

SUPPORTING INFORMATION

**Boradipyrromethenecyanines on the base of BODIPY nucleus
annelated with pyridone ring: a new approach to long-wavelength
dual fluorescent probe design**

Yuriy V. Zatsikha,^a Viktor P. Yakubovskiy,^a Mykola P. Shandura^a and Yuriy P. Kovtun^{*a}

*^a Institute of Organic Chemistry, National Academy of Sciences of Ukraine,
5 Murmanska str., 02660 Kyiv, Ukraine*

E-mail: kovtun@ioch.kiev.ua

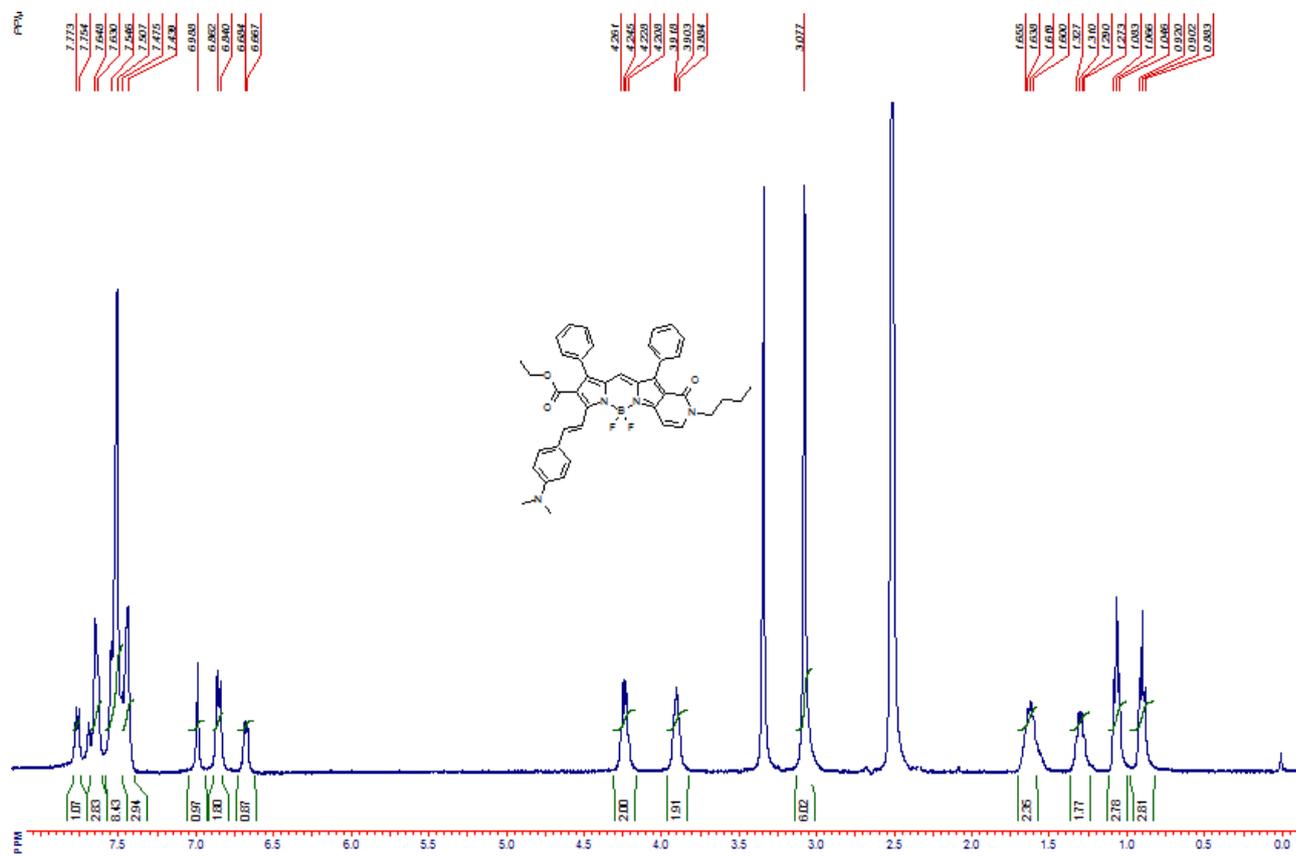


Figure 1. ¹H NMR spectrum of compound **2** in DMSO-d₆.

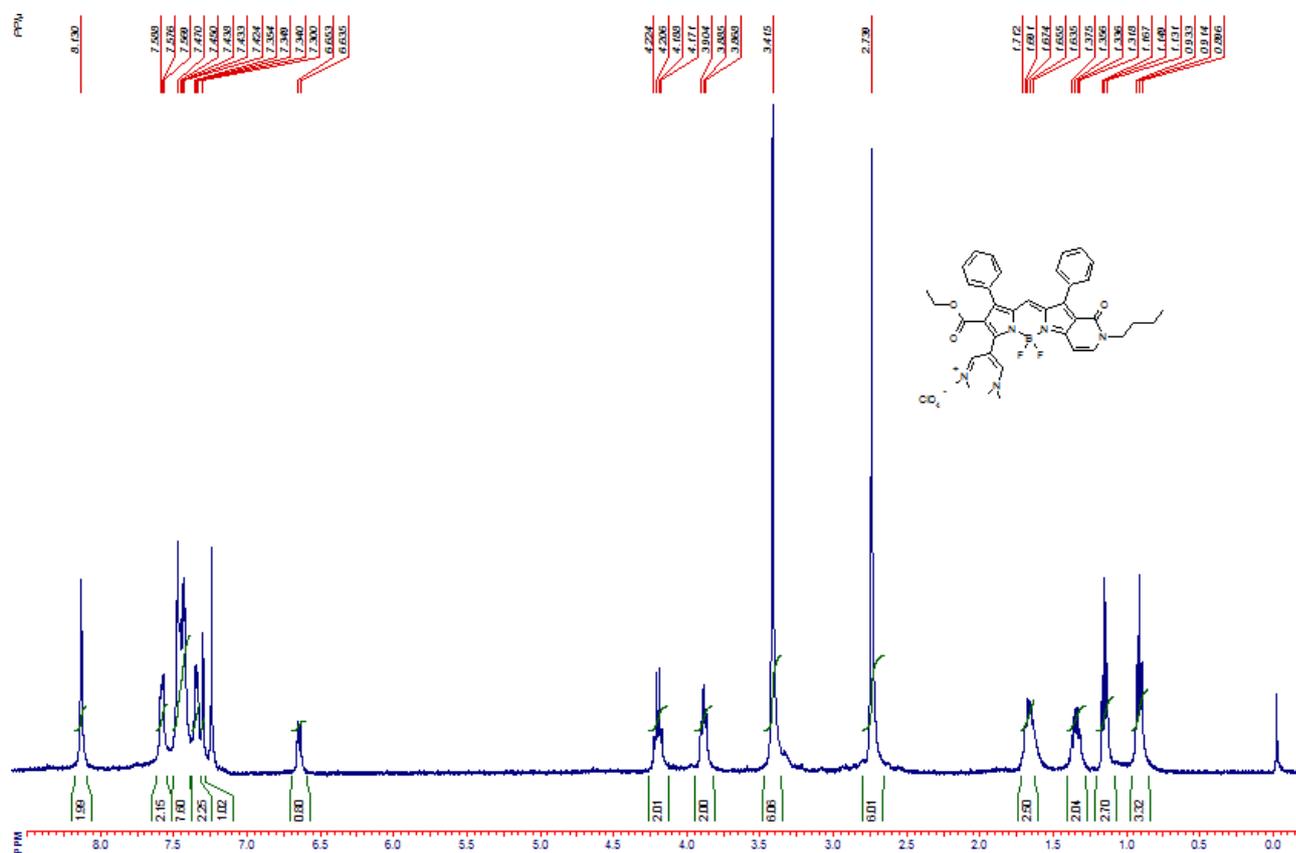


Figure 2. ¹H NMR spectrum of compound **3** in CDCl₃.

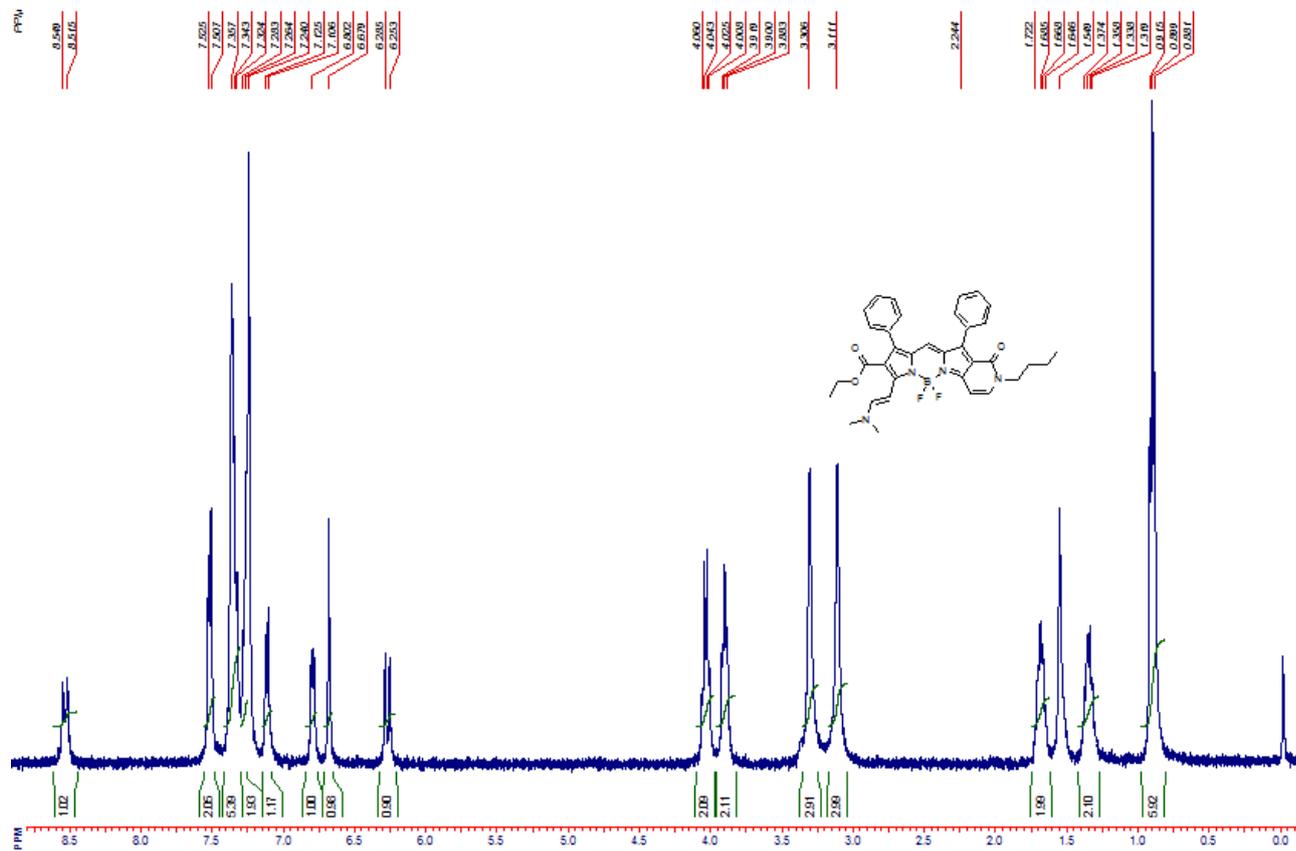


Figure 3. ¹H NMR spectrum of compound **4** in CDCl₃.

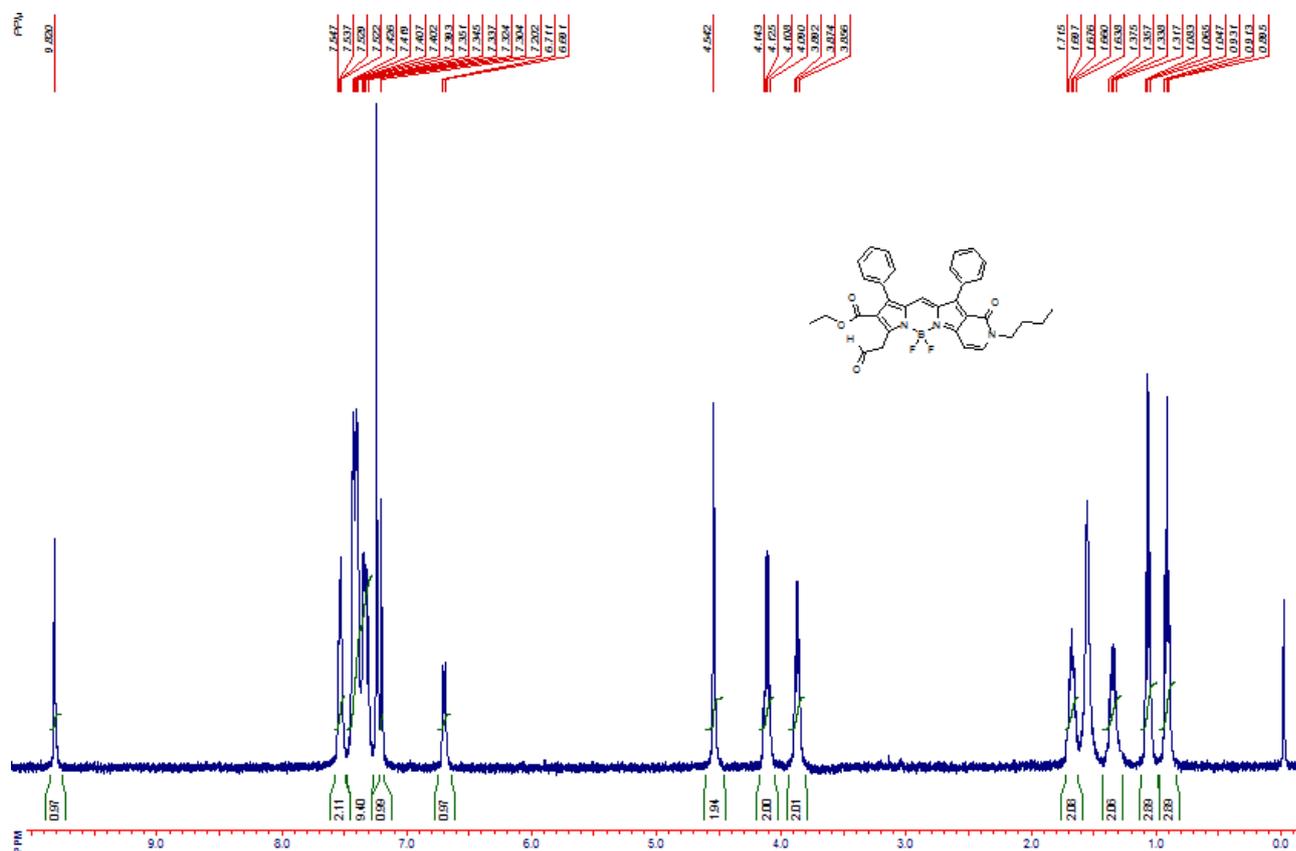


Figure 4. ¹H NMR spectrum of compound **5** in CDCl₃.

