

Supporting Information

Development of excellent long-wavelength BODIPY laser dyes with a strategy that combines extending π -conjugation and tuning ICT effect

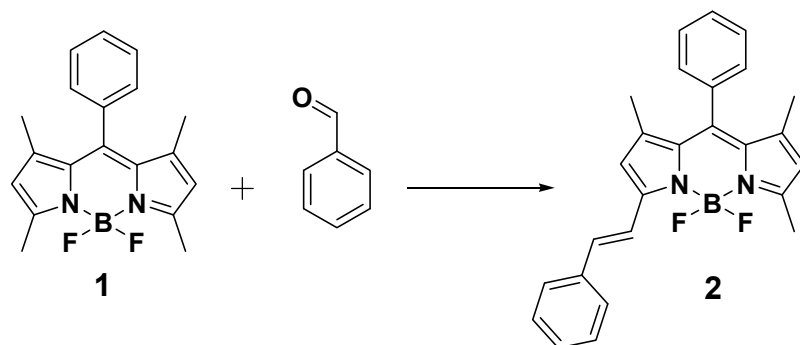
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M. Eugenia Perez-Ojeda,^b and Yi Xiao^{*a}

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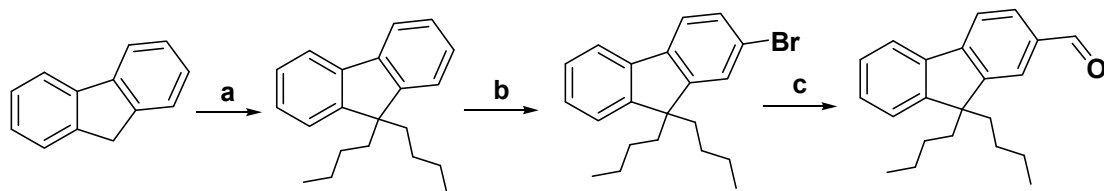
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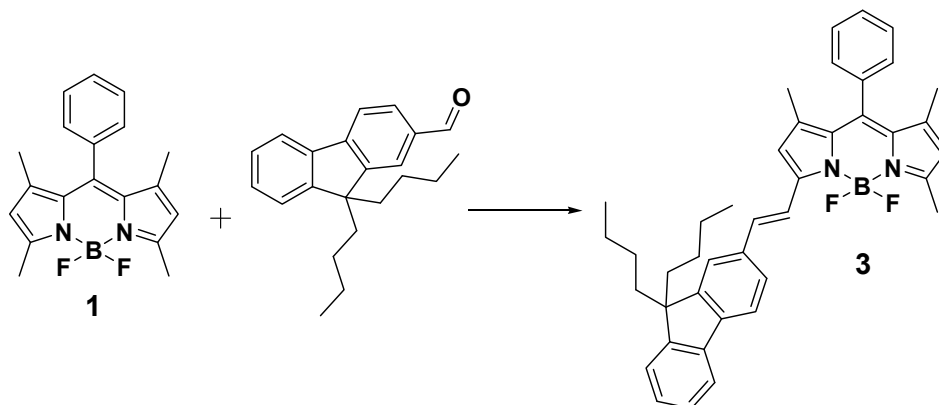
Routes for the synthesis of the new dyes



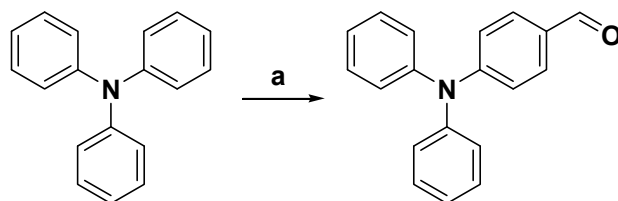
Routes to 9,9-dibutyl-9*H*-fluorene-2-carbaldehyde:



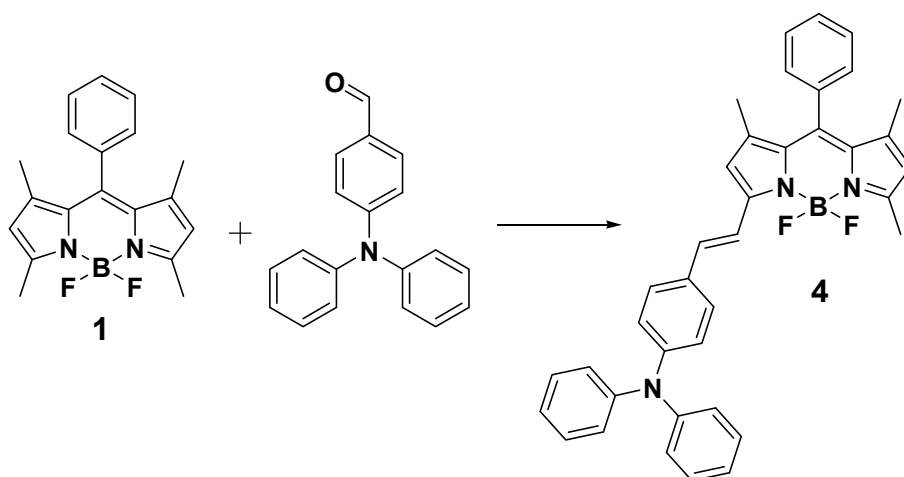
a. NaOH, DMSO, n-BuBr, 90°C, 80%. b. NBS, acetone, 80°C, 87%. c. n-BuLi, THF, -78°C-20°C, then, DMF, -78°C-20°C, 45%.



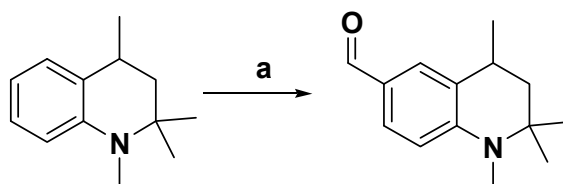
Routes to 4-(diphenylamino)benzaldehyde:



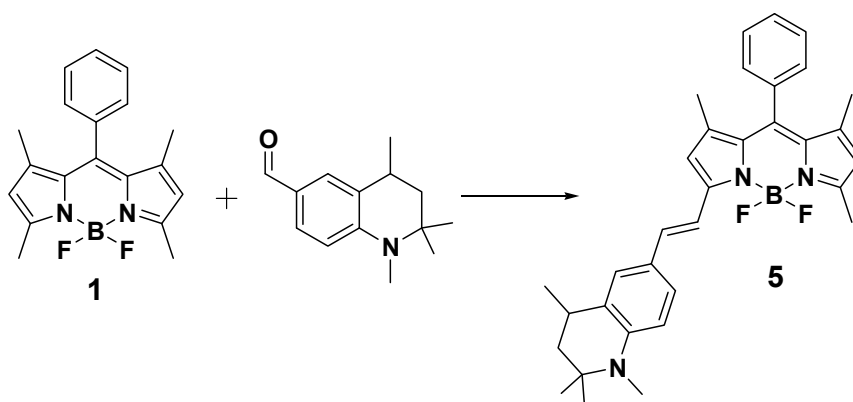
a. Vilsmeier reaction. POCl₃, DMF, 1h, rt, then, 2 h, 90°C, 80%.



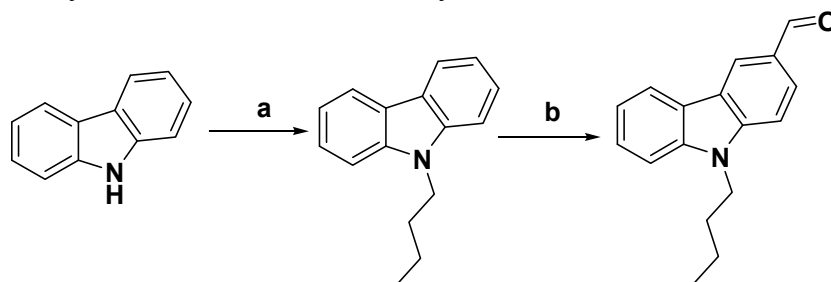
Routes to 1,2,2,4-tetramethyl-1,2,3,4-tetrahydroquinoline-6-carbaldehyde:



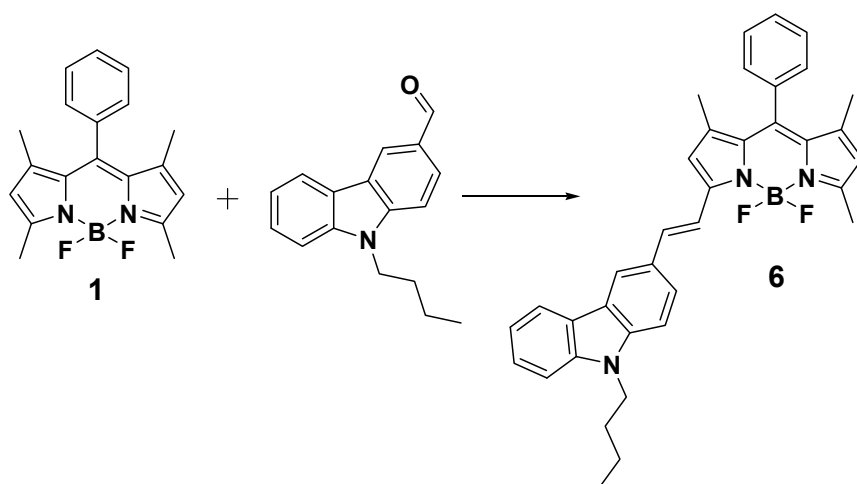
a. Vilsmeier reaction. POCl_3 , DMF, 2 h, 0°C , then, 6 h, 60°C , 50%.



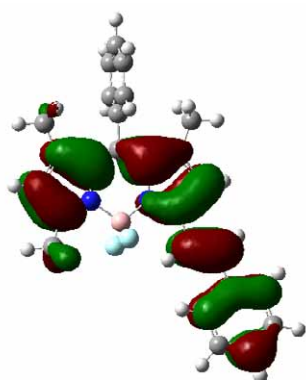
Routes to 9-butyl-9H-carbazole-3-carbaldehyde:



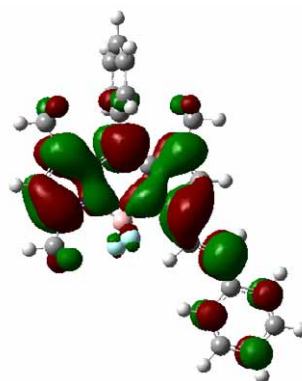
a. BuBr, KOH, Bu_4NBr , DMSO, 80°C , 90%. b. Vilsmeier reaction. POCl_3 , DMF, 0°C , 1 h then 100°C , 6 h, 65%.



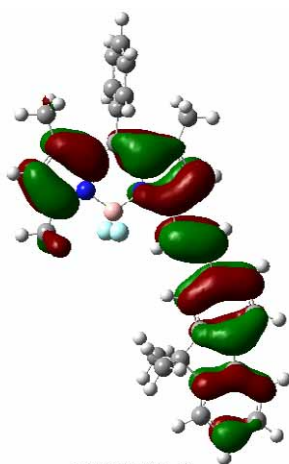
Diagrams showing the MOs levels of compounds 2-6



