

ELECTRONIC SUPPORTING INFORMATION (ESI)

to:

Formation, structure, and reactivity of meso-tetraaryl-chloro-lactones, porpholactams, and –chlorolactams, porphyrin and chlorin analogues incorporating oxazolone or imidazolone moieties

Joshua Akhigbe[†], John Haskoor[†], Jeanette A. Krause[‡],

Matthias Zeller[§], and Christian Brückner^{†,}*

Department of Chemistry, University of Connecticut, Storrs, CT 06269-3060, U.S.A.

Department of Chemistry, University of Cincinnati, Cincinnati, OH 45221-0172, U.S.A.

Department of Chemistry, Youngstown State University, Youngstown, OH 44555-3663, U.S.A.

* author to whom inquiries should be addressed to:

E-mail: c.bruckner@uconn.edu

Tel: +01 860-908-2743

ESI Table of Contents:

Figure 1.	^1H NMR Spectrum (400 MHz, CDCl_3) of 7a	4
Figure 2.	^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 3s) of 7a	5
Figure 3.	FT-IR Spectrum (neat, diffuse reflectance) of 7a	6
Figure 4.	^1H NMR Spectrum (400 MHz, CDCl_3) of 7b	7
Figure 5.	^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 5s) of 7b	8
Figure 6.	FT-IR Spectrum (neat, diffuse reflectance) of 7b	9
Figure 7.	^1H NMR Spectrum (400 MHz, CDCl_3) of 8a	10
Figure 8.	^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 3s) of 8a	11
Figure 9.	FT-IR Spectrum (neat, diffuse reflectance) of 8a	12
Figure 10.	^1H NMR Spectrum (400 MHz, CD_2Cl_2) of 8b	13
Figure 11.	^{13}C NMR Spectrum (100 MHz, CD_2Cl_2 , D1 = 5s) of 8b	14
Figure 12.	FT-IR Spectrum (neat, diffuse reflectance) of 8b	15
Figure 13.	^1H NMR Spectrum (400 MHz, CDCl_3) of 8c	16
Figure 14.	^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 5s) of 8c	17
Figure 15.	FT-IR Spectrum (neat, diffuse reflectance) of 8c	18
Figure 16.	^1H NMR Spectrum (400 MHz, CDCl_3) of 9a	19
Figure 17.	^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 3s) of 9a	20
Figure 18.	FT-IR Spectrum (neat, diffuse reflectance) of 9a	21
Figure 19.	^1H NMR Spectrum (400 MHz, CD_2Cl_2) of 9b	22
Figure 20.	^{13}C NMR Spectrum (100 MHz, CD_2Cl_2 , D1 = 5s) of 9b	23
Figure 21.	FT-IR Spectrum (neat, diffuse reflectance) of 9b	24
Figure 22.	^1H NMR Spectrum (400 MHz, CDCl_3) of 9c	25
Figure 23.	^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 5s) of 9c	26
Figure 24.	FT-IR Spectrum (neat, diffuse reflectance) of 9c	27
Figure 25.	^1H NMR Spectrum (400 MHz, CDCl_3) of 10a	28
Figure 26.	^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 3s) of 10a	29
Figure 27.	FT-IR Spectrum (neat, diffuse reflectance) of 10a	30
Figure 28.	^1H NMR Spectrum (400 MHz, CD_2Cl_2) of 10a	31
Figure 29.	^{13}C NMR Spectrum (100 MHz, CD_2Cl_2) of 10b	32
Figure 30.	FT-IR Spectrum (neat, diffuse reflectance) of 10b	33
Figure 31.	^1H NMR Spectrum (400 MHz, CDCl_3) of 10c	34

Figure 32.	^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 3s) of 10c	35
Figure 33.	FT-IR Spectrum (neat, diffuse reflectance) of 10c	36
Figure 34.	^1H NMR Spectrum (400 MHz, CDCl_3) of 11c	37
Figure 35.	^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 3s) of 11c	38
Figure 36.	FT-IR Spectrum (neat, diffuse reflectance) of 11c	39
Figure 37.	^1H NMR Spectrum (400 MHz, CDCl_3) of 15a	40
Figure 38.	^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 3s) of 15a	41
Figure 39.	FT-IR Spectrum (neat, diffuse reflectance) of 15a	42

