Electronic Supplementary Material (ESI) for RSC Advances.

Polyarylated Boron-Dipyrromethenes Containing Three Different Types of Aryl Groups

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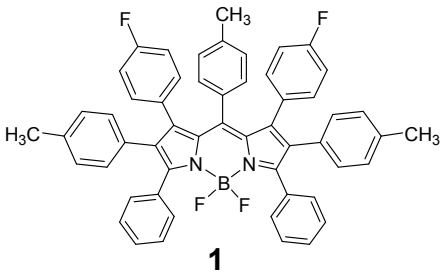

1

Indian Institute of Technology (B)

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omment	C54H39BF4N2		

cquisition Parameter

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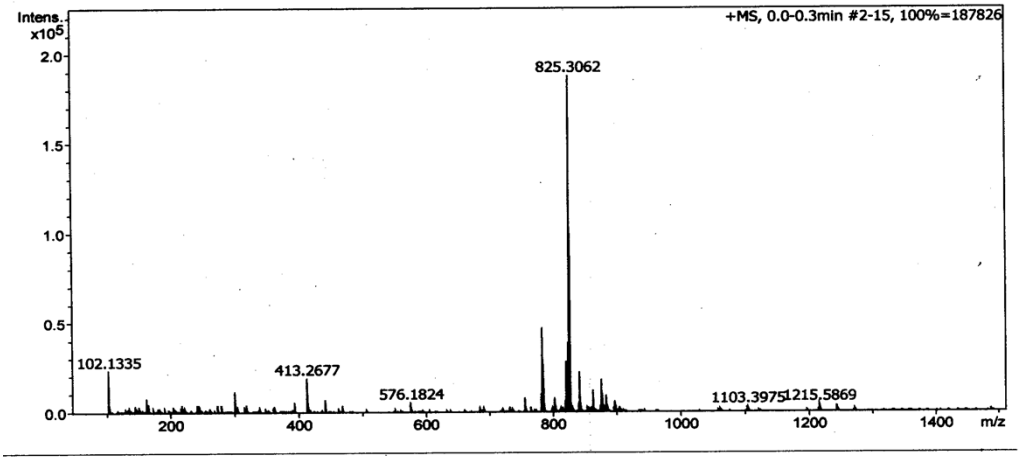

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Figure S1: HRMS of compound **1.**

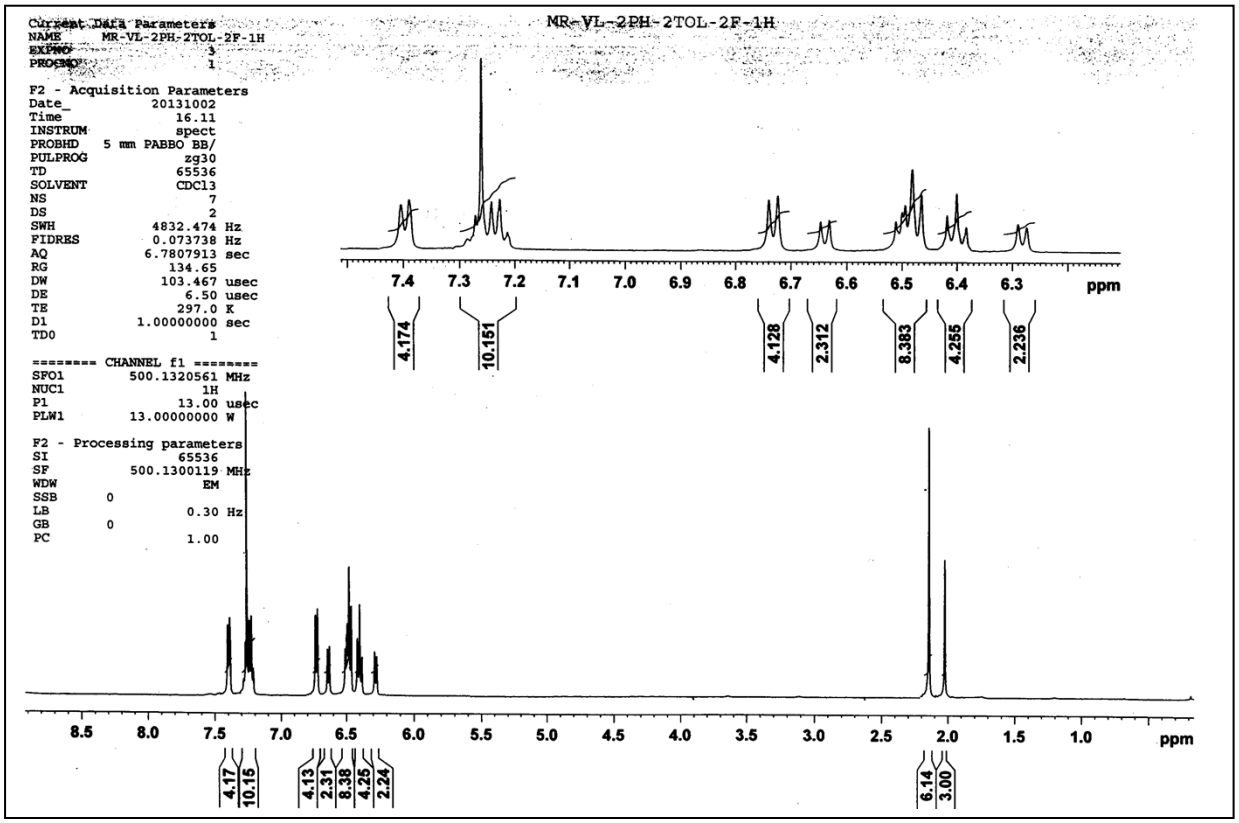


Figure S2: The ^{1}H NMR spectrum of compound **1** recorded in $CDCl_3$

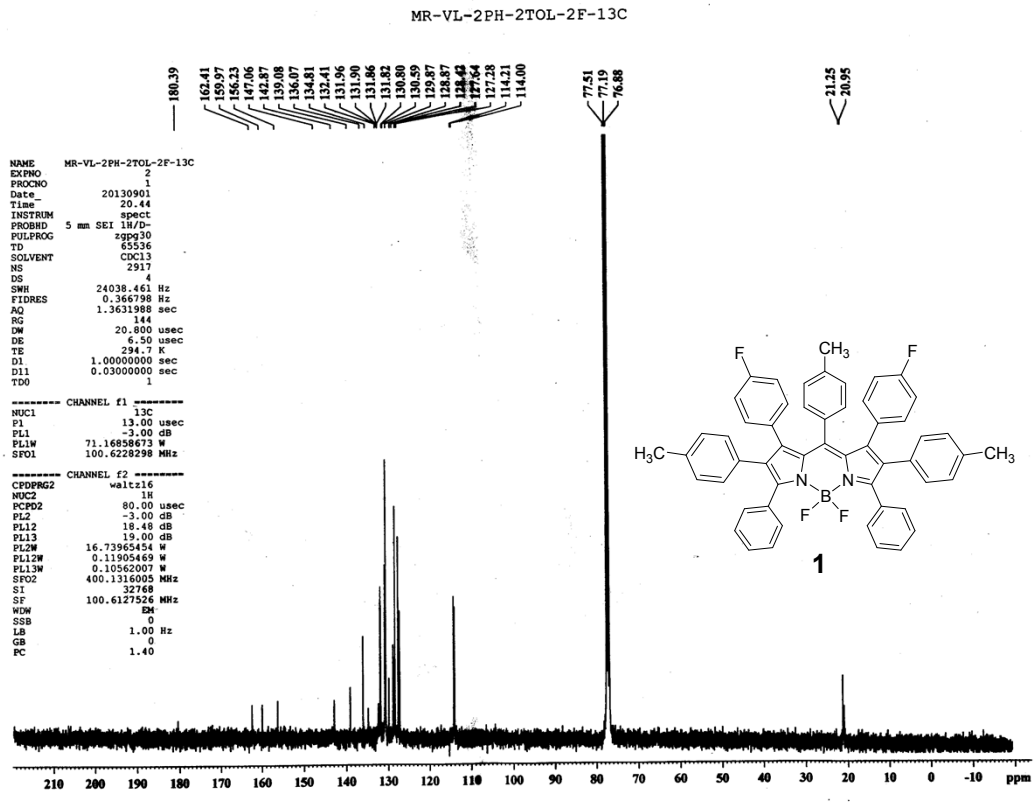


Figure S3: The ^{13}C NMR spectrum of compound **1** recorded in $CDCl_3$

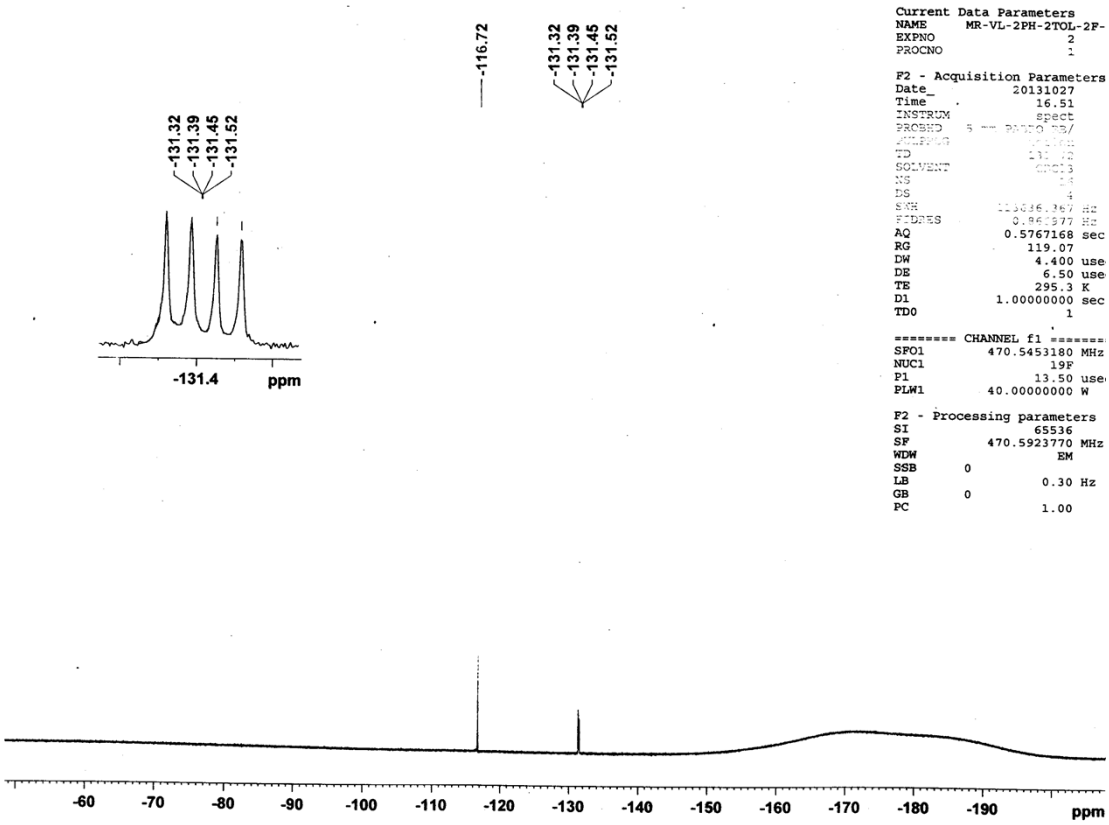


Figure S4: The ^{19}F NMR spectrum of compound **1** recorded in $CDCl_3$

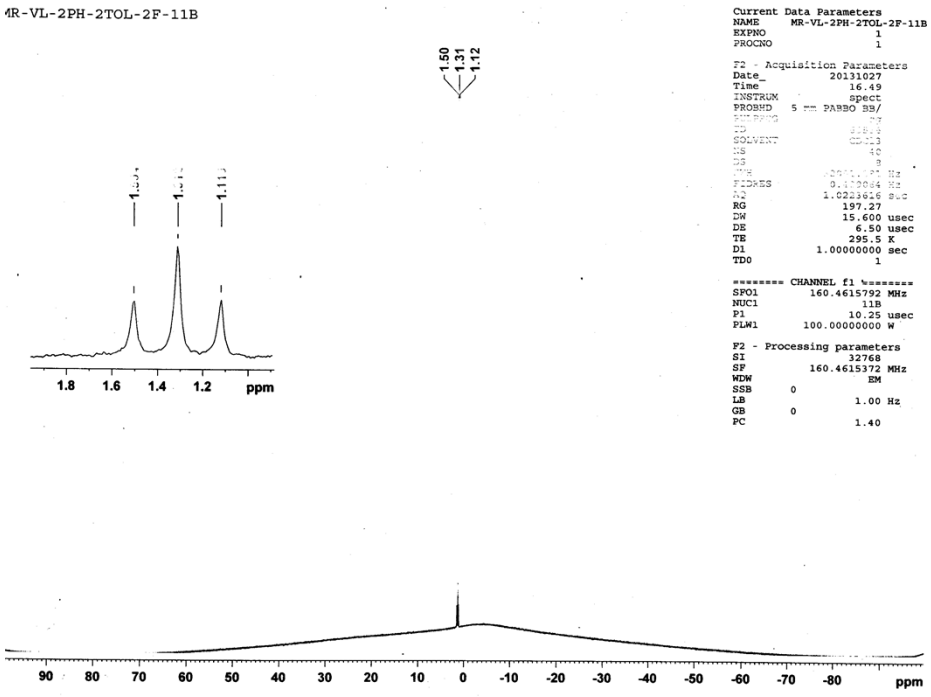
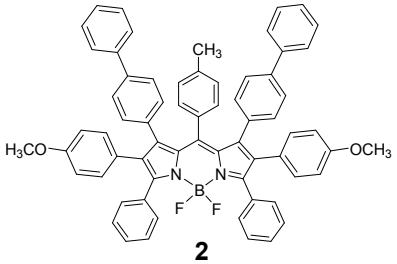


Figure S5: The ^{11}B NMR spectrum of compound **1** recorded in $CDCl_3$



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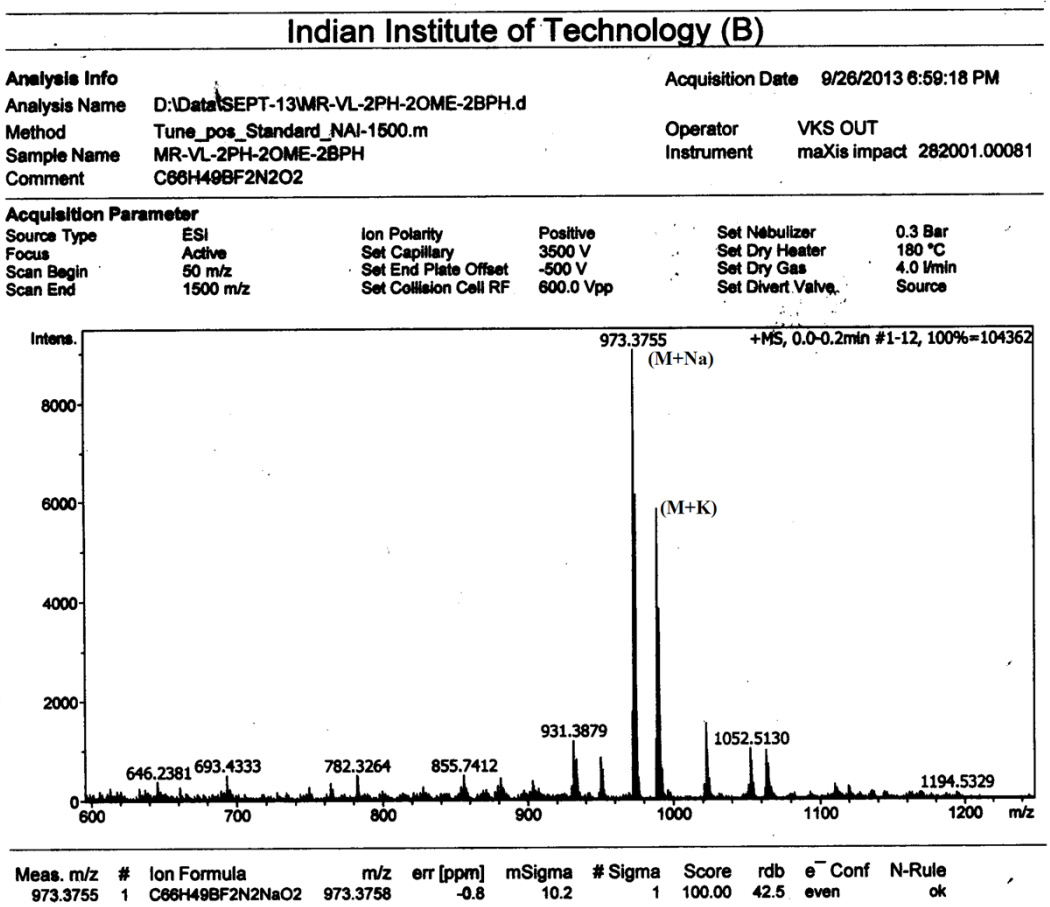


Figure S6: The HRMS spectrum of compound **2.**

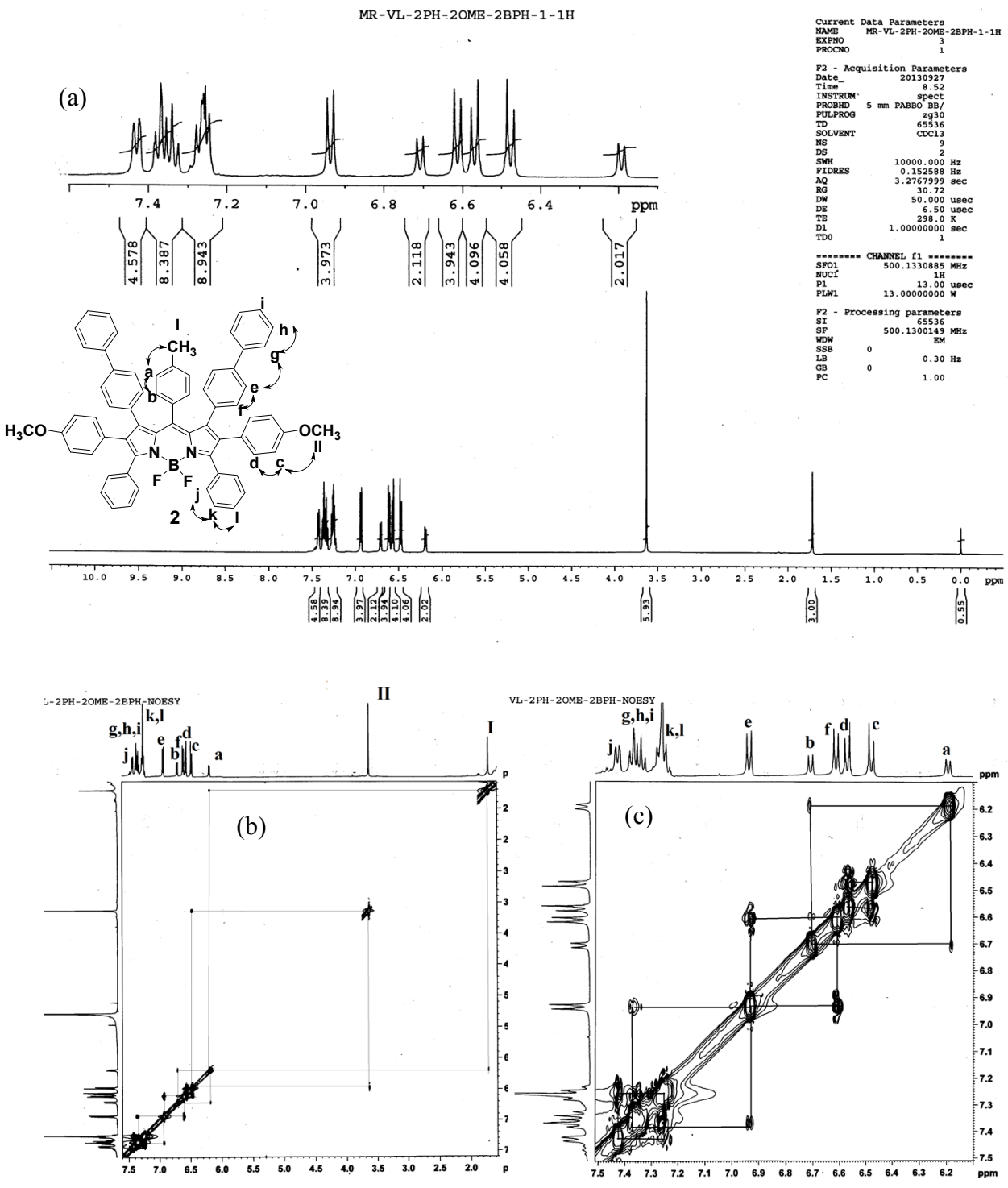


Figure S7: (a) The ^{1}H NMR spectrum of compound **2** recorded in $CDCl_3$. (b) The NOESY NMR spectrum of compound **2** recorded in $CDCl_3$. (c) The NOESY NMR spectrum of compound **2** in the selected region.

