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	800.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
685.2243	1	C42H33BF2KN2O2	685.2242	0.1	58.3	1	100.00	26.5	even	ok

Figure S36: The HRMS of compound 10



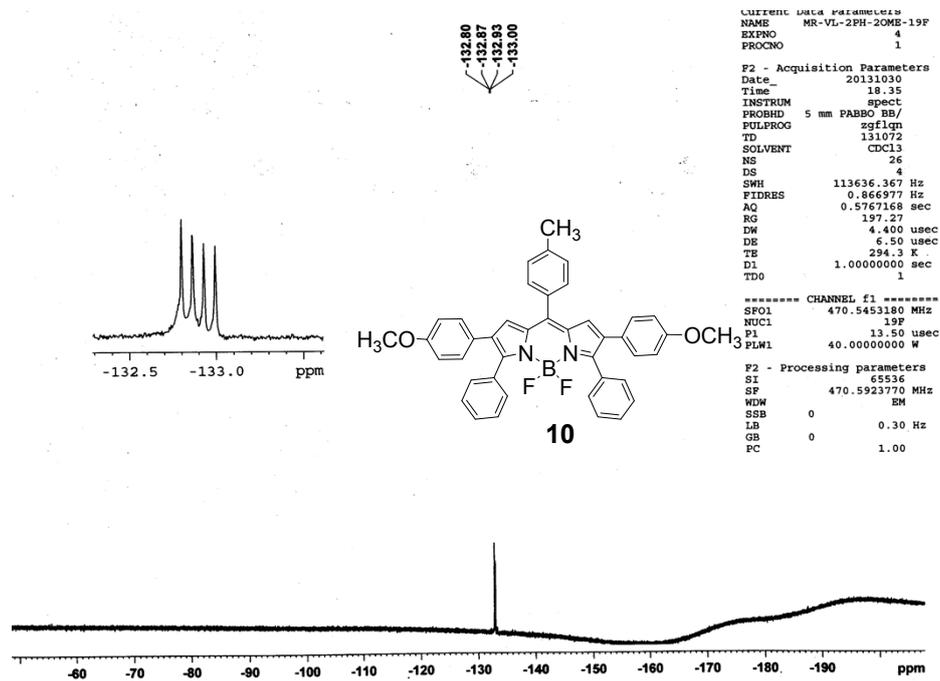


Figure S39: The ^{19}F NMR spectrum of compound **10** recorded in CDCl_3

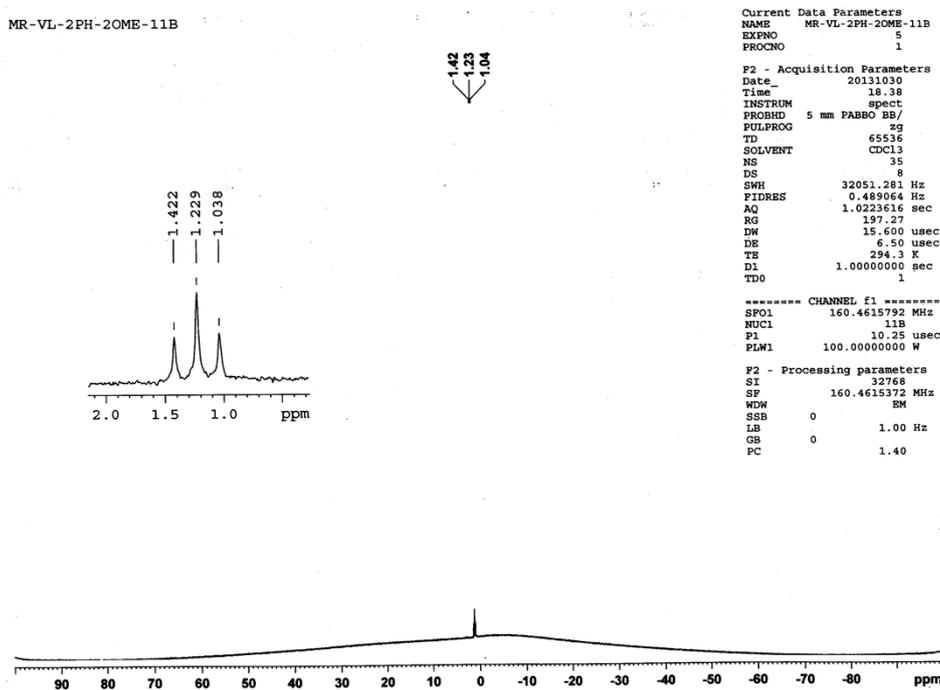
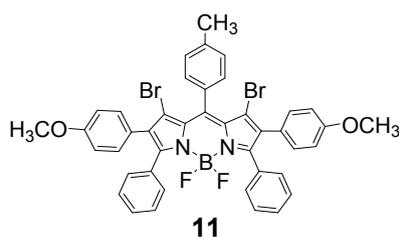


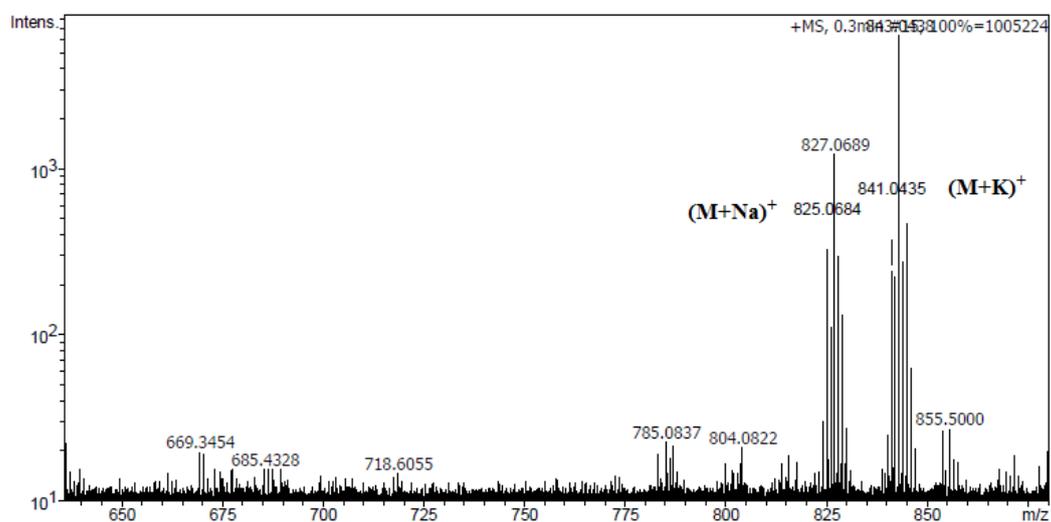
Figure S40: The ^{11}B NMR spectrum of compound **10** recorded in CDCl_3 .



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Analysis Info		Acquisition Date	
Analysis Name	D:\Data\SEPT-13\MR-VL-2OME-2BR-1.d	9/19/2013 8:23:35 PM	
Method	Tune_pos_Standard_NAI-1000.m	Operator	MR IN
Sample Name	MR-VL-2OME-2BR-1	Instrument	maXis impact 282001.00081
Comment	C42H31BBR2F2N2O2		

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 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	800.0 Vpp	Set Divert Valve	Source



Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
825.0684	1	C42H31BBR2F2N2NaO2	825.0713	-3.5	105.1	1	100.00	26.5	even	ok
841.0435	1	C42H31BBR2F2KN2O2	841.0452	-2.1	29.3	1	100.00	26.5	even	ok