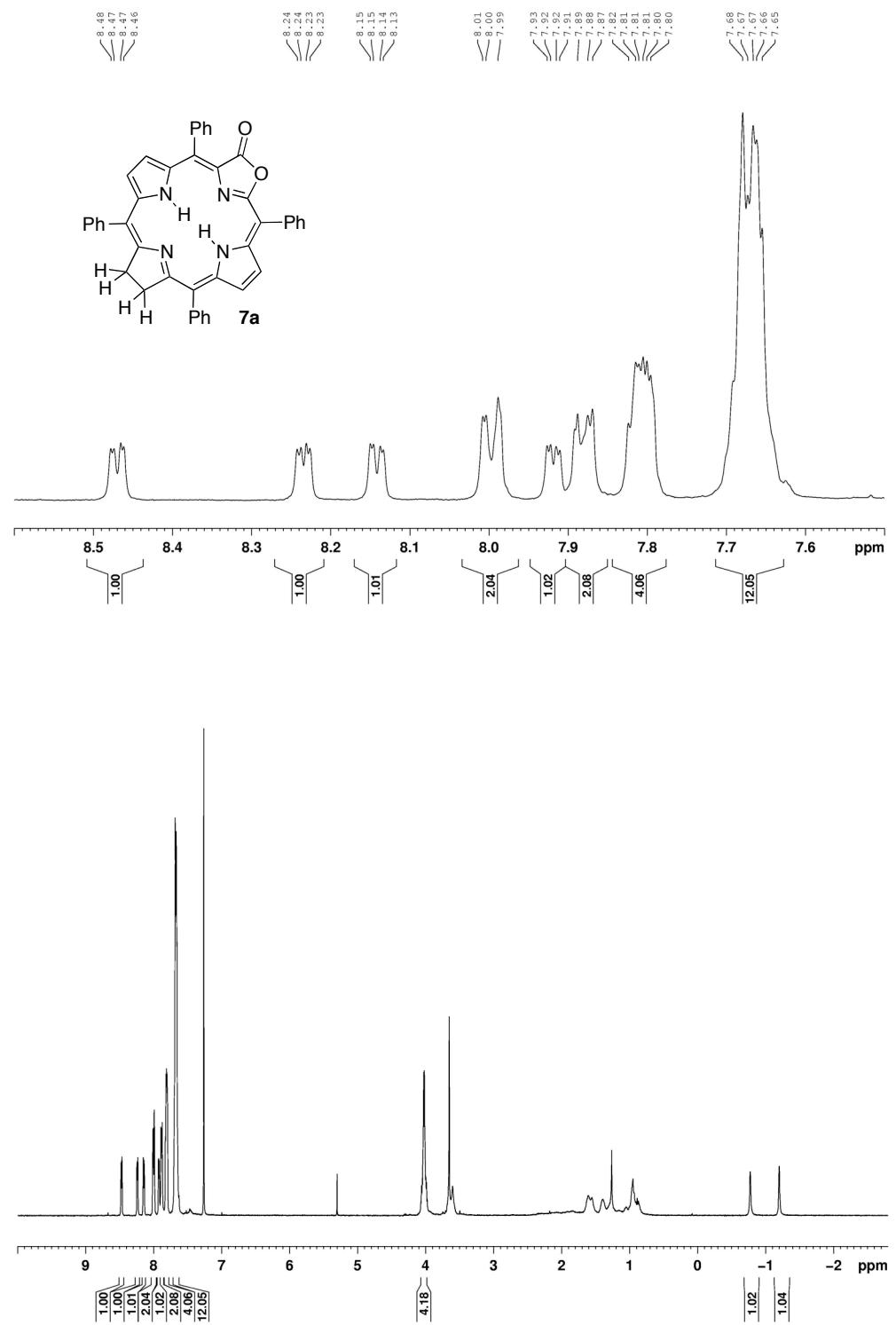


Figure 1. ^1H NMR Spectrum (400 MHz, CDCl_3) of **7a**