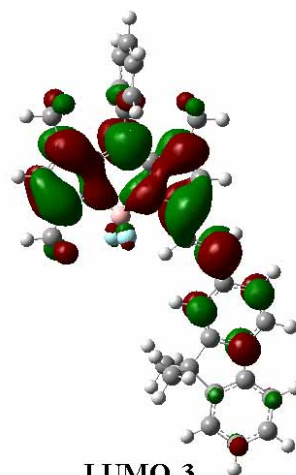
HOMO-2



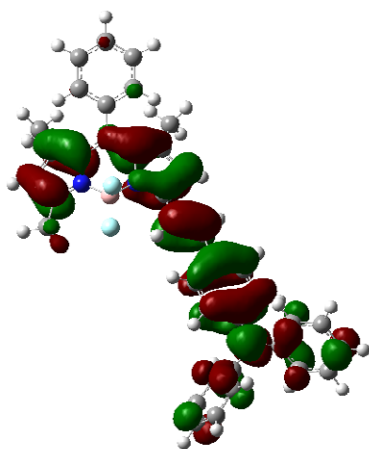
LUMO-2



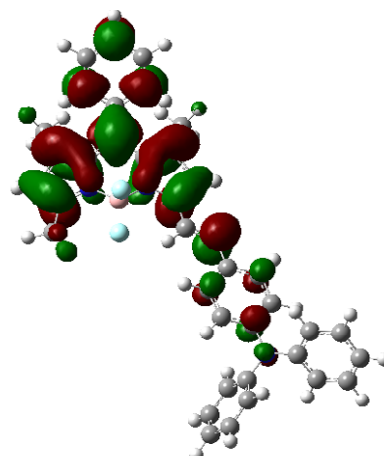
HOMO-3



LUMO-3



HOMO-4



LUMO-4

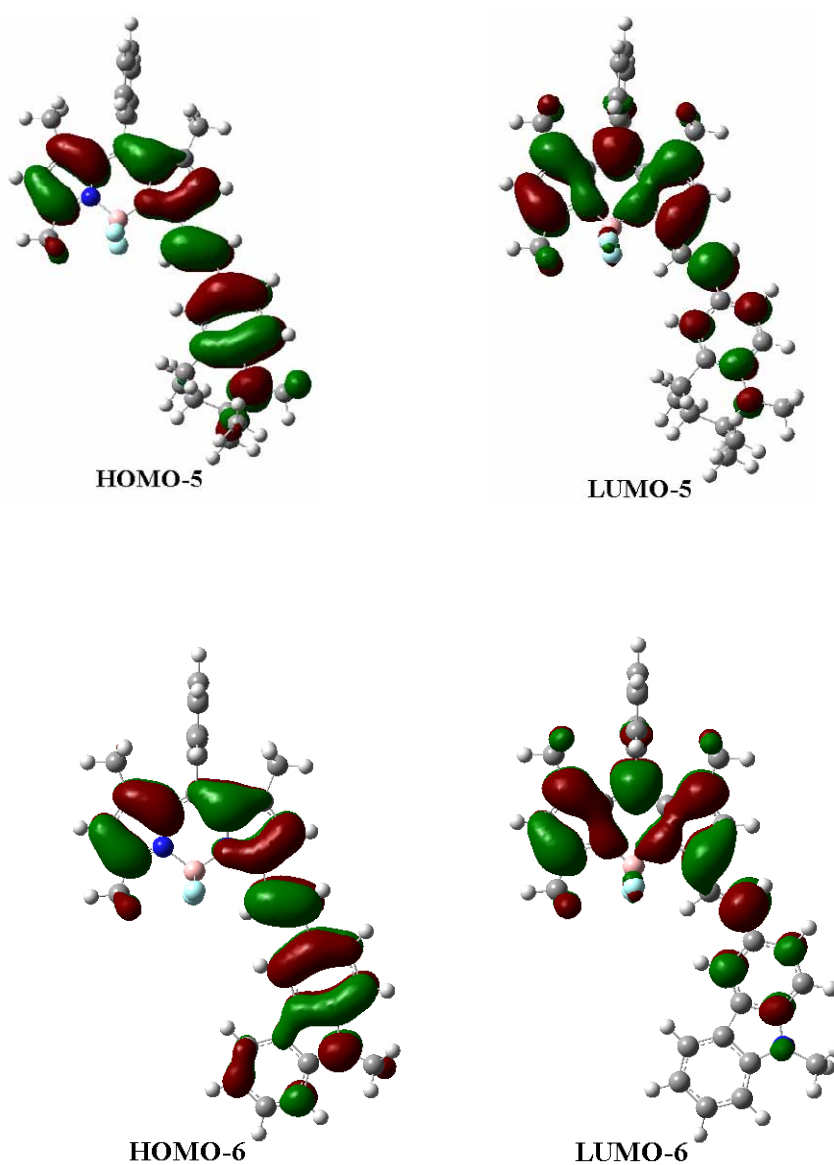


Figure. Diagrams showing the HOMO and LUMO levels of **2-6**. It is also an evidence for the difference of the electron-donating abilities which we can see from the electron density in HOMO and LUMO levels.