Figure S41: The HRMS of compound 11

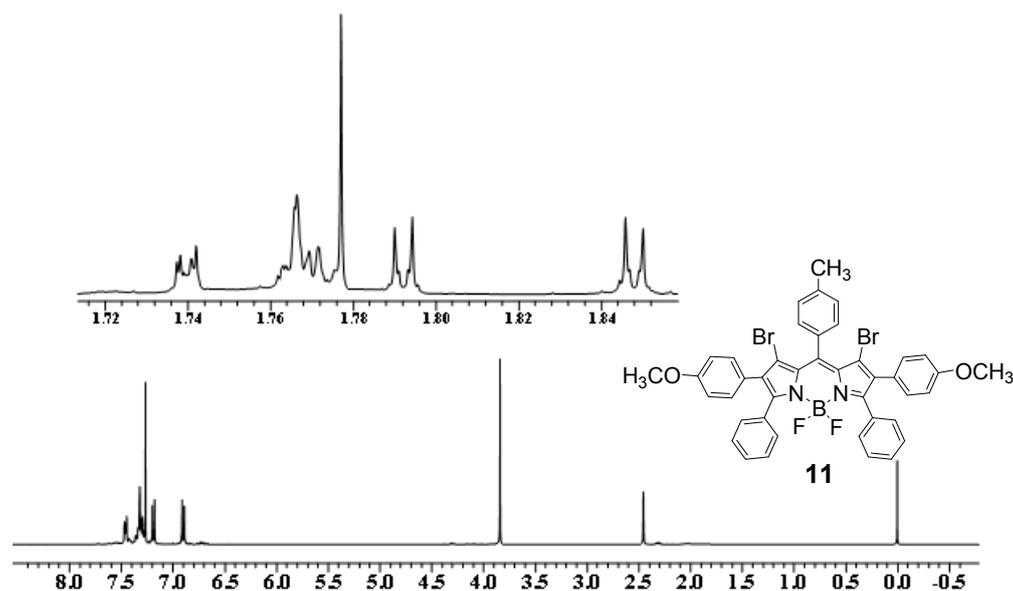


Figure S42: The ^1H NMR spectrum of compound **11** recorded in CDCl_3

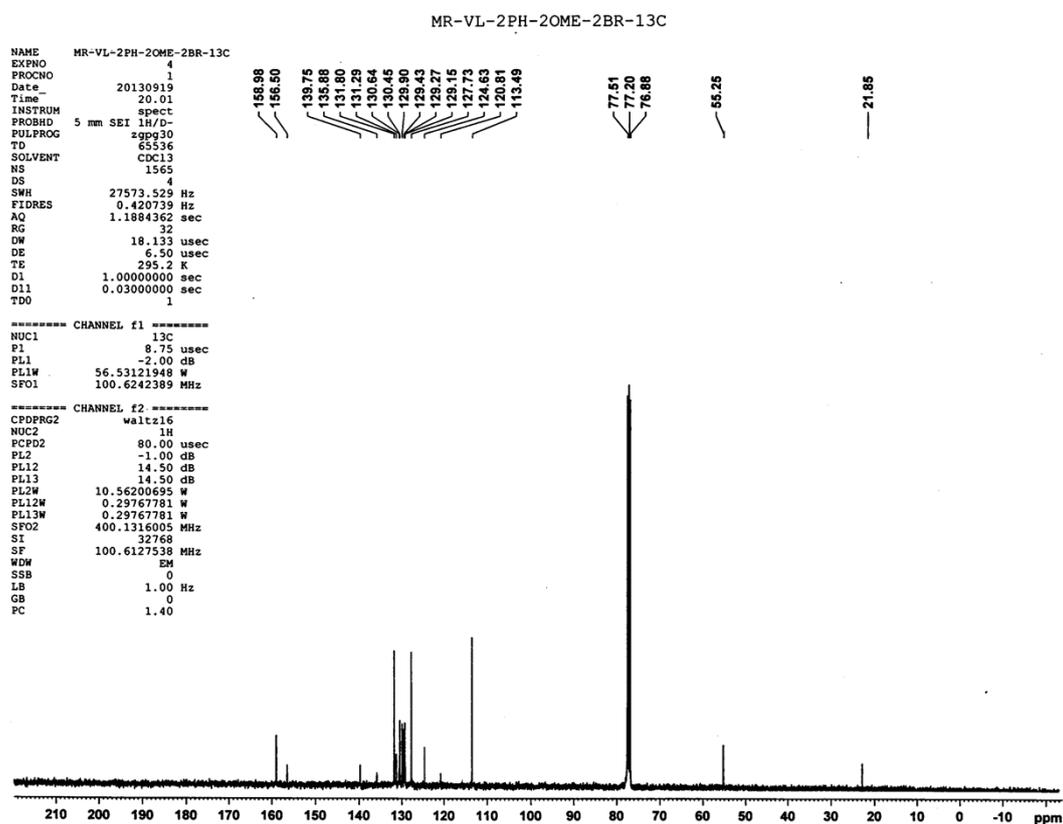
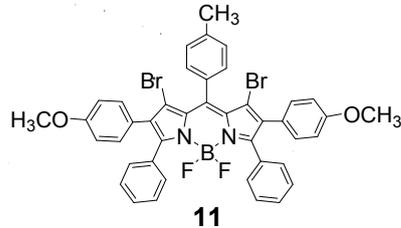
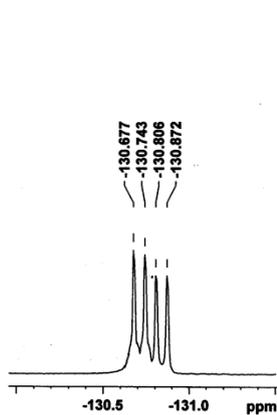


Figure S43: The ^{13}C NMR spectrum of compound **11** recorded in CDCl_3

mr-v1-2ome-2br-19f

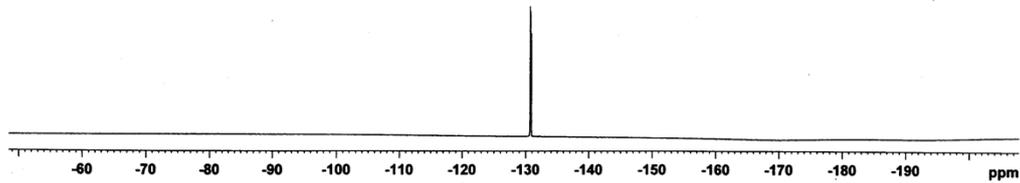


Current Data Parameters
 NAME mr-v1-2ome-2br-19f
 EXPNO 1
 PROCNO 1

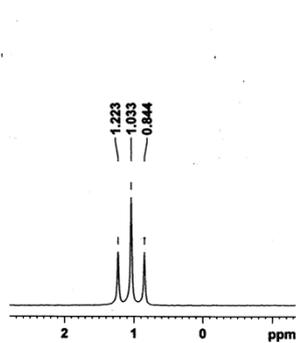
F2 - Acquisition Parameters
 Date_ 20130923
 Time 8.39
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zgfgqn
 TD 131072
 SOLVENT CDCl3
 NS 17
 DS 4
 SWH 113636.367 Hz
 FIDRES 0.866977 Hz
 AQ 0.5767168 sec
 RG 197.27
 DW 4.400 usec
 DE 6.50 usec
 TE 296.4 K
 D1 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 SF01 470.5453180 MHz
 NUC1 19F
 P1 13.50 usec
 PLW1 40.00000000 W

F2 - Processing parameters
 SI 65536
 SF 470.5923770 MHz
 WDW EM
 SSB 0
 LB 0.30 Hz
 GB 0
 PC 1.00

Figure S44: The ^{19}F NMR spectrum of compound **11** recorded in CDCl_3

mr-v1-2ome-2br-11B



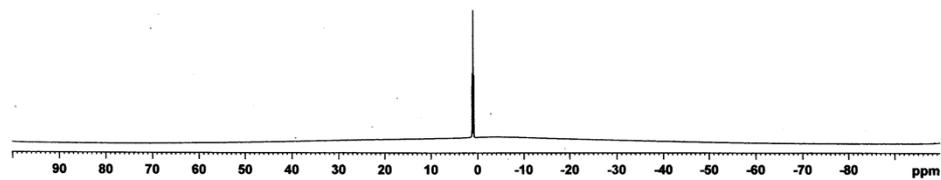
1.22
1.03
0.84

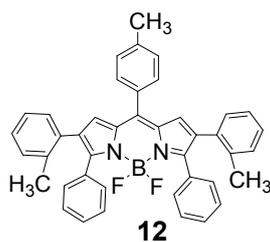
Current Data Parameters
 NAME mr-v1-2ome-2br-11B
 EXPNO 2
 PROCNO 1

F2 - Acquisition Parameters
 Date_ 20130923
 Time 8.42
 INSTRUM spect
 PROBHD 5 mm PABBO BB/
 PULPROG zg
 TD 65536
 SOLVENT CDCl3
 NS 15
 DS 8
 SWH 32051.281 Hz
 FIDRES 0.489064 Hz
 AQ 1.0223636 sec
 RG 197.27
 DW 15.600 usec
 DE 6.50 usec
 TE 296.4 K
 D1 1.00000000 sec
 TDO 1

----- CHANNEL f1 -----
 SF01 160.4615792 MHz
 NUC1 11B
 P1 10.25 usec
 PLW1 100.00000000 W

F2 - Processing parameters
 SI 32768
 SF 160.4615372 MHz
 WDW EM
 SSB 0
 LB 1.00 Hz
 GB 0
 PC 1.40