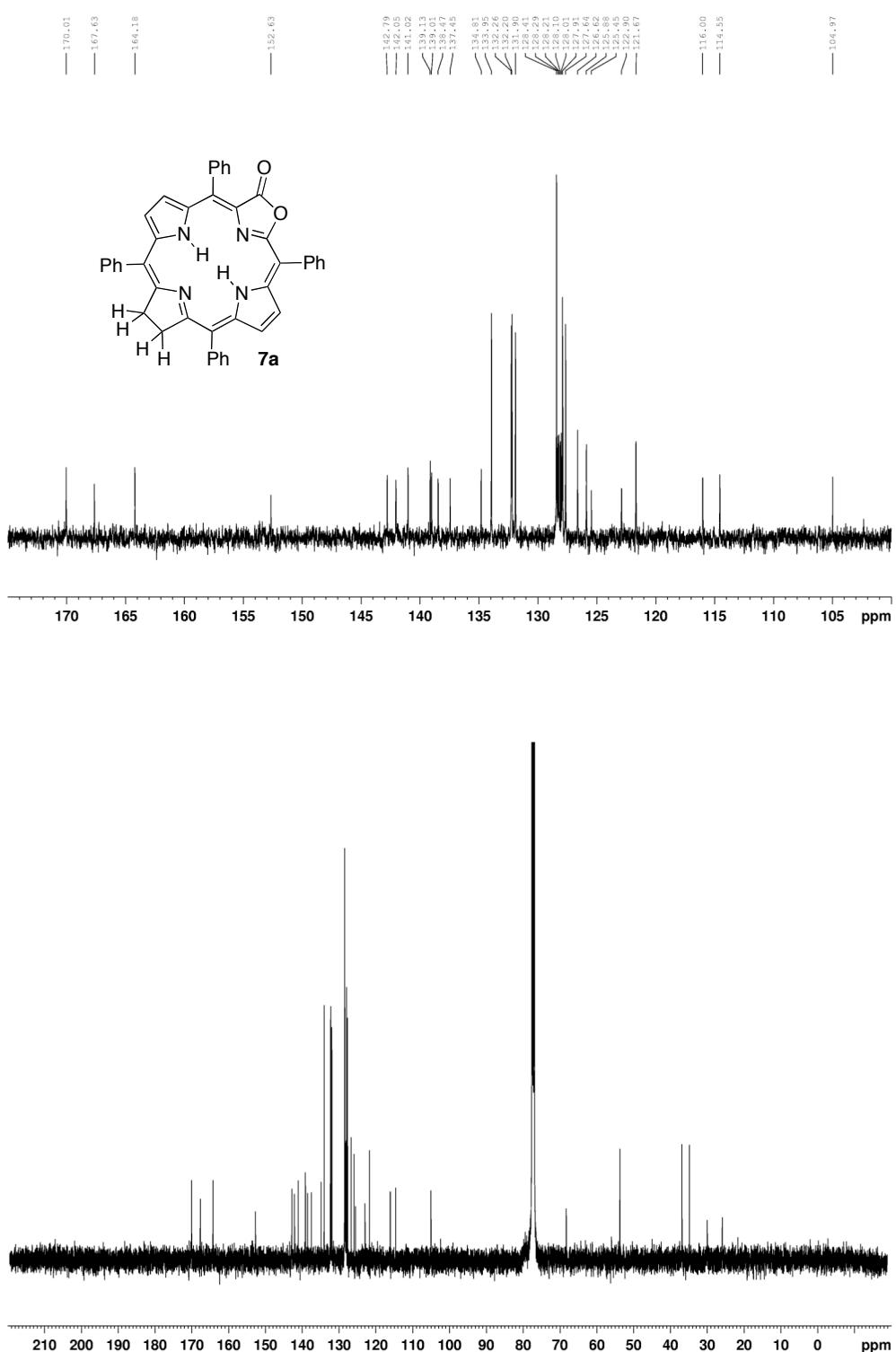


Figure 2. ^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 