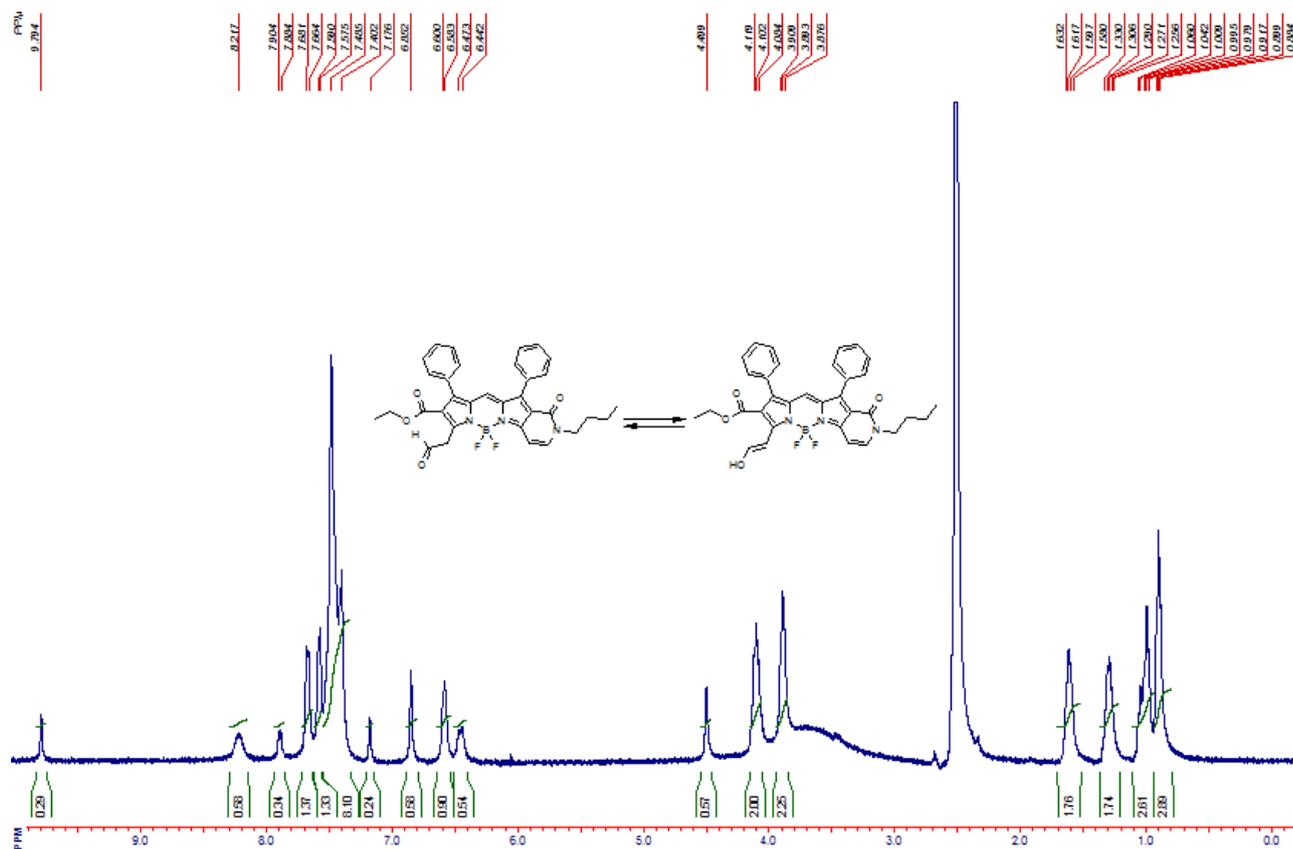


Figure 5. ¹H NMR spectrum of compound **5** in DMSO-d₆.

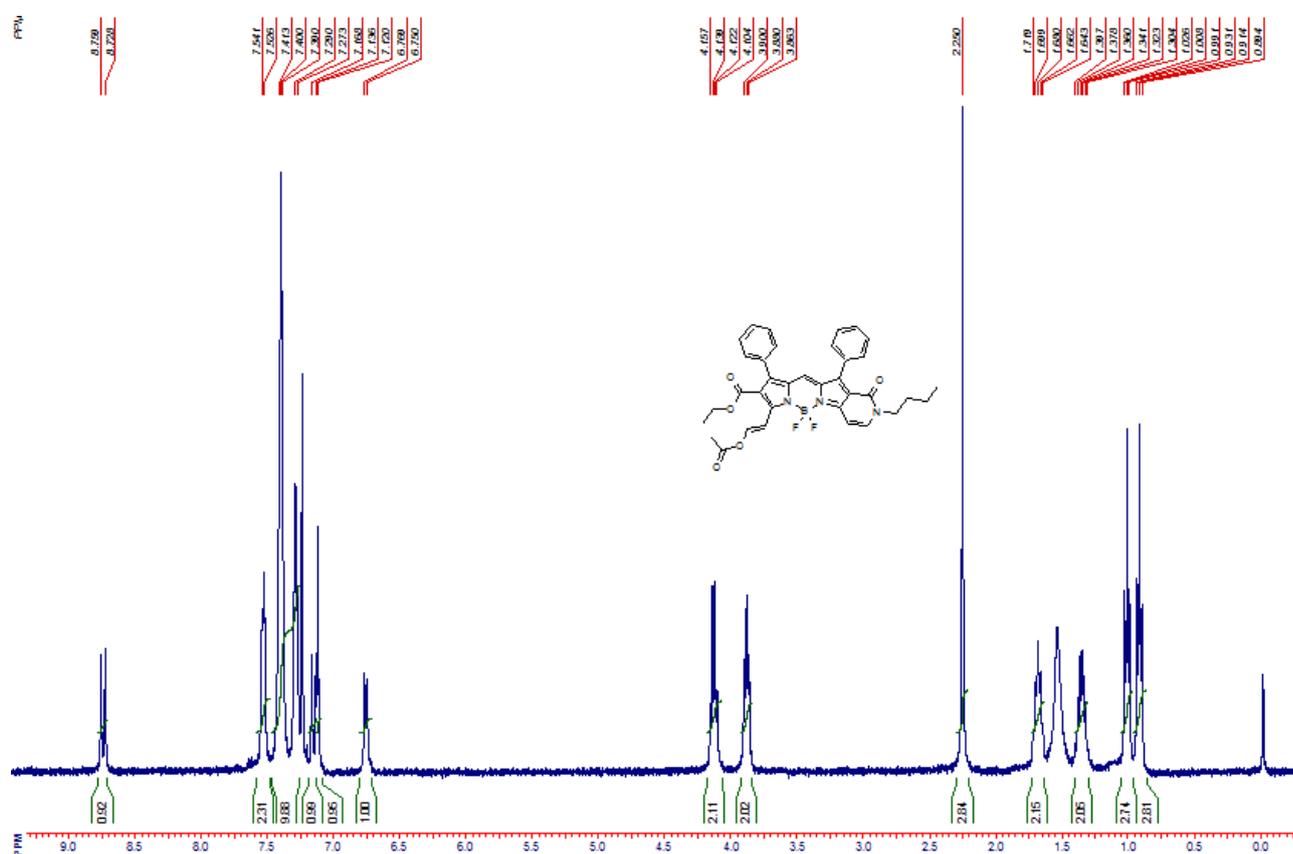


Figure 6. ¹H NMR spectrum of compound **6** in CDCl₃.

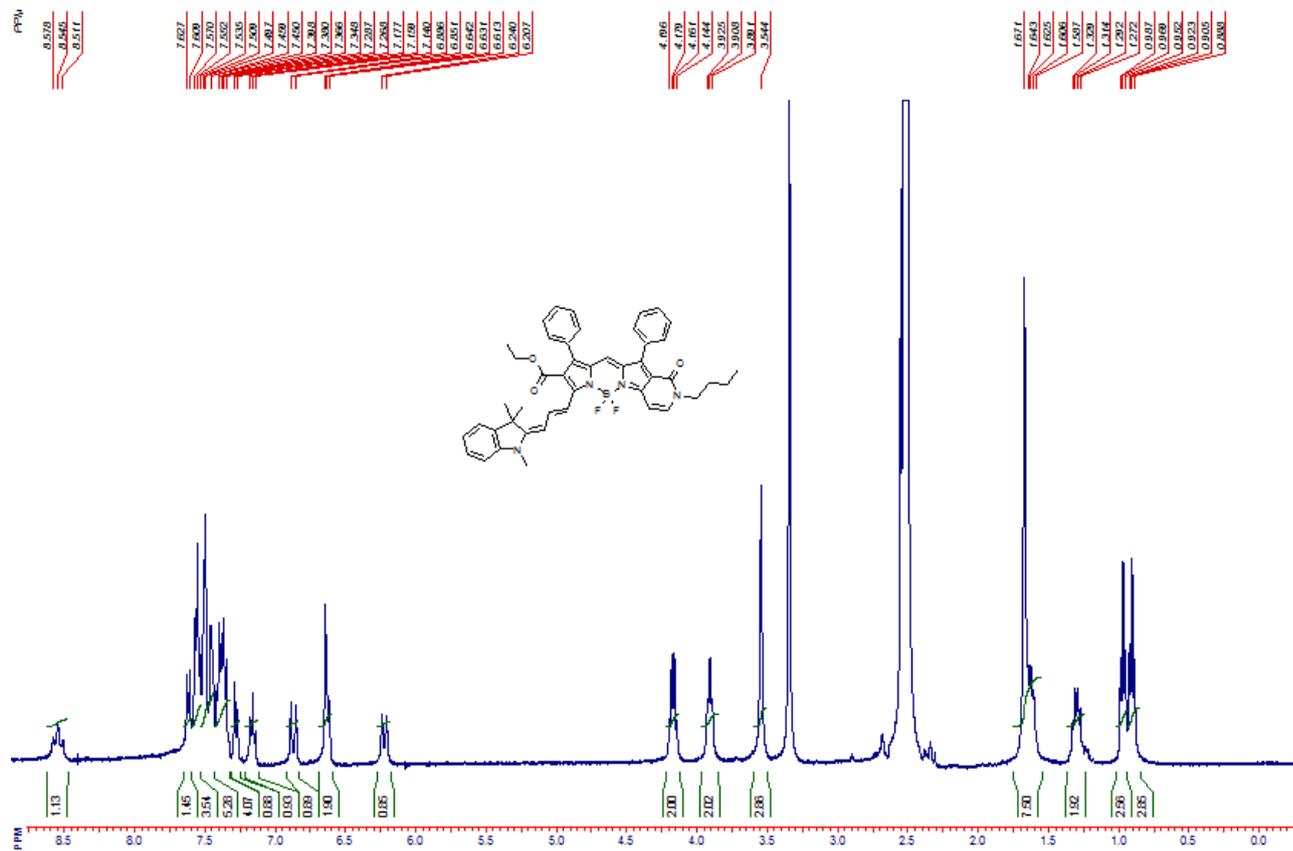


Figure 7. ^1H NMR spectrum of compound **7** in DMSO-d_6 .

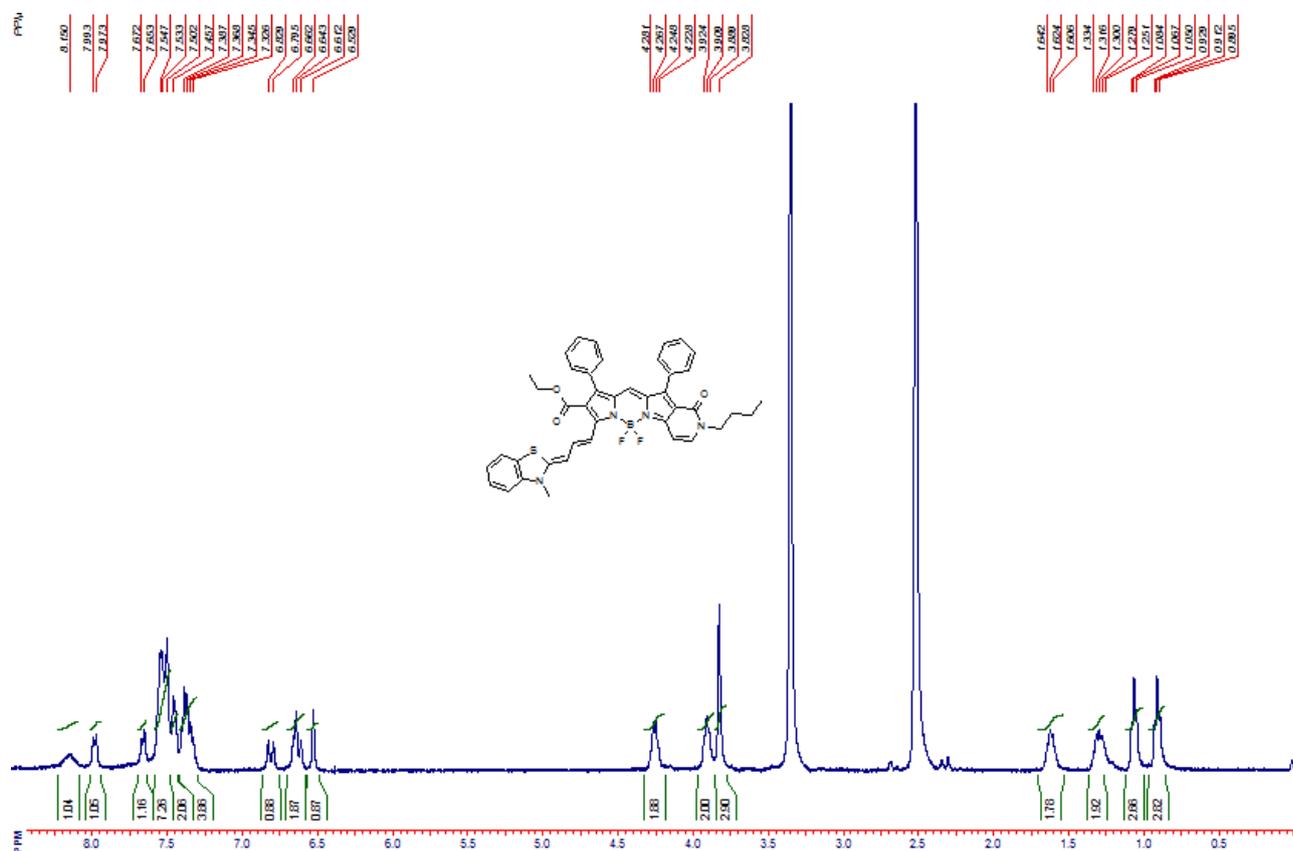


Figure 8. ^1H NMR spectrum of compound **8** in DMSO-d_6 .