Figure S1. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **2** in CDCl_3

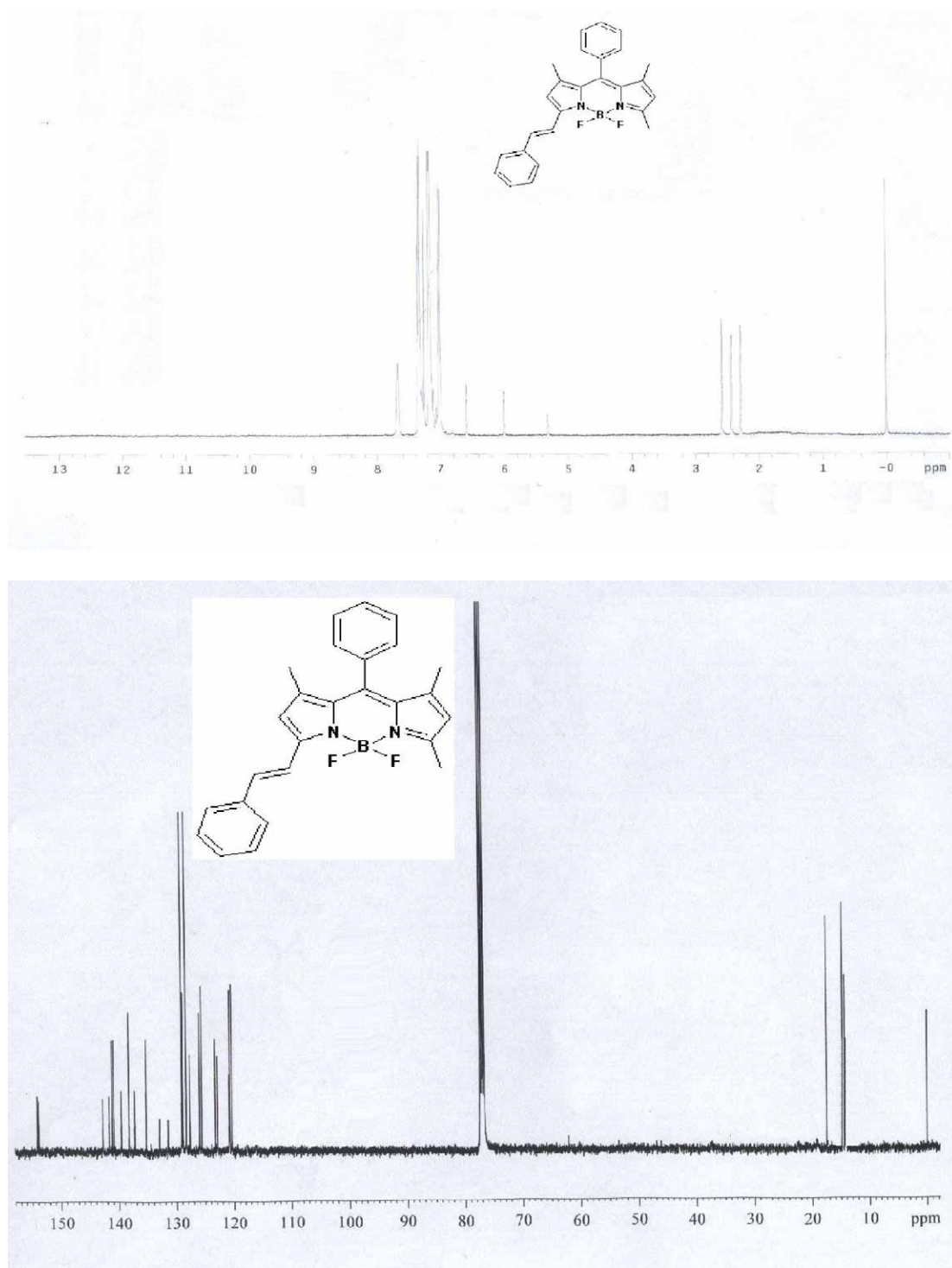