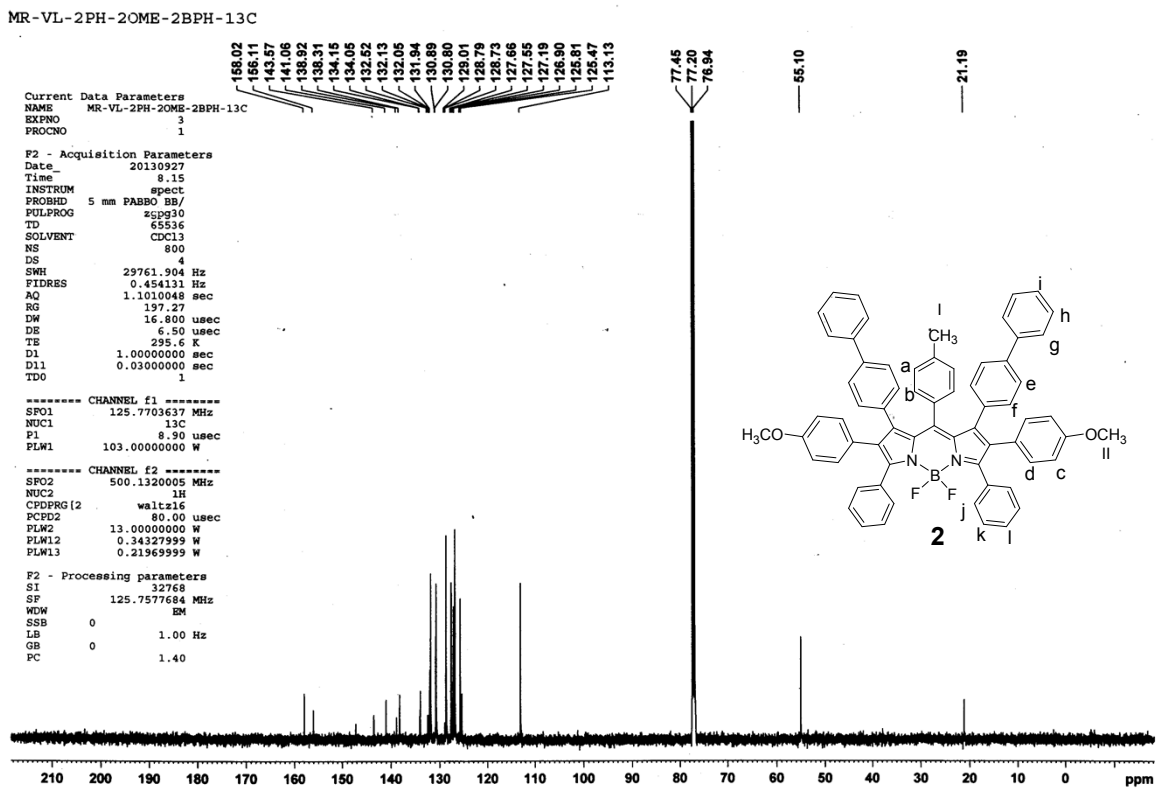


Figure S8: The ^{13}C NMR spectrum of compound **2** recorded in $CDCl_3$.

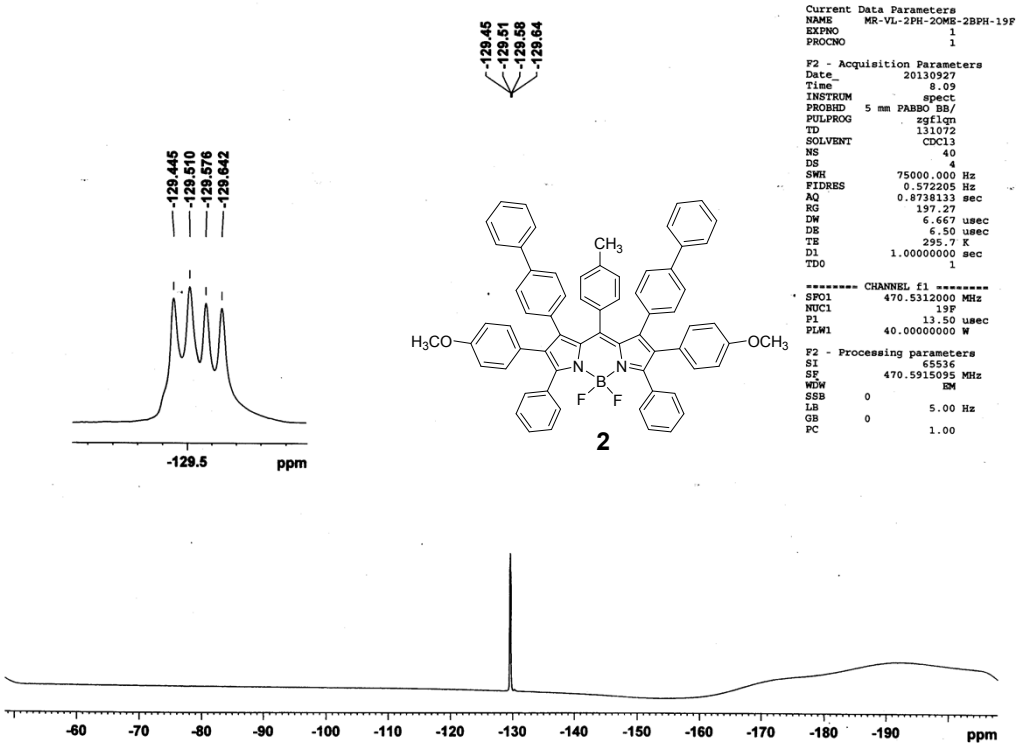


Figure S9: The ^{19}F NMR spectrum of compound **2** recorded in $CDCl_3$.

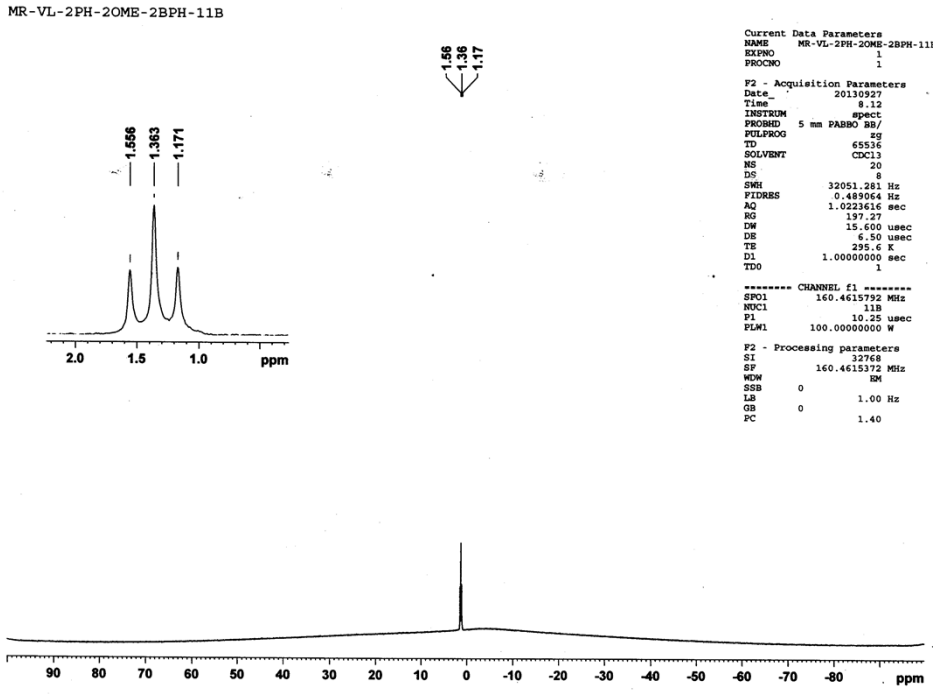
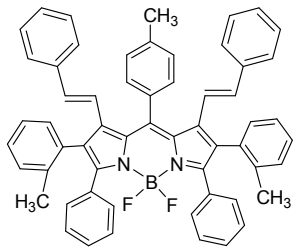


Figure S10: The ^{11}B NMR spectrum of compound **2** recorded in $CDCl_3$.



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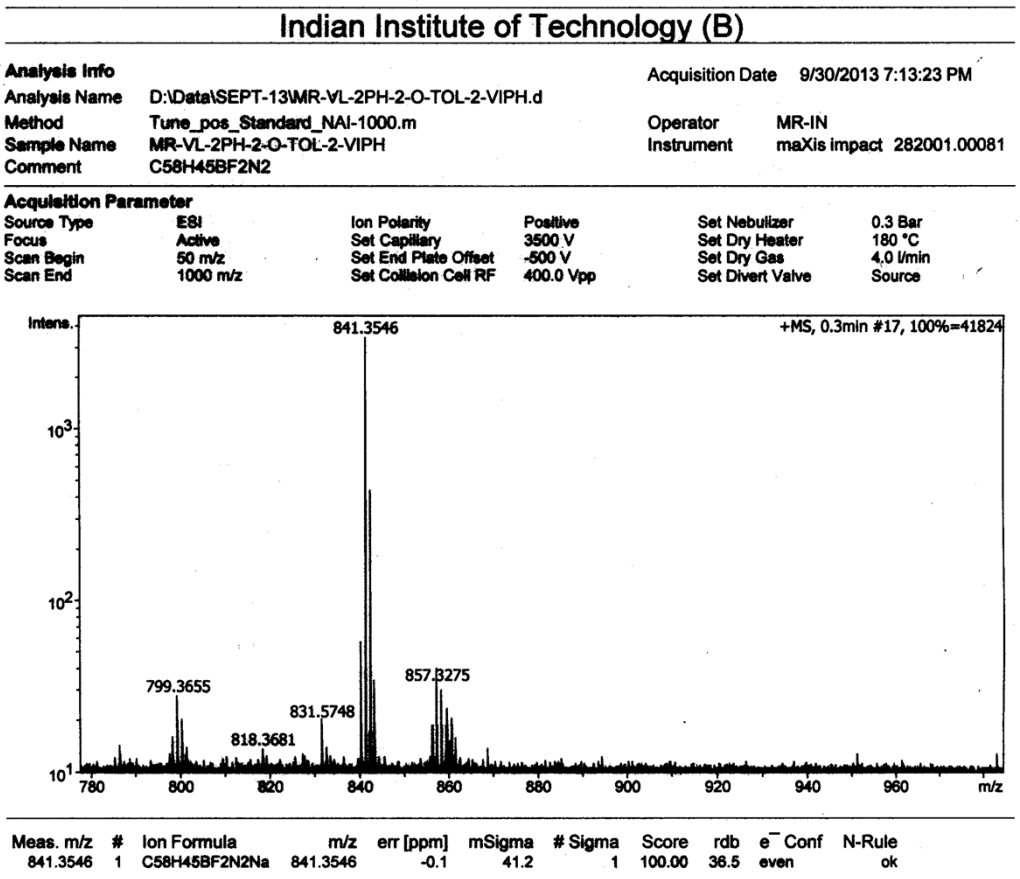


Figure S11: The HRMS spectrum of compound **3.**

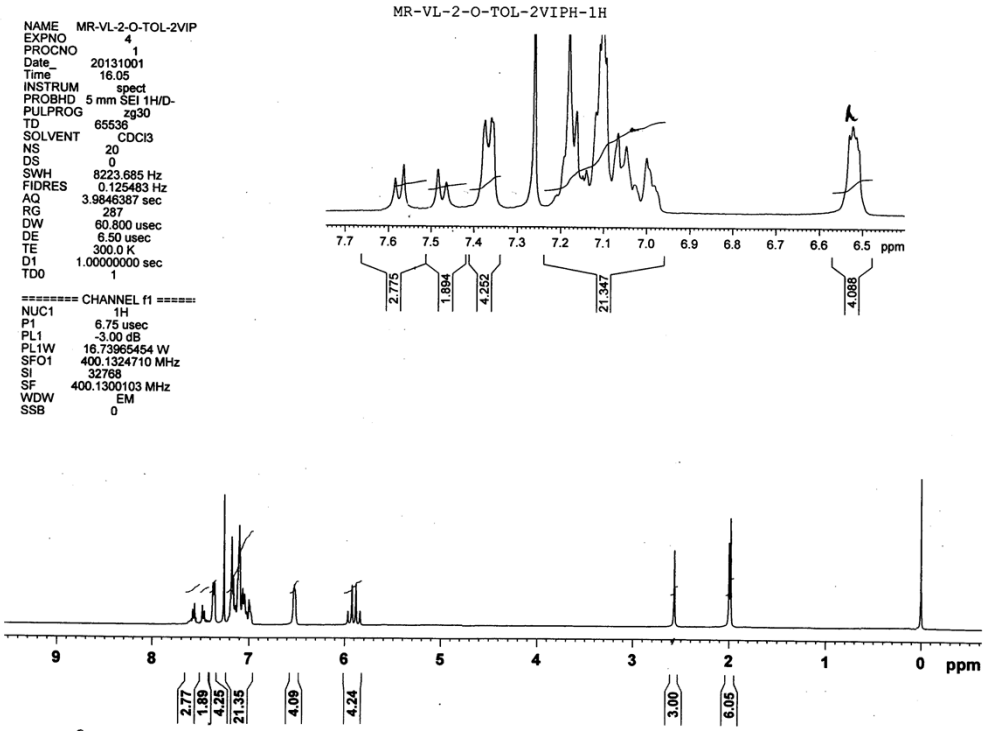


Figure S12: The ^{1}H NMR spectrum of compound **3** recorded in $CDCl_3$.

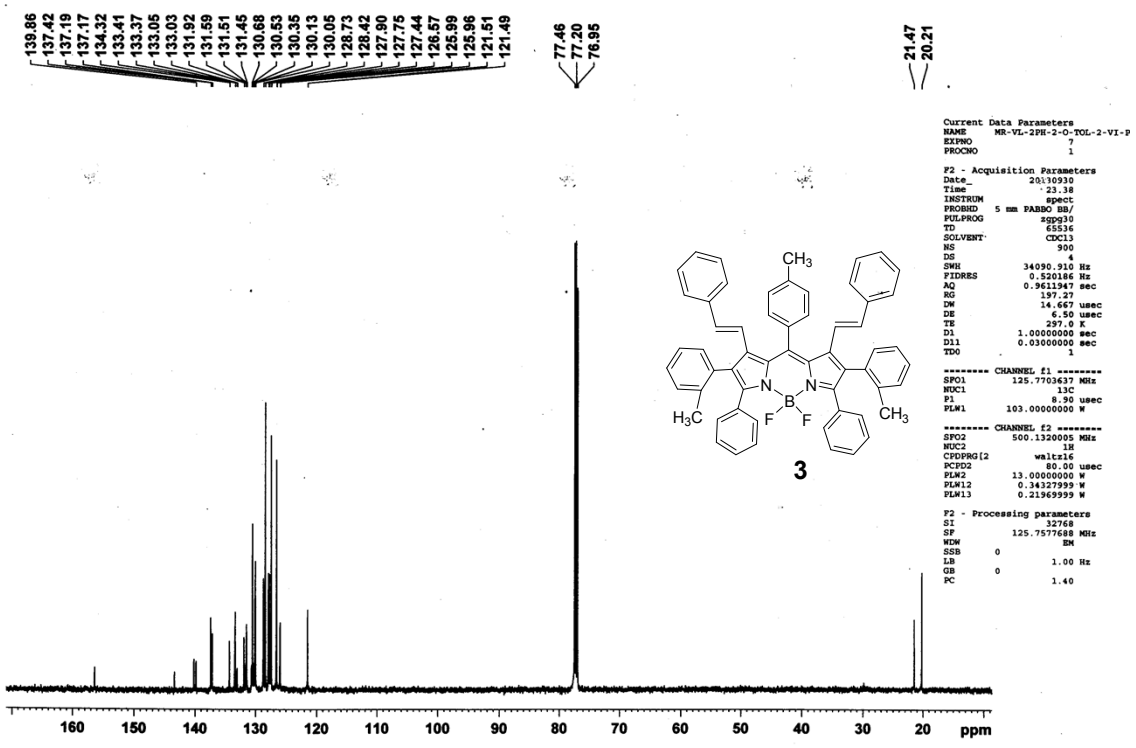


Figure S13: The ^{13}C NMR spectrum of compound **3** recorded in $CDCl_3$.

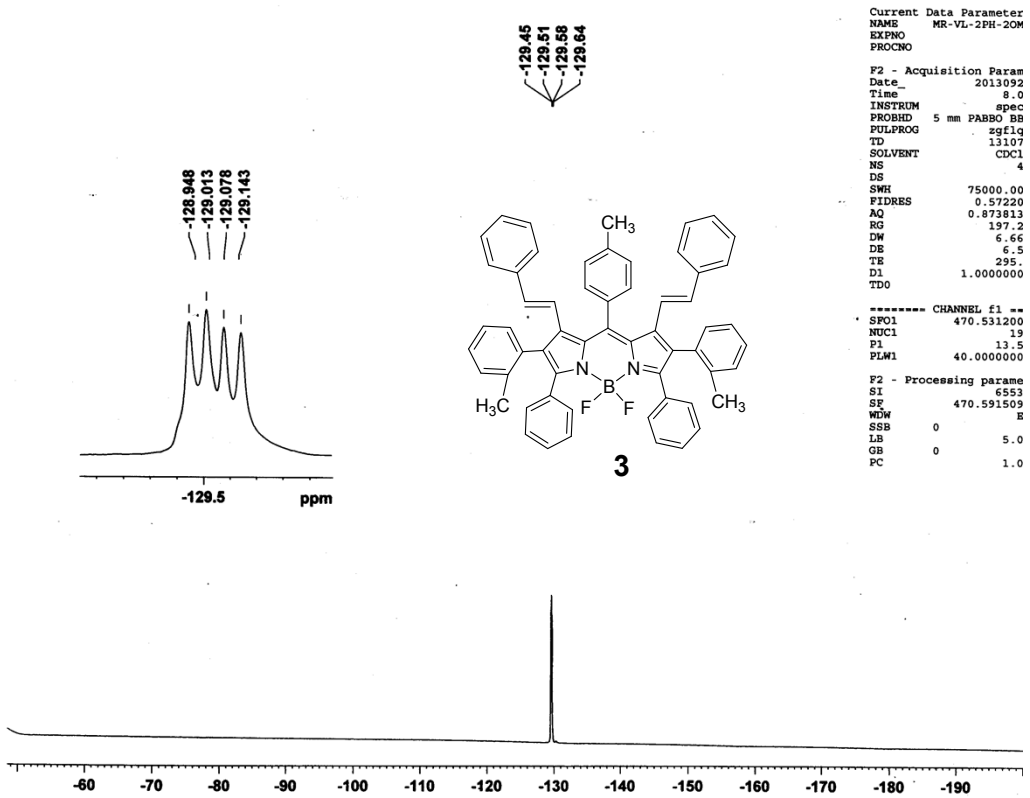


Figure S14: The ^{19}F NMR spectrum of compound **3** recorded in $CDCl_3$.

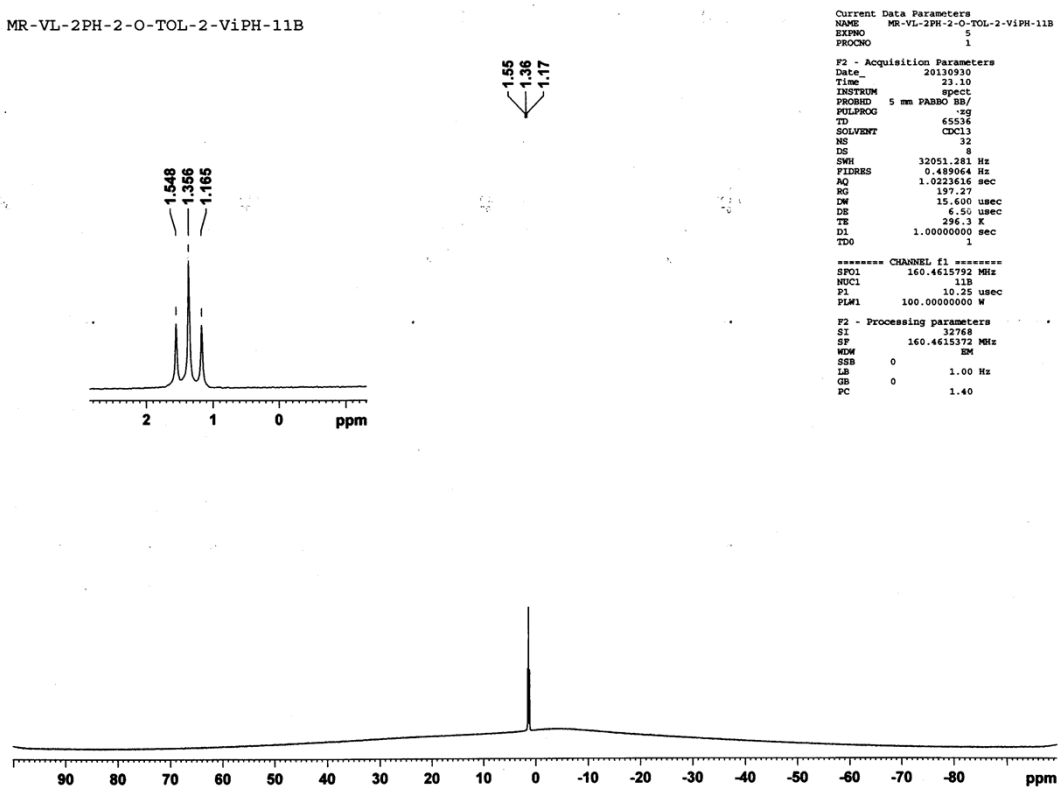
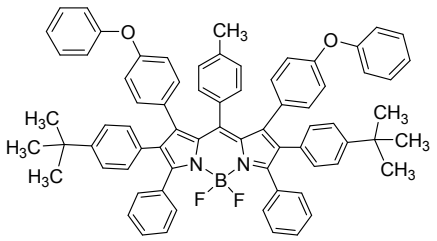


Figure S15: The ^{11}B NMR spectrum of compound **3** recorded in $CDCl_3$.