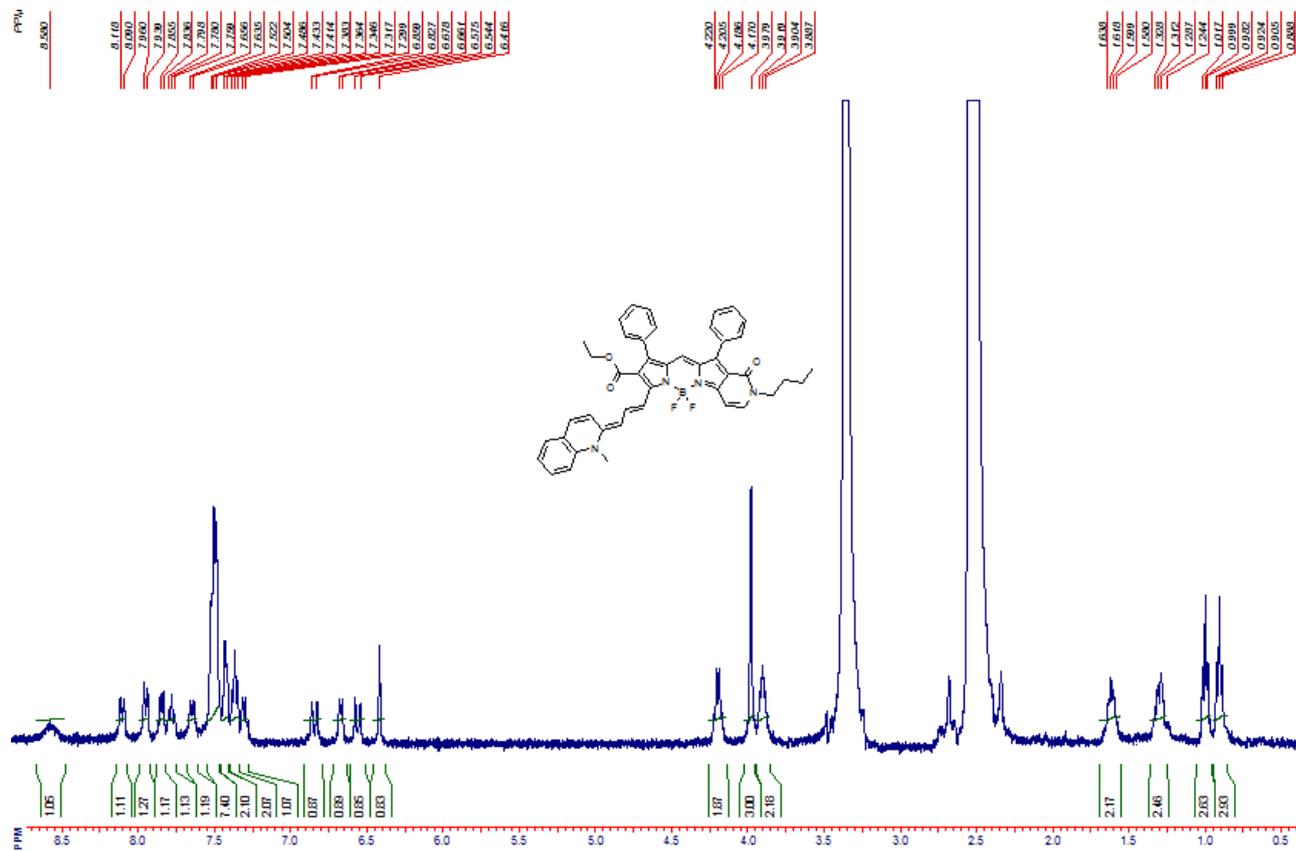


Figure 9. ^1H NMR spectrum of compound **9** in DMSO-d_6 .

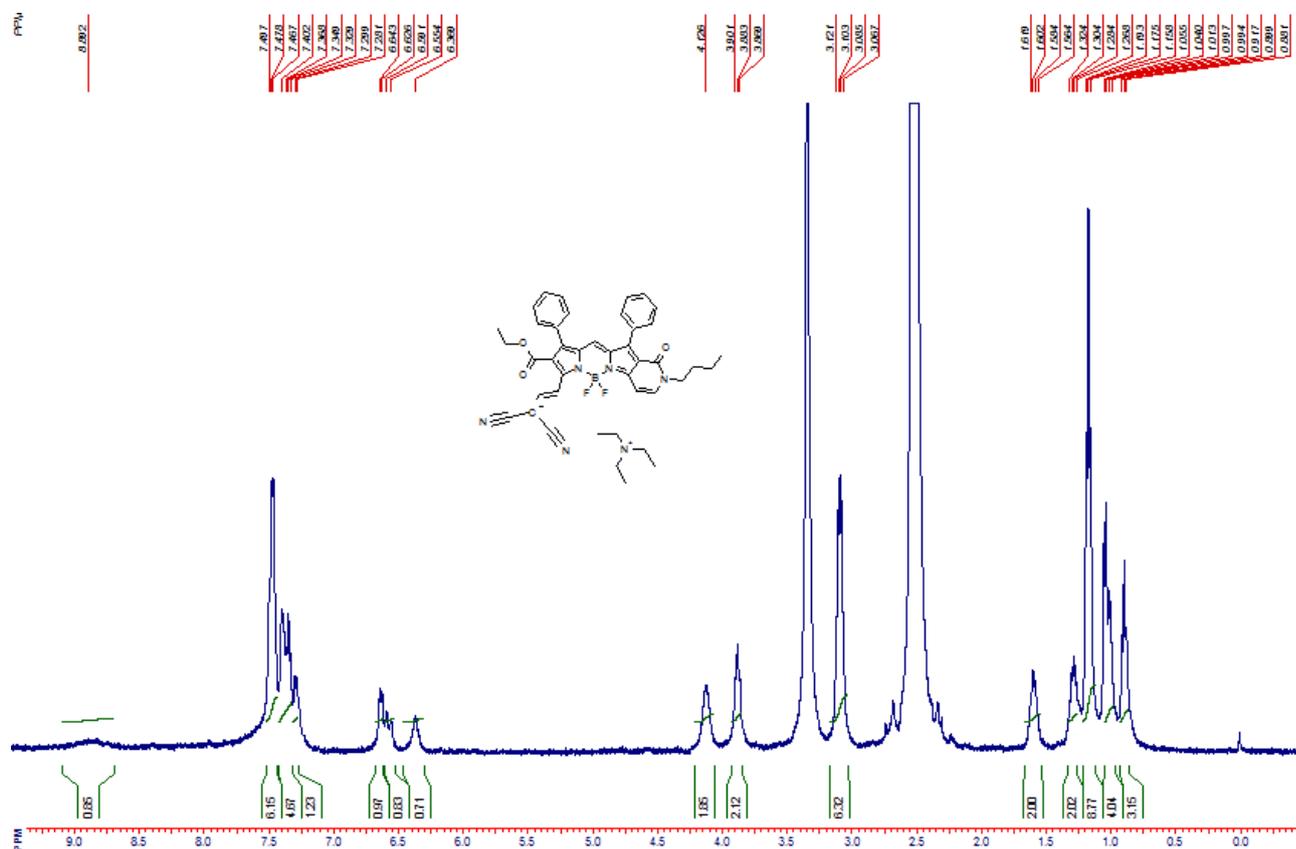


Figure 10. ^1H NMR spectrum of compound **10a** in DMSO-d_6 .

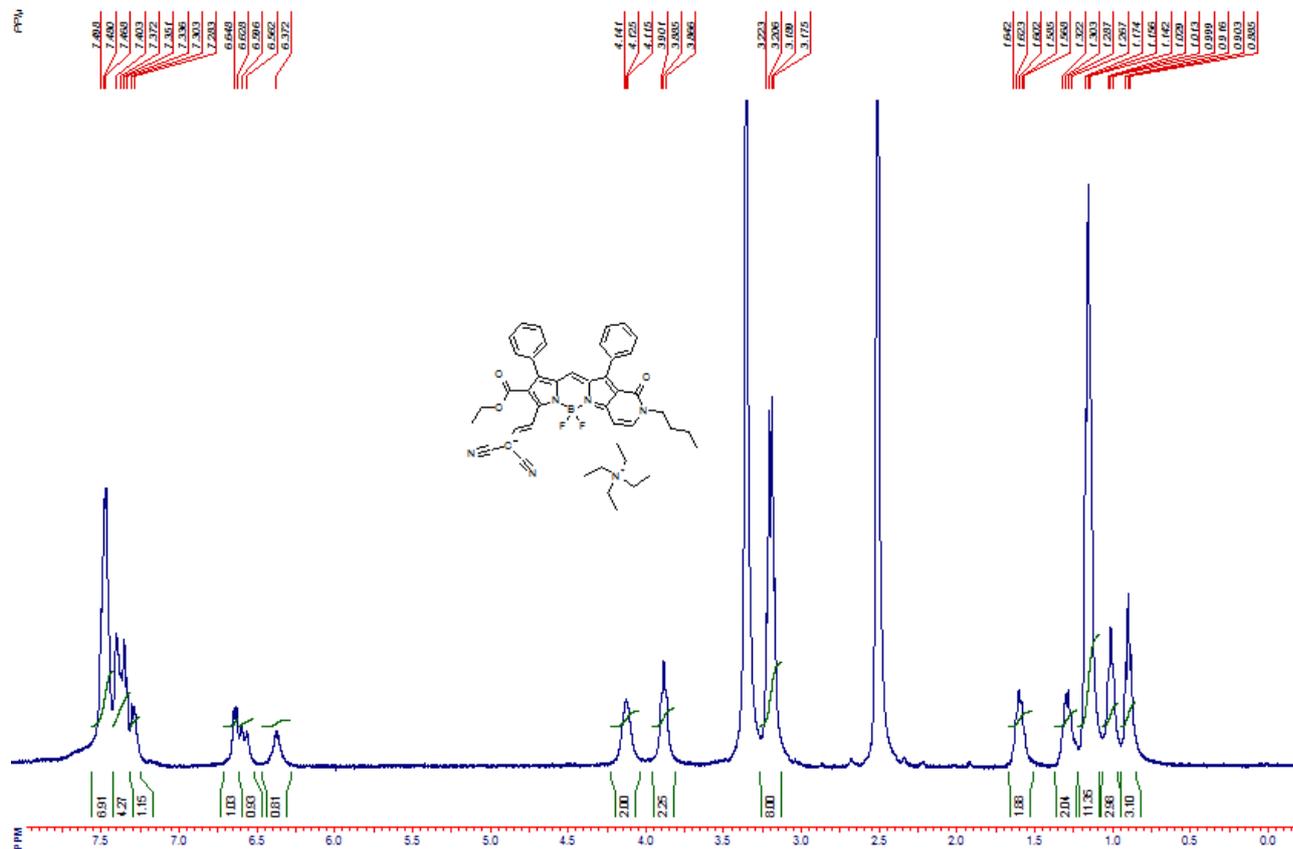


Figure 13. ¹H NMR spectrum of compound **10b** in DMSO-d₆.

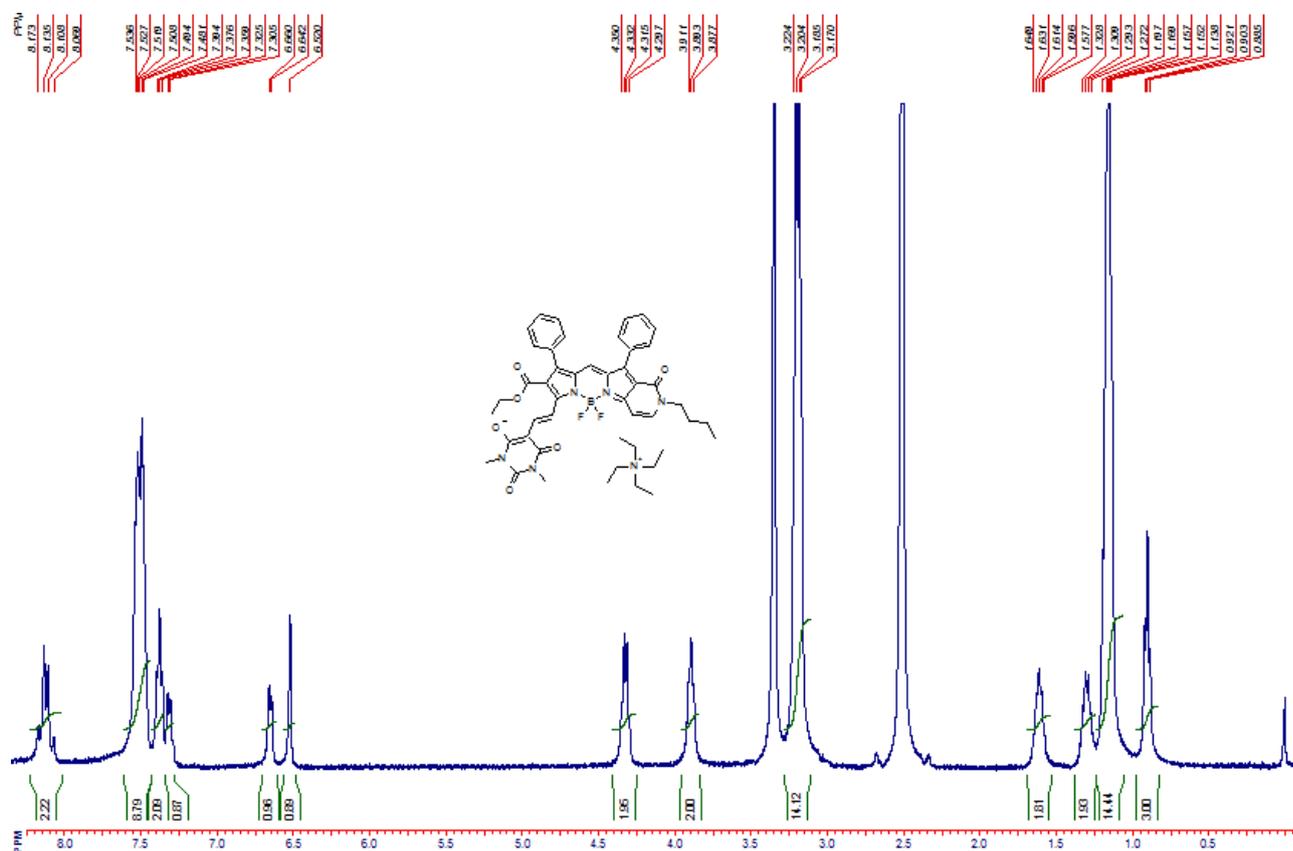


Figure 14. ¹H NMR spectrum of compound **11b** in DMSO-d₆.

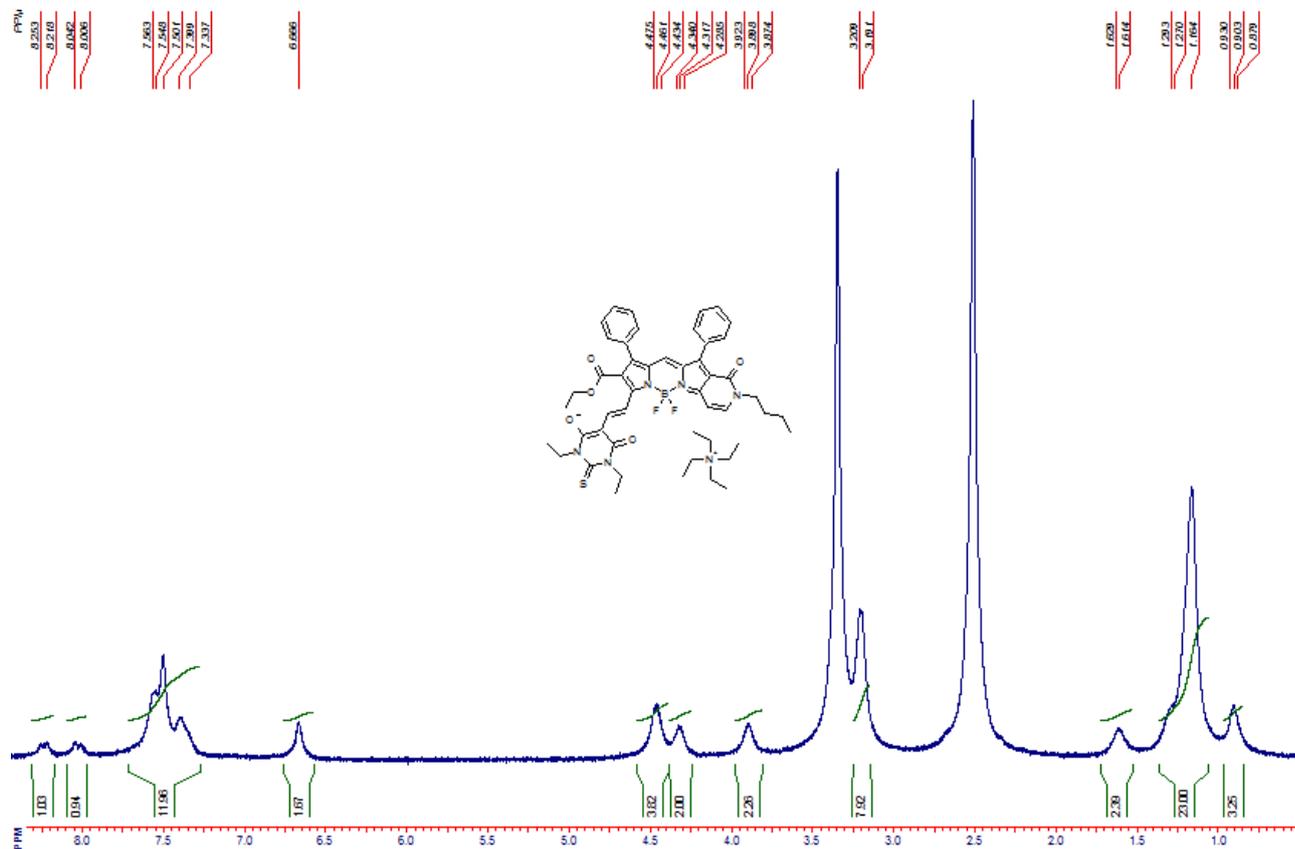


Figure 15. ¹H NMR spectrum of compound **12b** in DMSO-d₆.