Figure S2. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **3** in CDCl_3

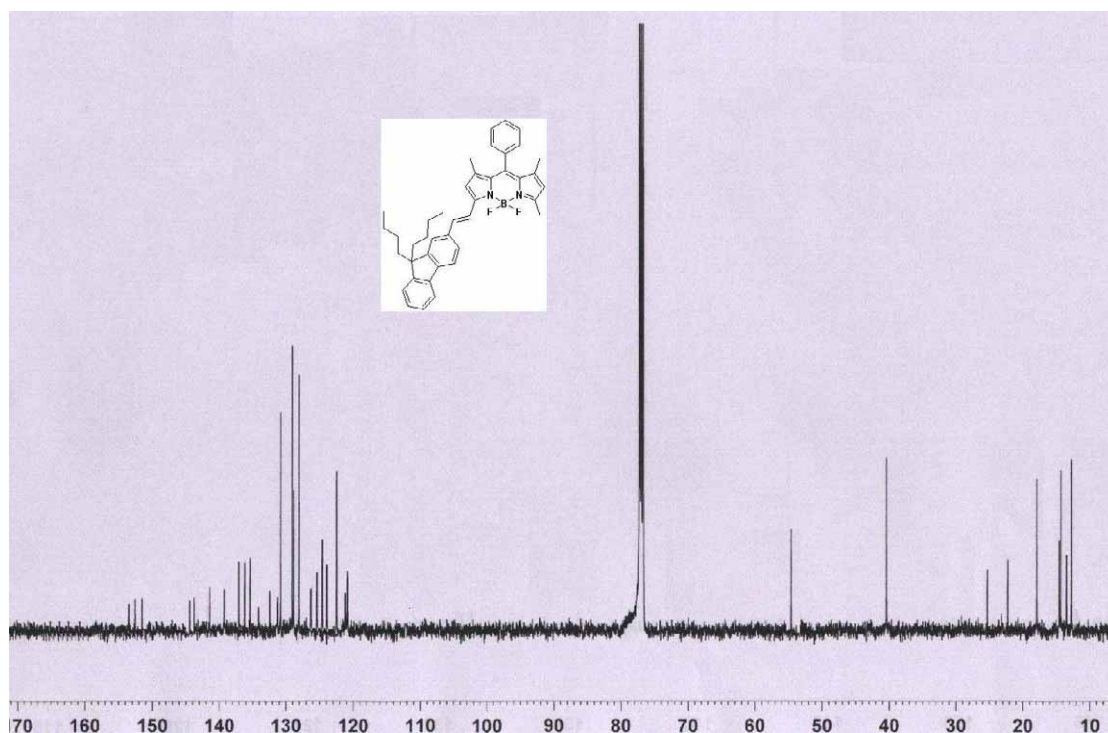
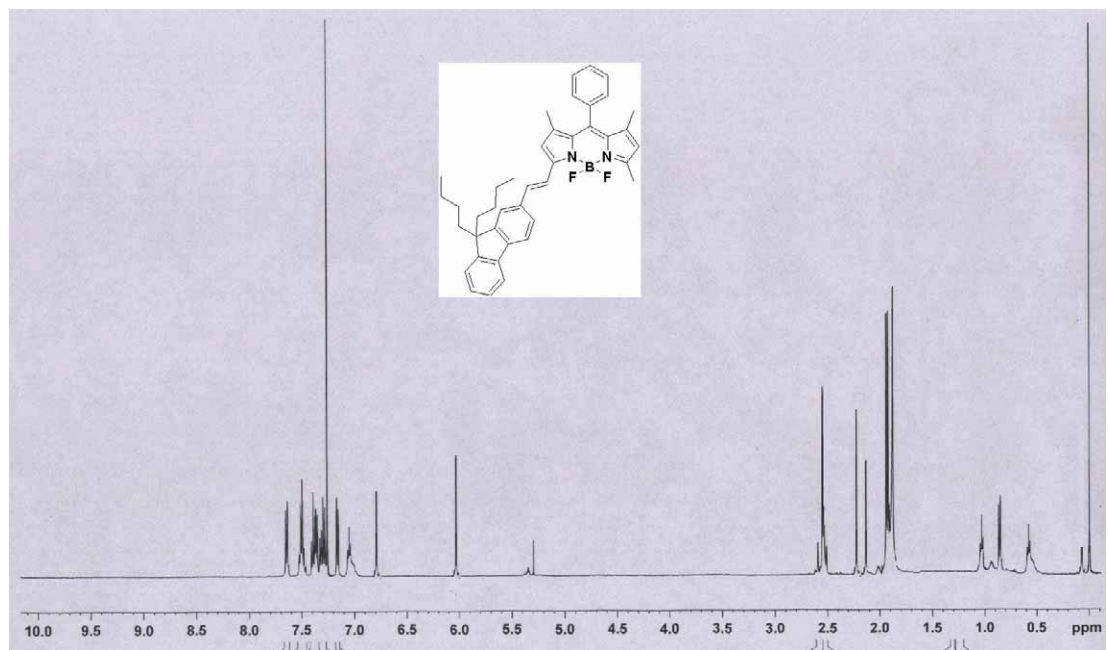