4

Indian Institute of Technology (B)

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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

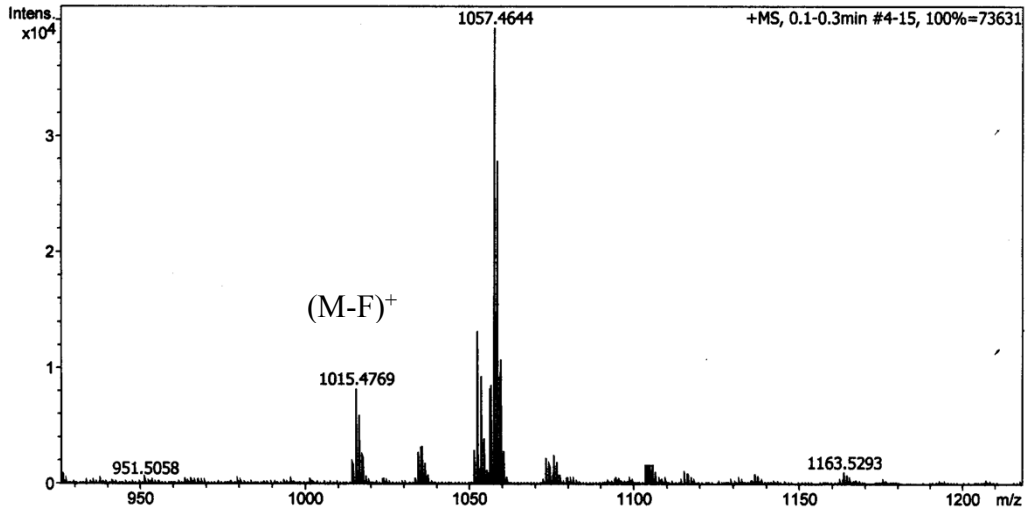

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Figure S16: The HRMS of compound **4.**

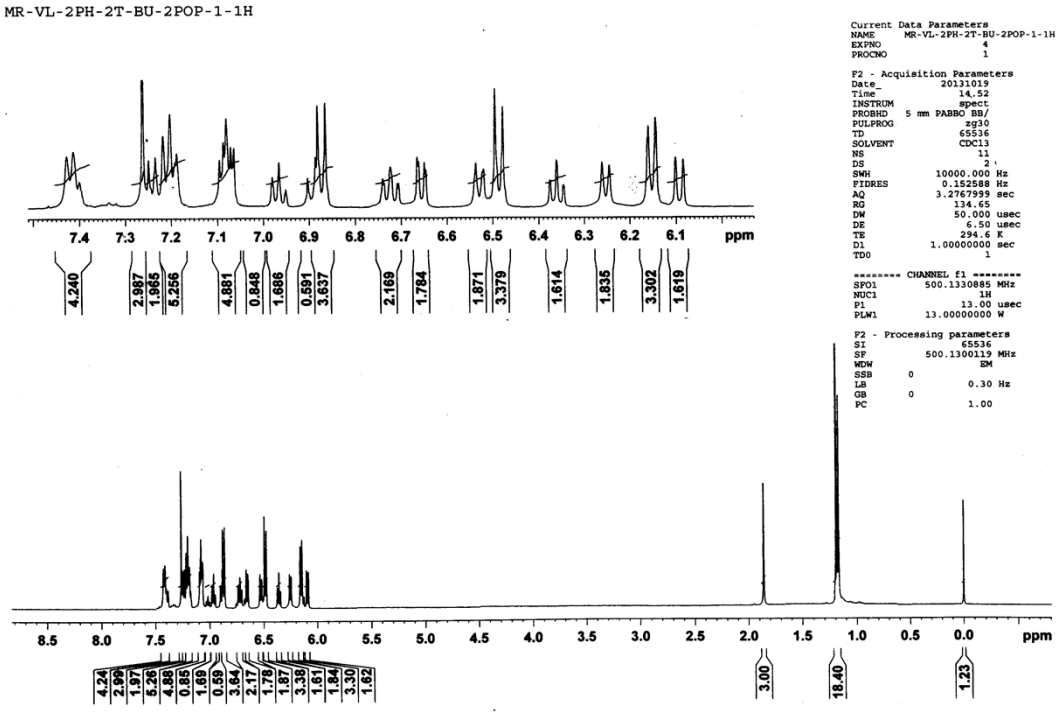


Figure S17: The ^{1}H NMR spectrum of compound **4** recorded in $CDCl_3$.

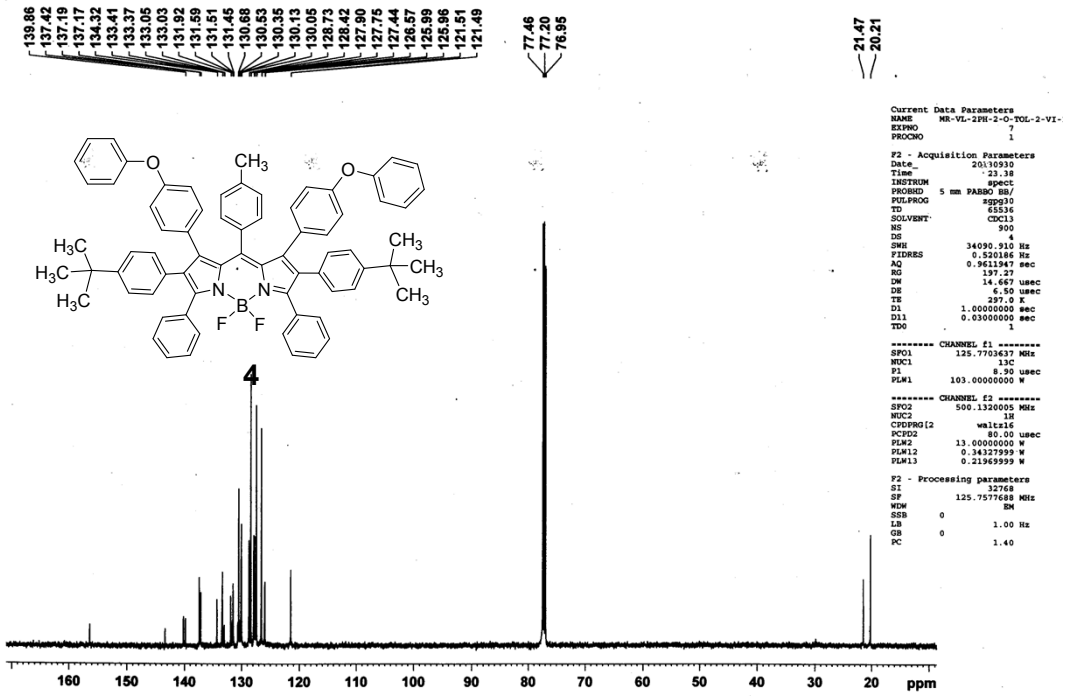


Figure S18: The ^{13}C NMR spectrum of compound **4** recorded in $CDCl_3$.

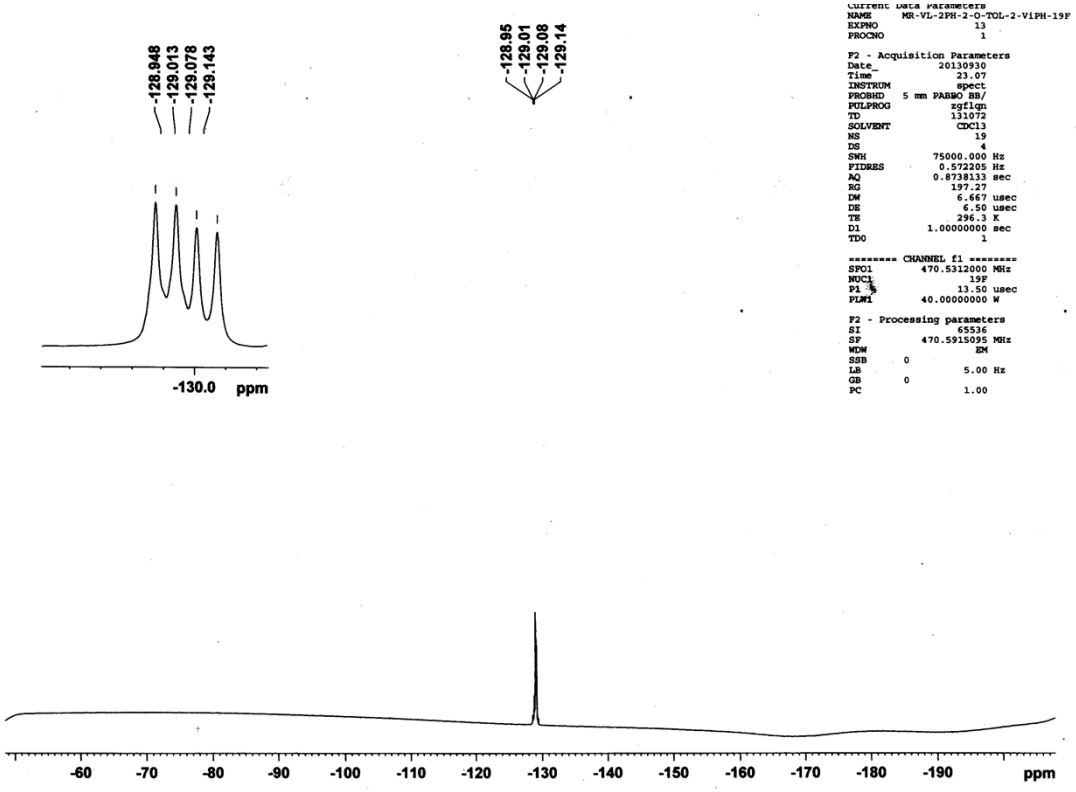


Figure S19: The ^{19}F NMR spectrum of compound **4** recorded in $CDCl_3$.

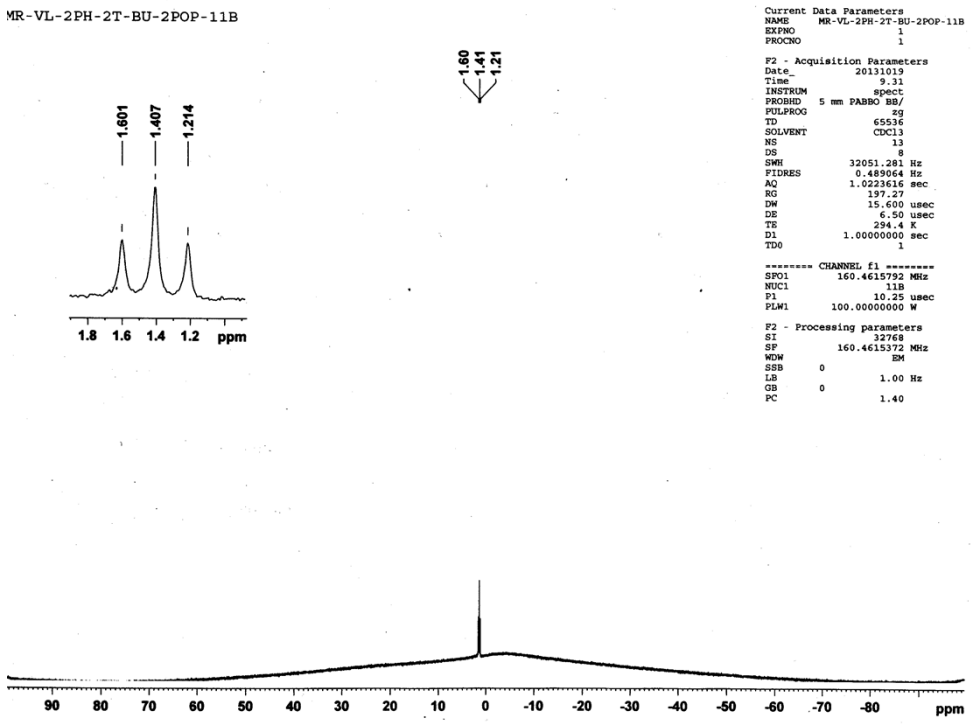
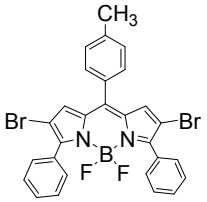


Figure S20: The ^{11}B NMR spectrum of compound **4** recorded in $CDCl_3$.



7

Indian Institute of Technology (B)

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Comment	C28H19BBr2F2N2		

Acquisition Parameter

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

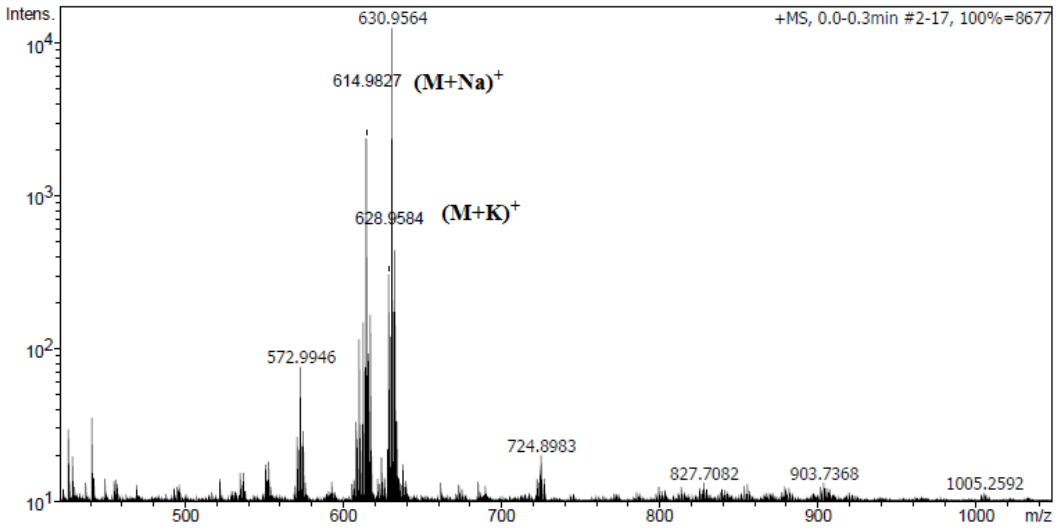

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Figure S21: The HRMS of compound **7**

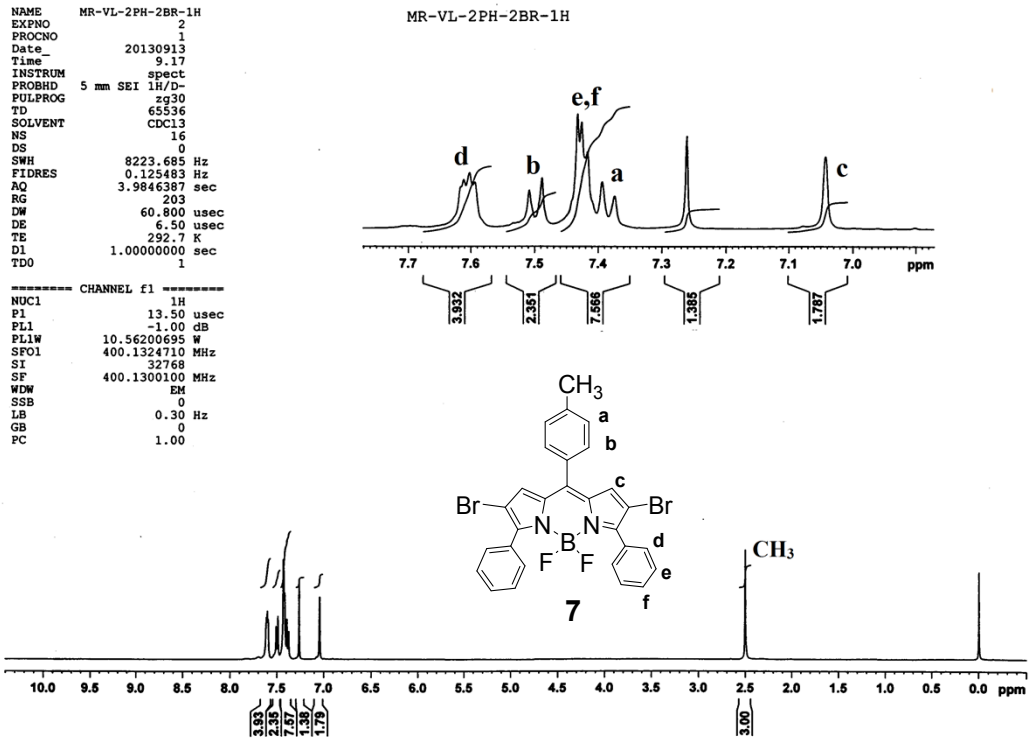


Figure S22: The ^{1}H NMR spectrum of compound **7** recorded in $CDCl_3$.

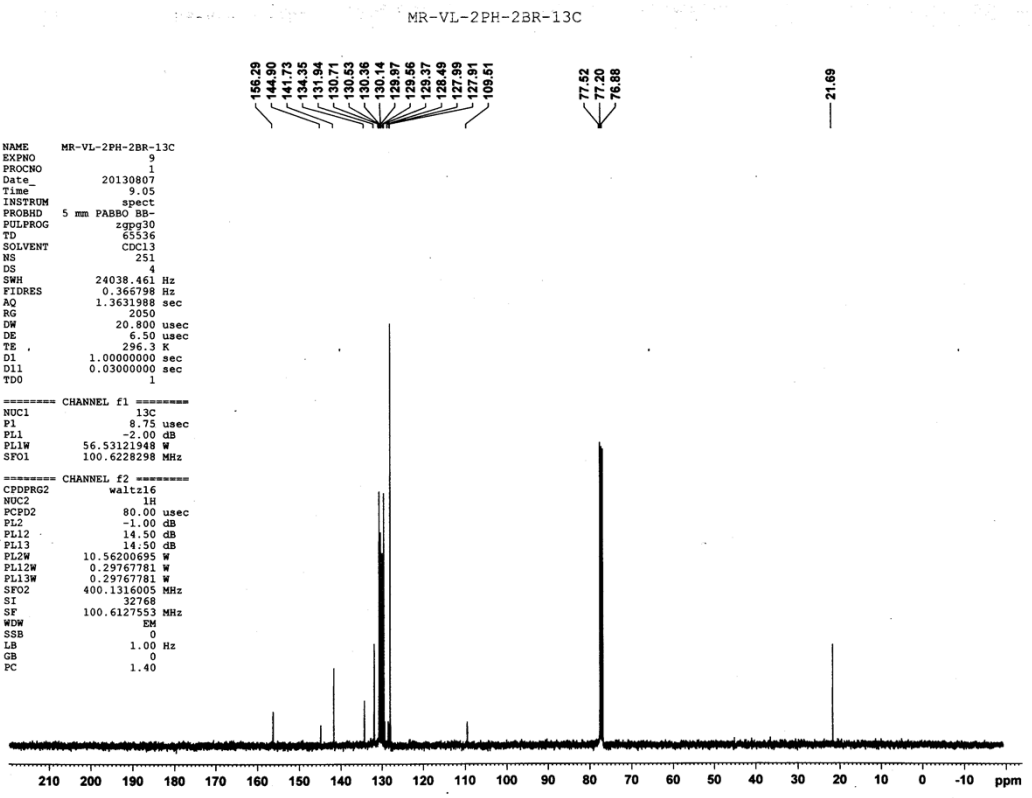


Figure S23: The ^{13}C NMR spectrum of compound **7** recorded in $CDCl_3$.

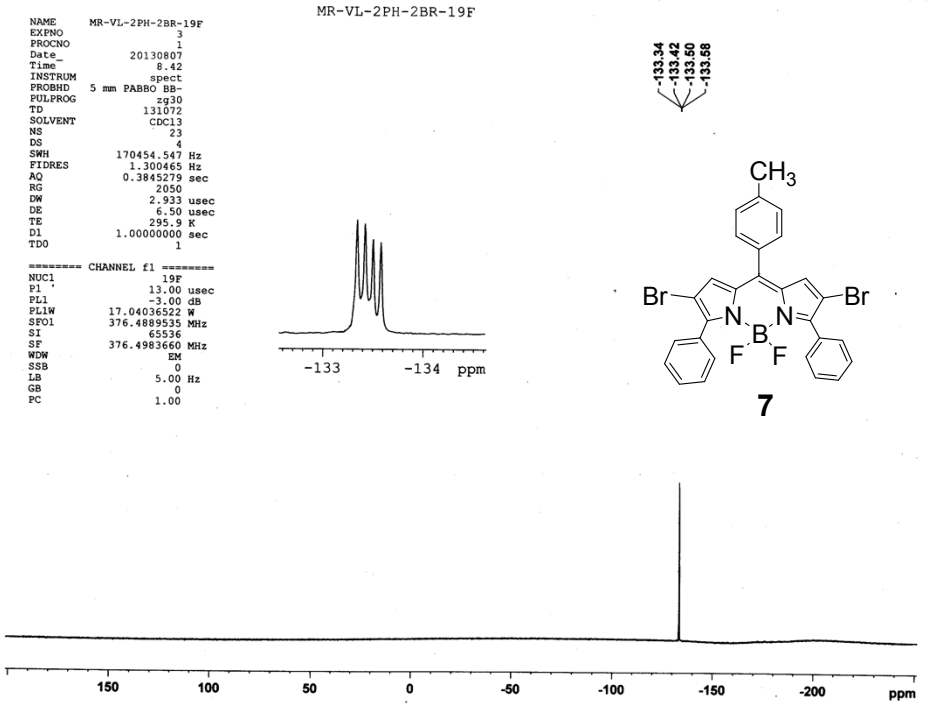


Figure S24: The ^{19}F NMR spectrum of compound **7** recorded in $CDCl_3$.