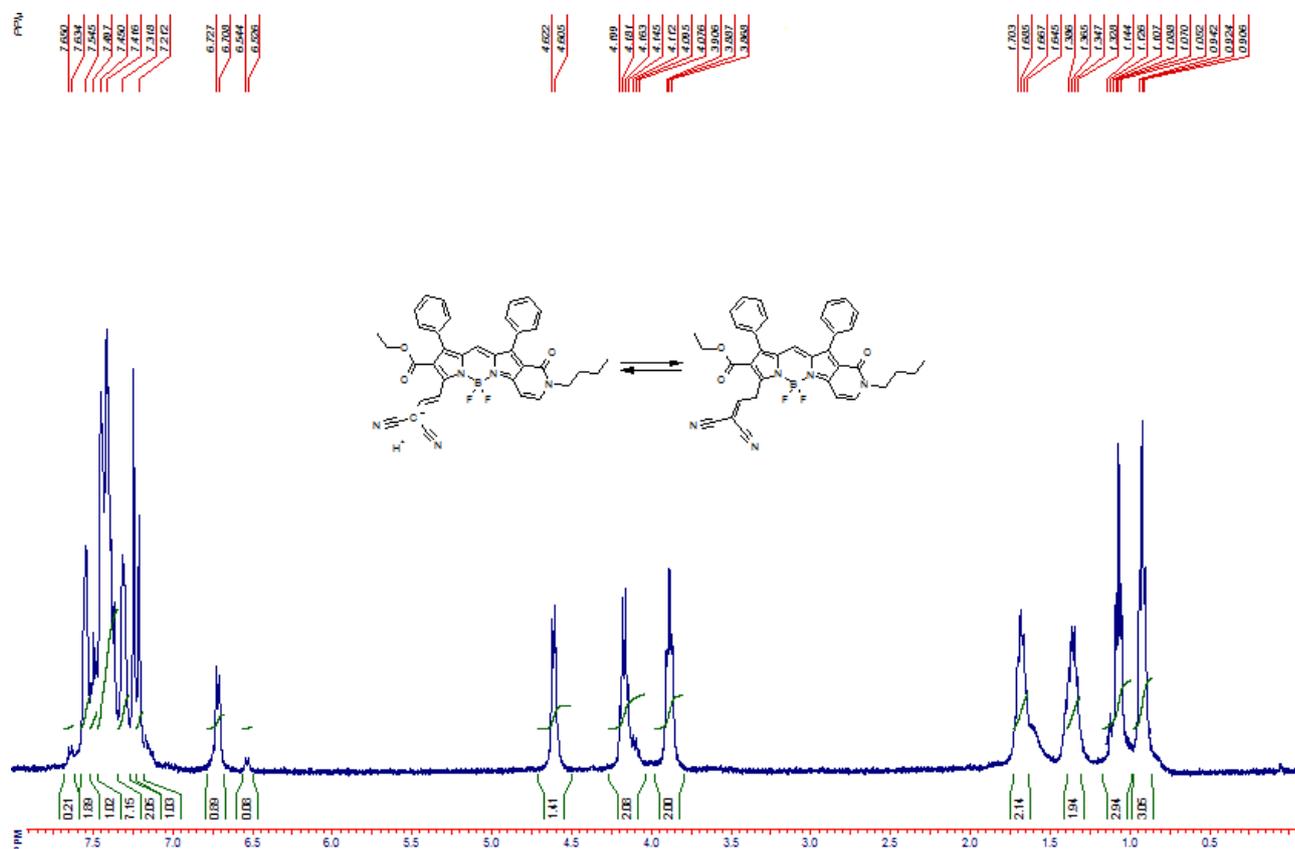


Figure 16. ¹H NMR spectrum of compound **13** in CDCl₃.

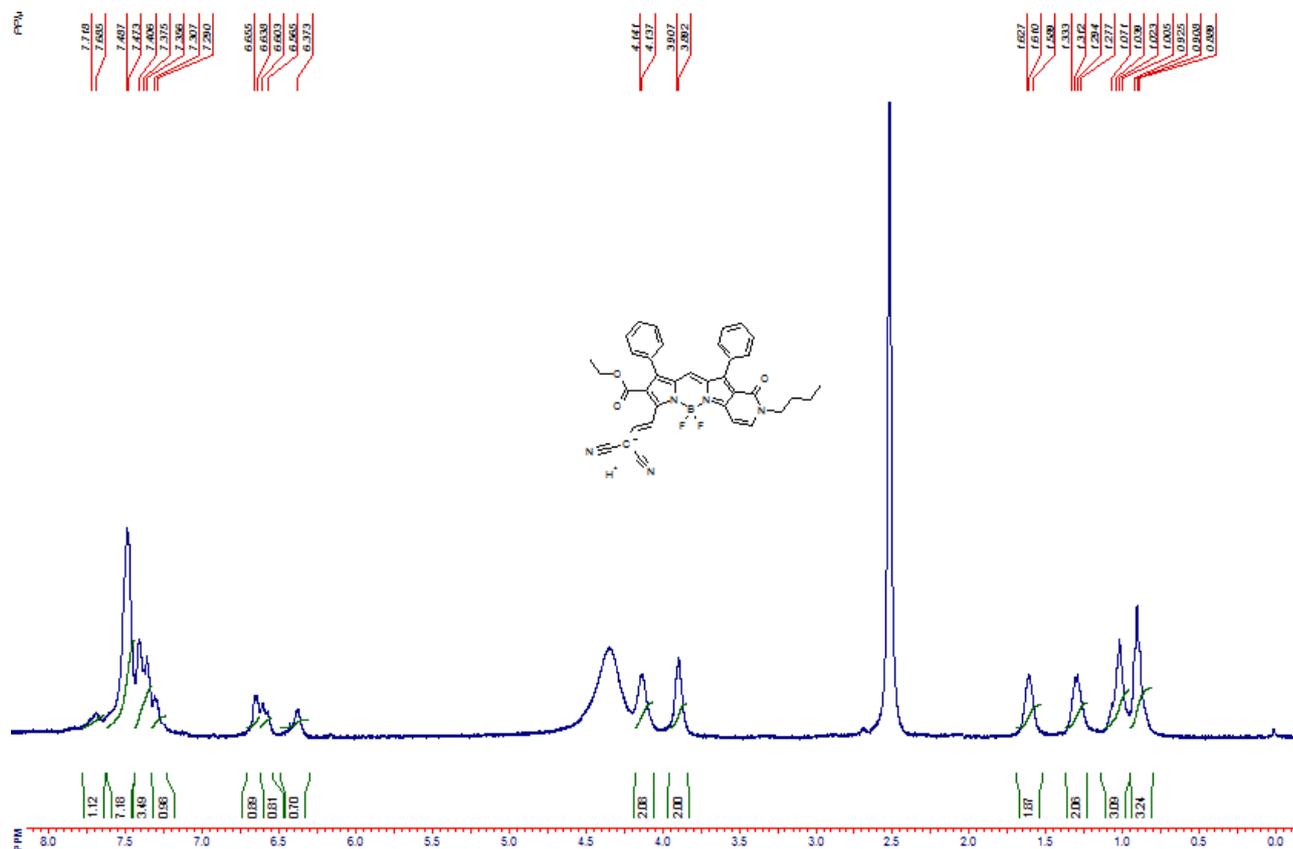


Figure 17. ¹H NMR spectrum of compound **13** in DMSO-d₆.

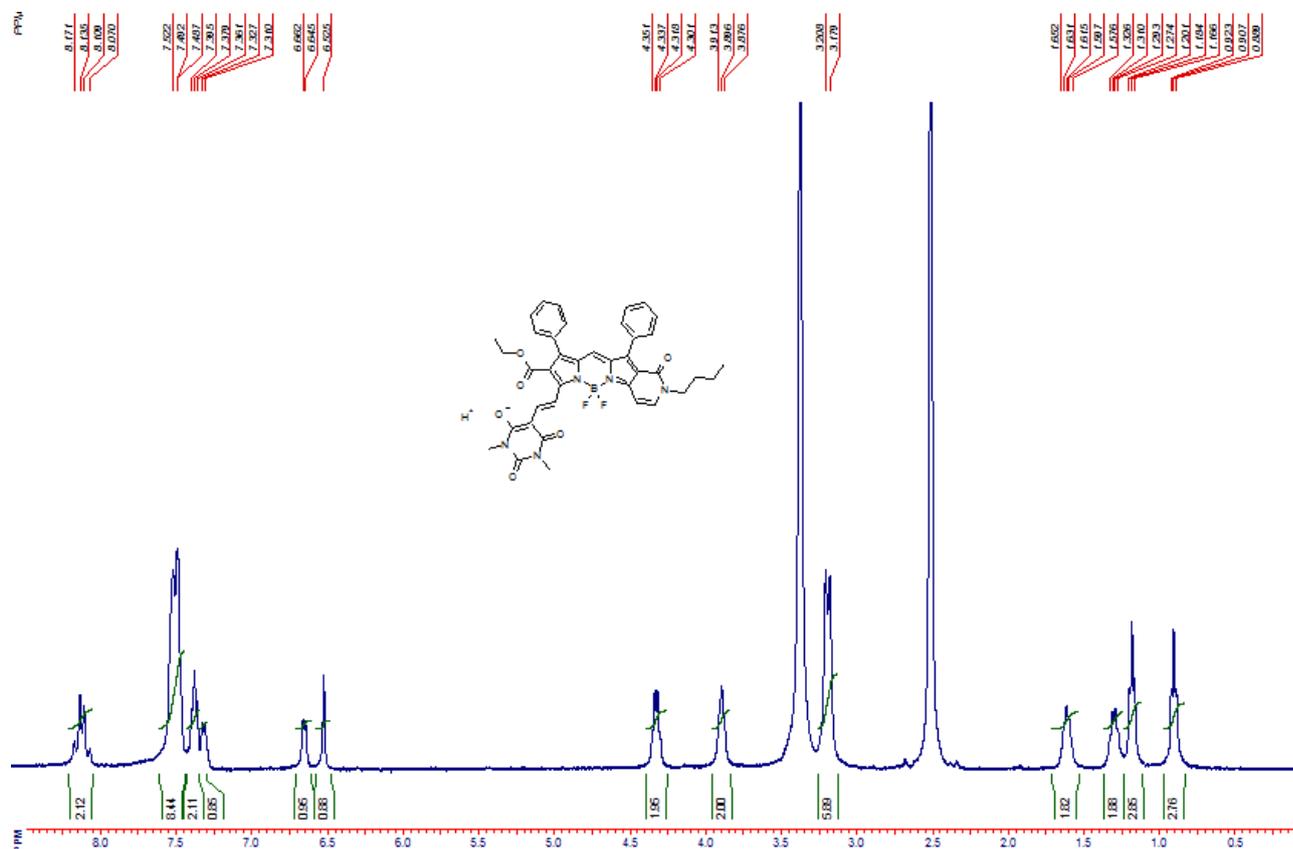


Figure 18. ¹H NMR spectrum of compound **14** in DMSO-d₆.

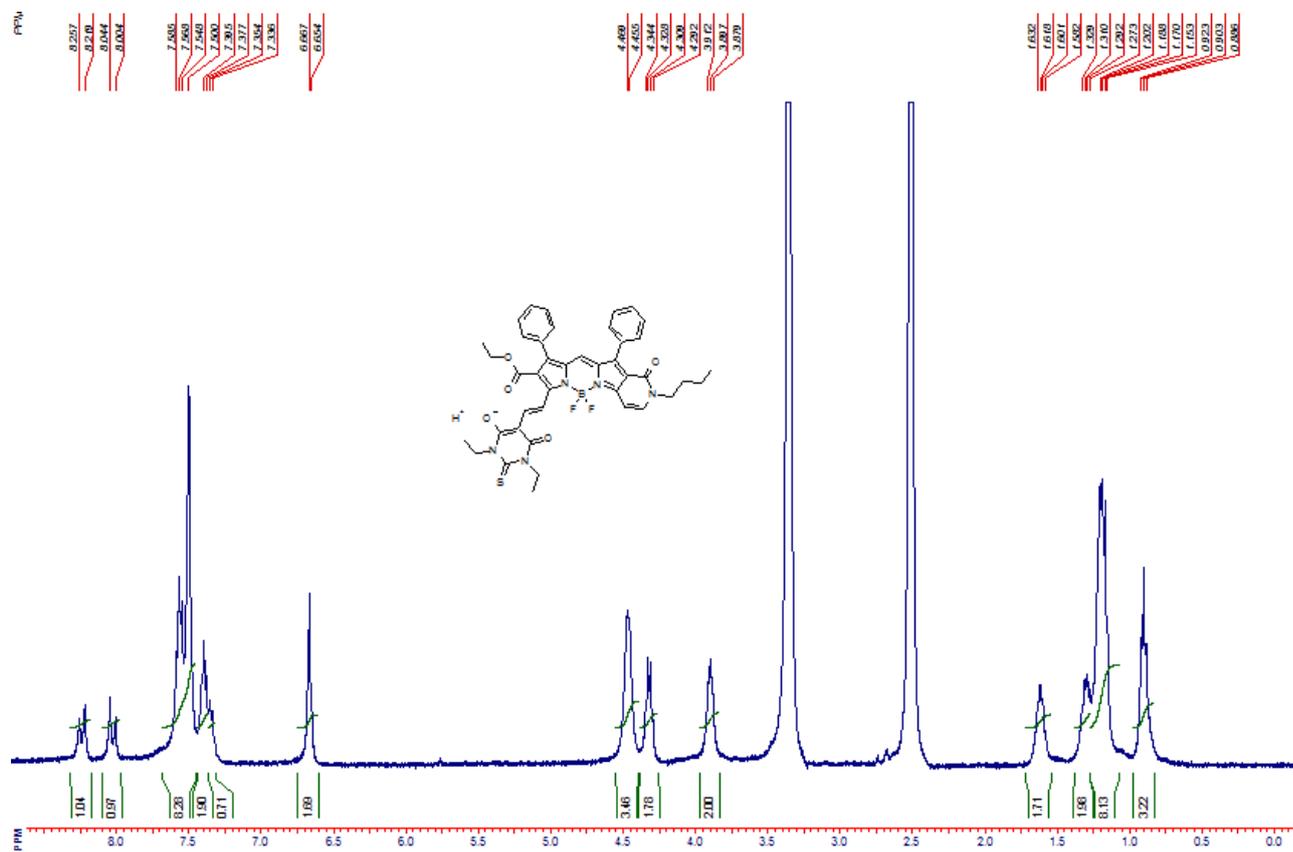


Figure 19. ¹H NMR spectrum of compound **15** in DMSO-d₆.