3s) of **7a**

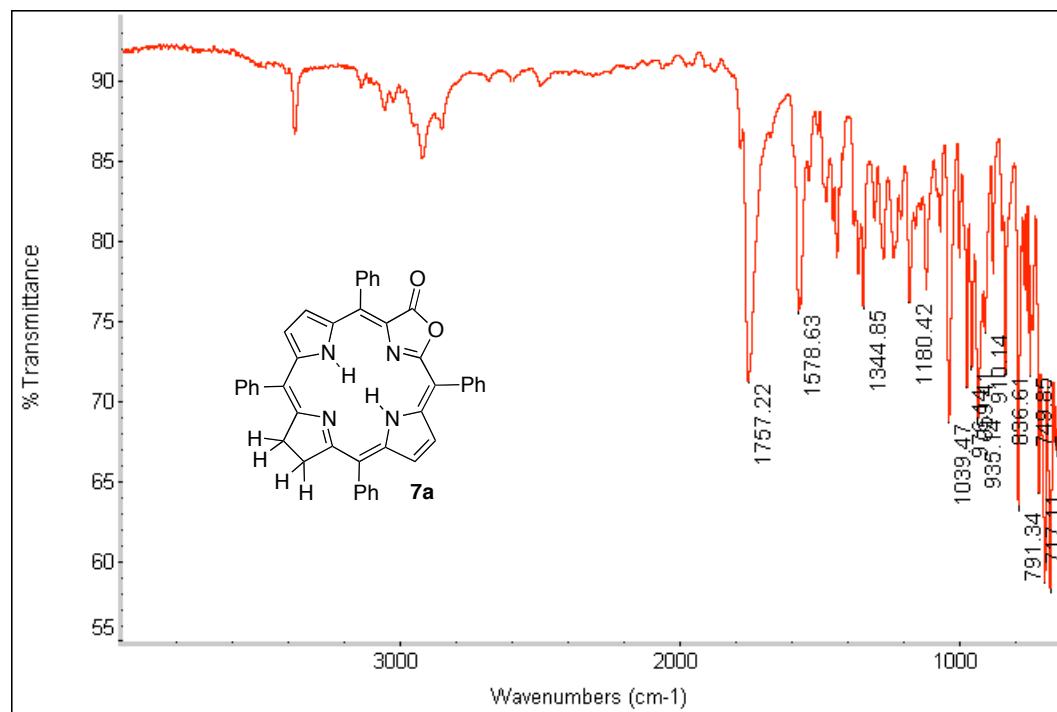


Figure 3. FT-IR Spectrum (neat, diffuse