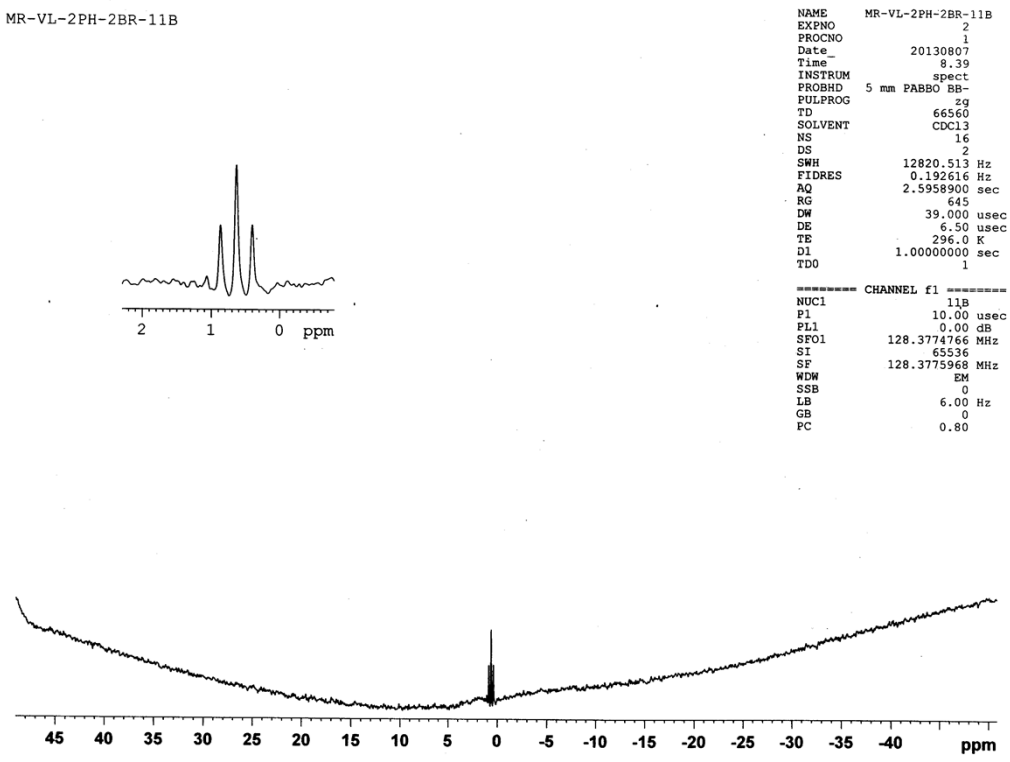
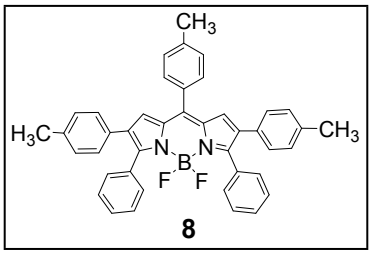


Figure S25: The ^{11}B NMR spectrum of compound **7** recorded in $CDCl_3$.



Indian Institute of Technology (B)

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Comment	C42H33BF2N2		

Acquisition Parameter

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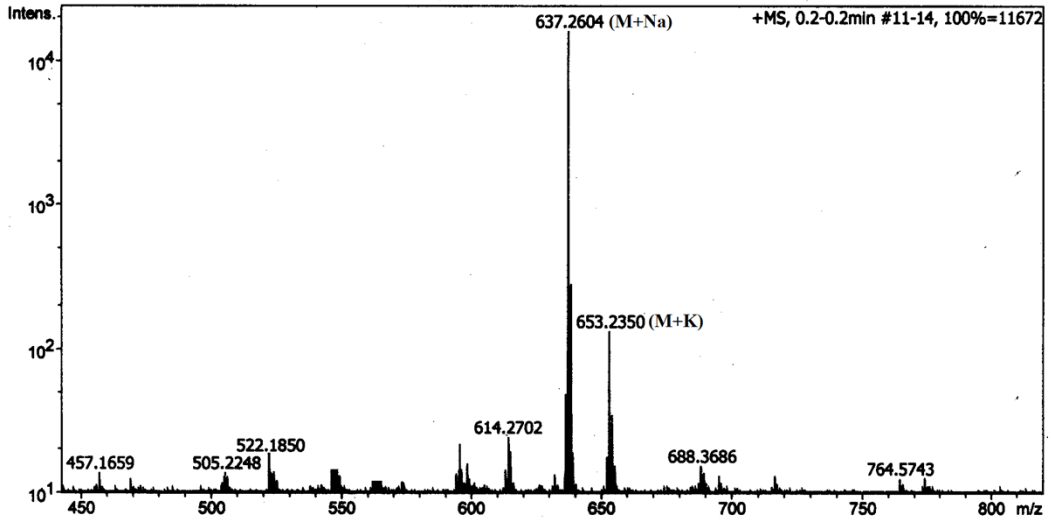

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637.260431	1	C42H33BF2N2Na	100.00	637.260423	-0.0	-0.0	8.4	26.5	even	ok	M+Na

Figure 26: The HRMS of compound **8**.

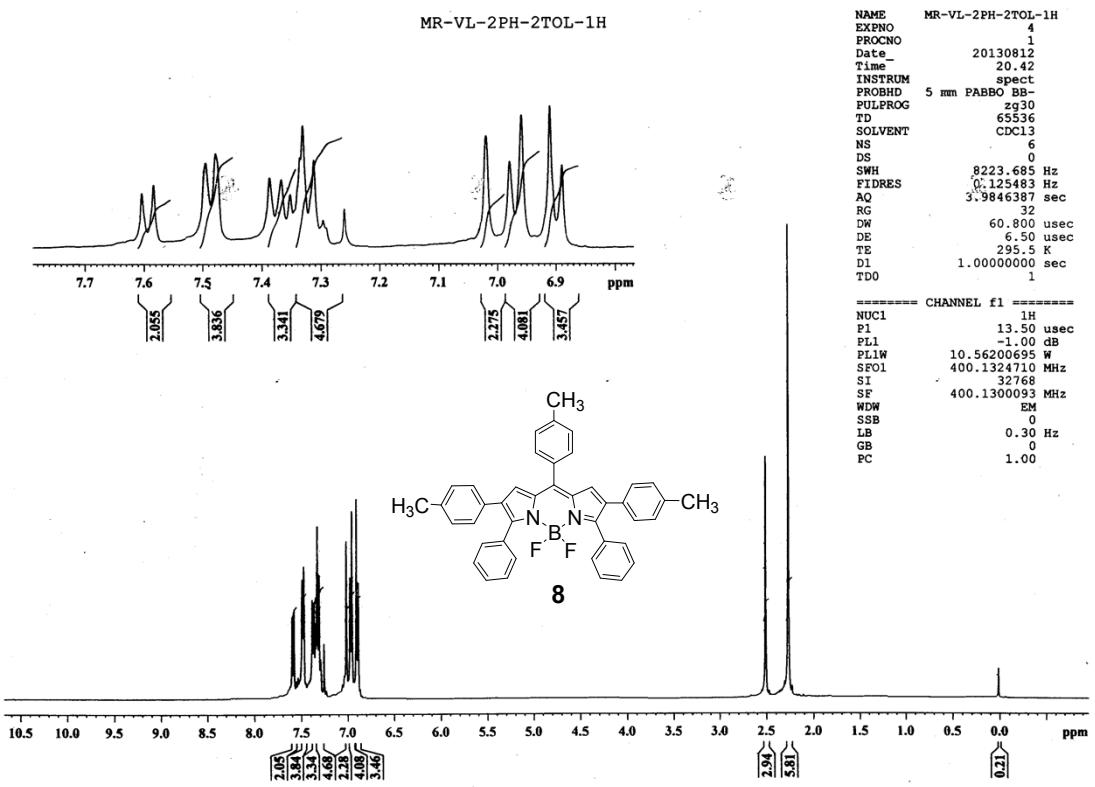


Figure S27: The ^{1}H NMR spectrum of compound **8** recorded in $CDCl_3$.

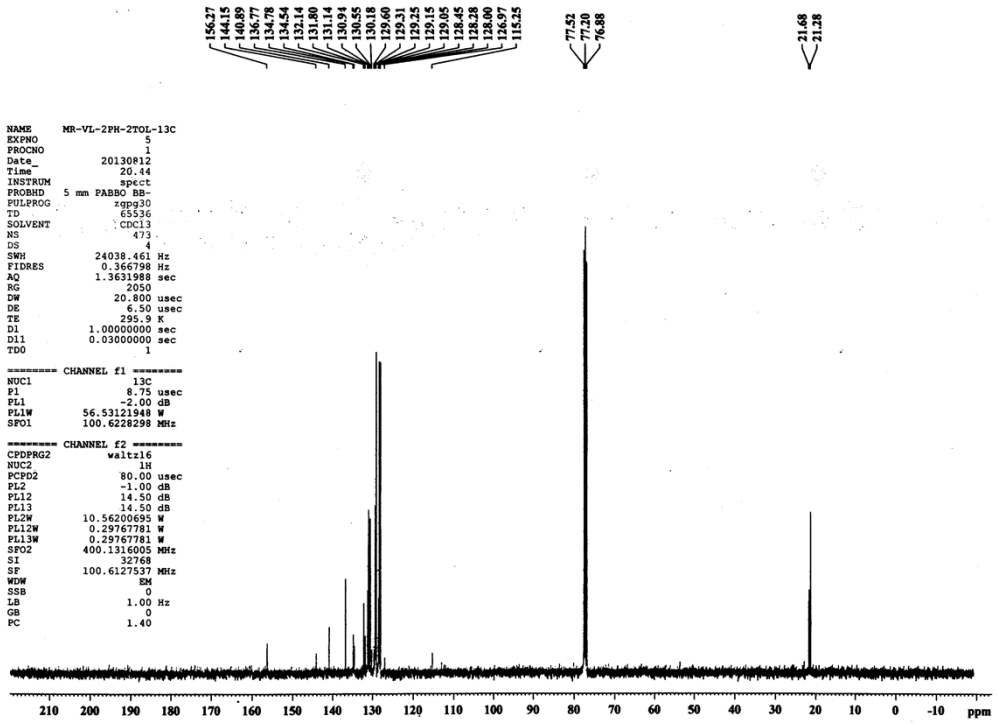


Figure S28: The ^{13}C NMR spectrum of compound **8** recorded in $CDCl_3$.

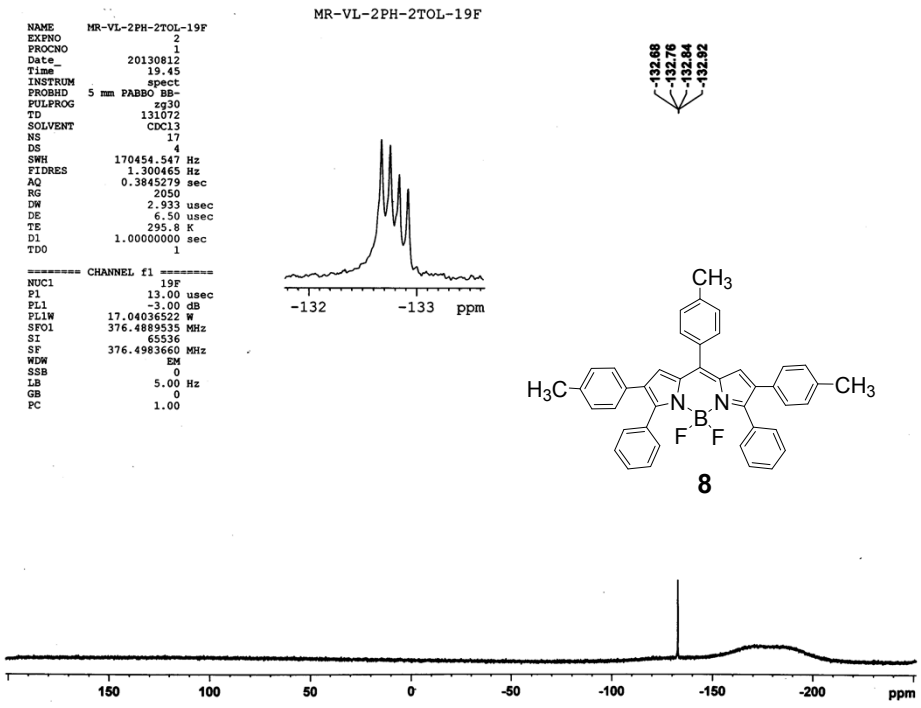


Figure S29: The ^{19}F NMR spectrum of compound **8** recorded in $CDCl_3$.

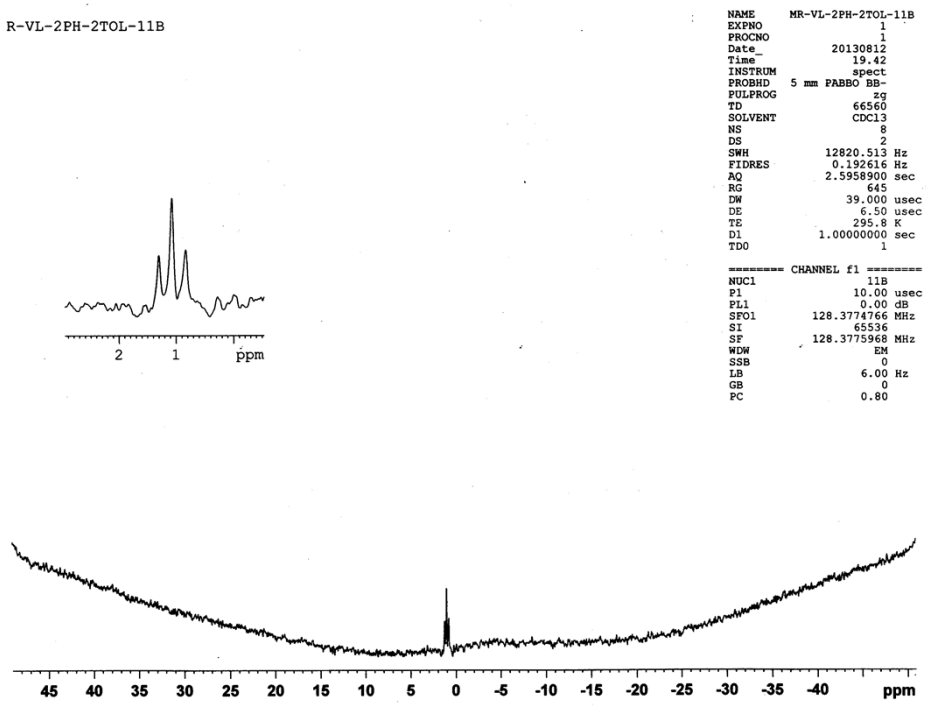
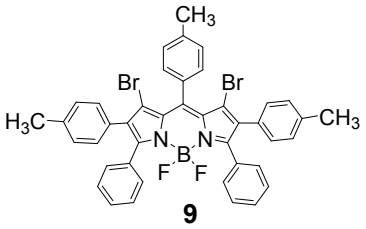


Figure S30: The ^{11}B NMR spectrum of compound **8** recorded in $CDCl_3$.



9

Indian Institute of Technology (B)

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Sample Name	MR-vl-2-PH-2TOL-2BR	Instrument	maXis impact 282001.00081
Comment	C42H31BBr2F2N2		

Acquisition Parameter

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Scan End	1000 m/z	Set Collision Cell RF	800.0 Vpp	Set Divert Valve	Source

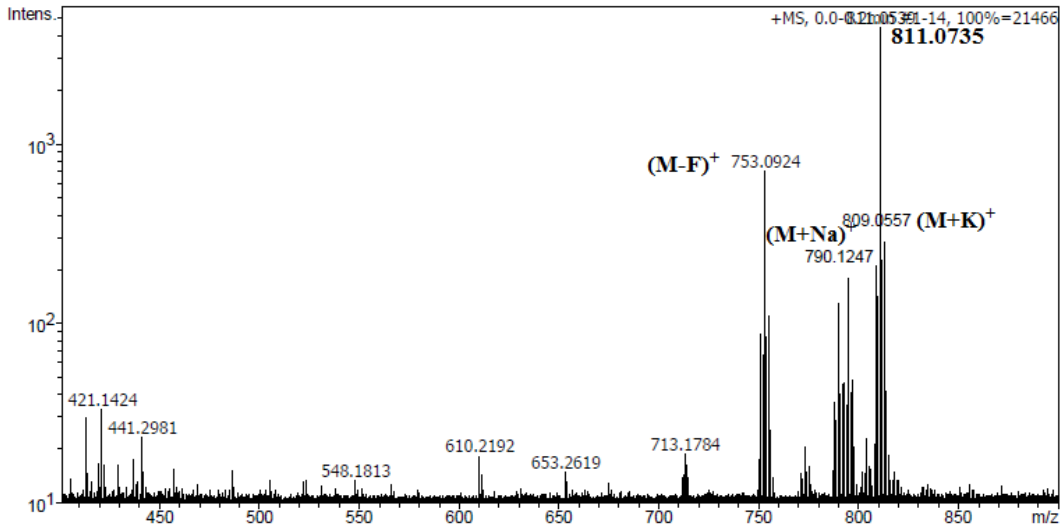

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Figure S31: The HRMS of compound **9.**

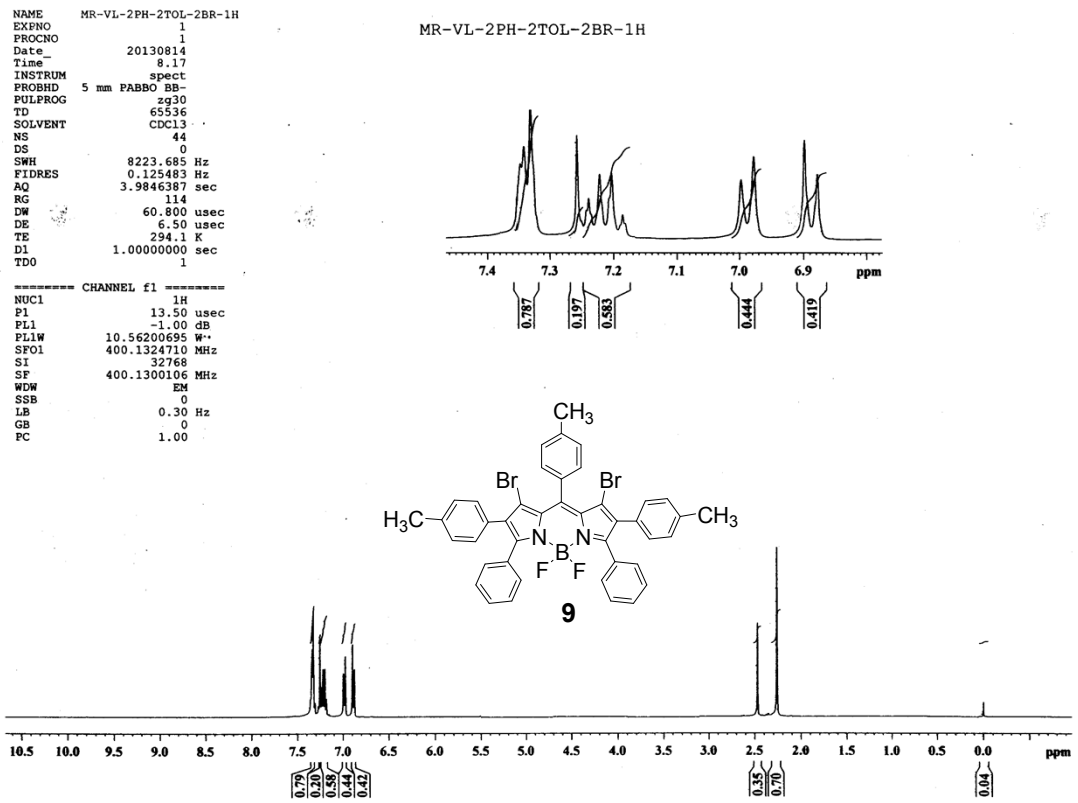


Figure S32: The ^{1}H NMR spectrum of compound **9** recorded in $CDCl_3$

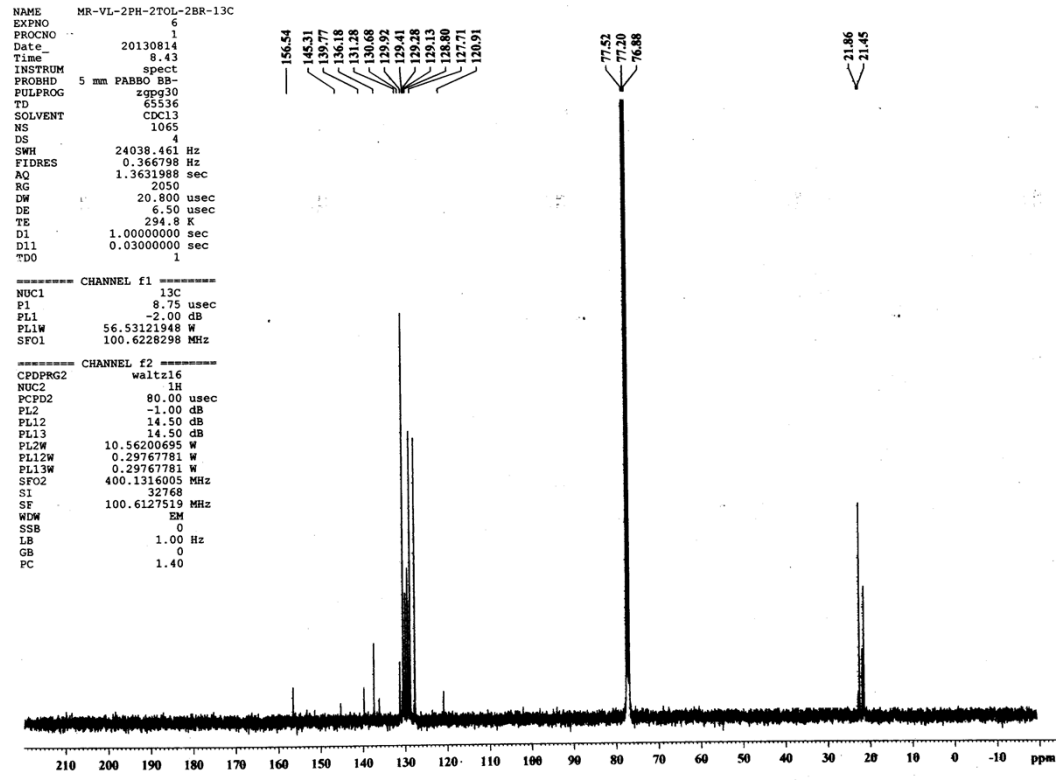


Figure S33: The ^{13}C NMR spectrum of compound **9** recorded in $CDCl_3$.