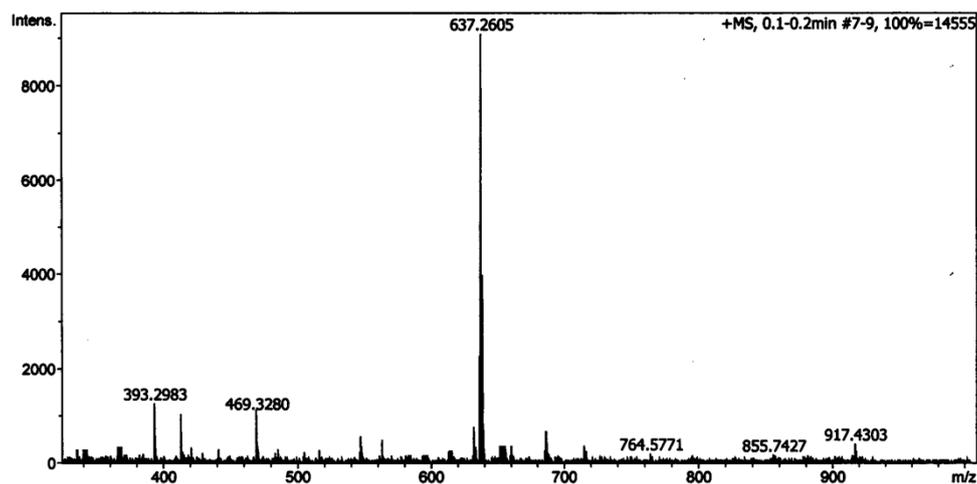
Figure S45: The ^{11}B NMR spectrum of compound **11** recorded in CDCl_3



Indian Institute of Technology (B)

Analysis Info		Acquisition Date	9/26/2013 7:50:52 PM
Analysis Name	D:\Data\SEPT-13\WR-VL-2PH-2-TOLYL.d	Operator	VKS OUT
Method	Tune_pos_Standard_NAI-1000.m	Instrument	maXis impact 282001.00081
Sample Name	MR-VL-2PH-2-TOLYL - <i>ortho</i>		
Comment	C42H33BF2N2		

Acquisition Parameter					
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 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
637.2605	1	C42H33BF2N2Na	637.2604	0.1	14.2	1	100.00	26.5	even	ok

Figure S46: The HRMS of compound 12.