reflectance) of **7a**

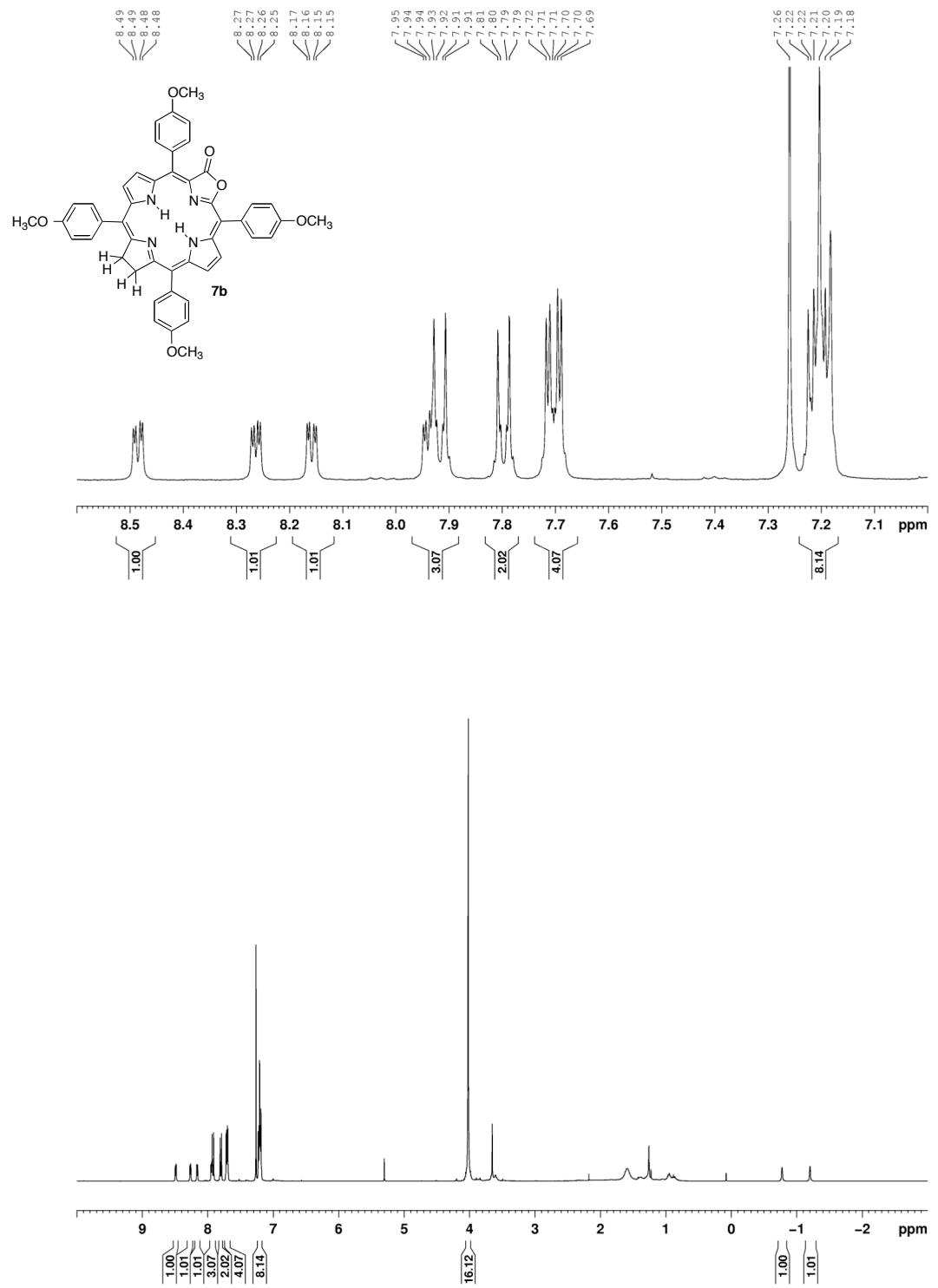


Figure 4. ^1H NMR Spectrum (400 MHz, CDCl_3) of **7b**