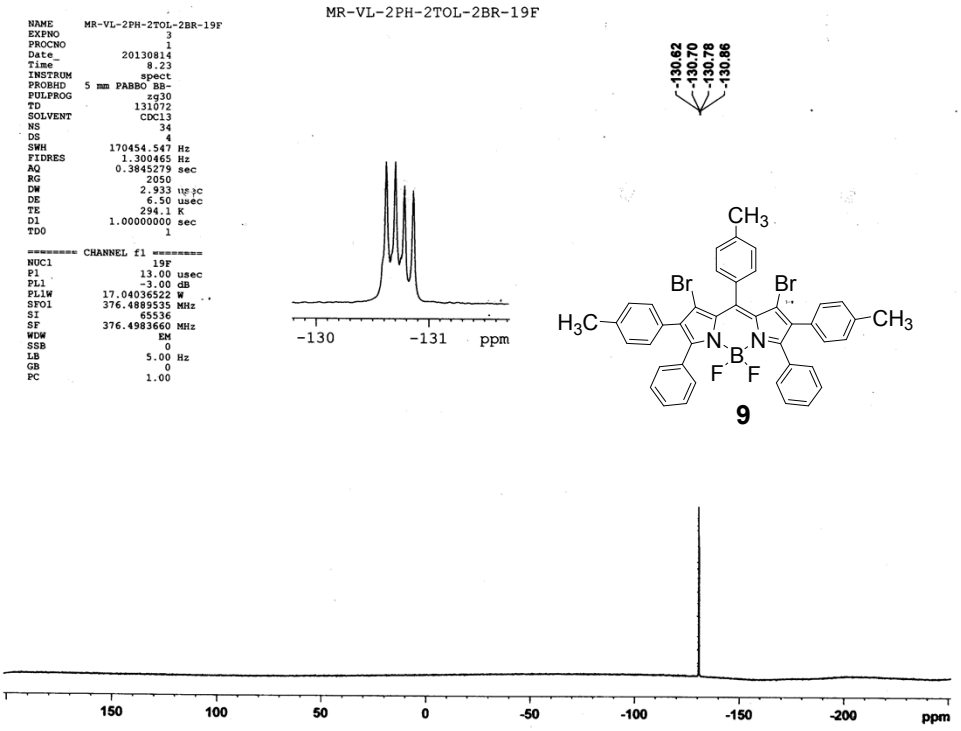


Figure S34: The ^{19}F NMR spectrum of compound **9** recorded in $CDCl_3$.

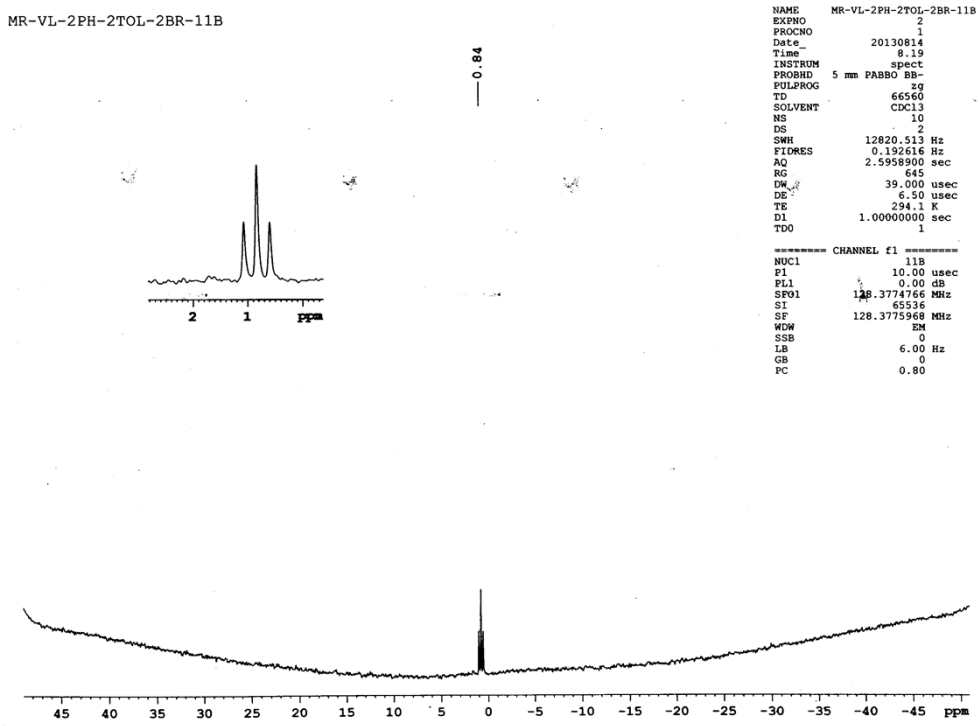
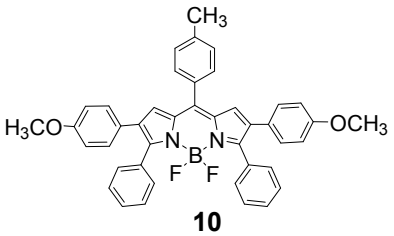


Figure S35: The ^{11}B NMR spectrum of compound **9** recorded in $CDCl_3$.



10

Indian Institute of Technology (B)

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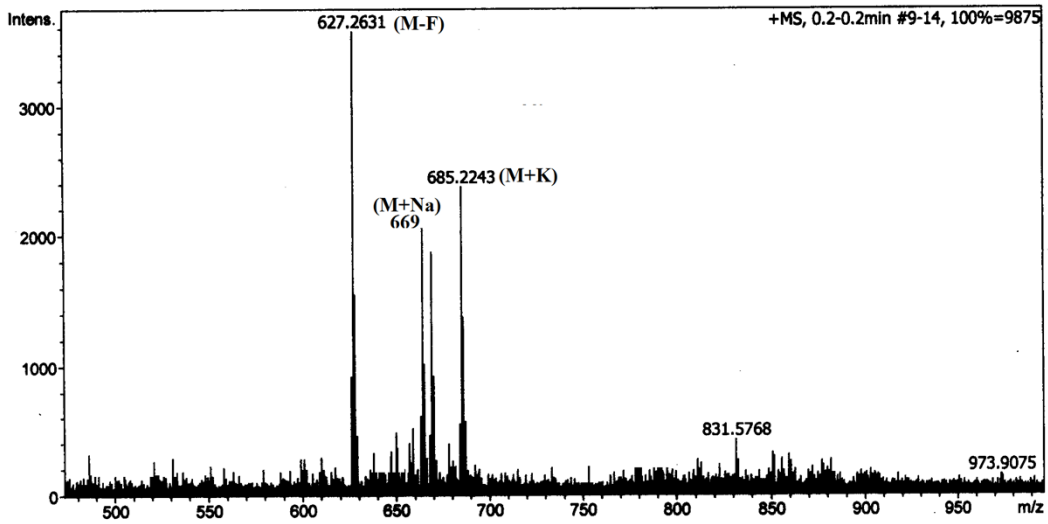
Comment	C42H33BF2N2O2		

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**

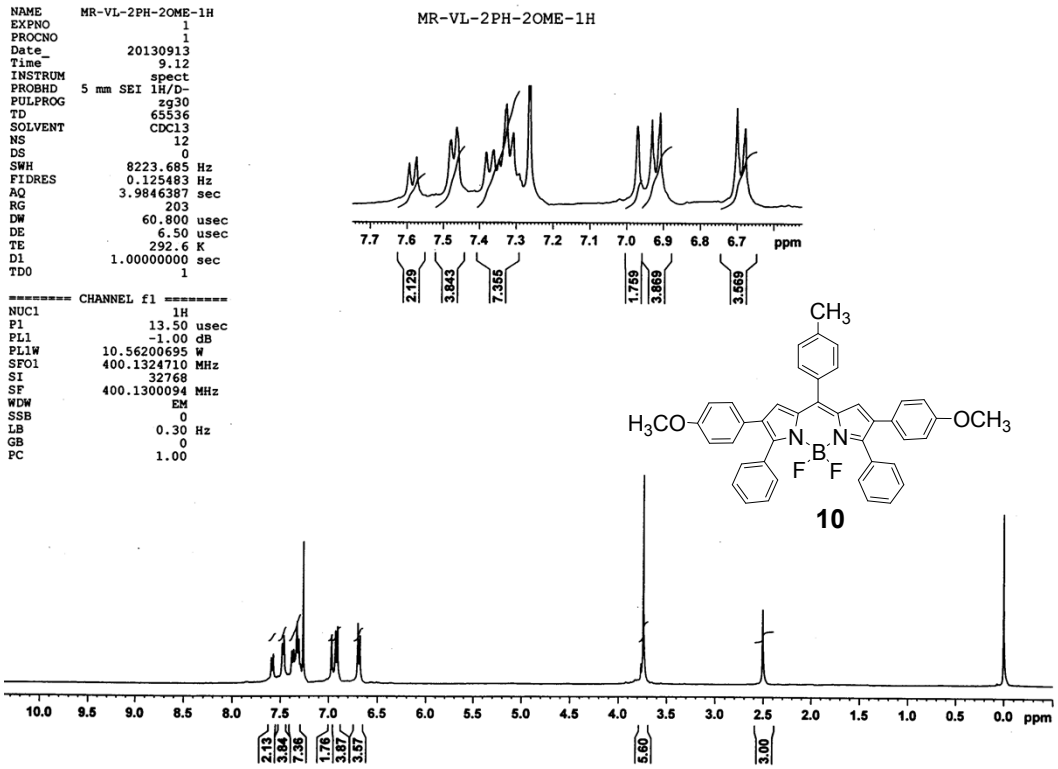


Figure S37: The ^{1}H NMR spectrum of compound **10** recorded in $CDCl_3$.

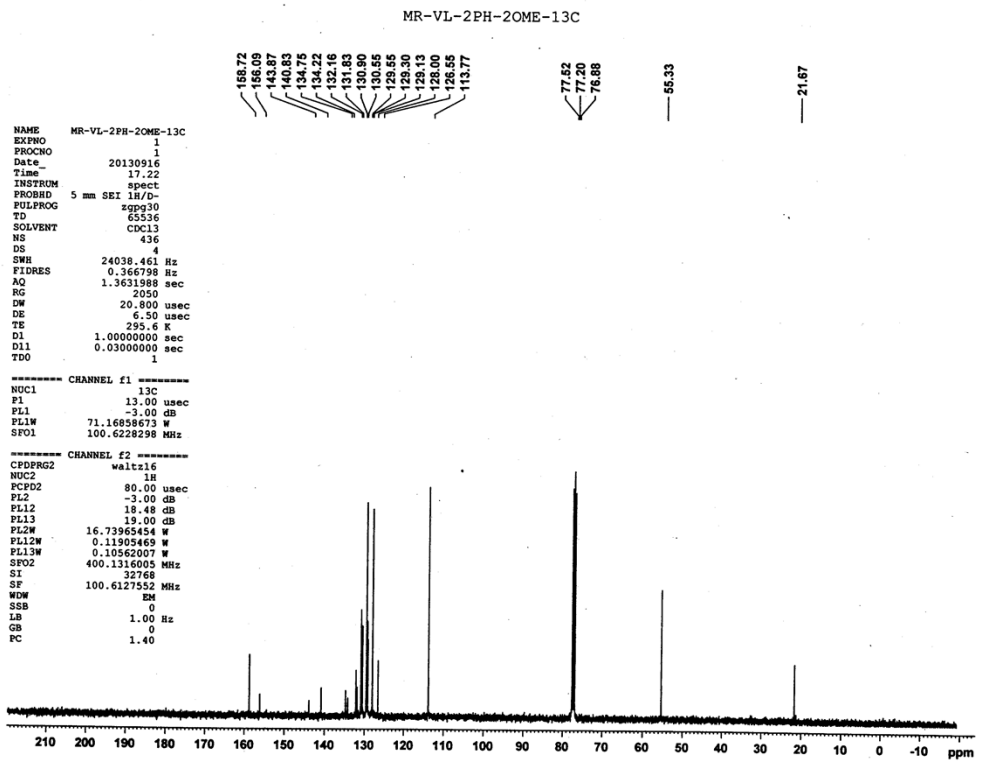


Figure S38: The ^{13}C NMR spectrum of compound **10** recorded in $CDCl_3$.

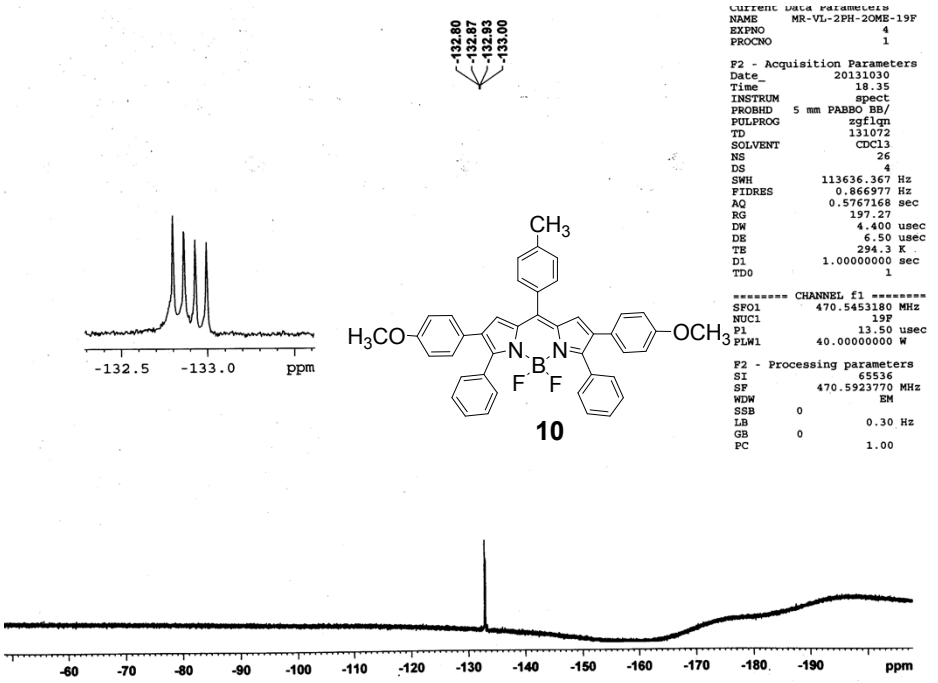


Figure S39: The ^{19}F NMR spectrum of compound **10** recorded in $CDCl_3$

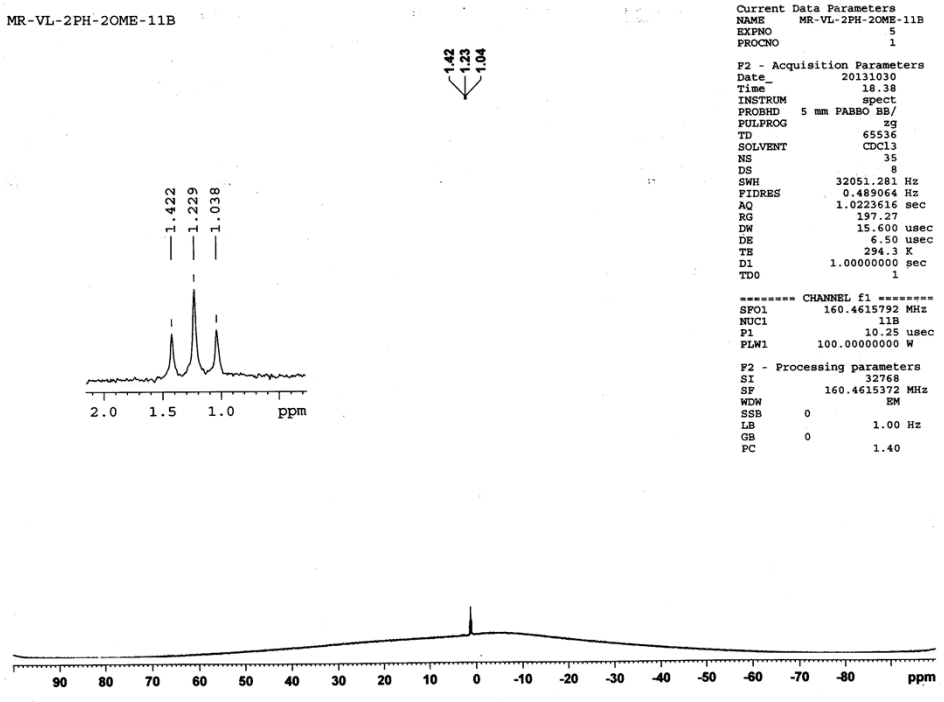
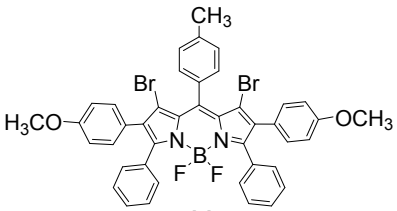


Figure S40: The ^{11}B NMR spectrum of compound **10** recorded in $CDCl_3$.