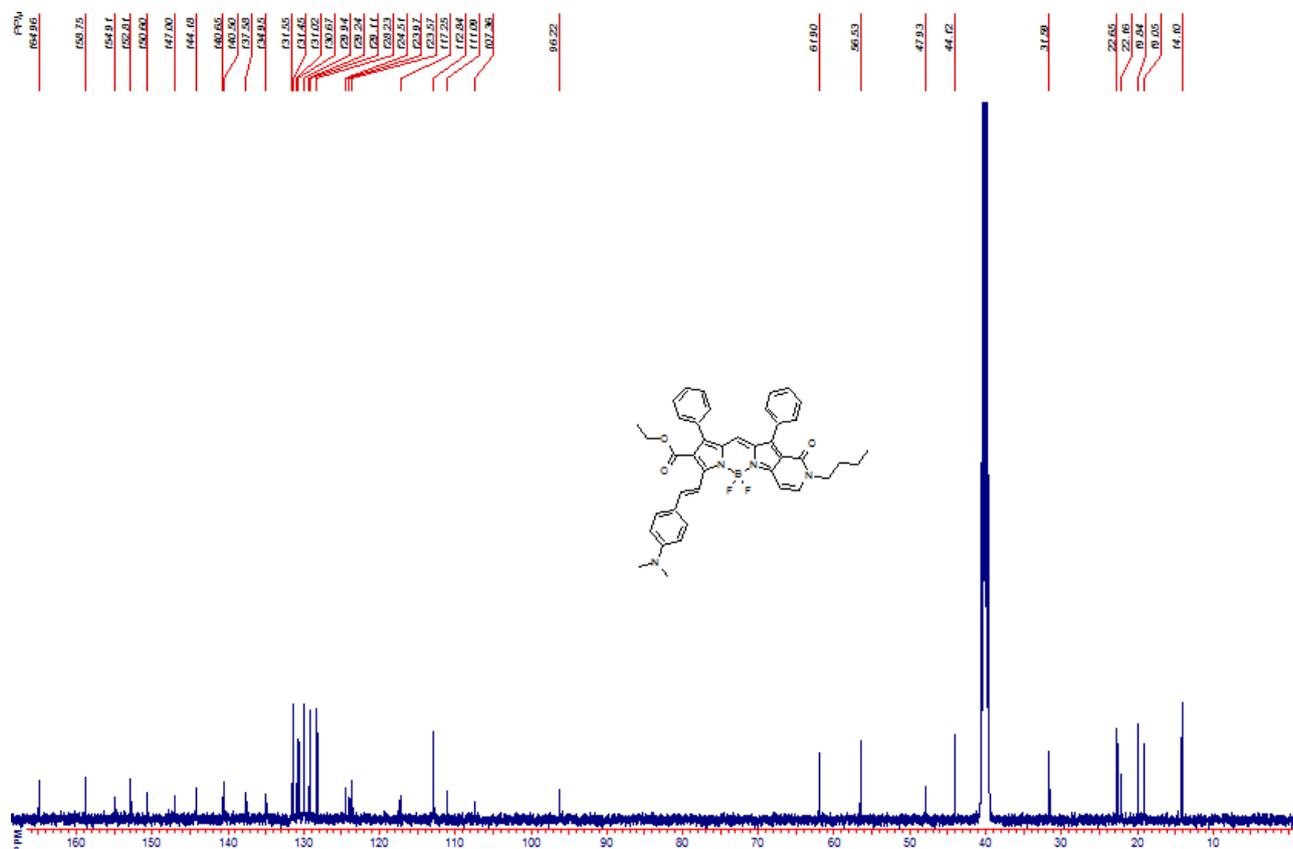


Figure 20. ¹³C NMR spectrum of compound **2** in DMSO.

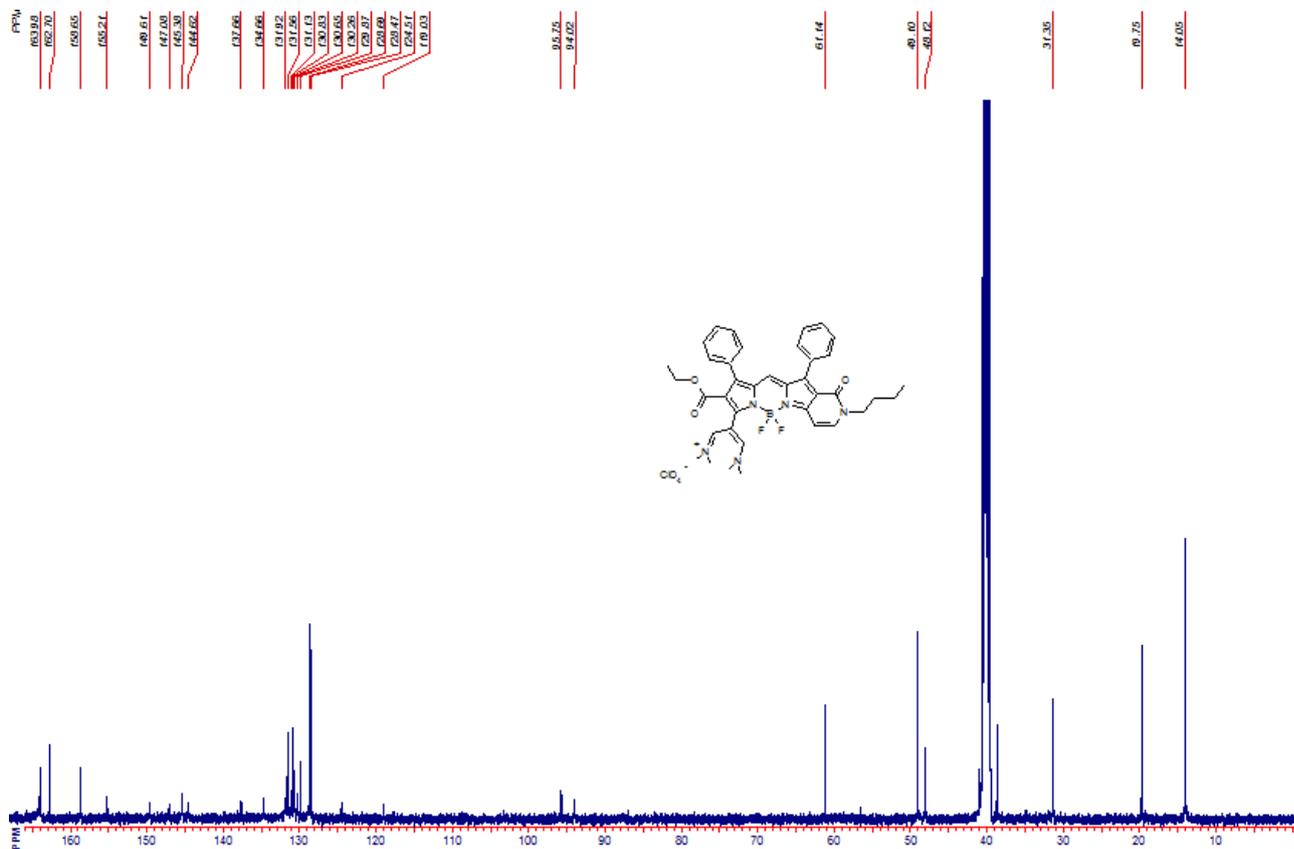


Figure 21. ¹³C NMR spectrum of compound **3** in DMSO.

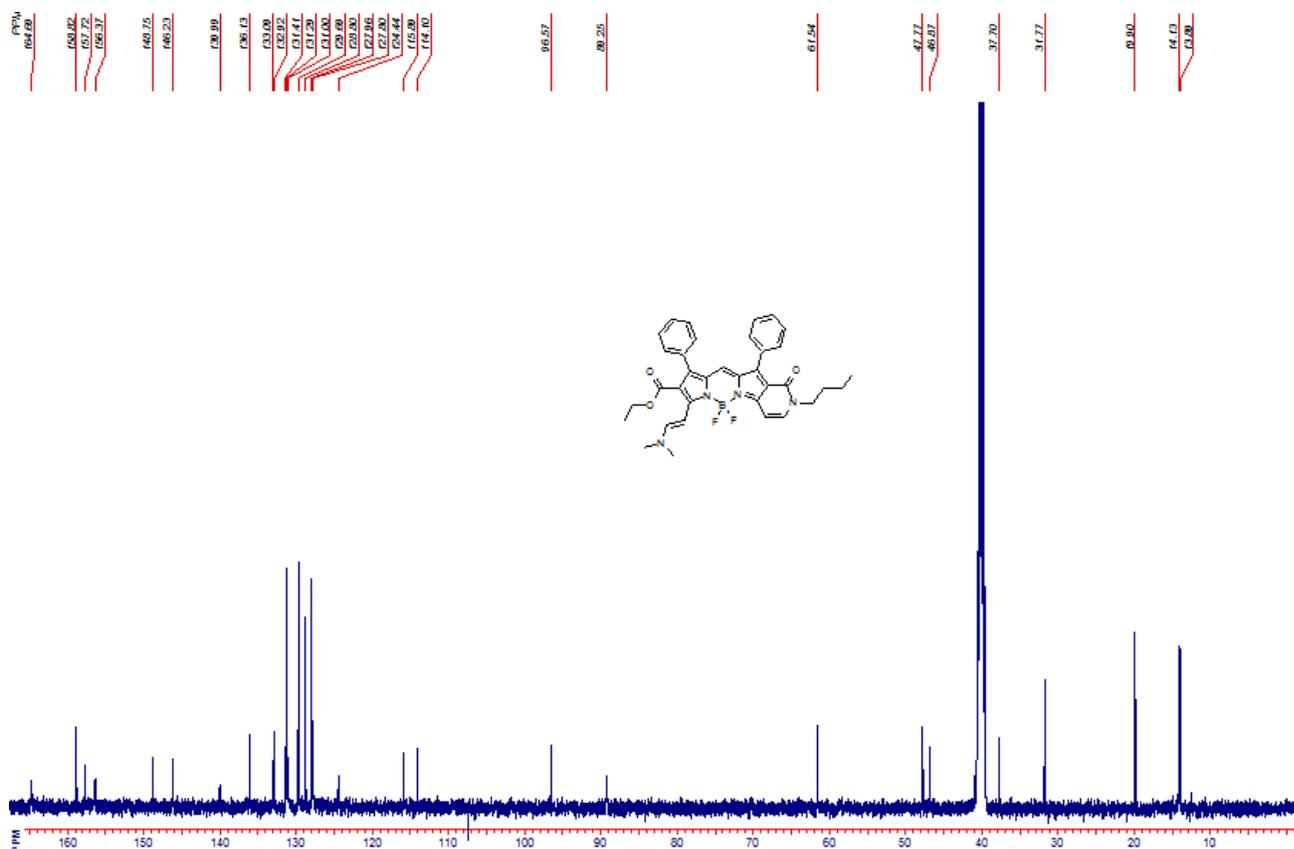


Figure 22. ¹³C NMR spectrum of compound **4** in DMSO.

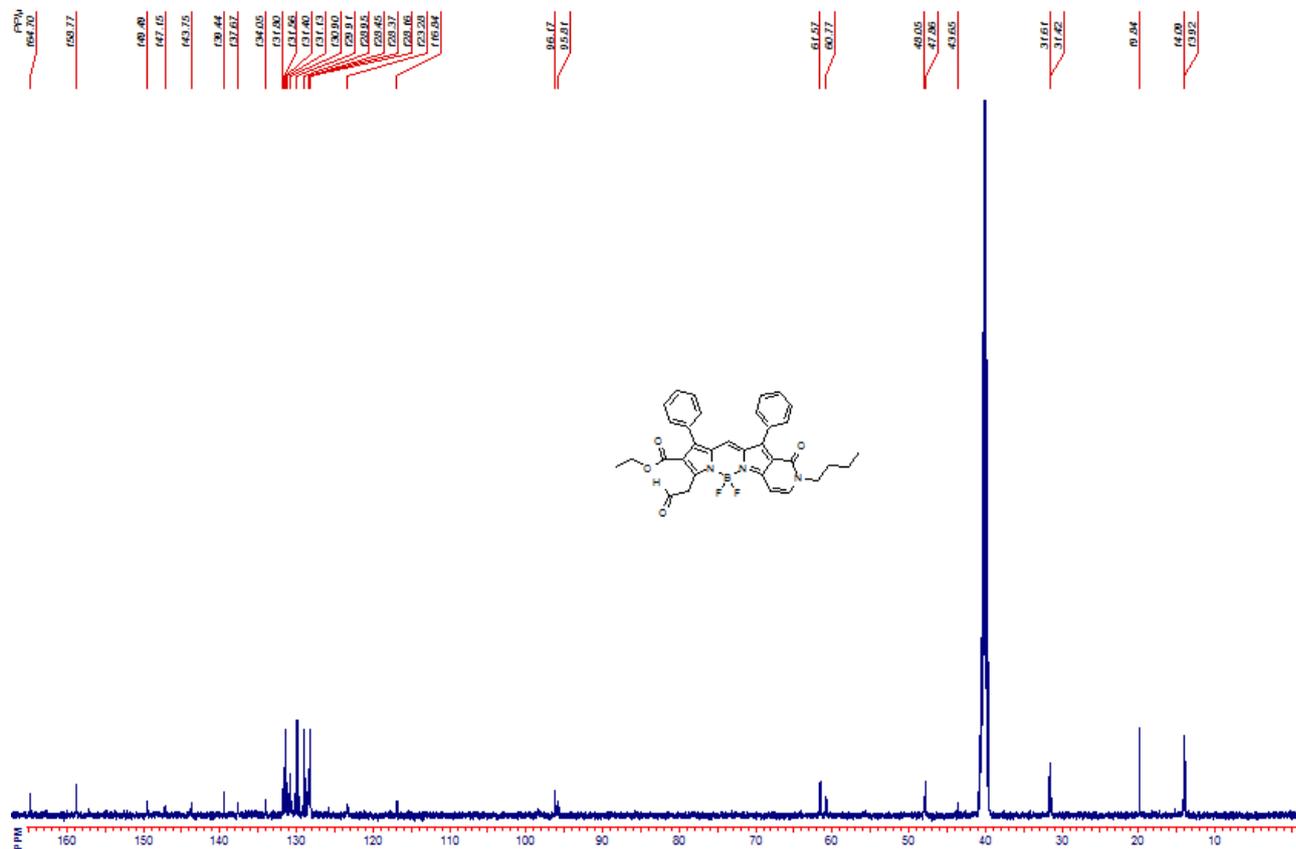


Figure 23. ¹³C NMR spectrum of compound **5** in DMSO.