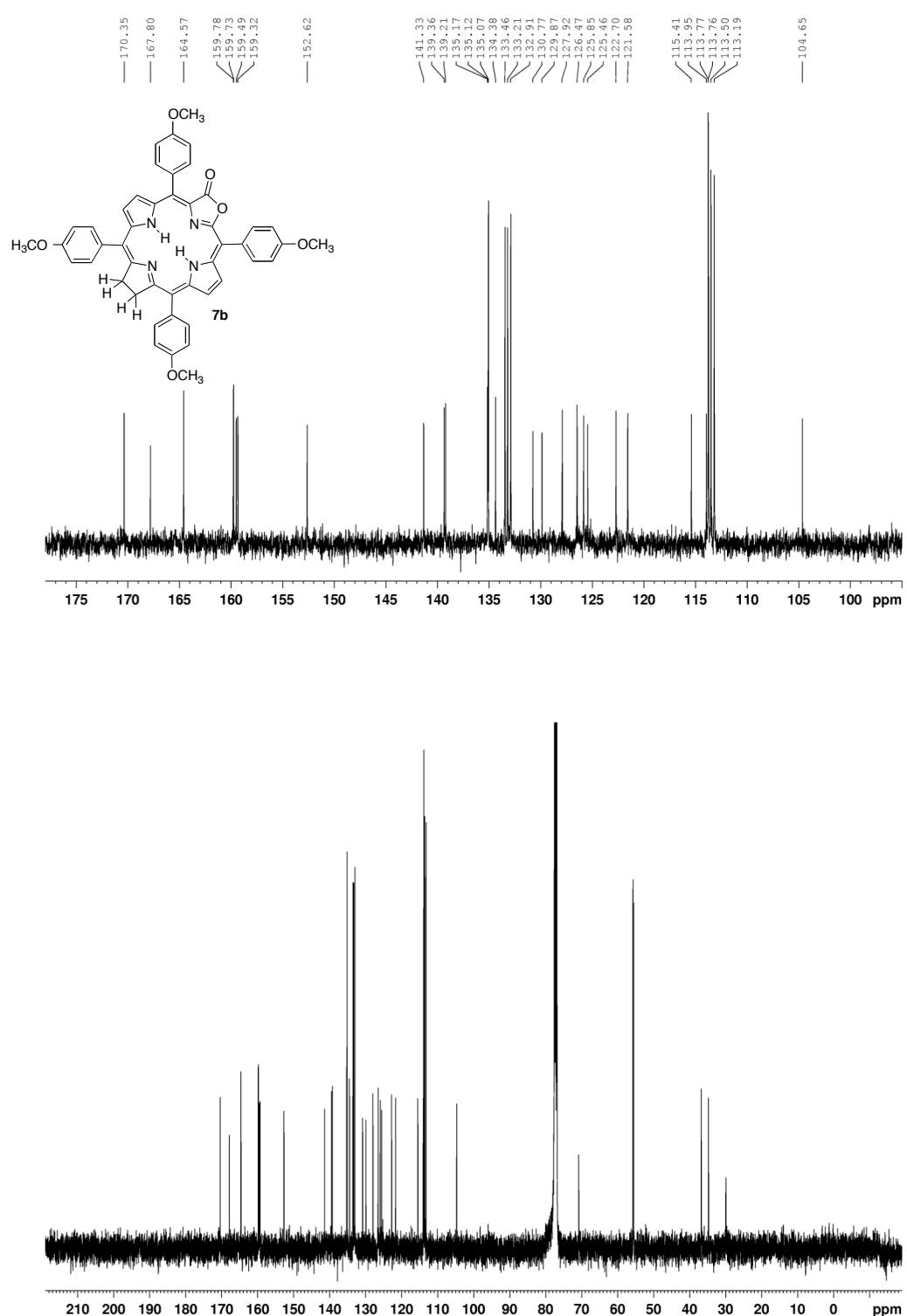


Figure 5. ¹³C NMR Spectrum (100 MHz, CDCl₃, D1 = 5s) of **7b**

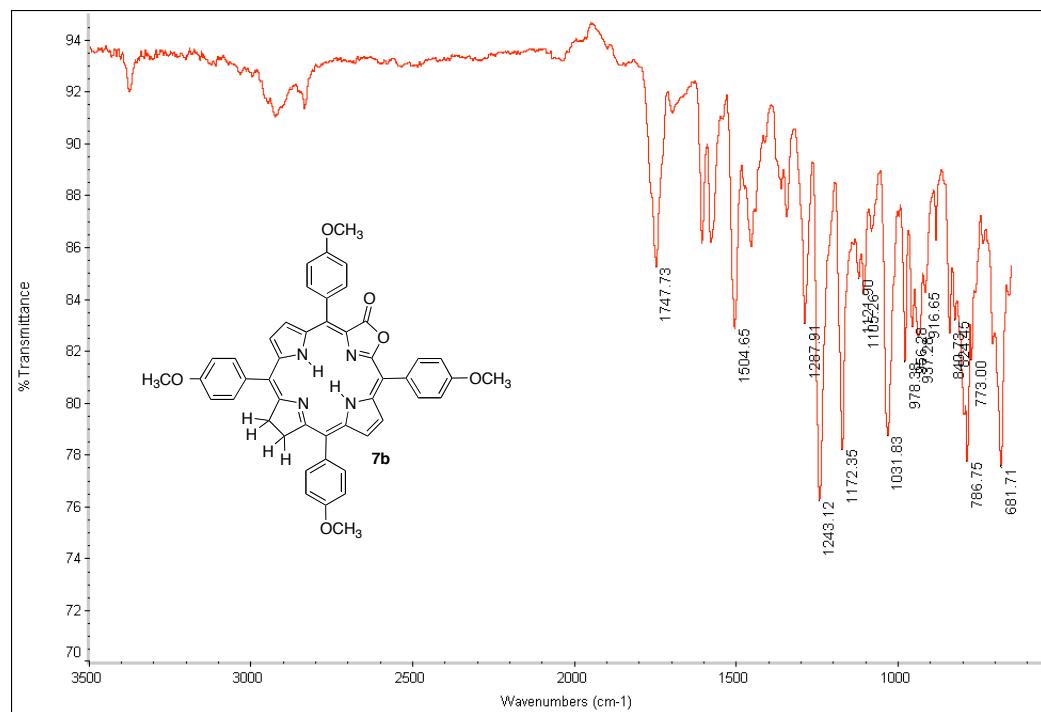
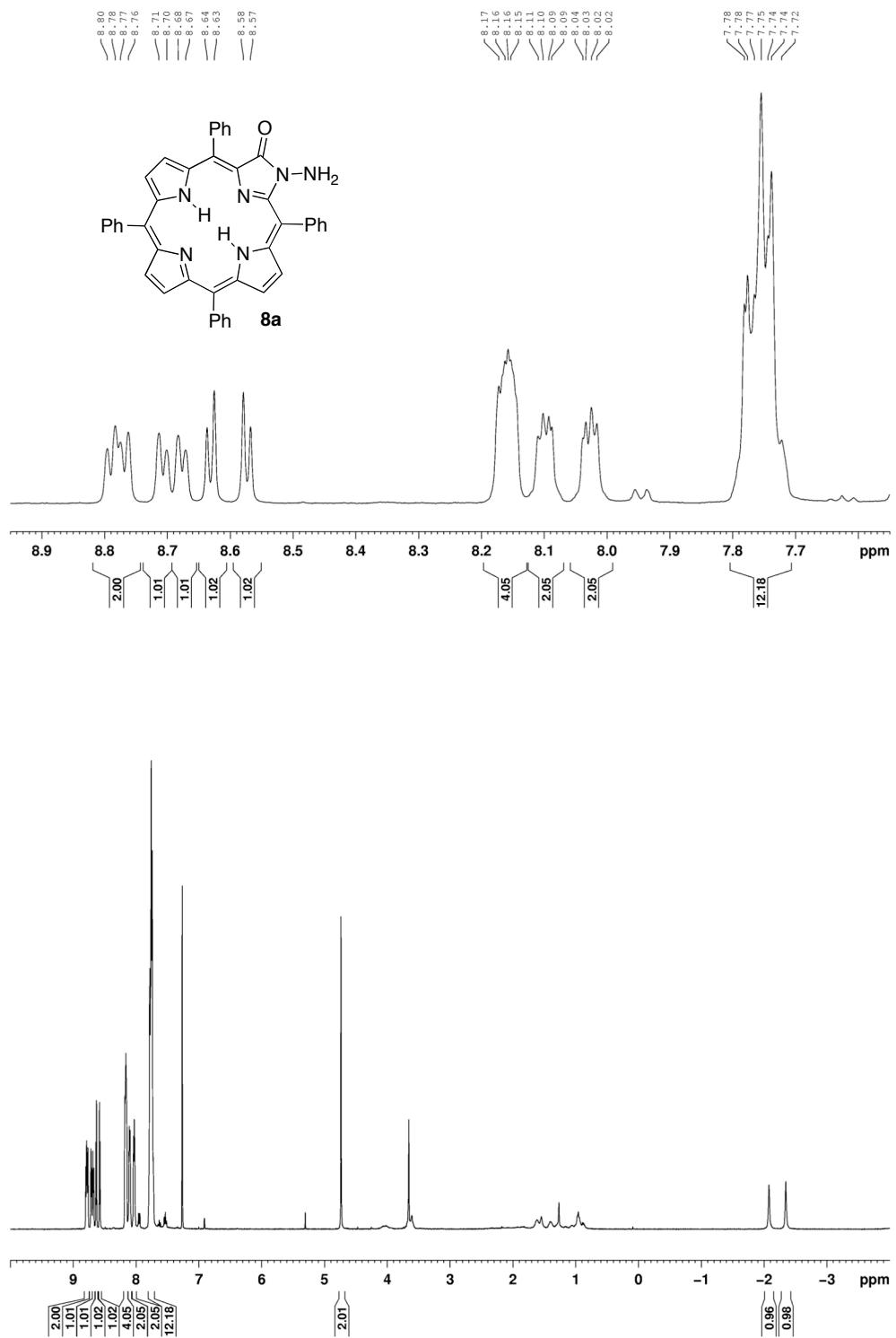