11

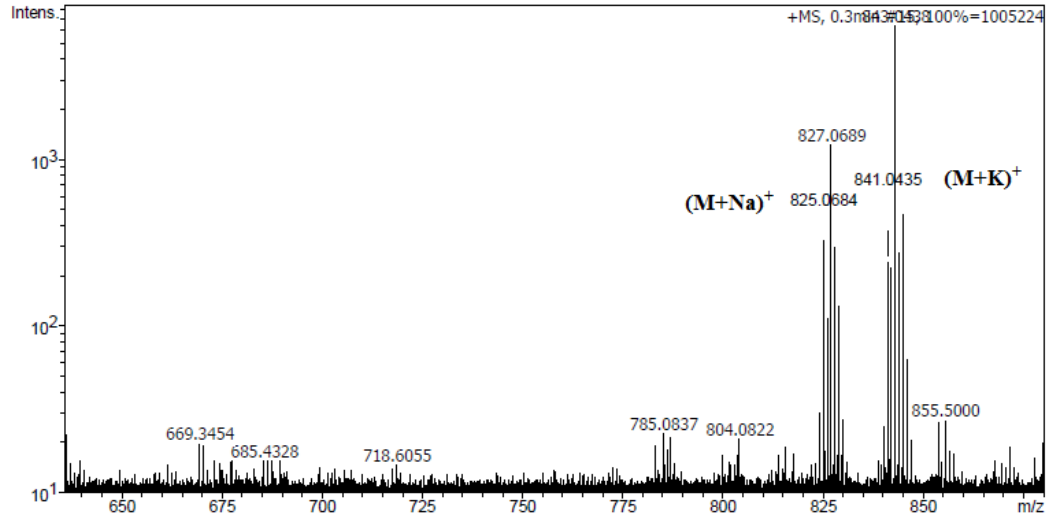
Indian Institute of Technology (B)

Analysis Info

Analysis Name	D:\Data\SEPT-13\MR-VL-2OME-2BR-1.d	Acquisition Date	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**

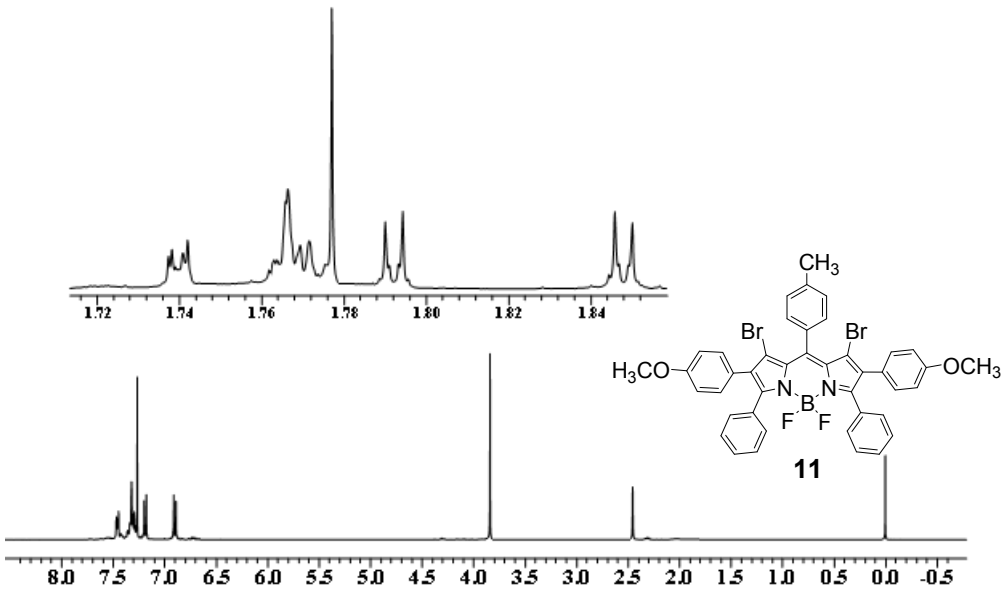


Figure S42: The ^{1}H NMR spectrum of compound **11** recorded in $CDCl_3$

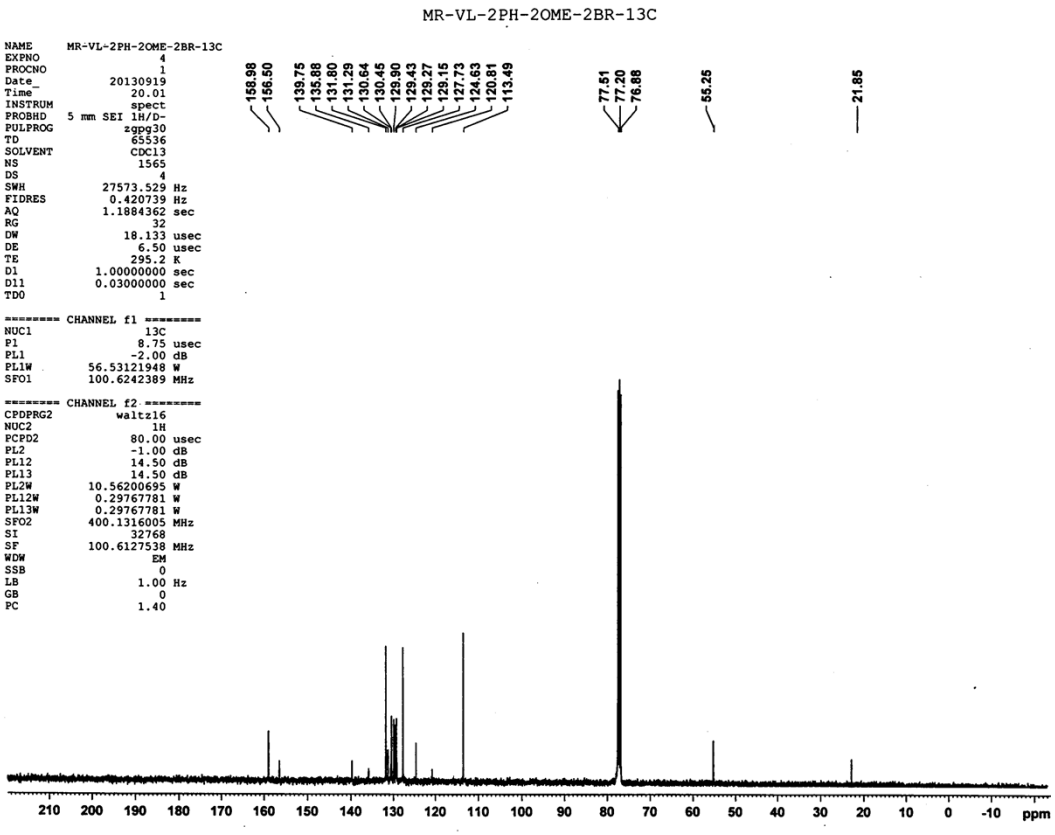


Figure S43: The ^{13}C NMR spectrum of compound **11** recorded in $CDCl_3$

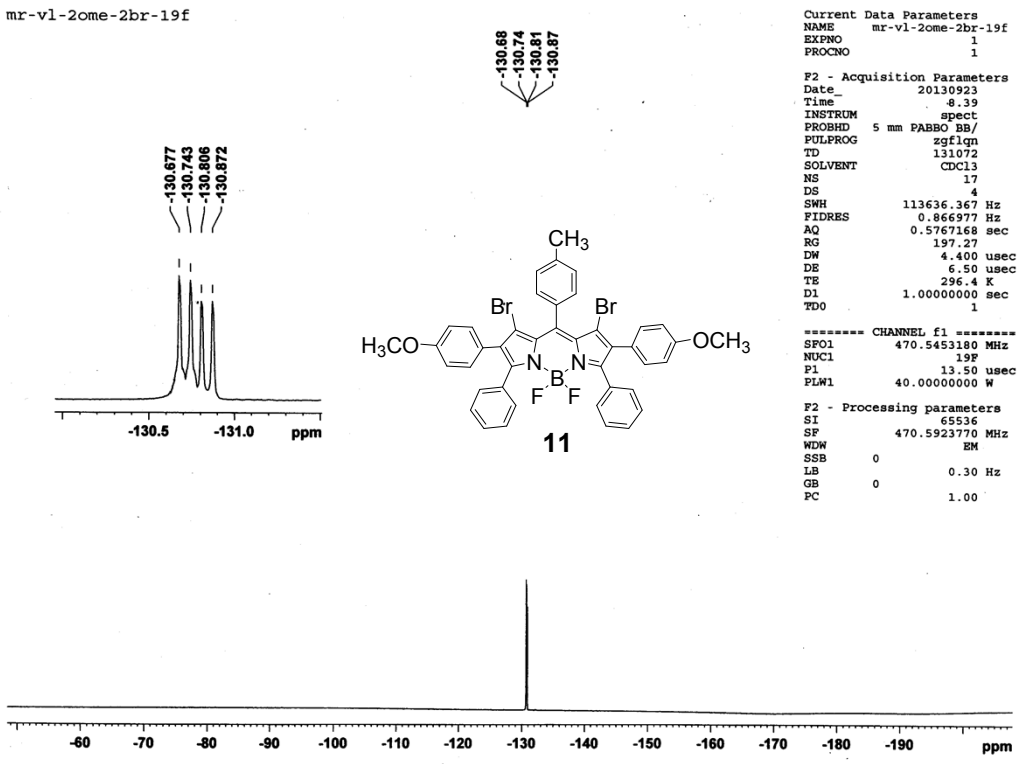


Figure S44: The ^{19}F NMR spectrum of compound **11** recorded in $CDCl_3$

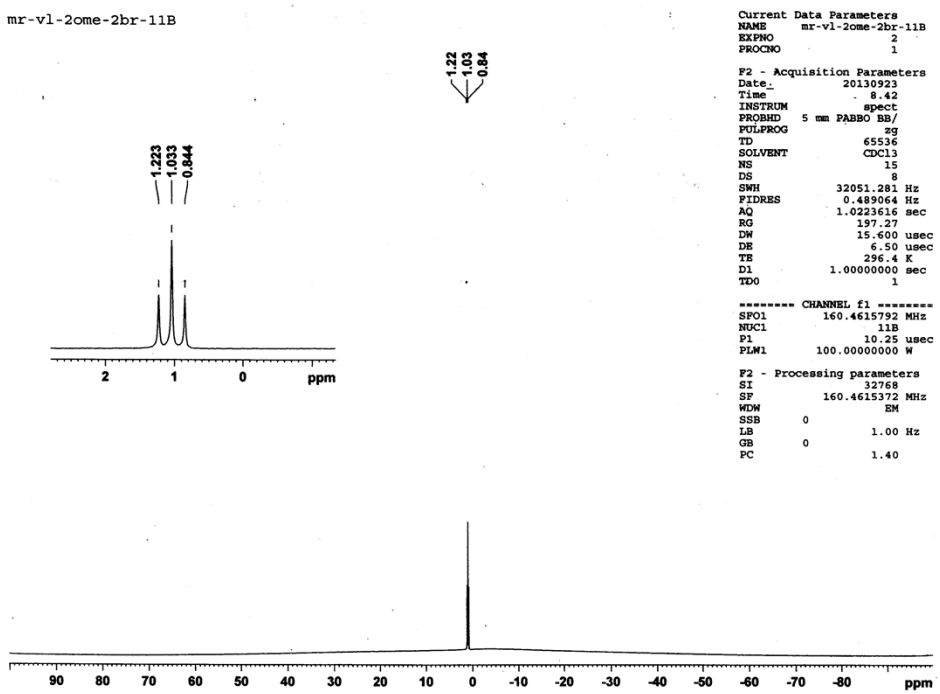
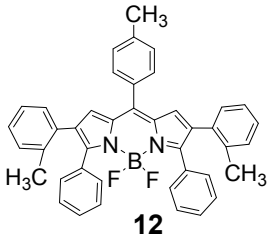


Figure S45: The ^{11}B NMR spectrum of compound **11** recorded in $CDCl_3$



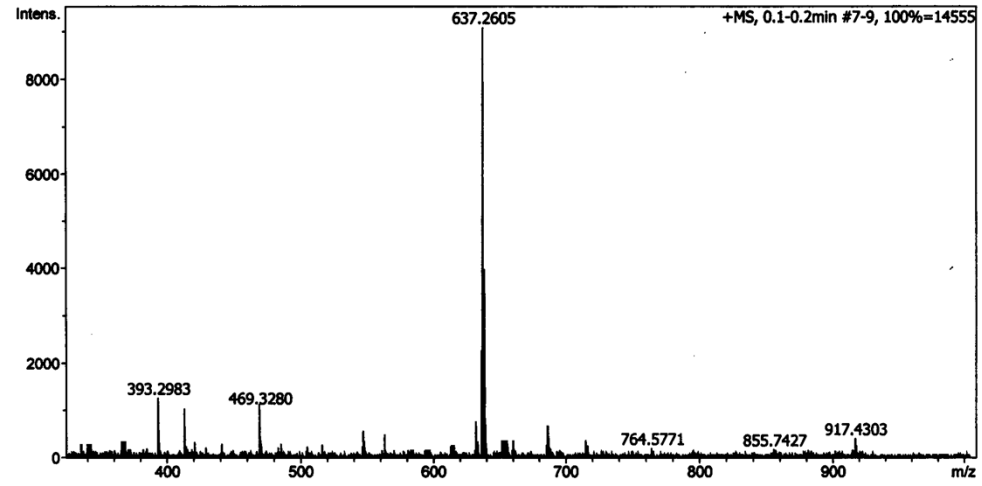
12

Indian Institute of Technology (B)

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

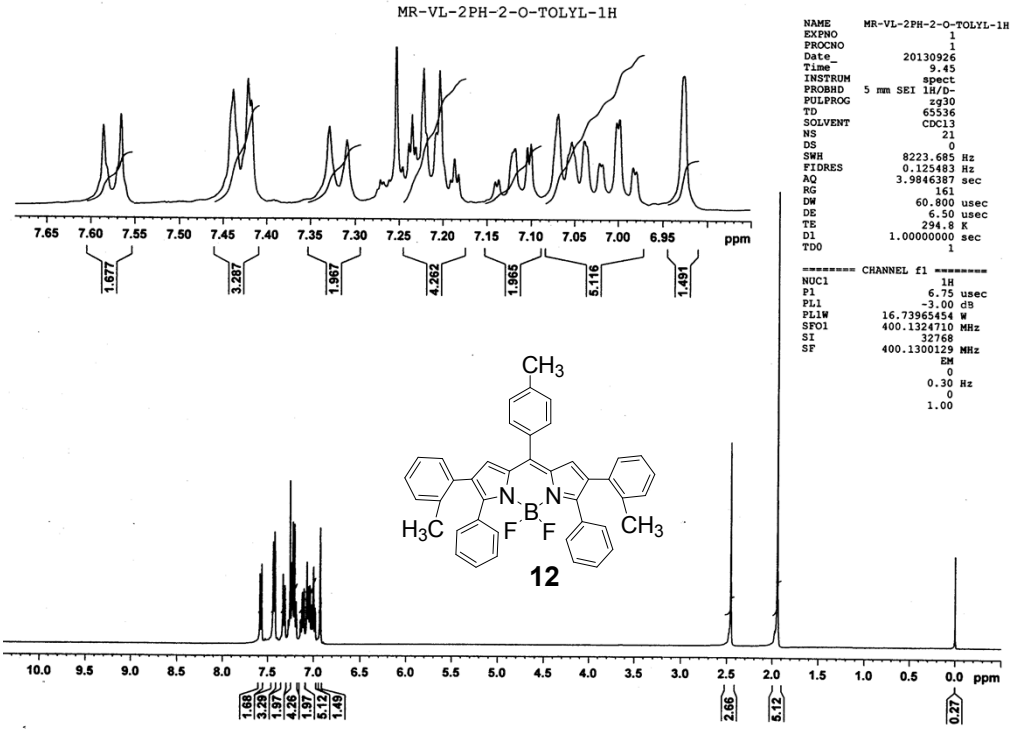


Figure S47: The ^{1}H NMR spectrum of compound **12** recorded in $CDCl_3$

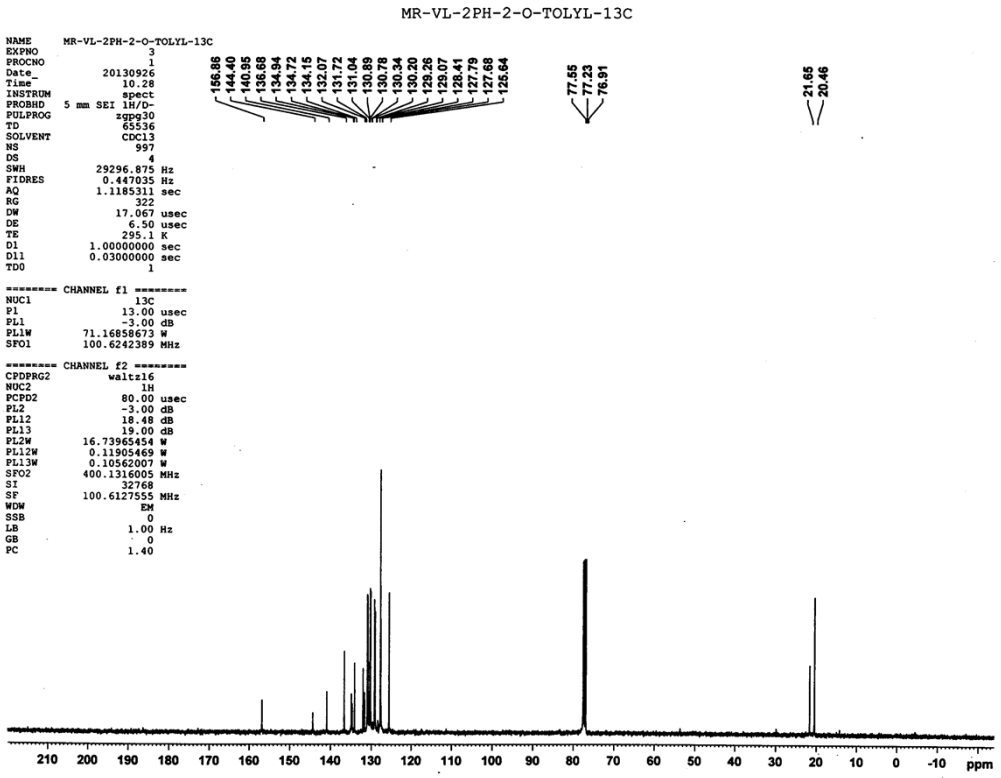


Figure S48: The ^{13}C NMR spectrum of compound **12** recorded in $CDCl_3$

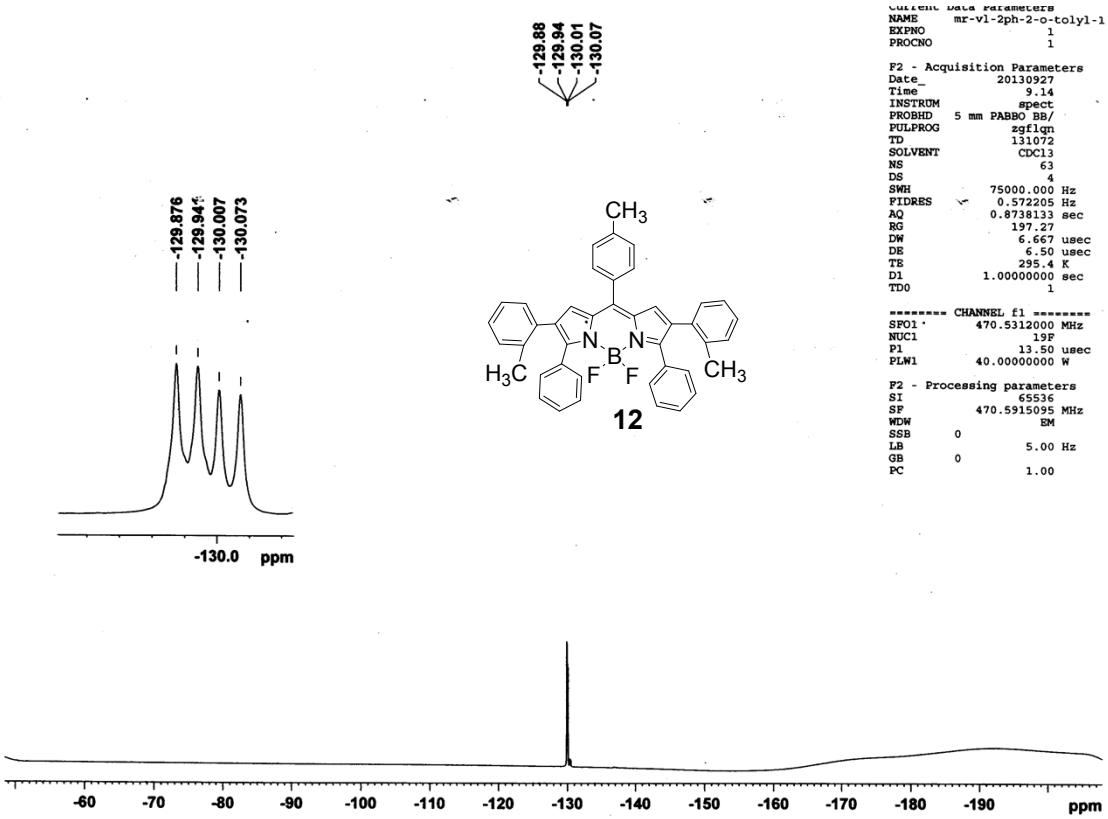


Figure S49: The ^{19}F NMR spectrum of compound **12** recorded in $CDCl_3$

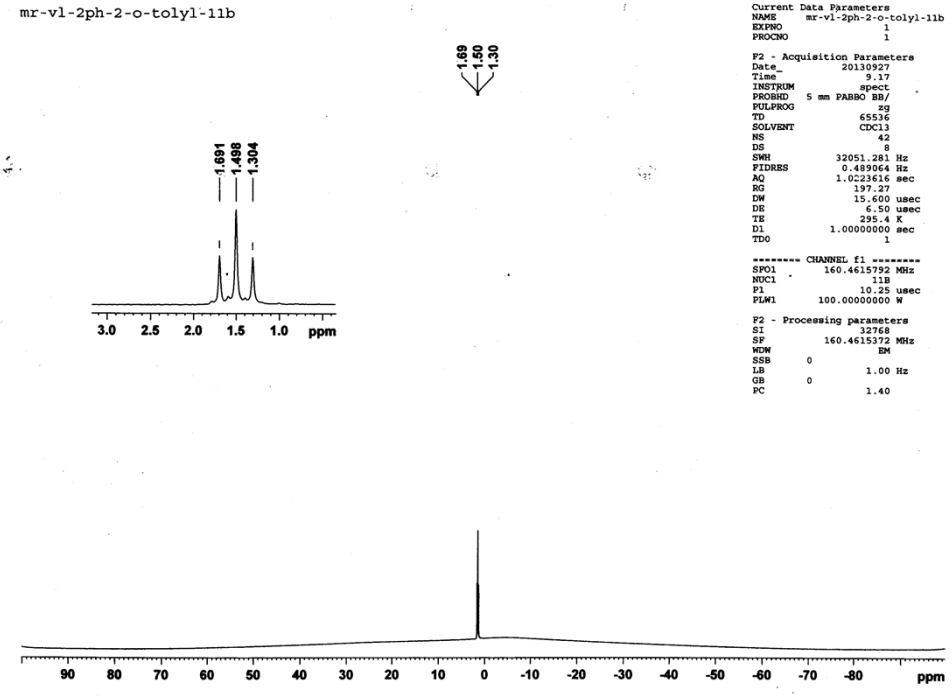
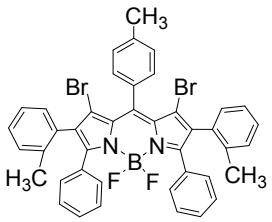


Figure S50: The ^{11}B NMR spectrum of compound **12** recorded in $CDCl_3$



13

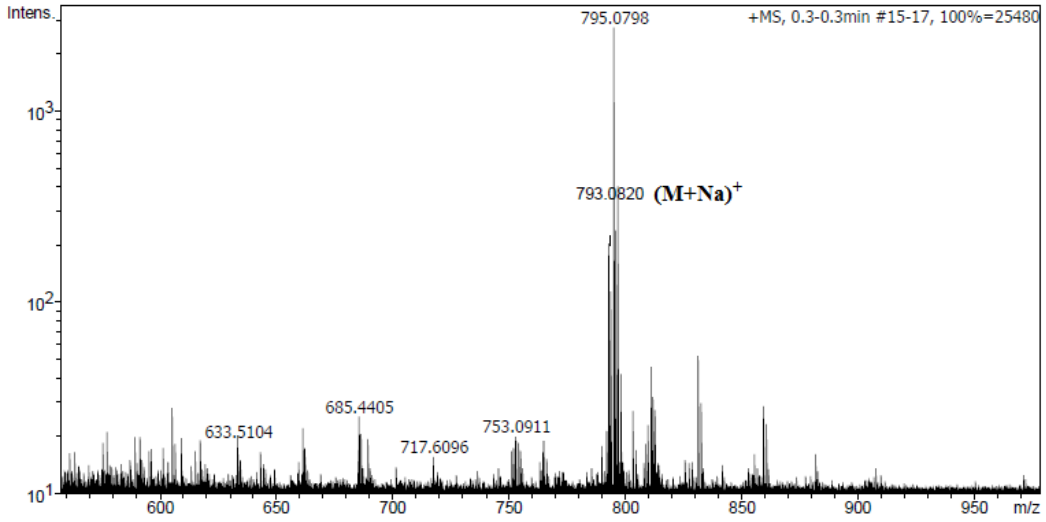
Indian Institute of Technology (B)

Analysis Info

Analysis Name	D:\Data\SEPT-13\MR-VL-2PH-2-O-TOL-2BR.d	Acquisition Date	9/30/2013 6:50:53 PM
Method	Tune_pos_Standard_NAI-1000.m	Operator	KPK- OUT
Sample Name	MR-VL-2PH-2-O-TOL-2BR	Instrument	maXis impact 282001.00081
Comment	C42H31BBR2F2N2		

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**.