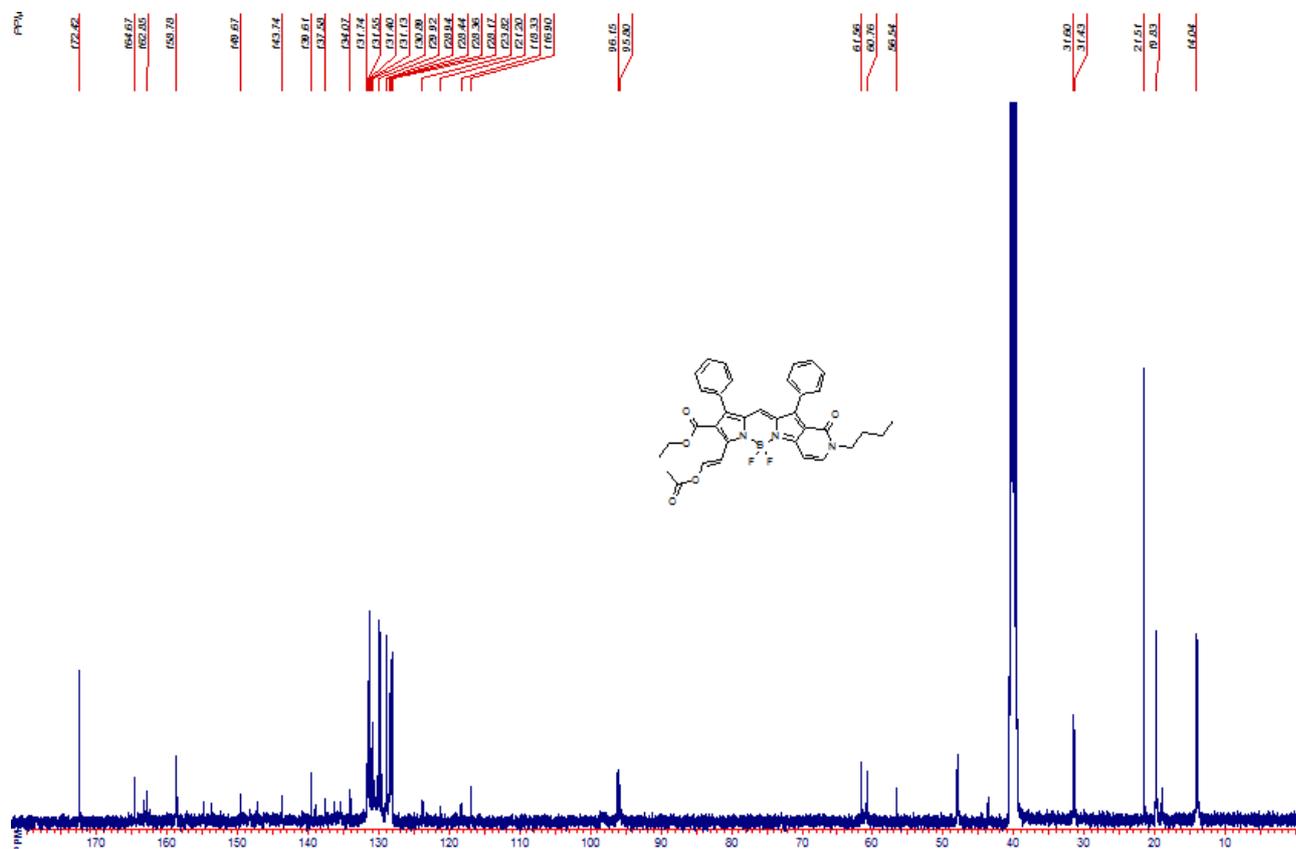


Figure 24. ¹³C NMR spectrum of compound **6** in DMSO.

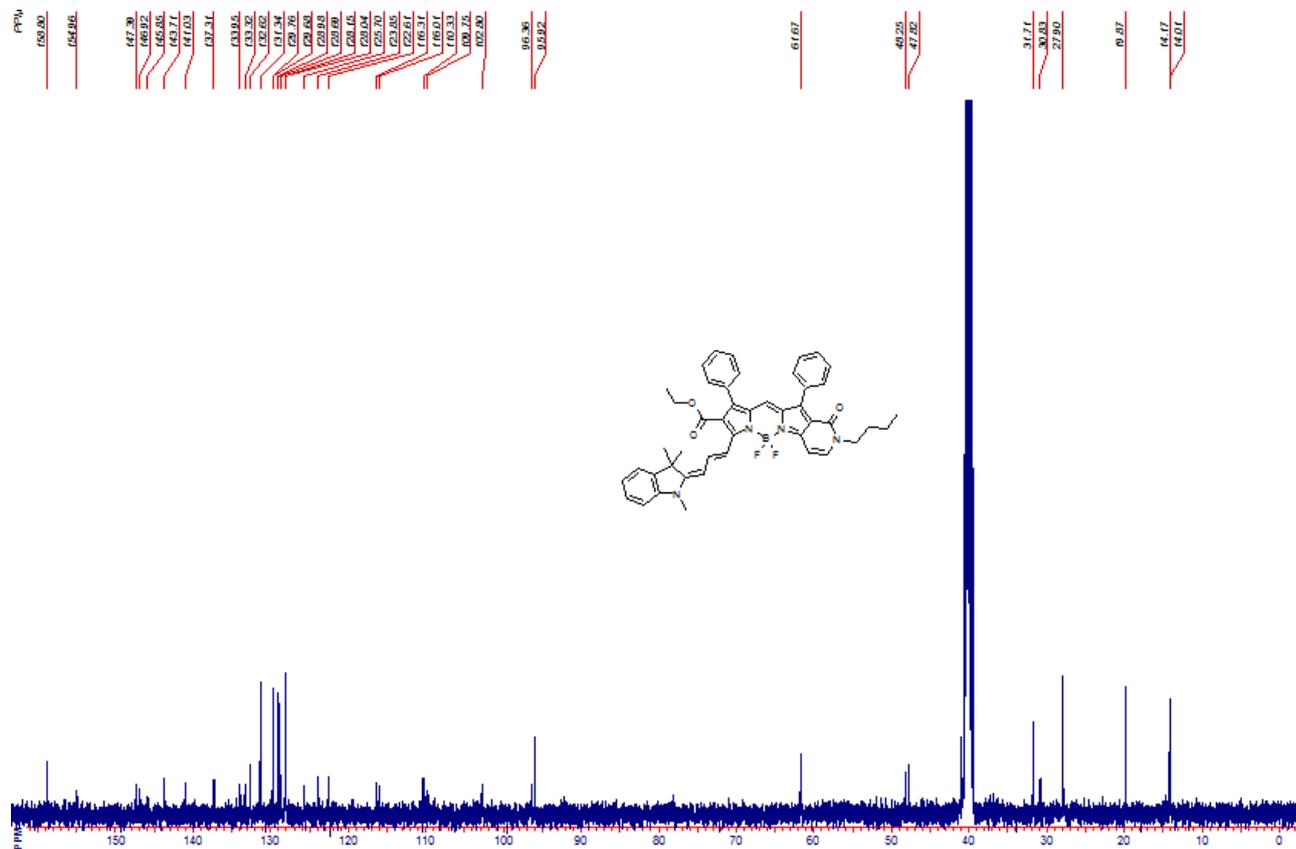


Figure 25. ^{13}C NMR spectrum of compound **7** in DMSO.

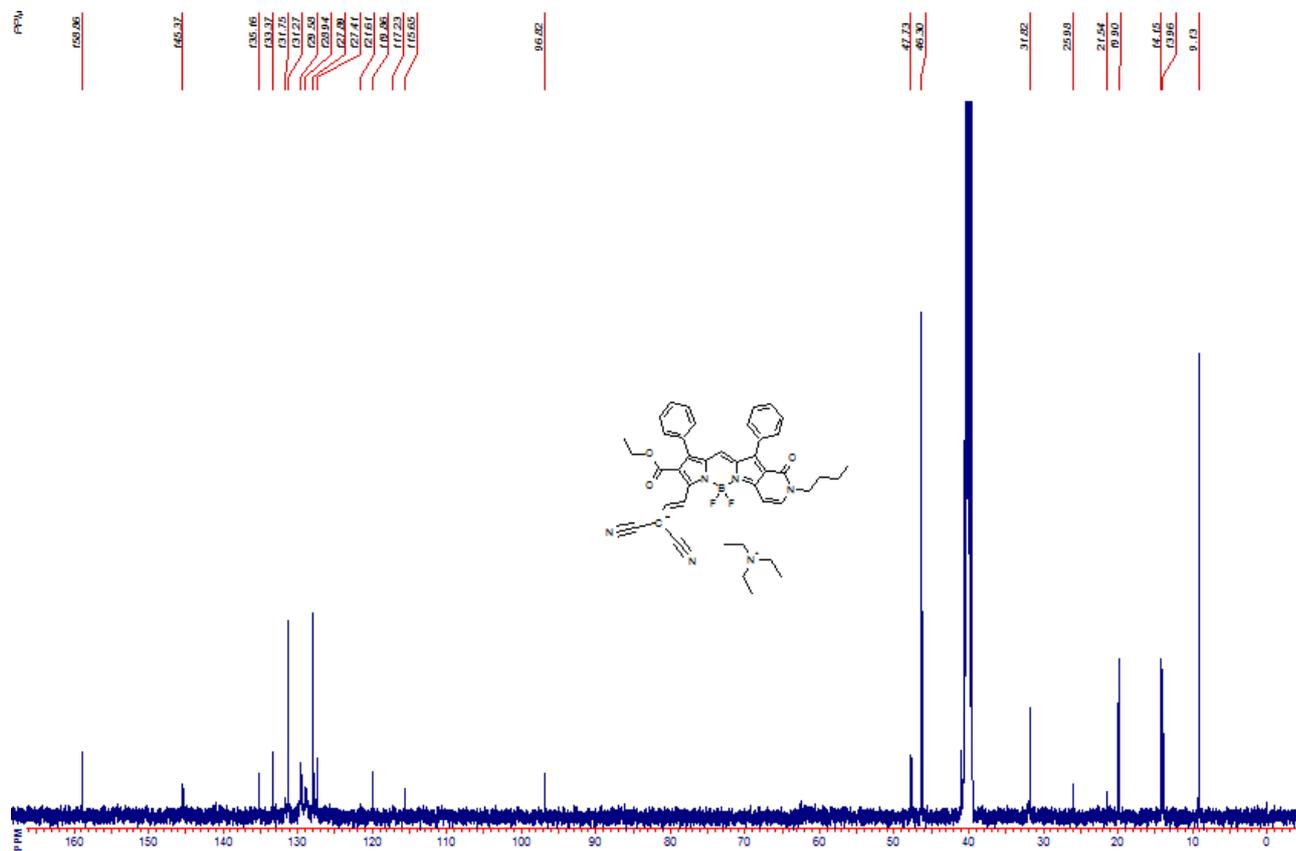


Figure 26. ^{13}C NMR spectrum of compound **10a** in DMSO.

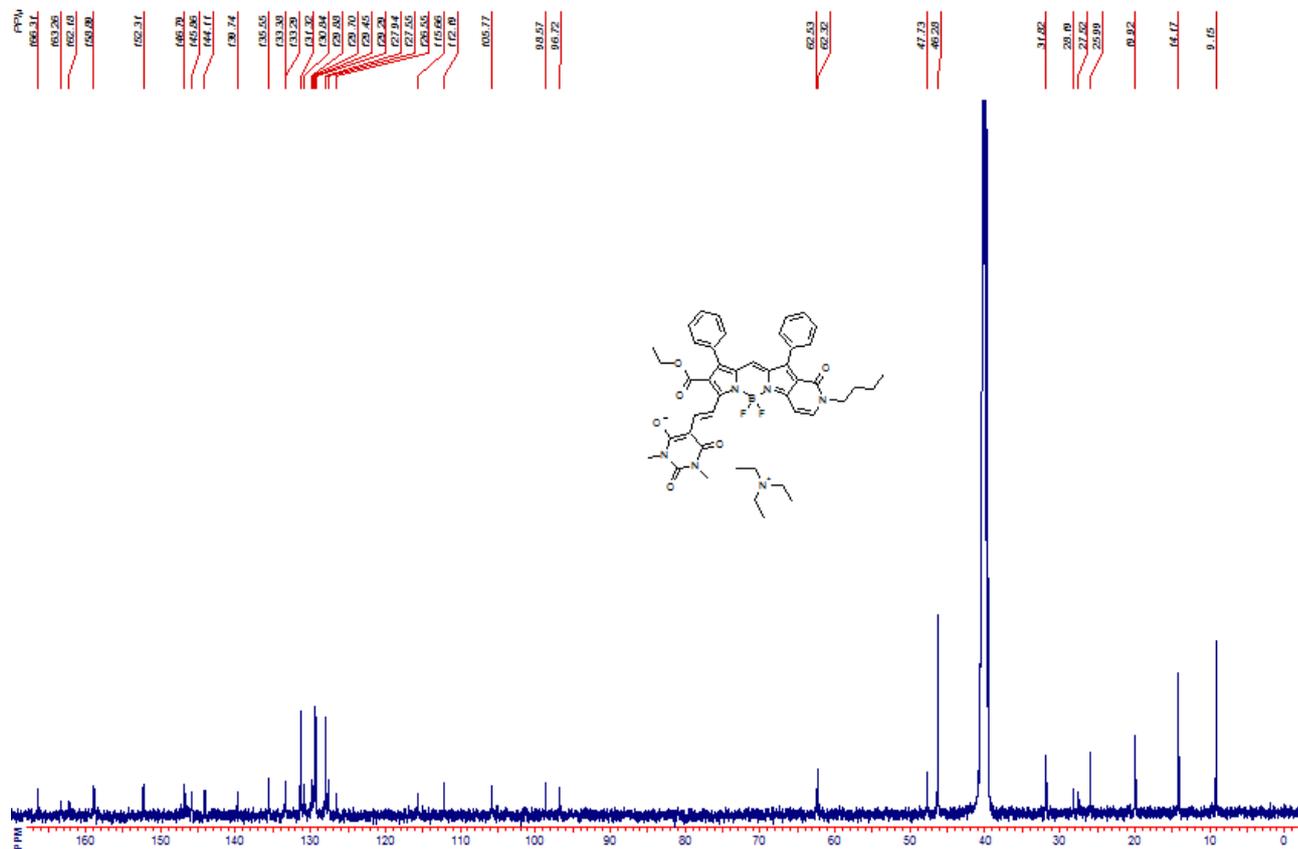


Figure 27. ^{13}C NMR spectrum of compound **11a** in DMSO.