Figure S3. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **4** in CDCl_3

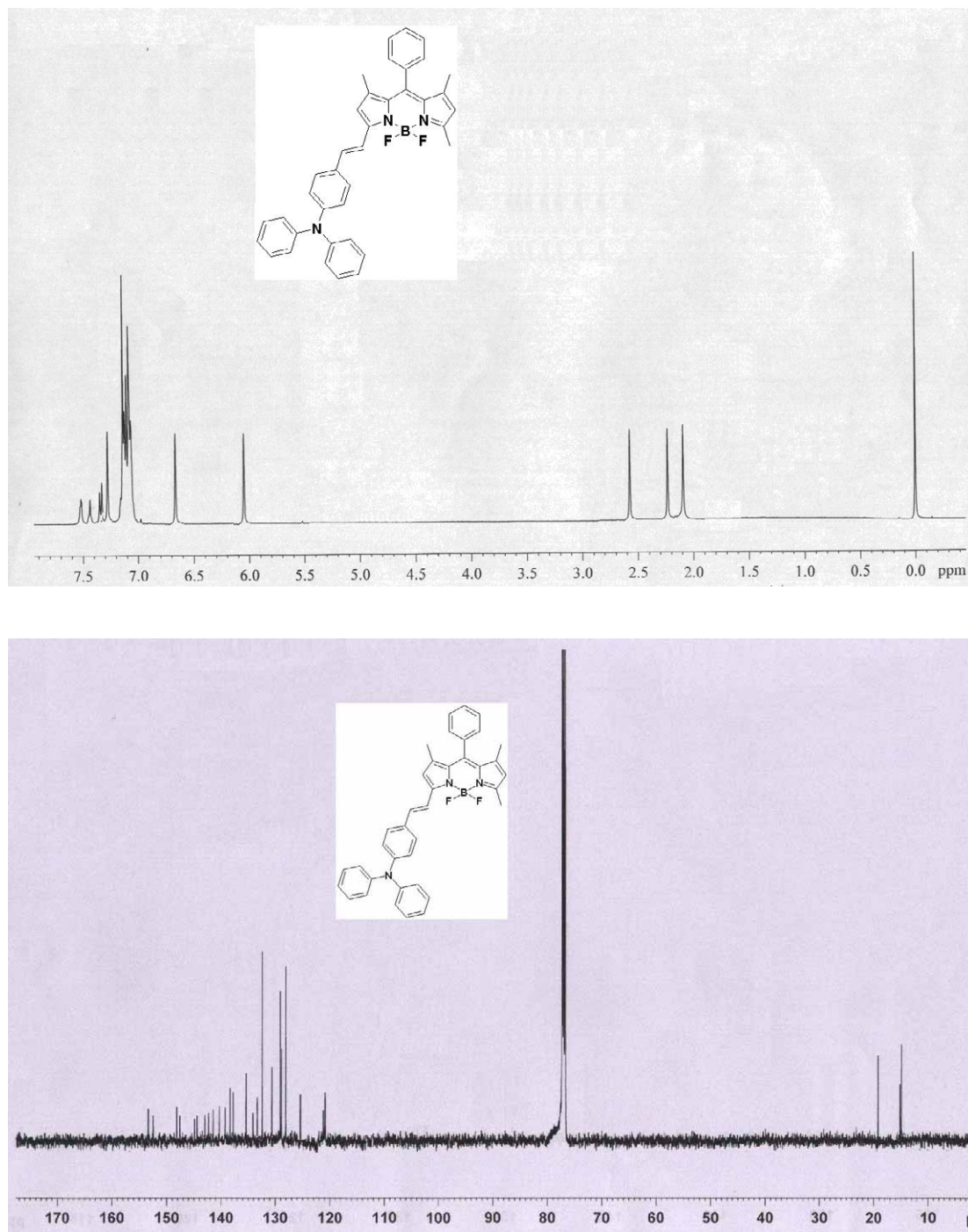


Figure S4. ^1H NMR (400 MHz) and ^{13}C NMR (100 MHz) spectra of compound **5** in CDCl_3