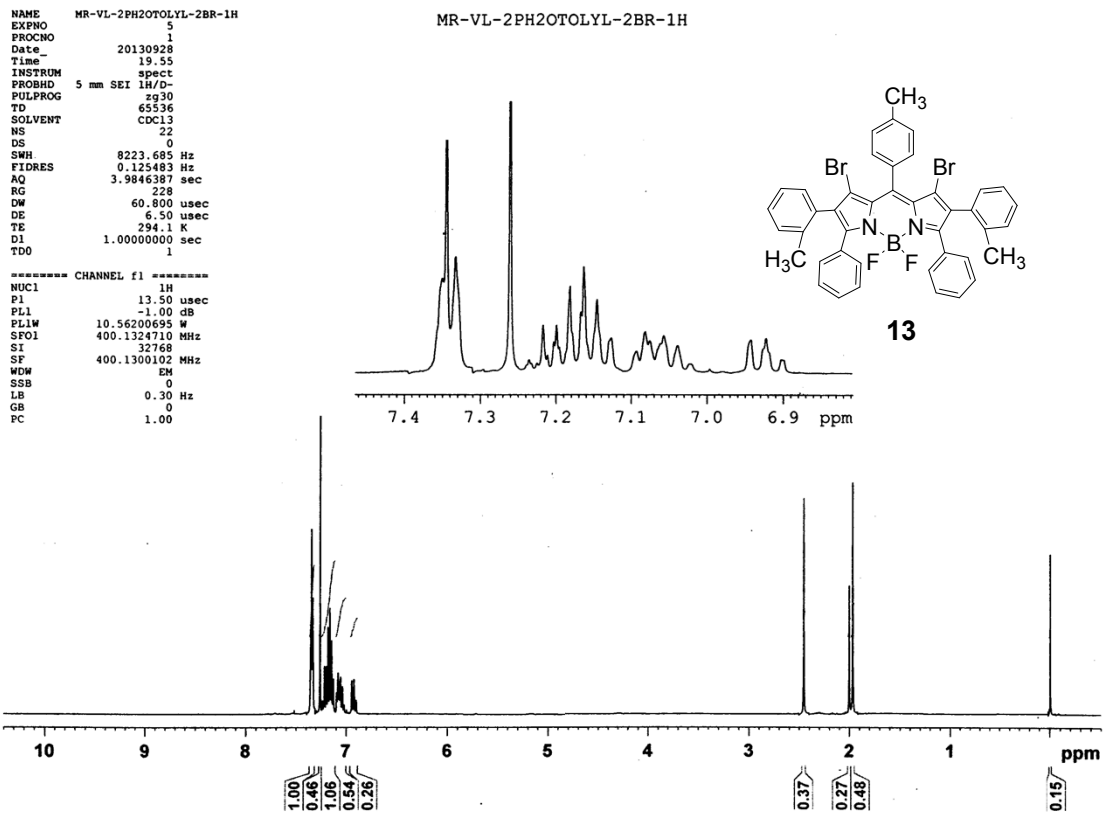


Figure S52: The ^{1}H NMR spectrum of compound **13** recorded in $CDCl_3$.

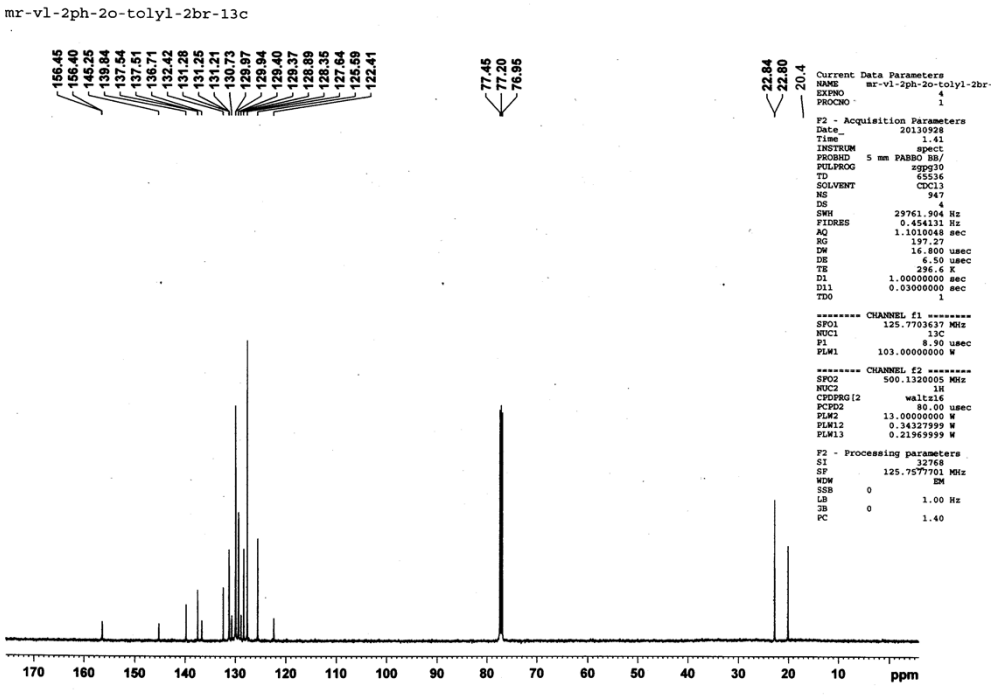


Figure S53: The ^{13}C NMR spectrum of compound **13** recorded in $CDCl_3$.

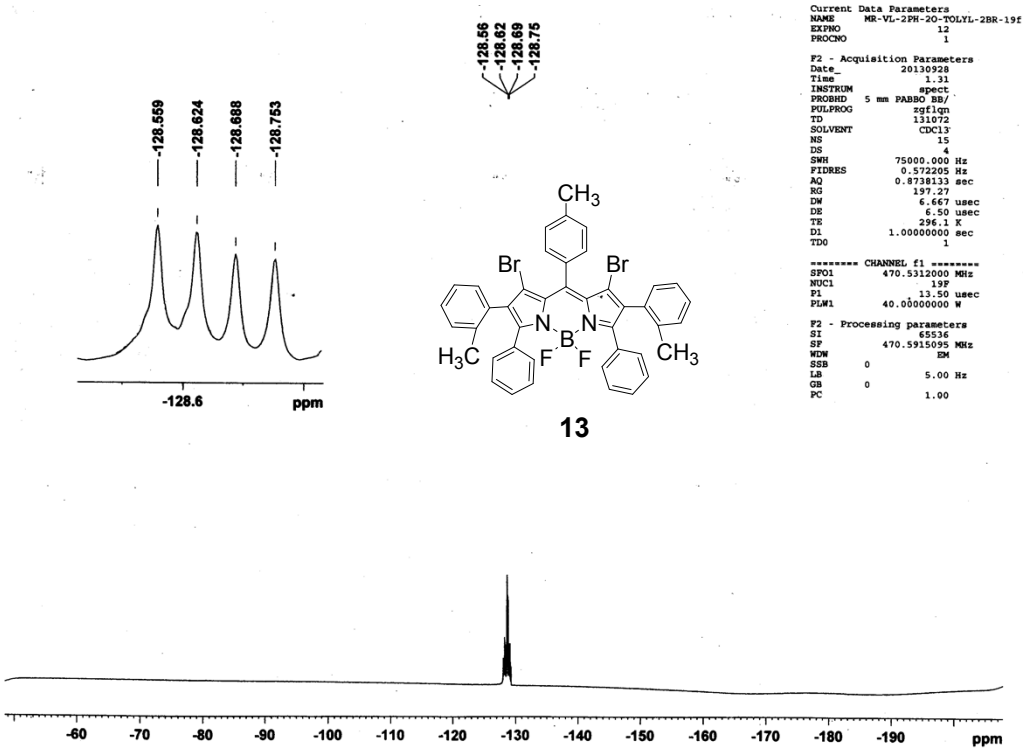


Figure S54: The ^{19}F NMR spectrum of compound **13** recorded in $CDCl_3$.

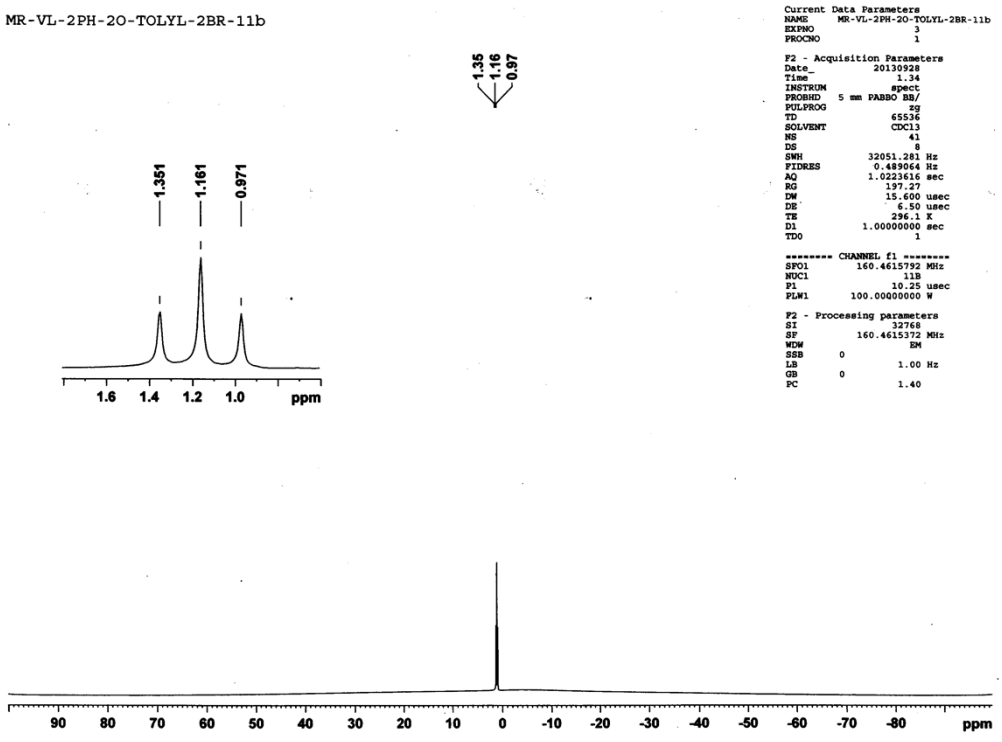
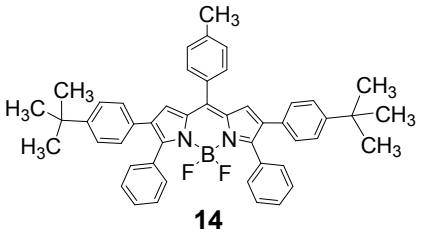


Figure S55: The ^{11}B NMR spectrum of compound **13** recorded in $CDCl_3$.



14

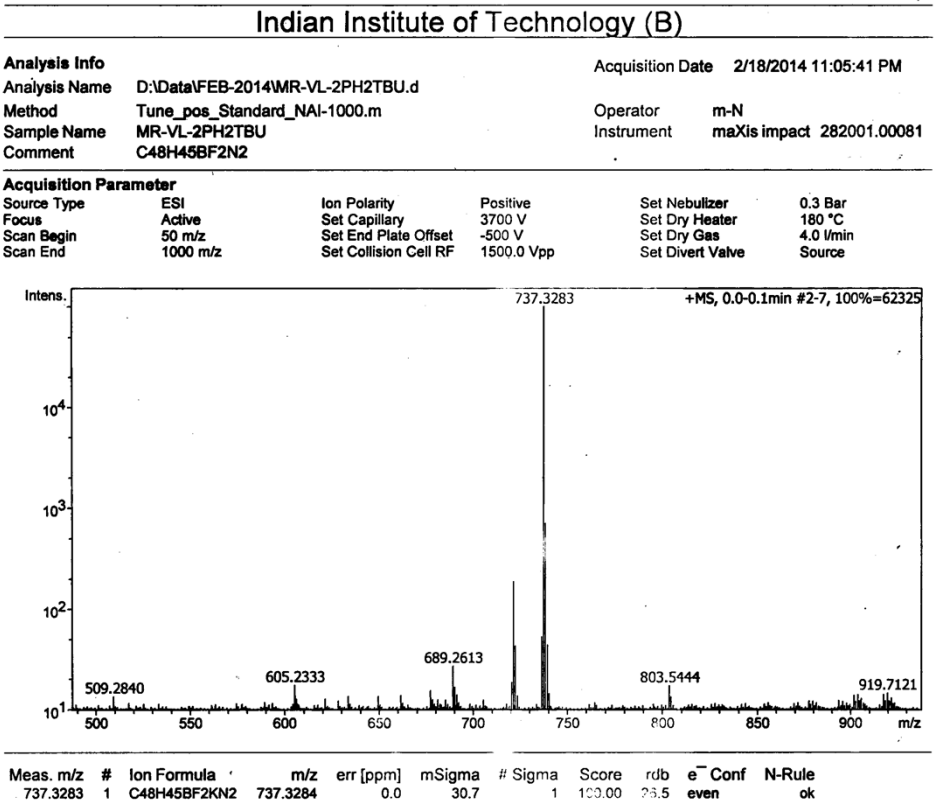


Figure S56: The HRMS of compound **14.**

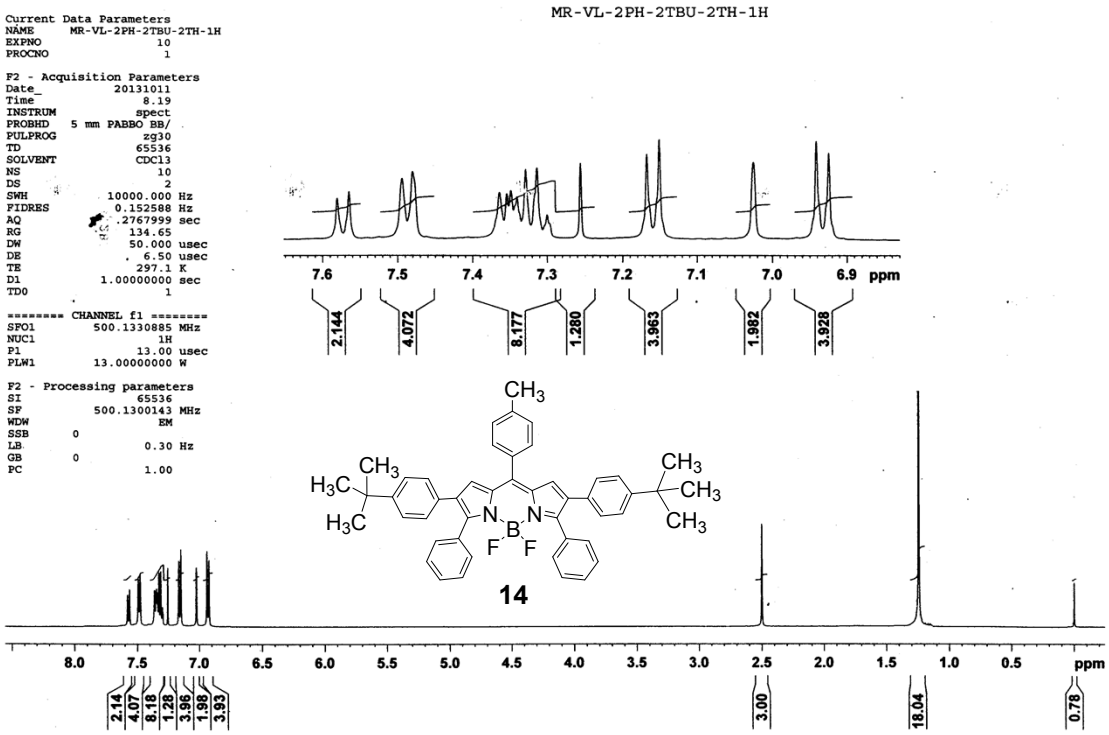


Figure S57: The ^{1}H NMR spectrum of compound **14** recorded in $CDCl_3$.

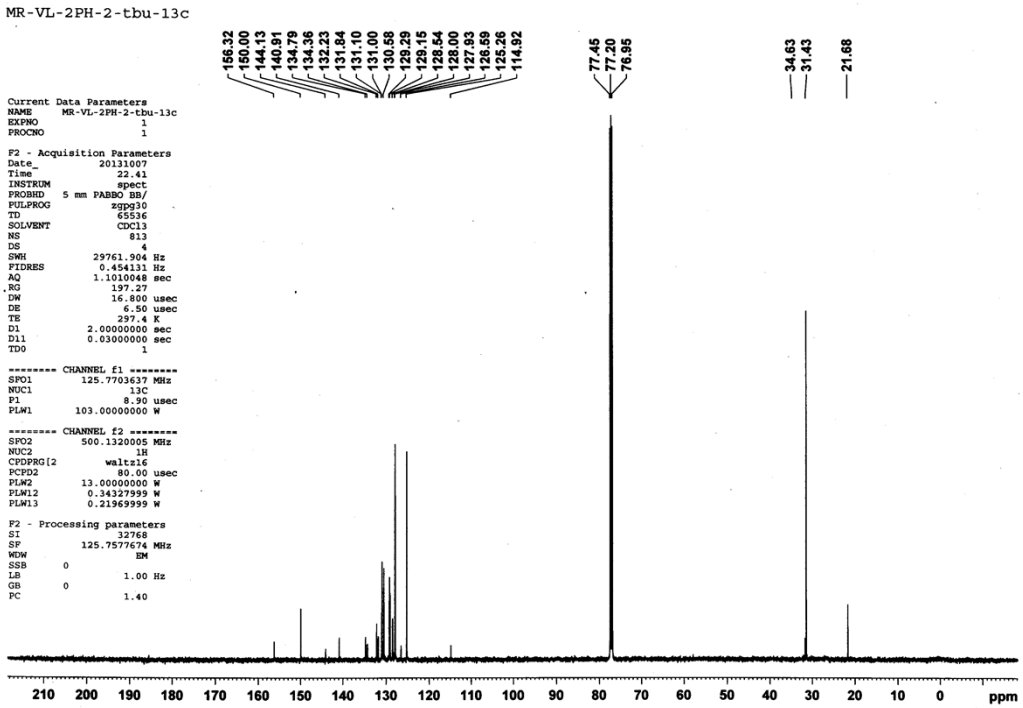


Figure S58: The ^{13}C NMR spectrum of compound **14** recorded in $CDCl_3$.