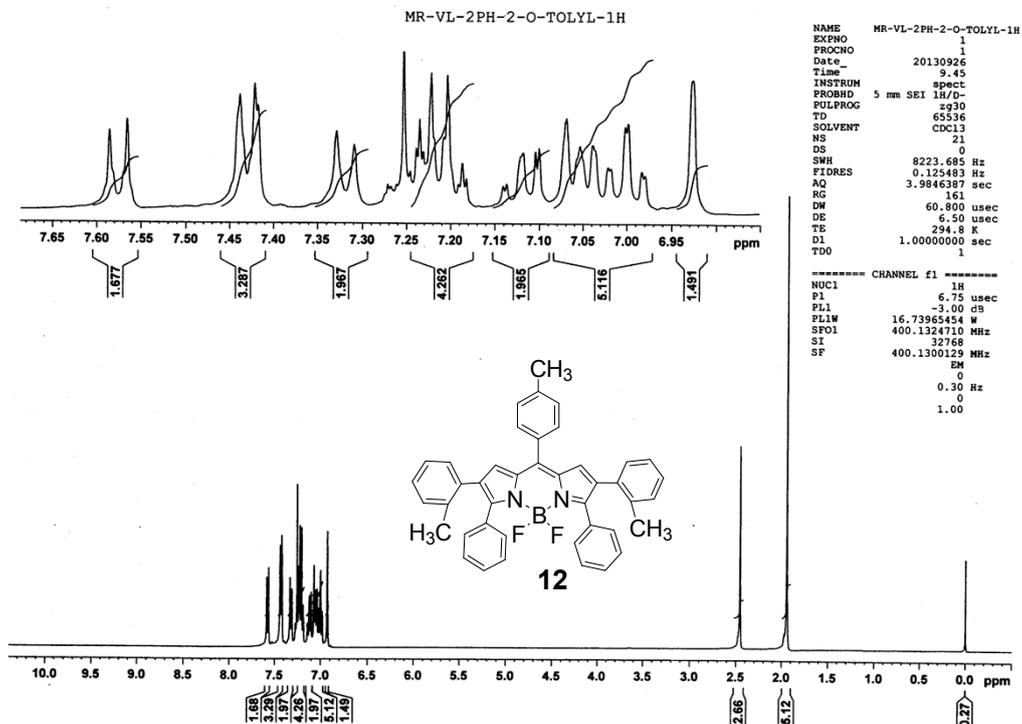


Figure S47: The ^1H NMR spectrum of compound **12** recorded in CDCl_3

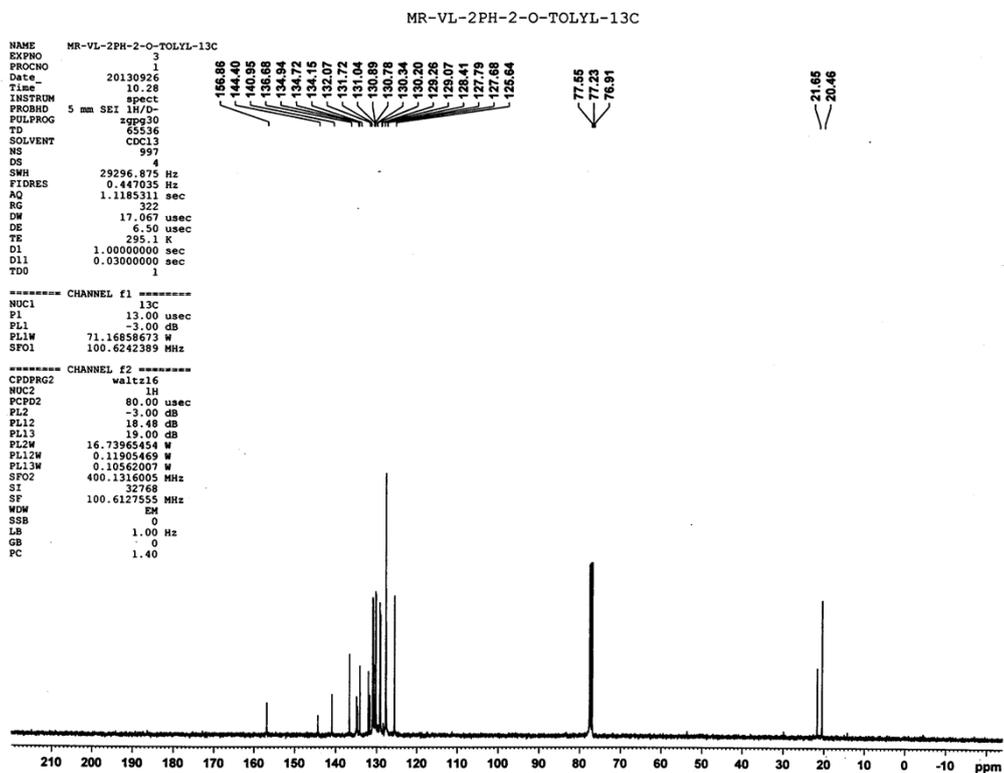


Figure S48: The ^{13}C NMR spectrum of compound **12** recorded in CDCl_3

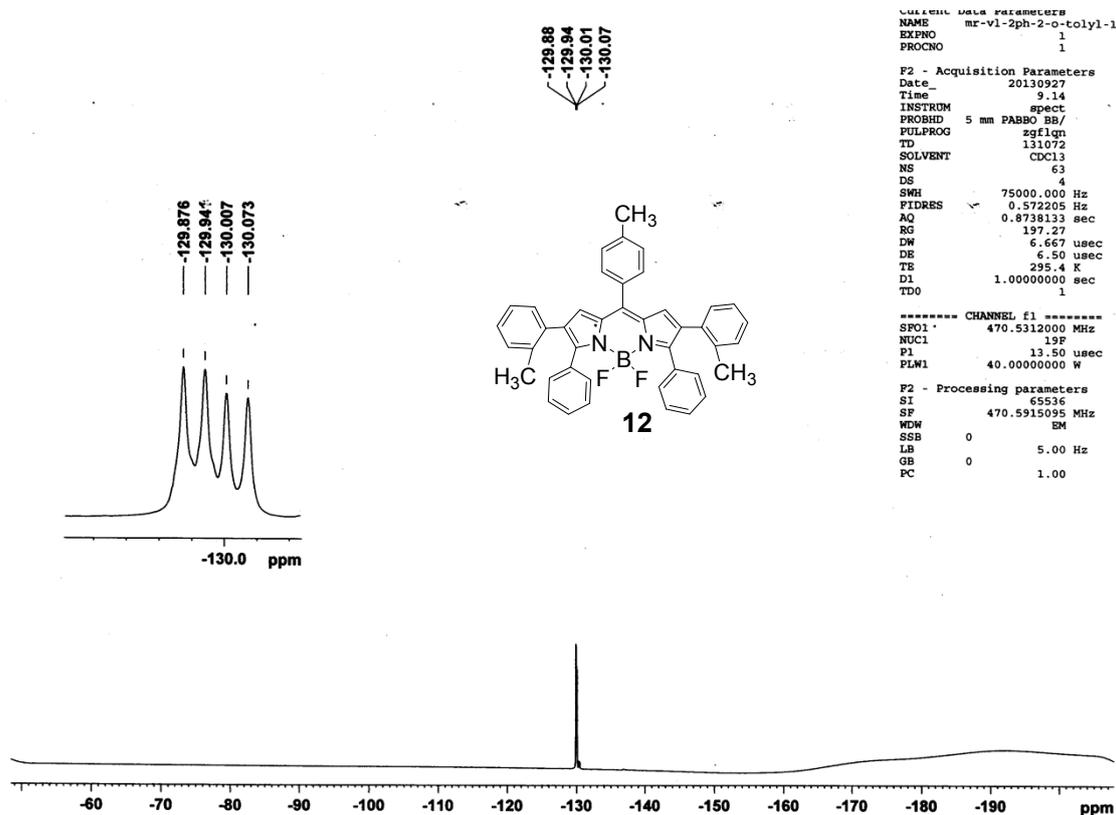


Figure S49: The ¹⁹F NMR spectrum of compound **12** recorded in CDCl₃

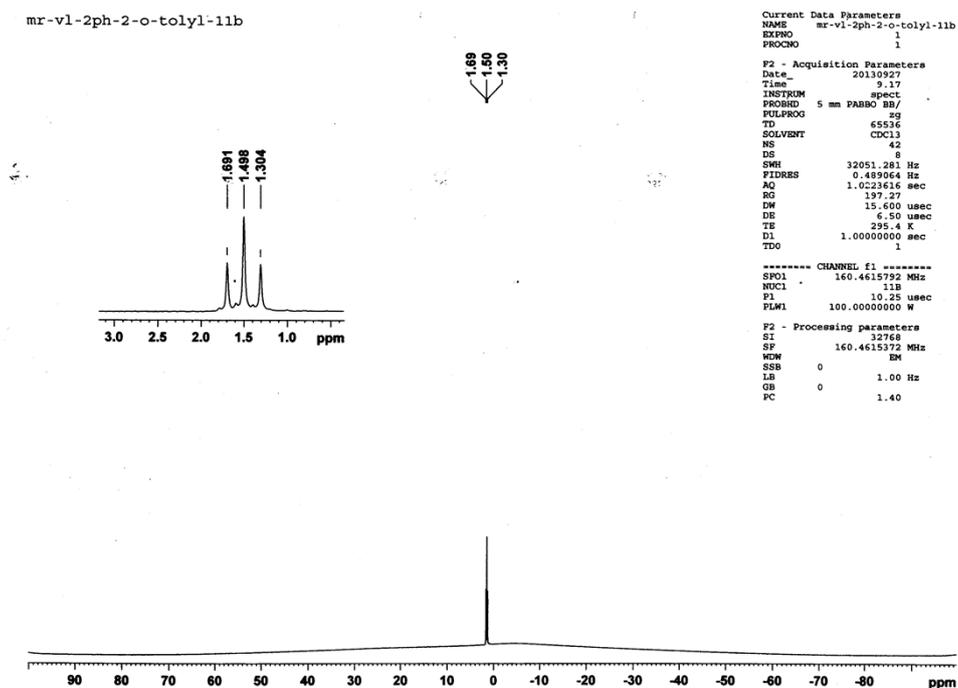
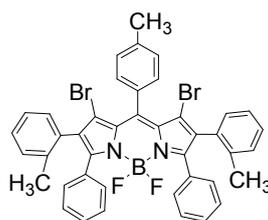


Figure S50: The ¹¹B NMR spectrum of compound **12** recorded in CDCl₃



13

 Indian Institute of Technology (B)

Analysis Info

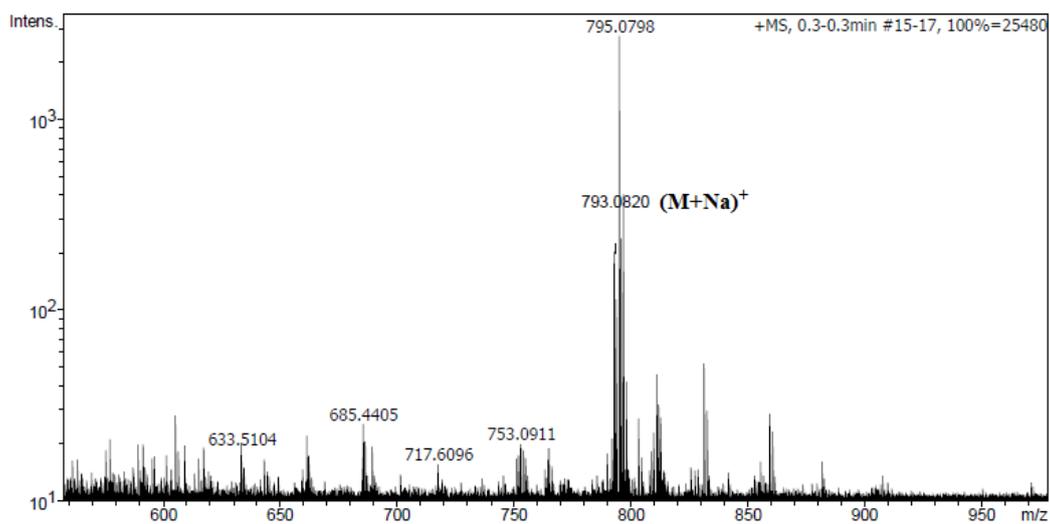
Analysis Name D:\Data\SEPT-13\MR-VL-2PH-2-O-TOL-2BR.d
 Method Tune_pos_Standard_NAI-1000.m
 Sample Name MR-VL-2PH-2-O-TOL-2BR
 Comment C42H31BBR2F2N2

Acquisition Date 9/30/2013 6:50:53 PM

Operator KPK- OUT
 Instrument maXis impact 282001.00081

Acquisition Parameter

Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 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
793.0820	1	C42H31BBR2F2N2Na	793.0814	-0.6	42.9	1	100.00	26.5	even	ok

Figure S51: The HRMS of compound 13.