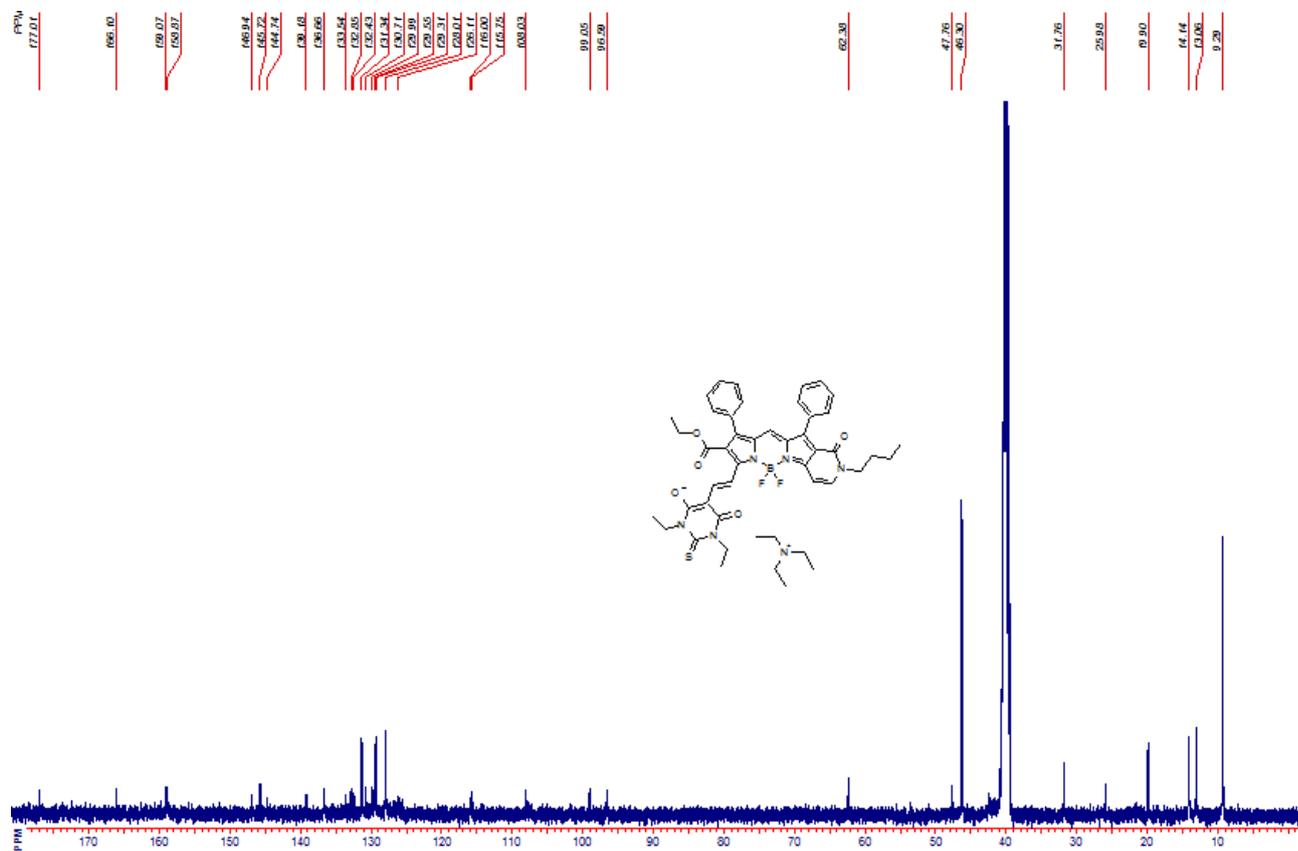


Figure 28. ^{13}C NMR spectrum of compound **12a** in DMSO.

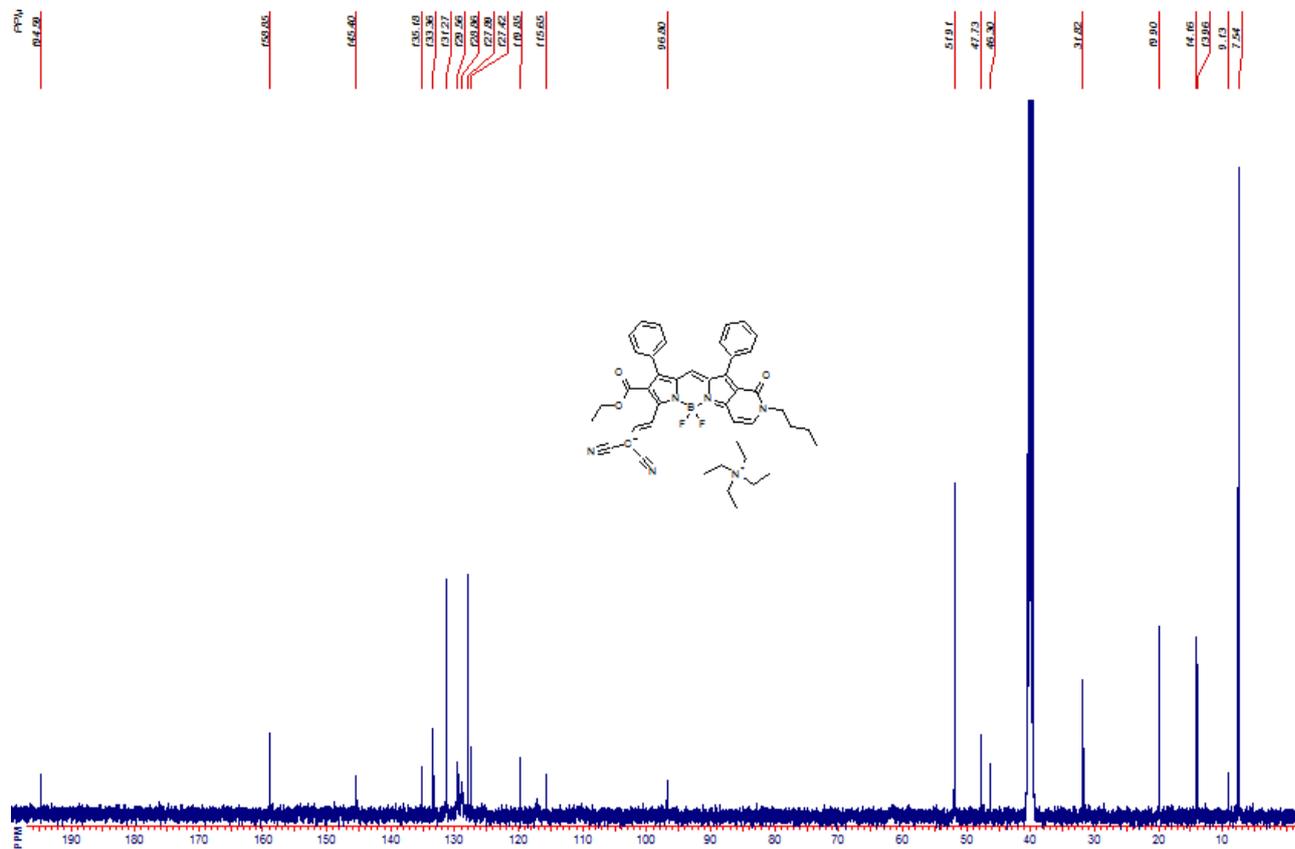


Figure 29. ^{13}C NMR spectrum of compound **10b** in DMSO.

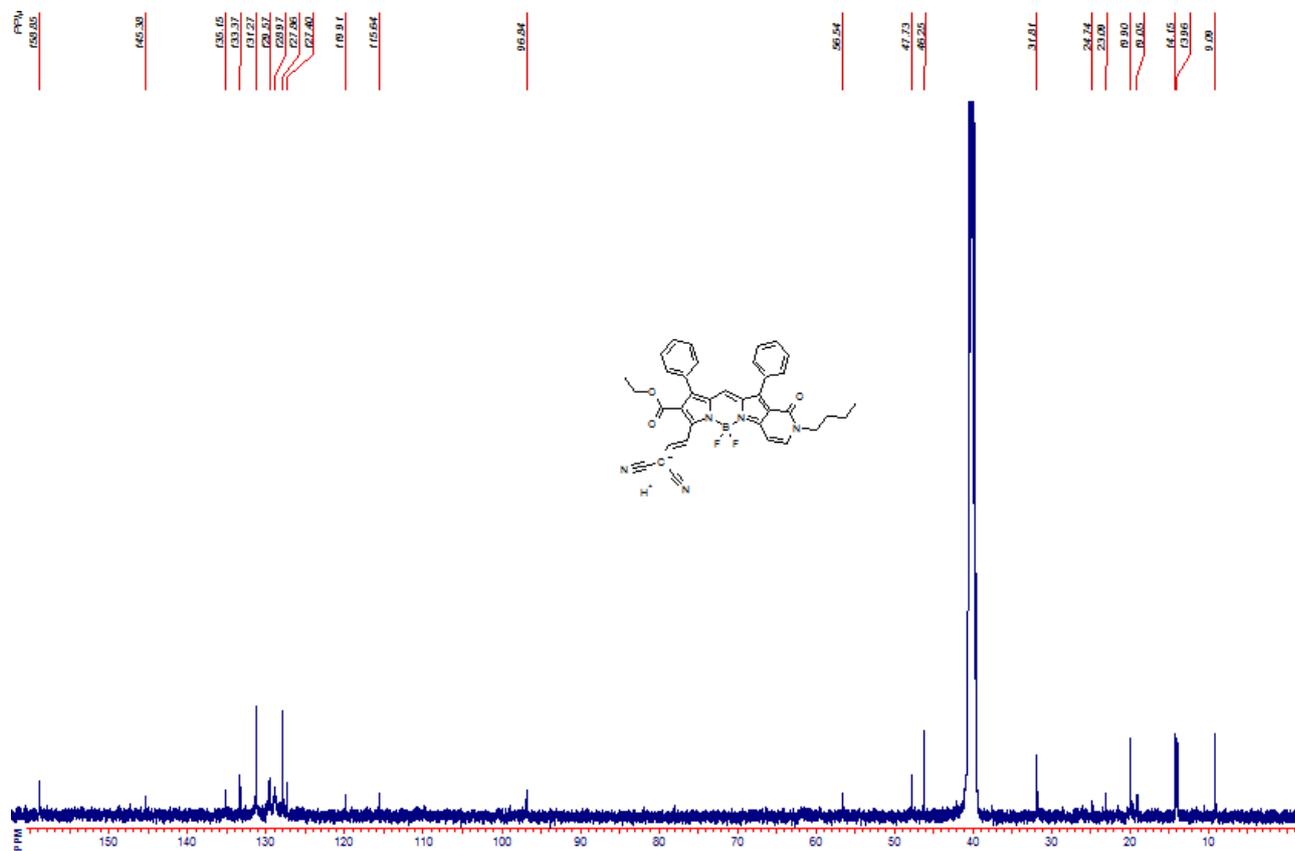


Figure 30. ^{13}C NMR spectrum of compound **13** in DMSO.

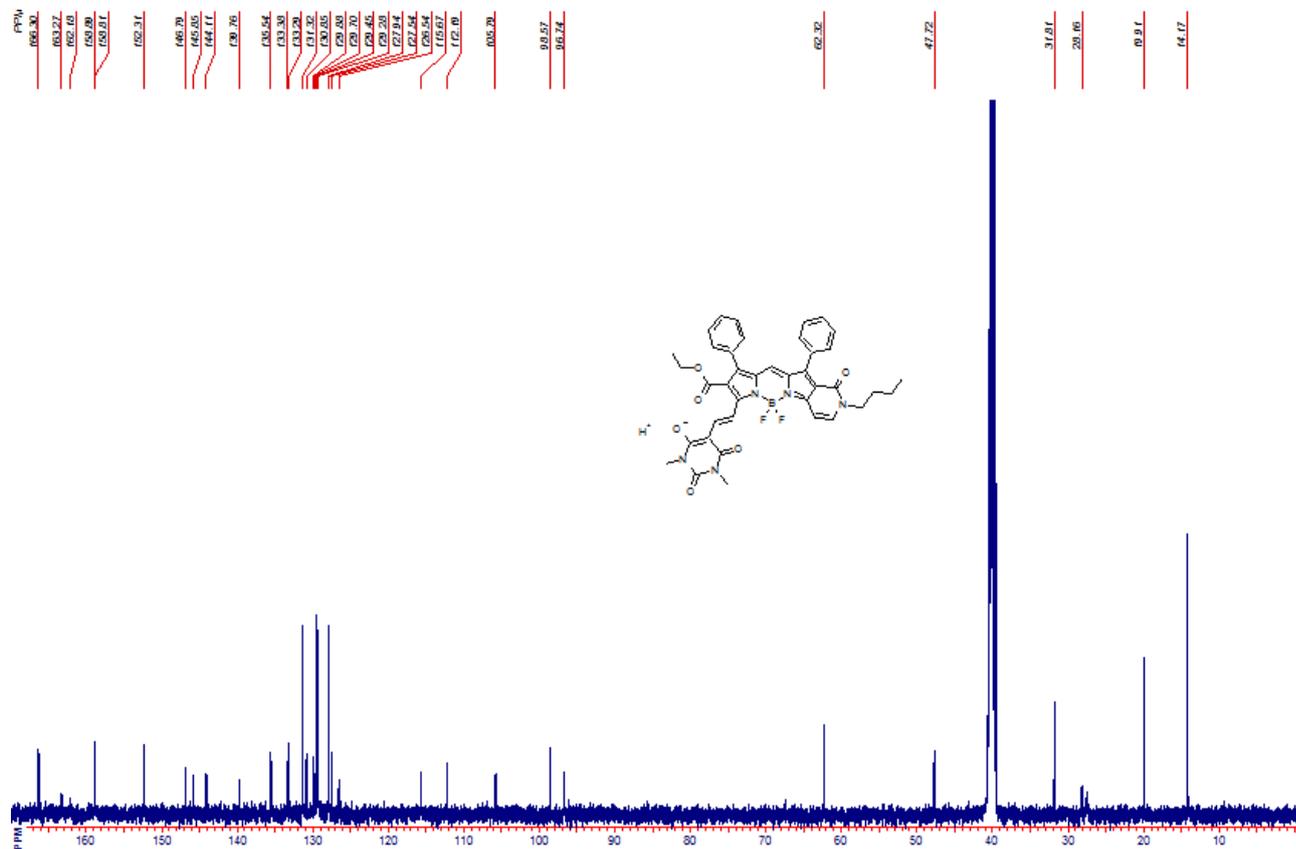


Figure 31. ^{13}C NMR spectrum of compound **14** in DMSO.

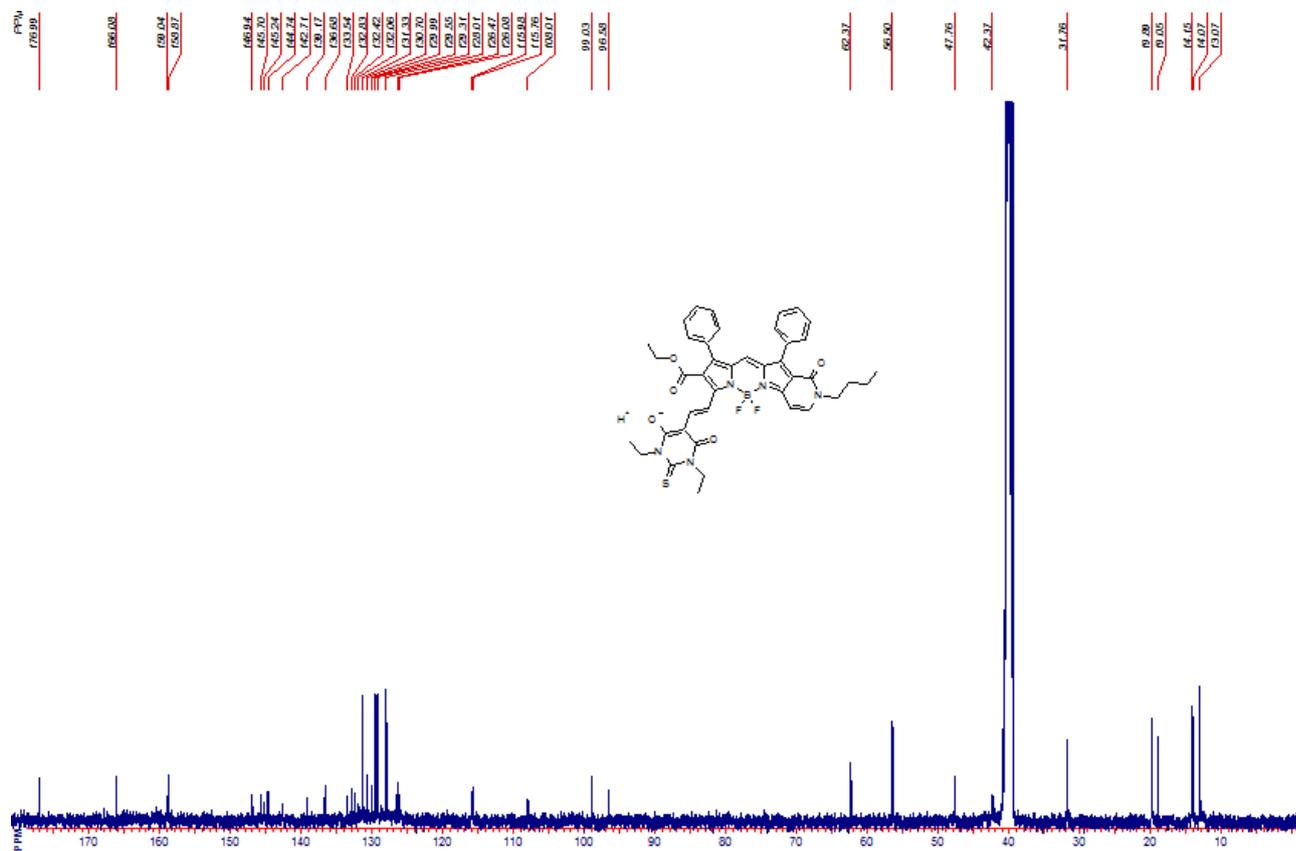


Figure 32. ^{13}C NMR spectrum of compound **15** in DMSO.