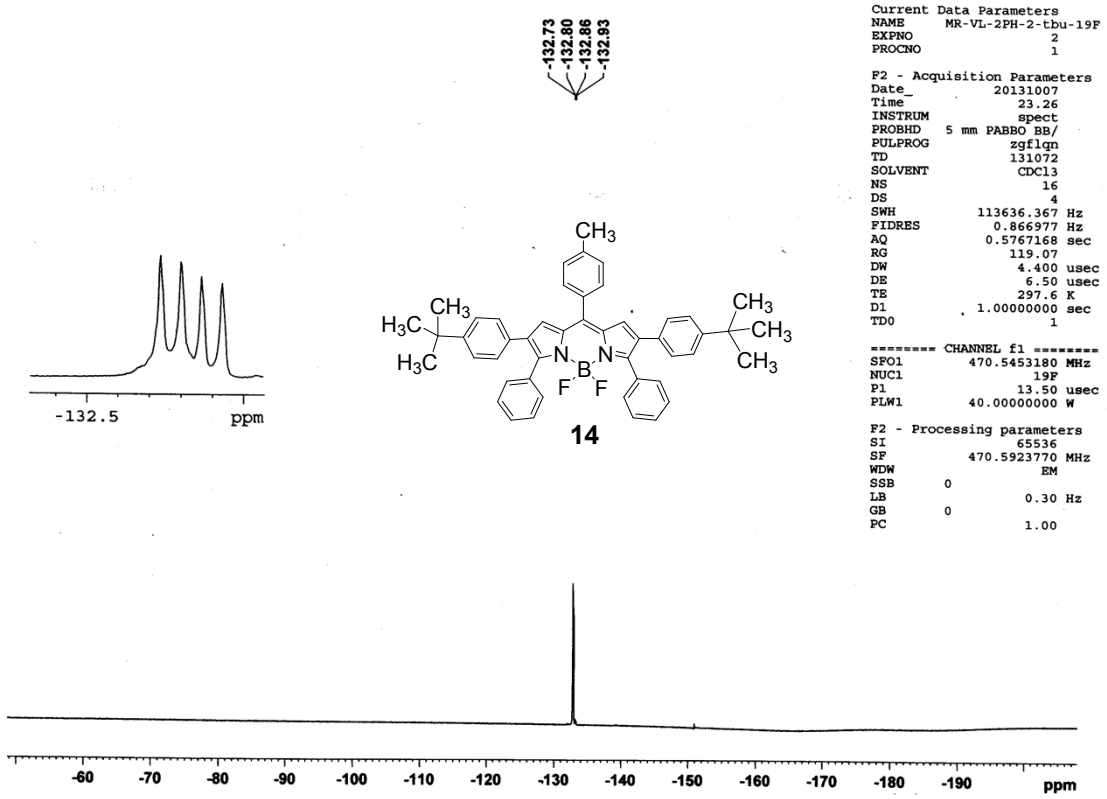


Figure S59: The ^{19}F NMR spectrum of compound **14** recorded in $CDCl_3$.

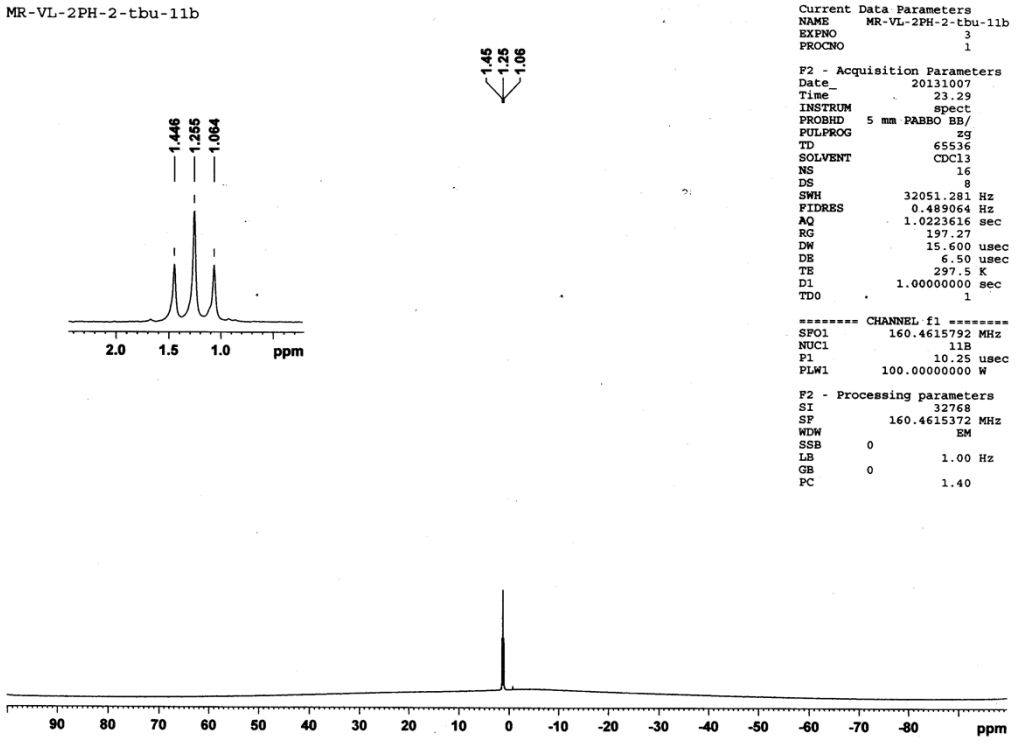
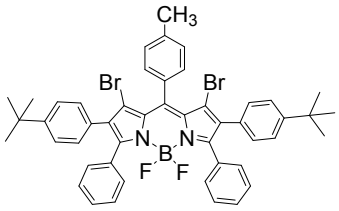


Figure S60: The ^{11}B NMR spectrum of compound **14** recorded in $CDCl_3$.



15

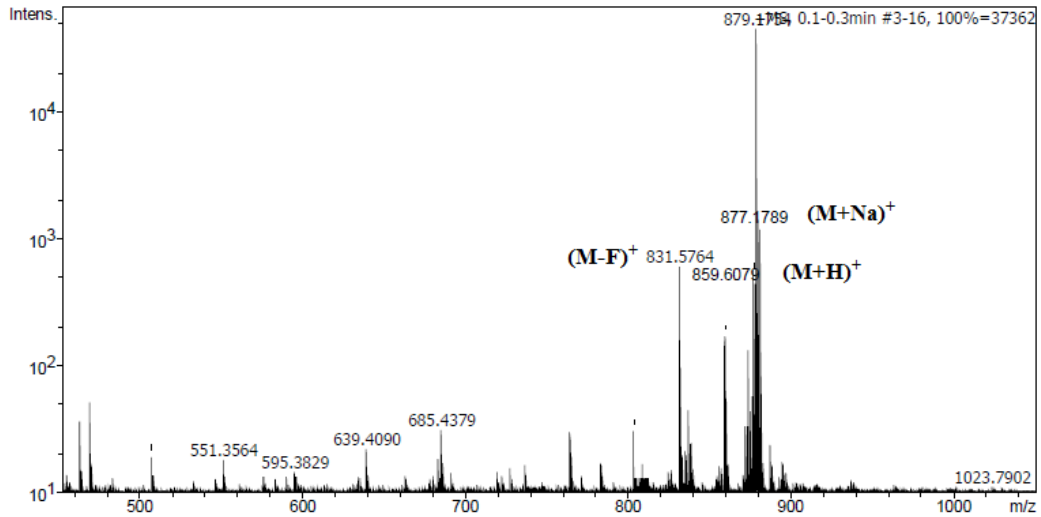
Indian Institute of Technology (B)

Analysis Info

Analysis Name	D:\Data\OCT-13\MR-VL-2PH-2T-BU-2BR.d	Acquisition Date	10/22/2013 7:35:14 PM
Method	Tune_pos_Standard_NAI-1500.m	Operator	SSK OUT
Sample Name	MR-VL-2PH-2T-BU-2BR	Instrument	maXis impact 282001.00081
Comment	C48H43BBr2F2N2		

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.**

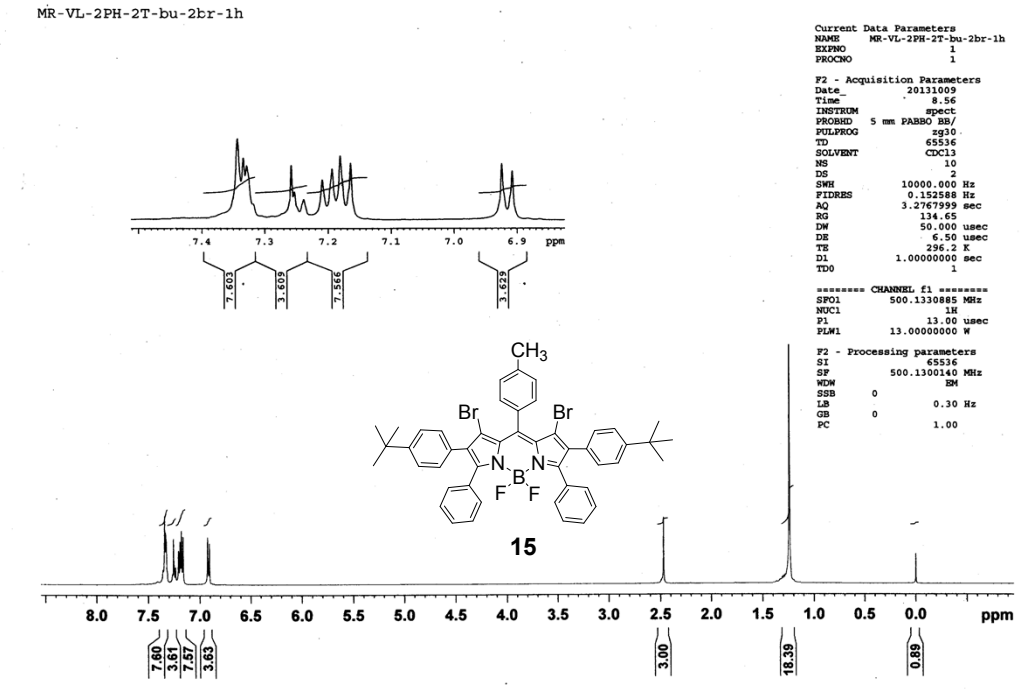


Figure S62: The ^{1}H NMR spectrum of compound **15** recorded in $CDCl_3$.

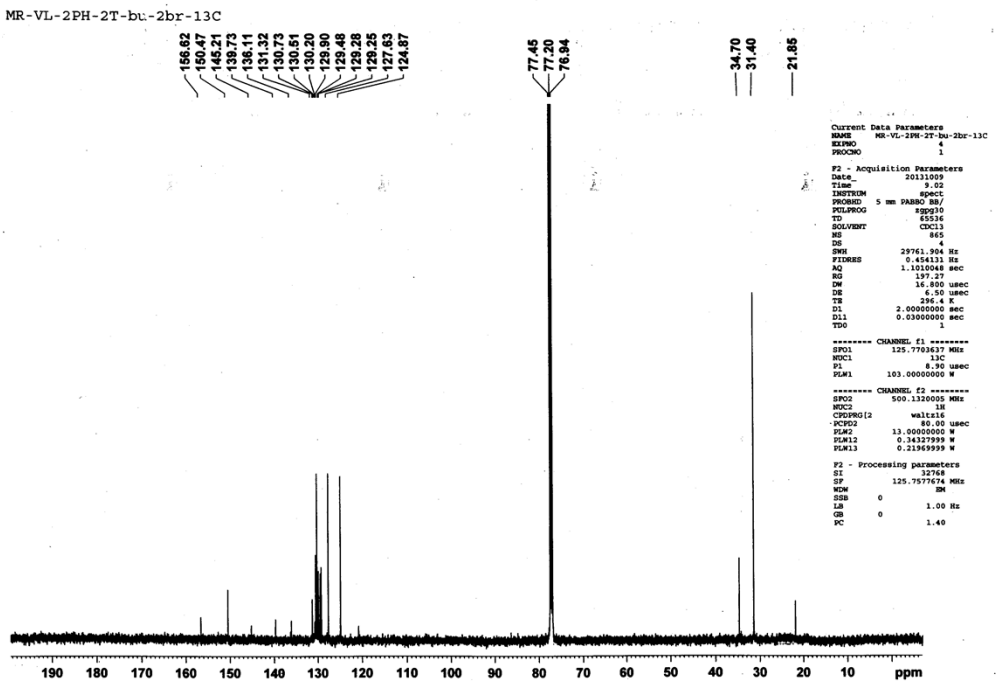


Figure S63: The ^{13}C NMR spectrum of compound **15** recorded in $CDCl_3$.

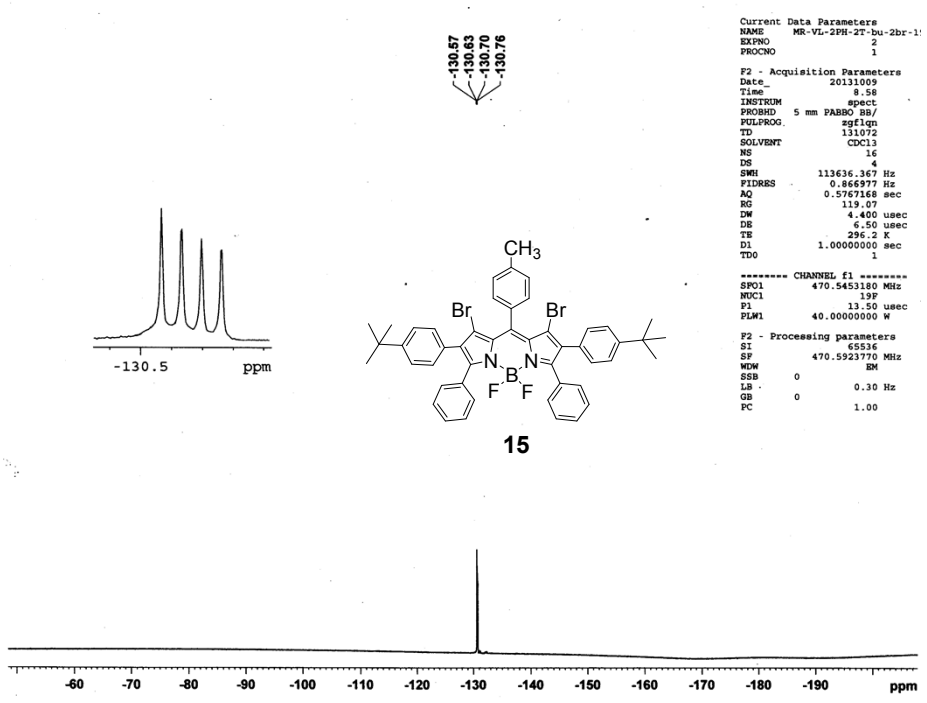


Figure S64: The ^{19}F NMR spectrum of compound **15** recorded in $CDCl_3$.

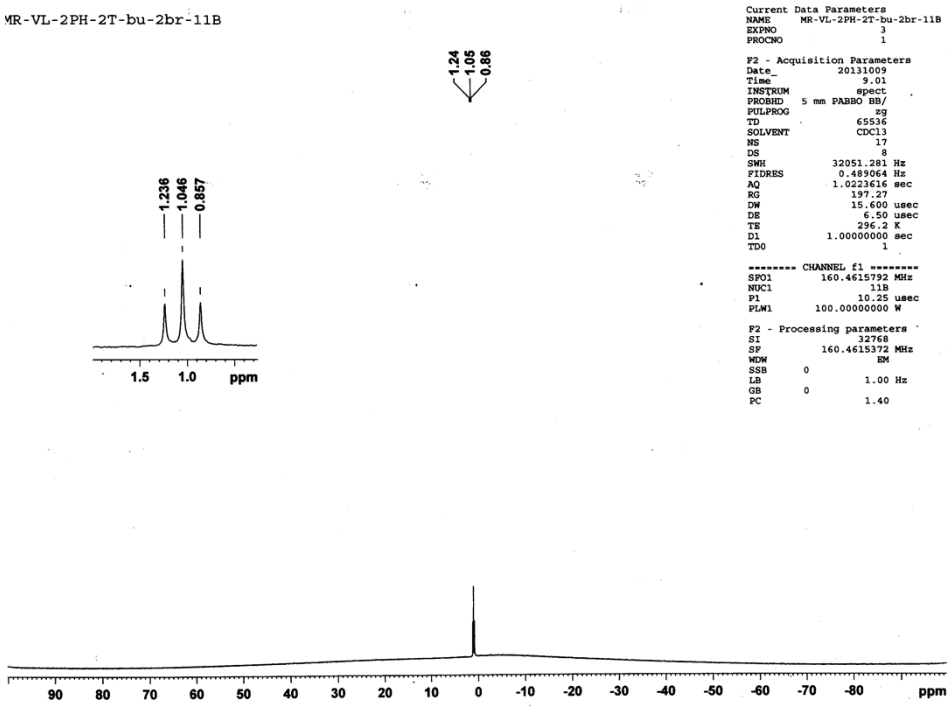


Figure S65: The ^{11}B NMR spectrum of compound **15** recorded in $CDCl_3$.

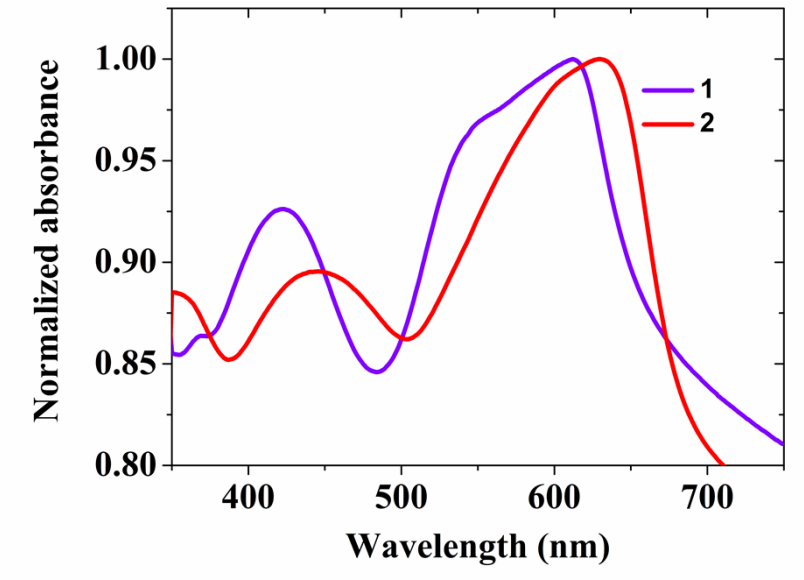


Figure S66: The normalized absorption spectra of compounds **1** (violet) and **2** (red) in solid state.

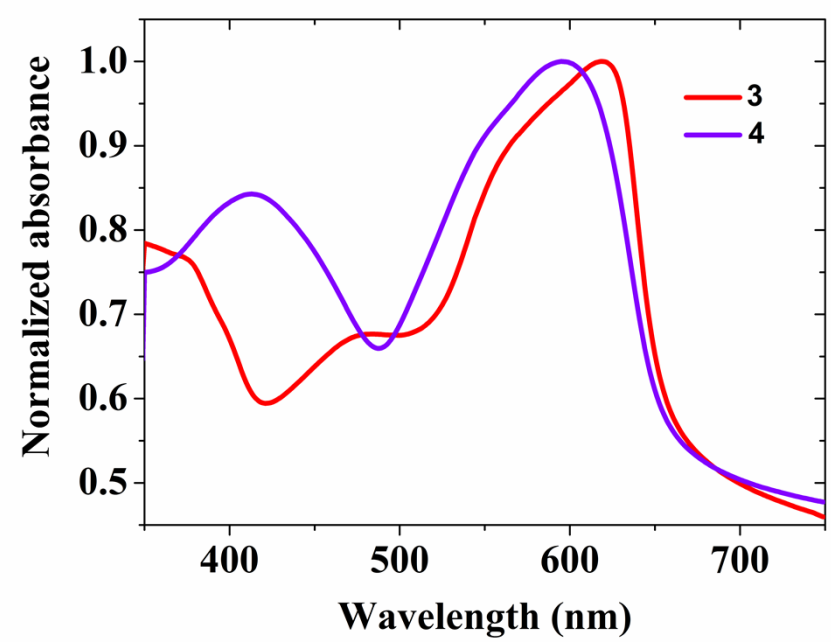


Figure S67: The normalized absorption spectra of compounds **3** (red) and **4** (violet) in solid state.

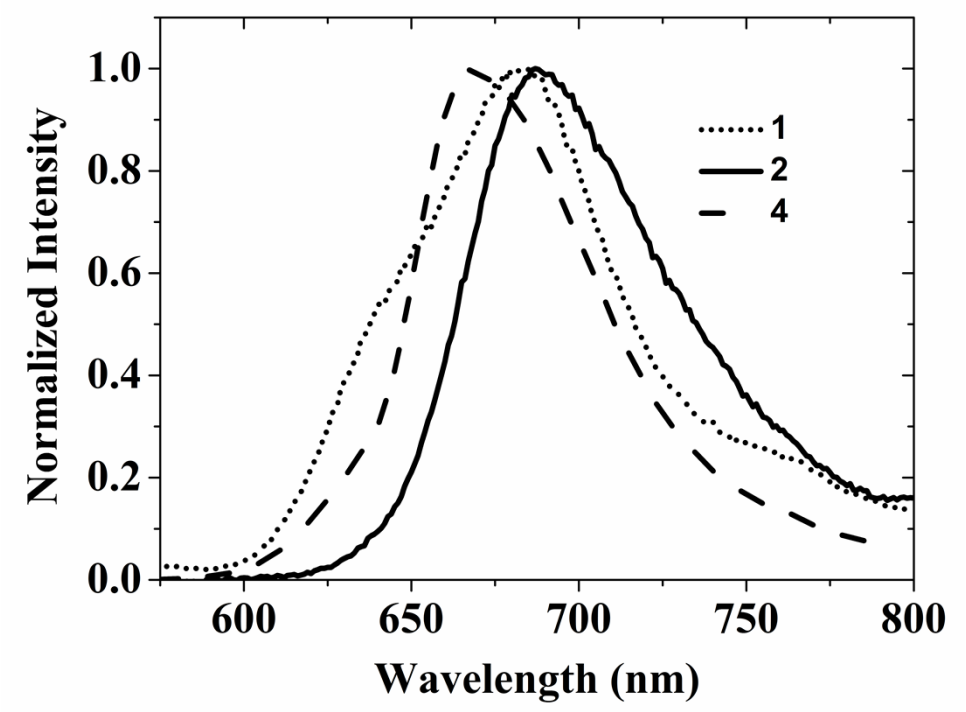


Figure S68: The normalized emission spectra of compounds **1** (dotted line), **2** (solid line) and **4** (dashed line) in solid state.