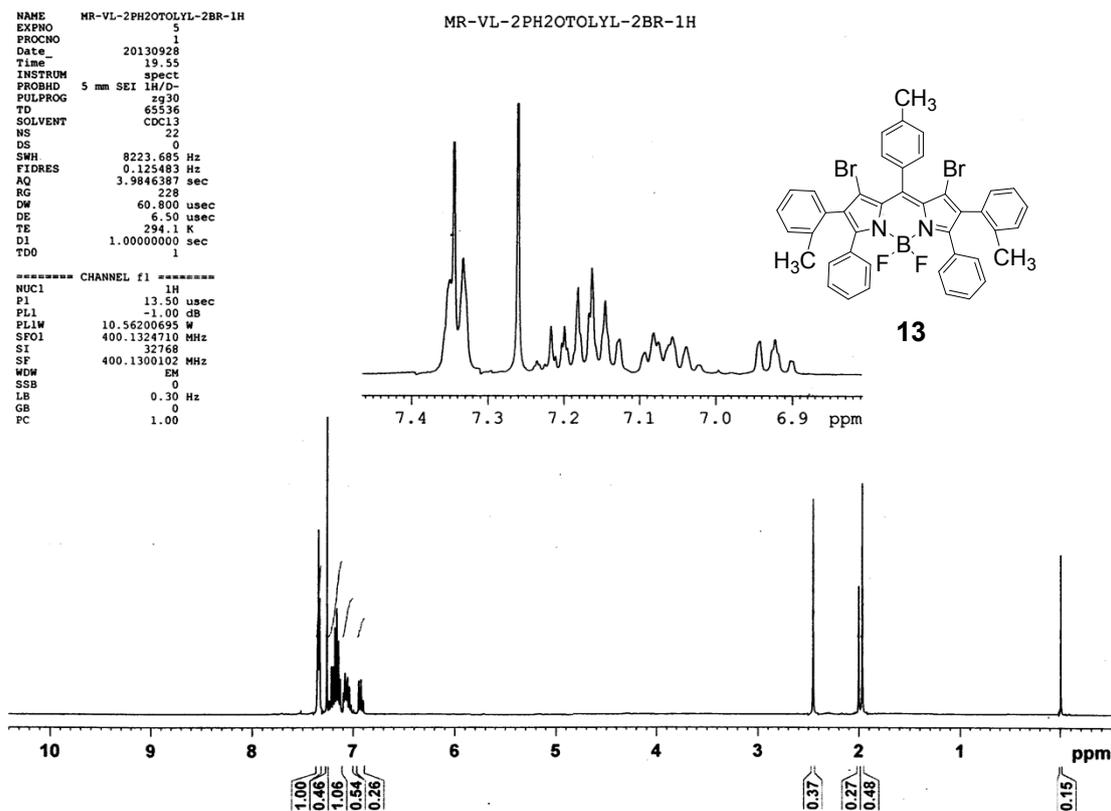


Figure S52: The ^1H NMR spectrum of compound **13** recorded in CDCl_3 .

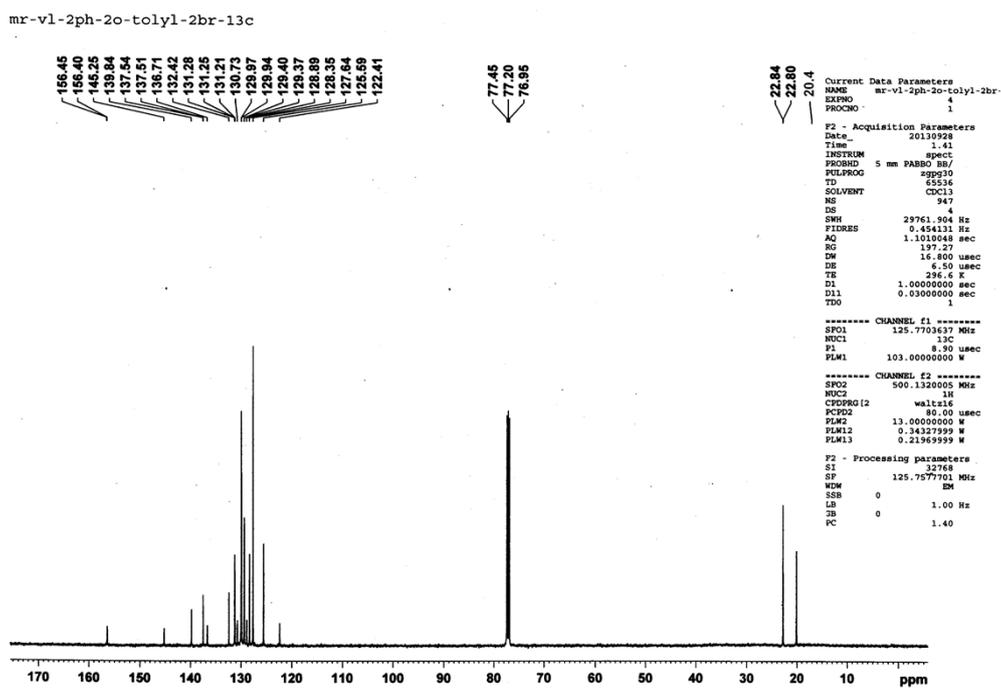


Figure S53: The ^{13}C NMR spectrum of compound **13** recorded in CDCl_3 .

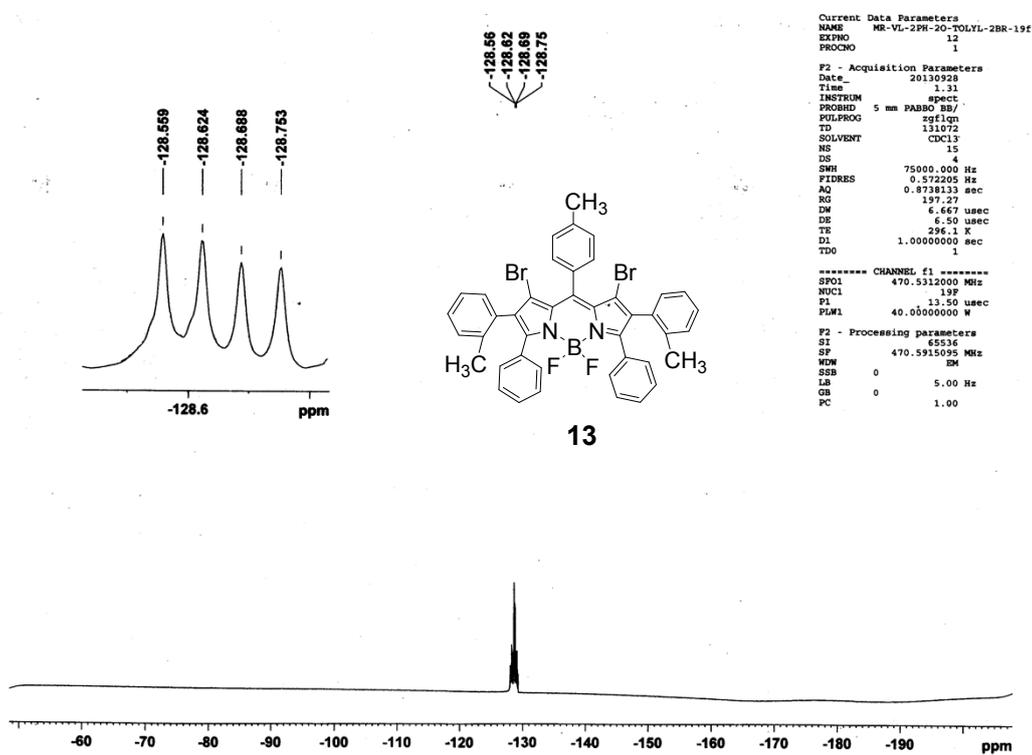


Figure S54: The ^{19}F NMR spectrum of compound **13** recorded in CDCl_3 .

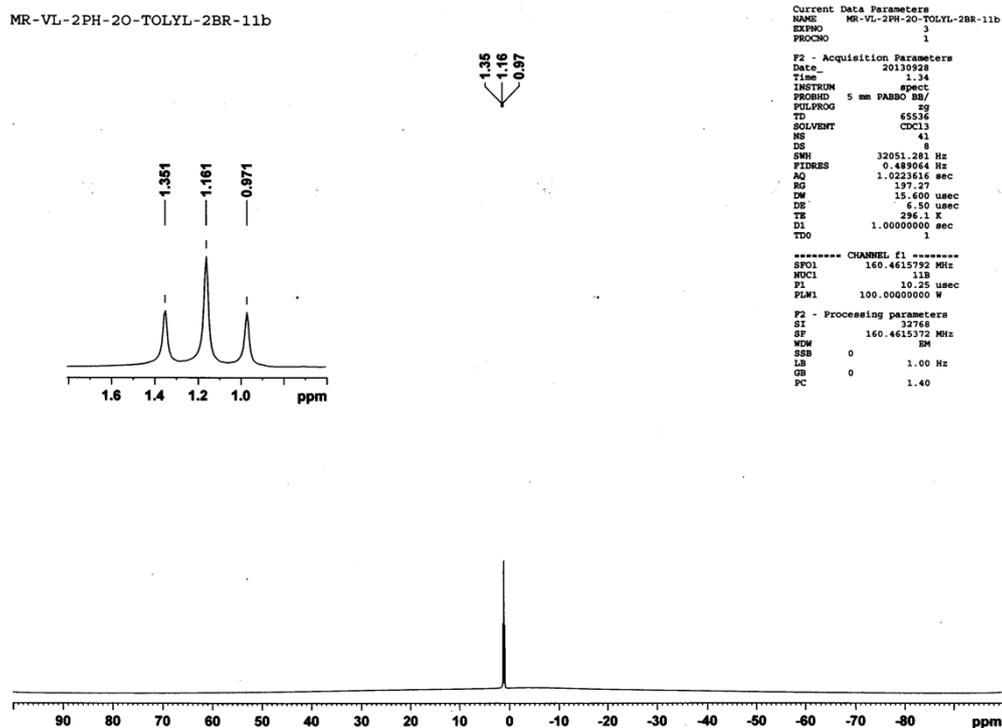
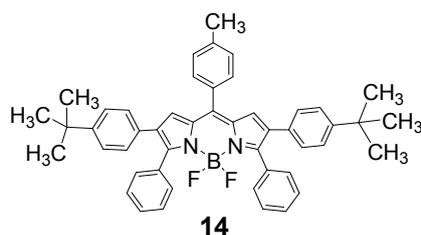