Absorption spectra

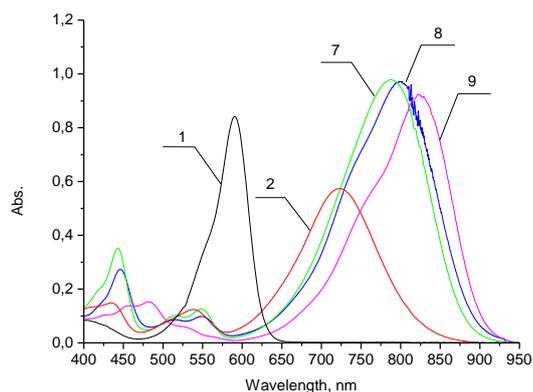


Figure 33. Absorption spectra of compounds **1,2** and **7-9** in DMF ($C_M = 1 \cdot 10^{-5}$)

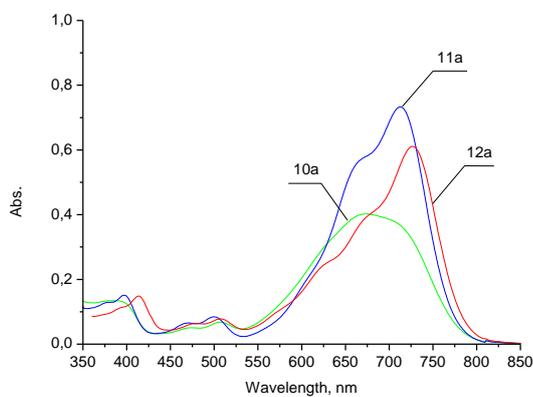


Figure 34. Absorption spectra of compounds **10a-12a** in DMF ($C_M = 1 \cdot 10^{-5}$)

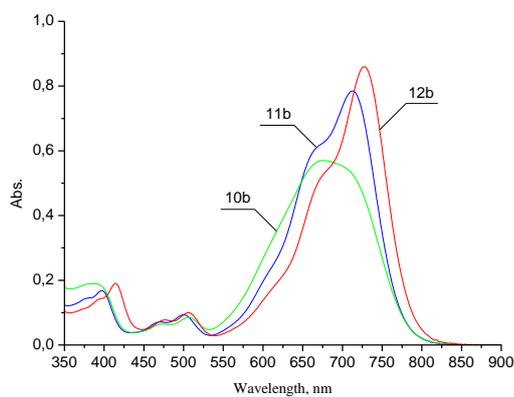


Figure 35. Absorption spectra of compounds **10b-12b** in DMF ($C_M = 1 \cdot 10^{-5}$)

Fluorescence spectra

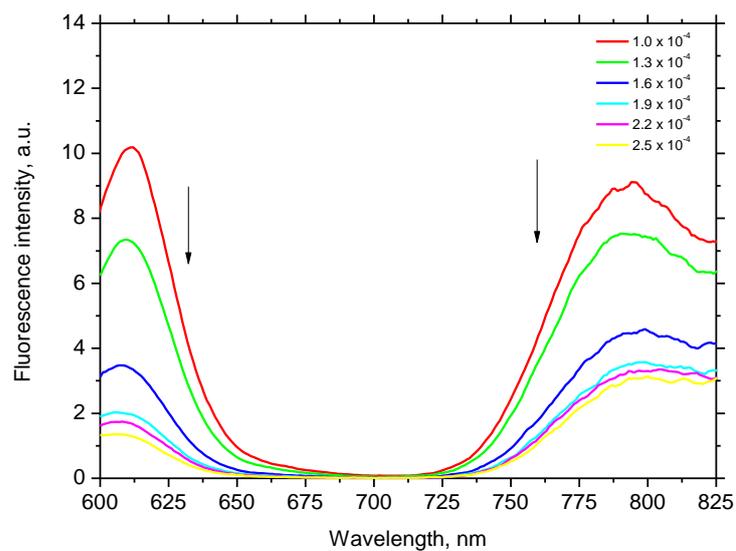


Figure.36. Fluorescence spectra of compound **14** in MeCN in different concentrations at 25 °C. Initial concentration of the dye is 1.0×10^{-4} M, final – 2.5×10^{-4} M. Excitation wavelength is 590 nm.

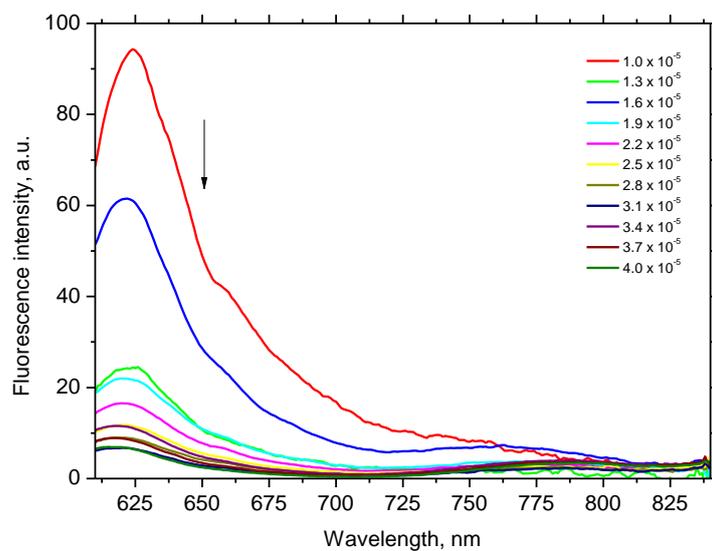


Figure.37. Fluorescence spectra of compound **14** in MeCN in different concentrations at 25 °C. Initial concentration of the dye is 1.0×10^{-5} M, final – 4.0×10^{-5} M. Excitation wavelength is 600 nm.

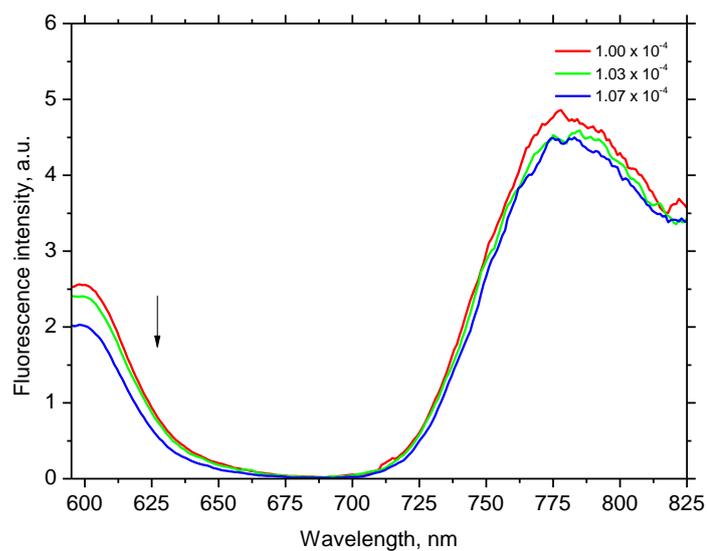


Figure.38. Fluorescence spectra of compound **14** in MeOH in different concentrations at 25 °C. Initial concentration of the dye is 1.00×10^{-4} M, final – 1.07×10^{-4} M. Excitation wavelength is 590 nm.

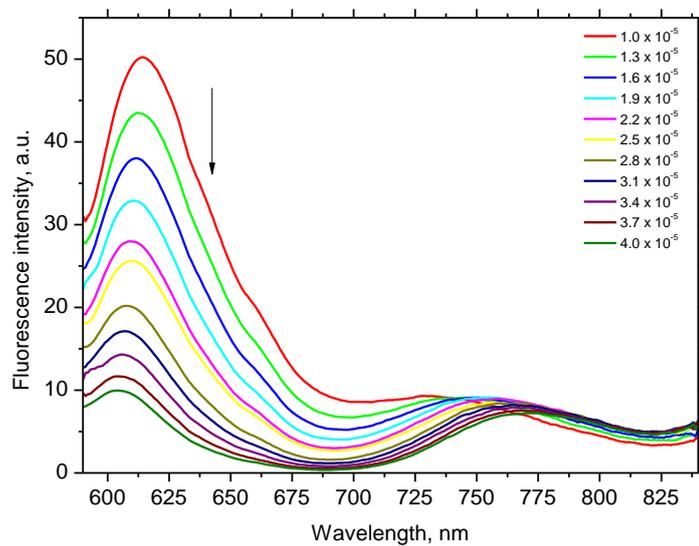


Figure.39. Fluorescence spectra of compound **14** in MeOH in different concentrations at 25 °C. Initial concentration of the dye is 1.0×10^{-5} M, final – 4.0×10^{-5} M. Excitation wavelength is 580 nm.

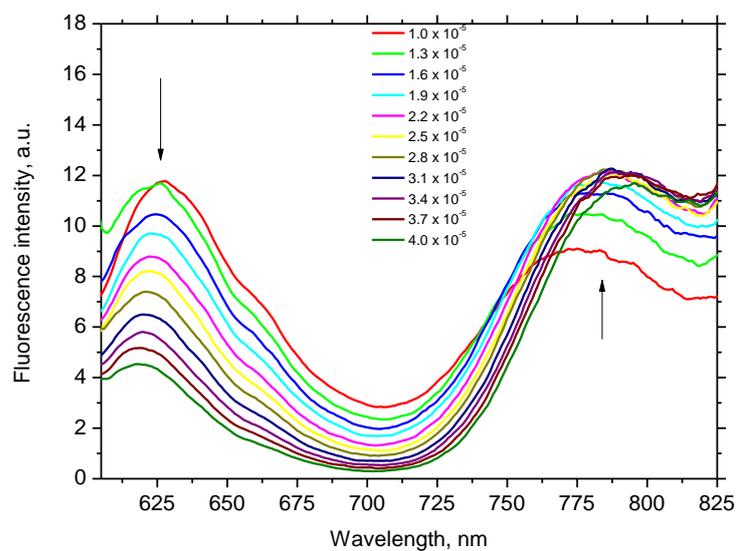


Figure.40. Fluorescence spectra of compound **14** in 50% DMSO aqueous solution in different concentrations at 25 °C. Initial concentration of the dye is 1.0×10^{-5} M, final – 4.0×10^{-5} M. Excitation wavelength is 590 nm.

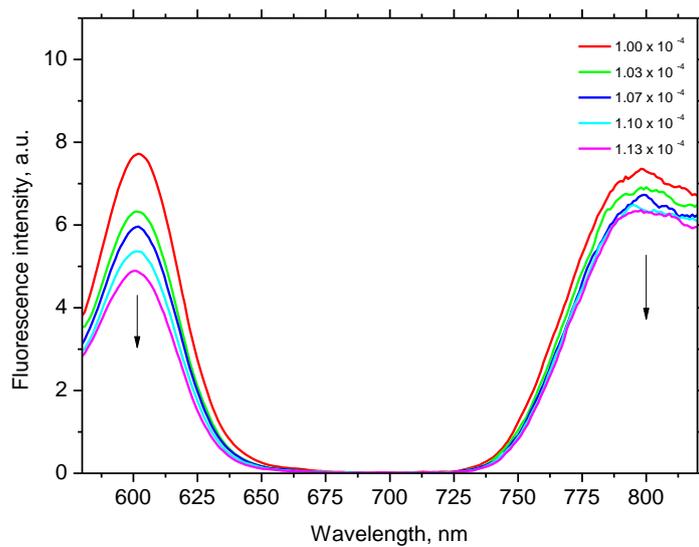


Figure.41. Fluorescence spectra of compound **15** in MeOH in different concentrations at 25 °C. Initial concentration of the dye is 1.00×10^{-4} M, final – 1.13×10^{-4} M. Excitation wavelength is 570 nm.

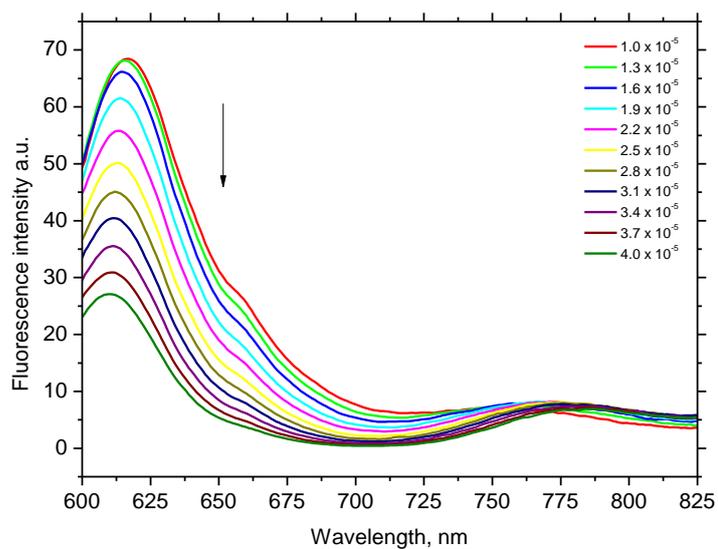


Figure.42. Fluorescence spectra of compound **15** in MeOH in different concentrations at 25 °C. Initial concentration of the dye is 1.0×10^{-5} M, final – 4.0×10^{-5} M. Excitation wavelength is 590 nm.

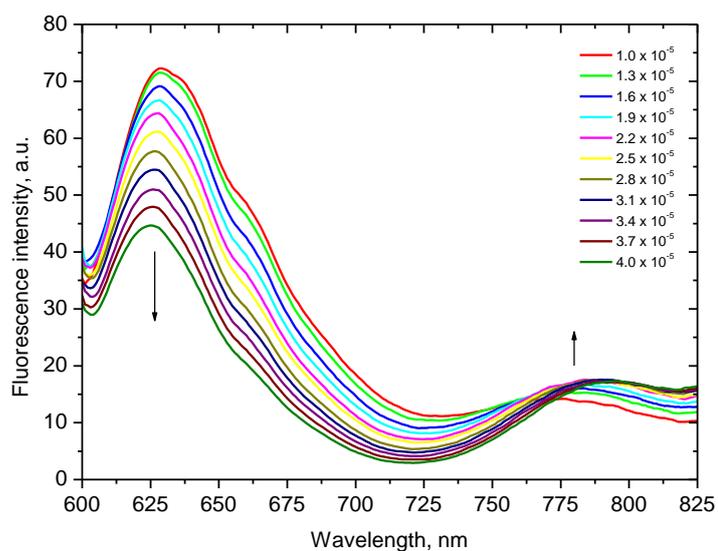


Figure.43. Fluorescence spectra of compound **15** in 50% DMSO aqueous solution in different concentrations at 25 °C. Initial concentration of the dye is 1.0×10^{-5} M, final – 4.0×10^{-5} M. Excitation wavelength is 590 nm.