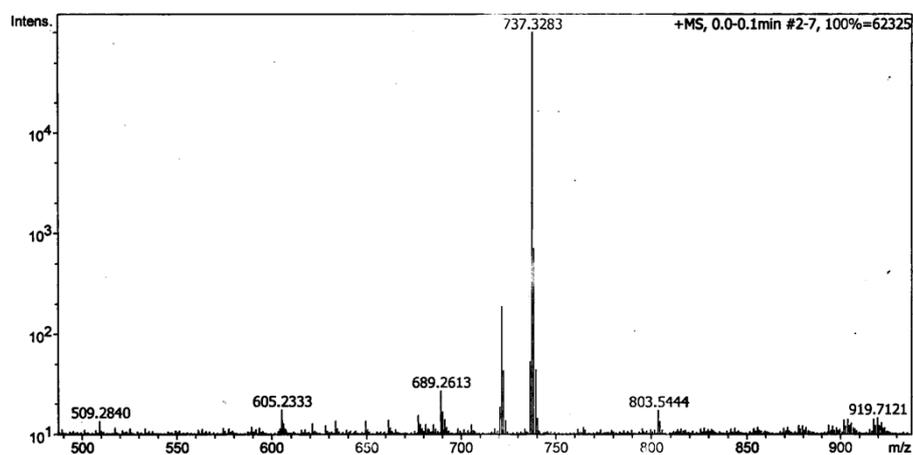
Figure S55: The ^{11}B NMR spectrum of compound **13** recorded in CDCl_3 .



Indian Institute of Technology (B)

Analysis Info		Acquisition Date	2/18/2014 11:05:41 PM
Analysis Name	D:\Data\FEB-2014\MR-VL-2PH2TBU.d	Operator	m-N
Method	Tune_pos_Standard_NAI-1000.m	Instrument	maXis impact 282001.00081
Sample Name	MR-VL-2PH2TBU		
Comment	C48H45BF2N2		

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	1000 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
737.3283	1	C48H45BF2KN2	737.3284	0.0	30.7	1	100.00	25.5	even	ok

Figure S56: The HRMS of compound 14.

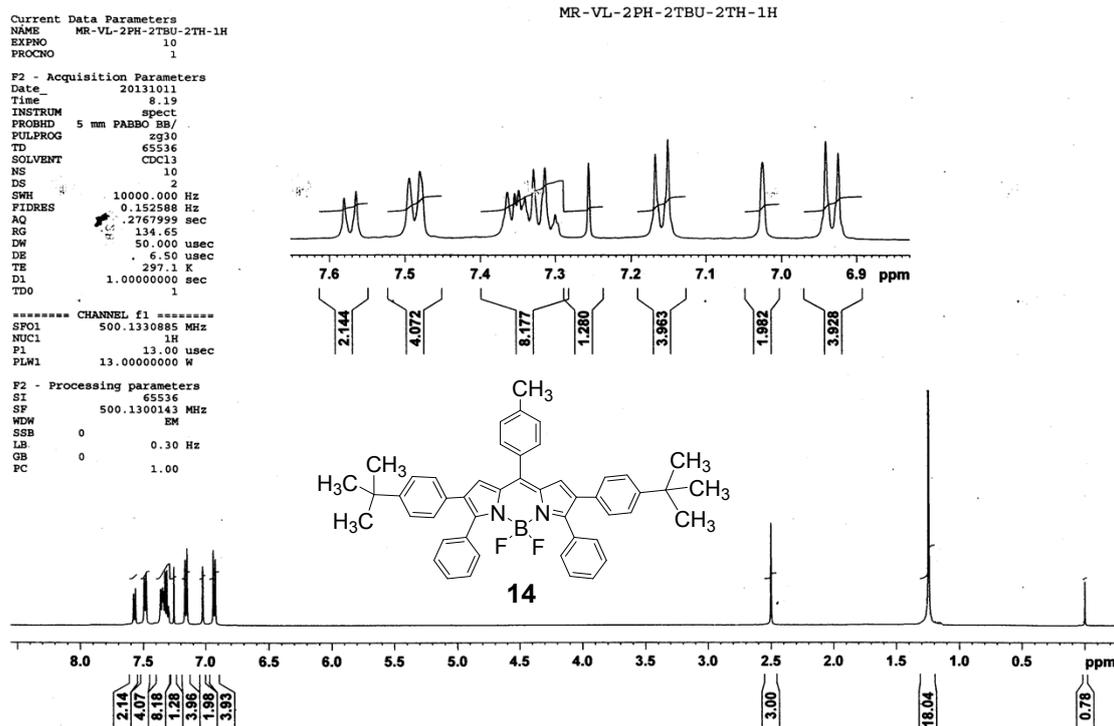


Figure S57: The ^1H NMR spectrum of compound 14 recorded in CDCl_3 .

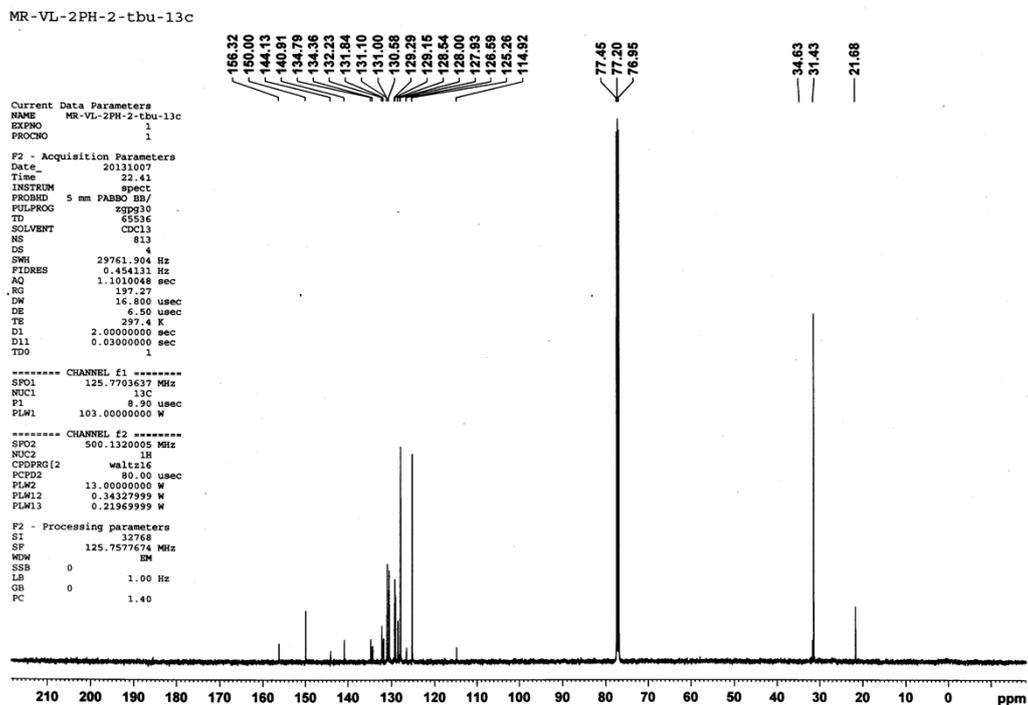
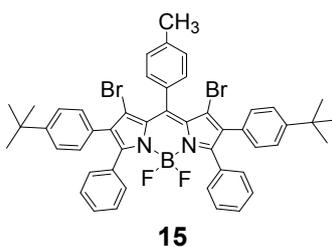


Figure S58: The ^{13}C NMR spectrum of compound 14 recorded in CDCl_3 .



Indian Institute of Technology (B)

Analysis Info

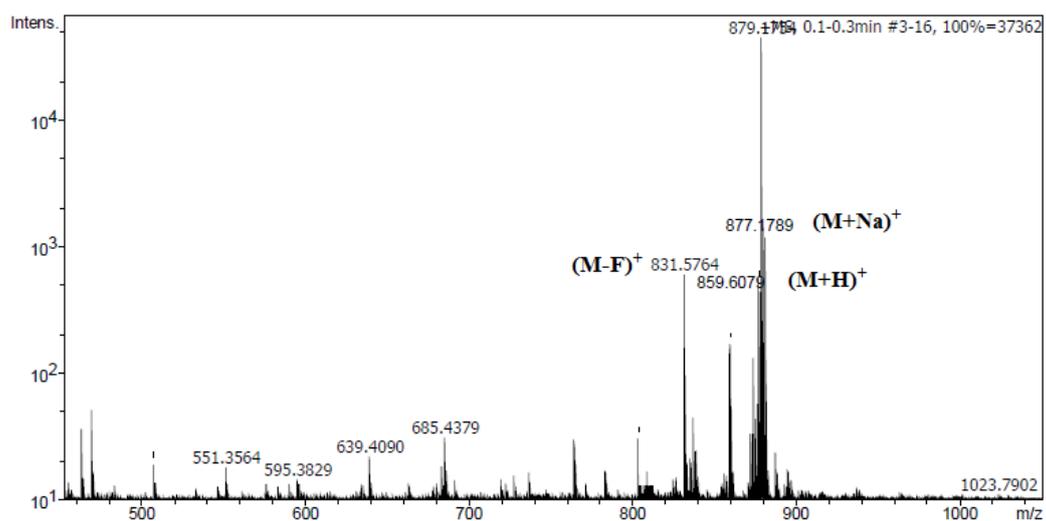
Analysis Name D:\Data\OCT-13\MR-VL-2PH-2T-BU-2BR.d
 Method Tune_pos_Standard_NAI-1500.m
 Sample Name MR-VL-2PH-2T-BU-2BR
 Comment C48H43BBR2F2N2

Acquisition Date 10/22/2013 7:35:14 PM

Operator SSK OUT
 Instrument maXis impact 282001.00081

Acquisition Parameter

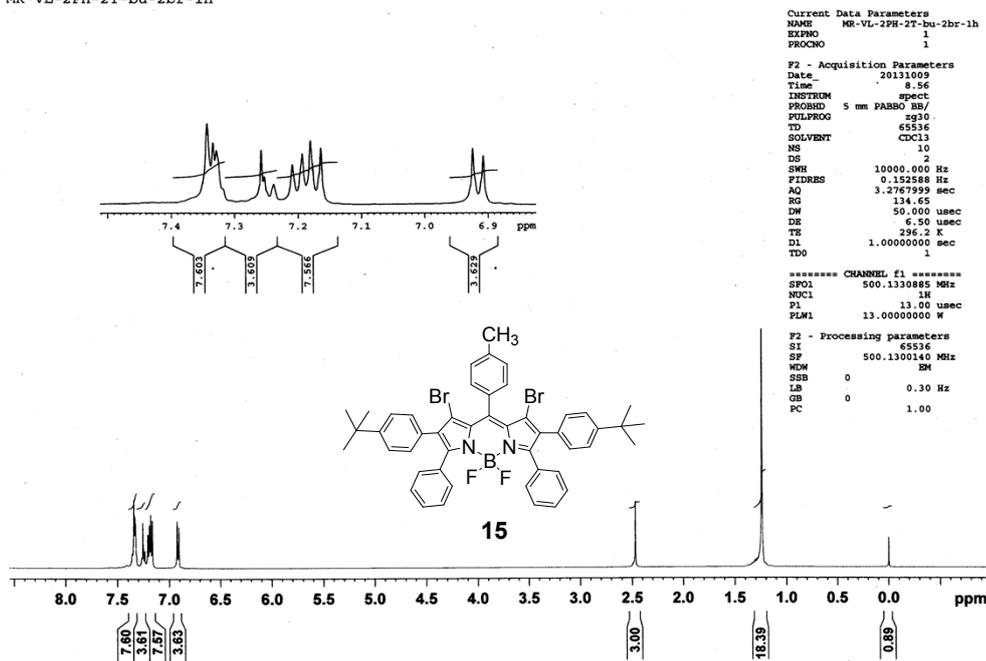
Source Type	ESI	Ion Polarity	Positive	Set Nebulizer	0.3 Bar
Focus	Active	Set Capillary	3500 V	Set Dry Heater	180 °C
Scan Begin	50 m/z	Set End Plate Offset	-500 V	Set Dry Gas	4.0 l/min
Scan End	1500 m/z	Set Collision Cell RF	600.0 Vpp	Set Divert Valve	Source



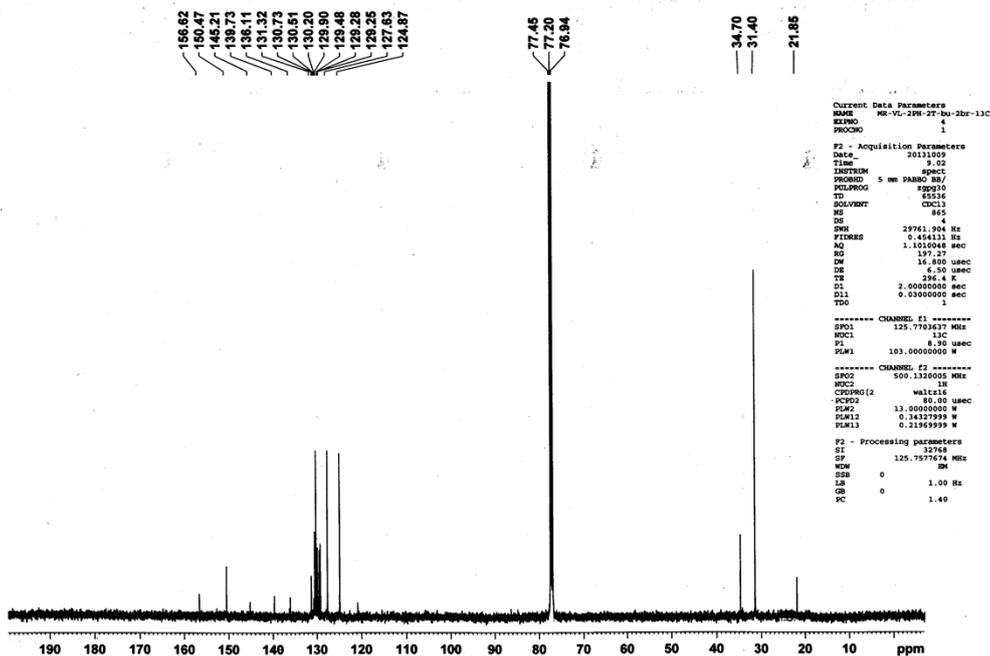
Meas. m/z	#	Ion Formula	m/z	err [ppm]	mSigma	# Sigma	Score	rdb	e ⁻ Conf	N-Rule
877.1789	1	C48H43BBR2F2N2Na	877.1754	-4.0	34.0	1	100.00	26.5	even	ok

Figure S61: The HRMS of compound **15**.

MR-VL-2PH-2T-bu-2br-1h



MR-VL-2PH-2T-bu-2br-13C



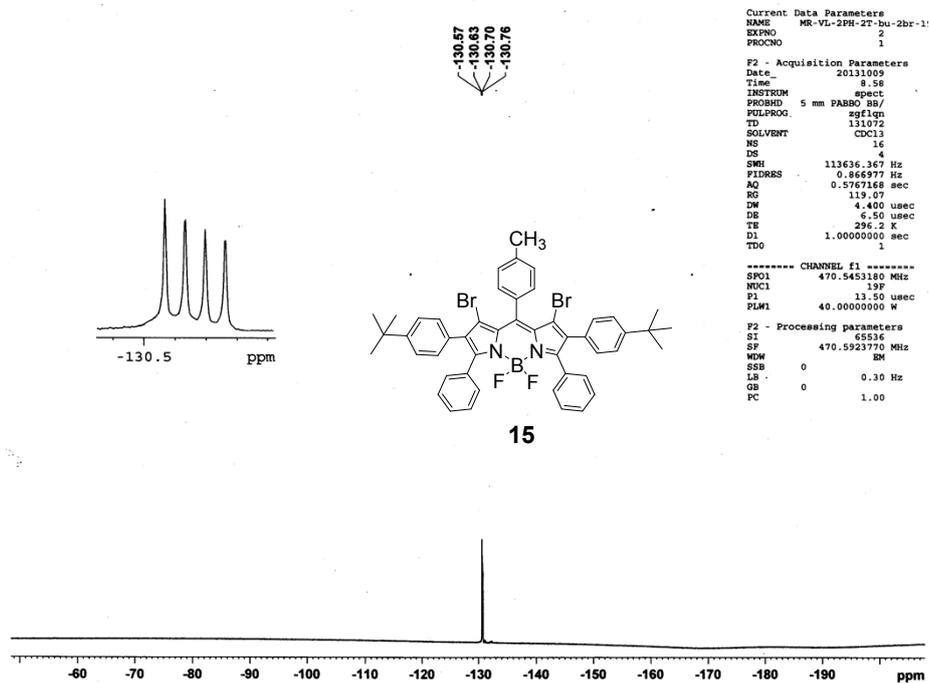


Figure S64: The ^{19}F NMR spectrum of compound 15 recorded in CDCl_3 .

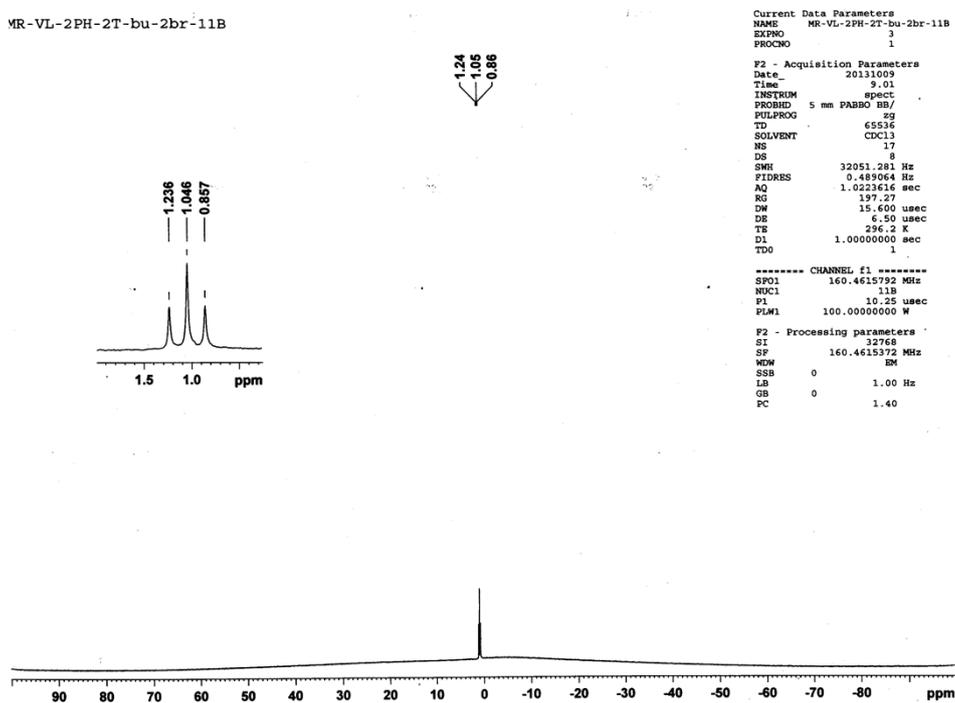


Figure S65: The ^{11}B NMR spectrum of compound 15 recorded in CDCl_3 .

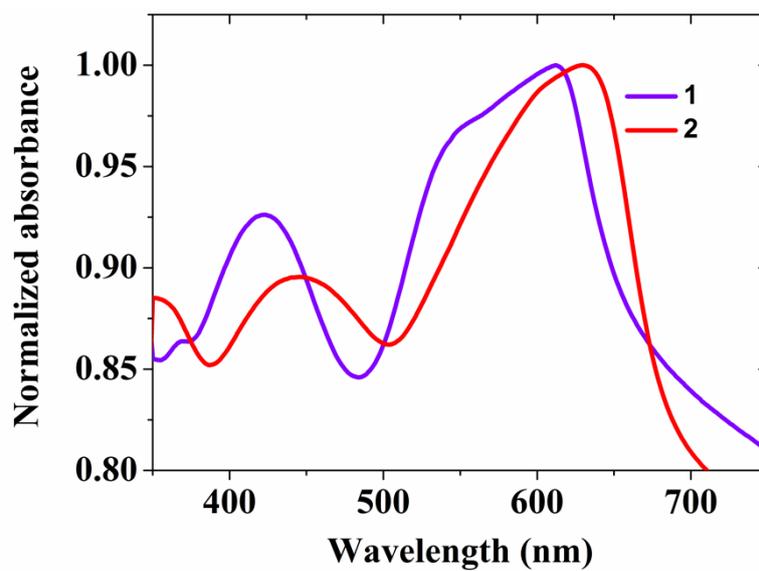


Figure S66: The normalized absorption spectra of compounds **1** (violet) and **2** (red) in solid state.

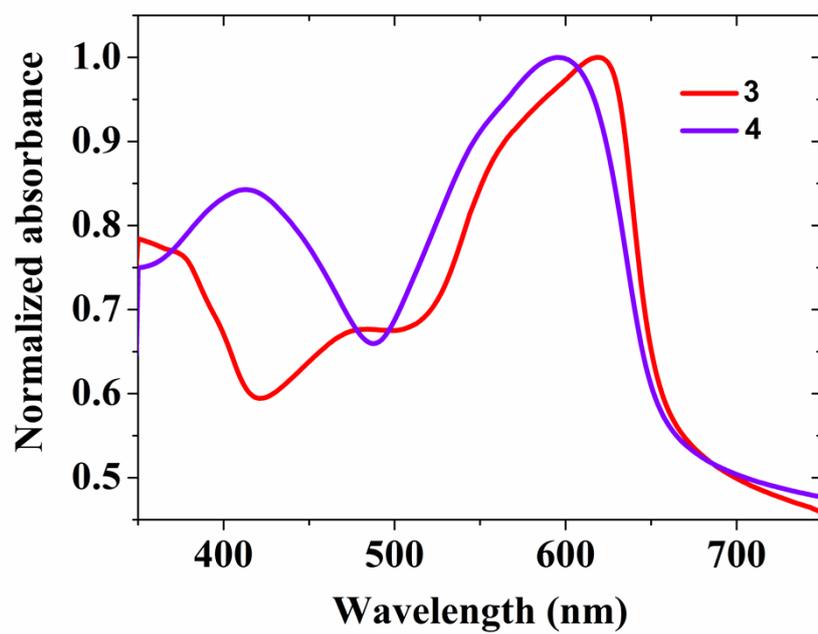


Figure S67: The normalized absorption spectra of compounds **3** (red) and **4** (violet) in solid state.

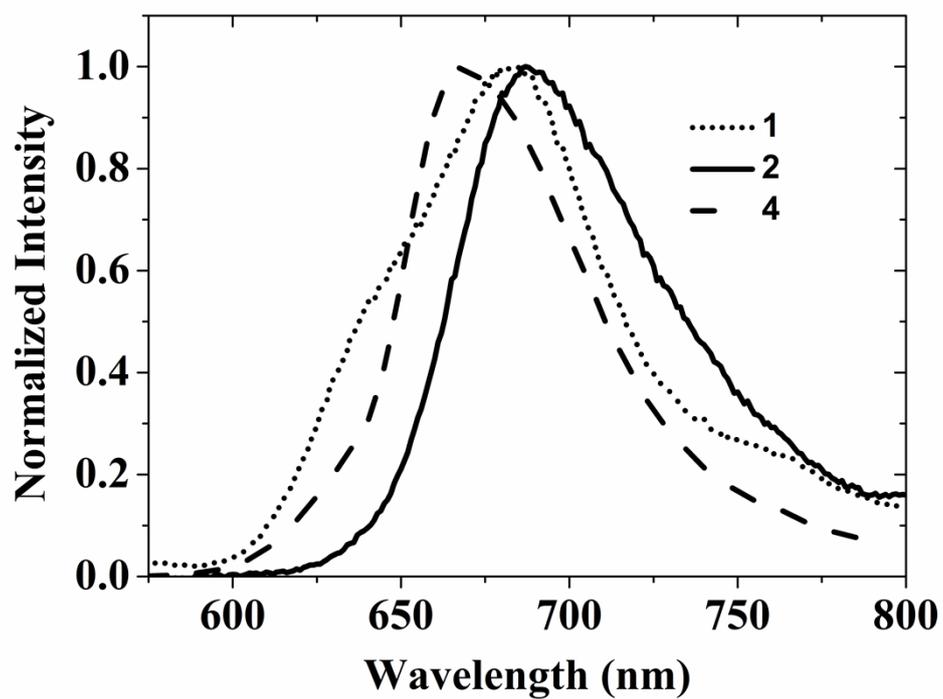


Figure S68: The normalized emission spectra of compounds **1** (dotted line), **2** (solid line) and **4** (dashed line) in solid state.