Figure 6. FT-IR Spectrum (neat, diffuse reflectance) of **7b**



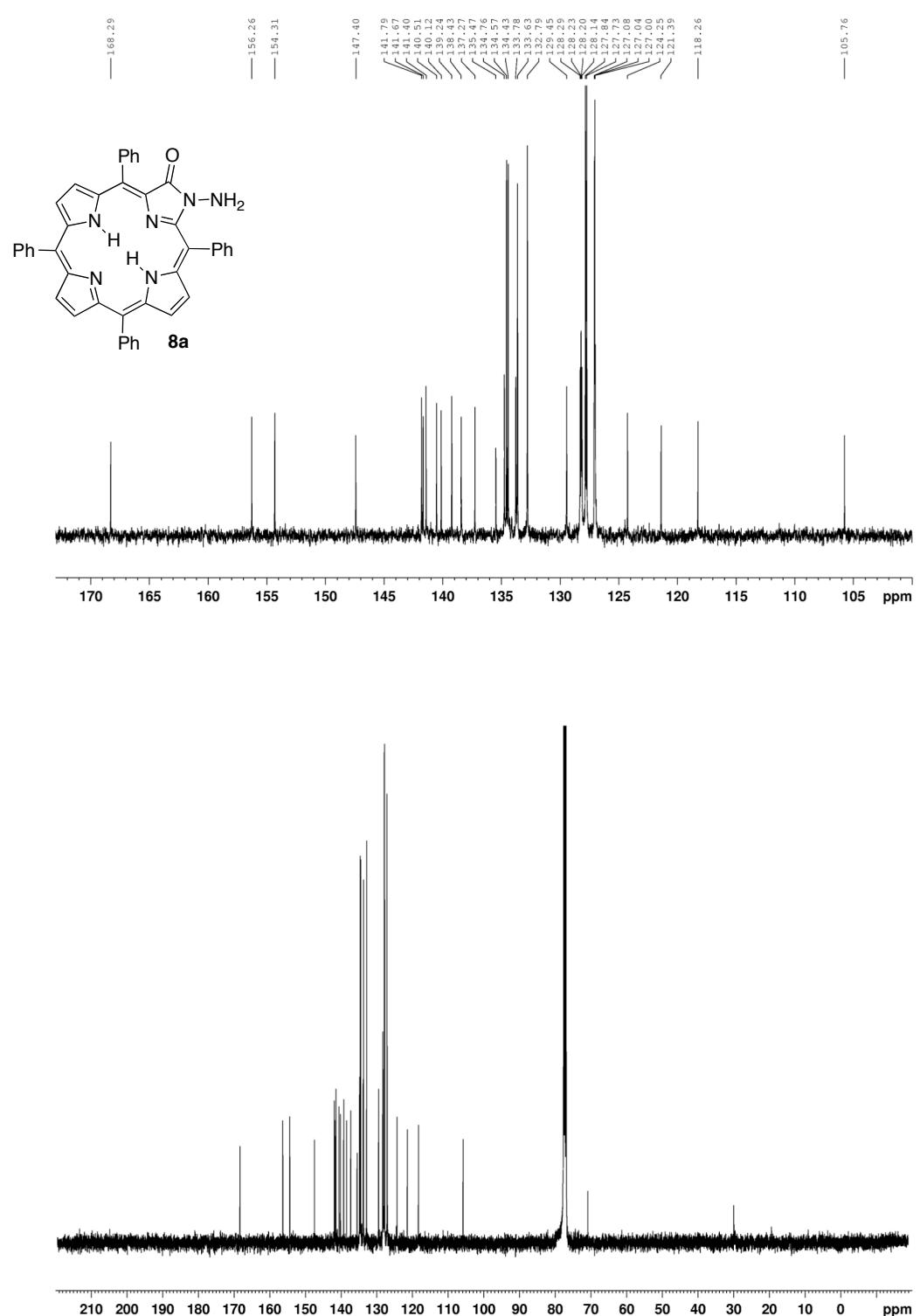


Figure 8. ^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 3s) of **8a**

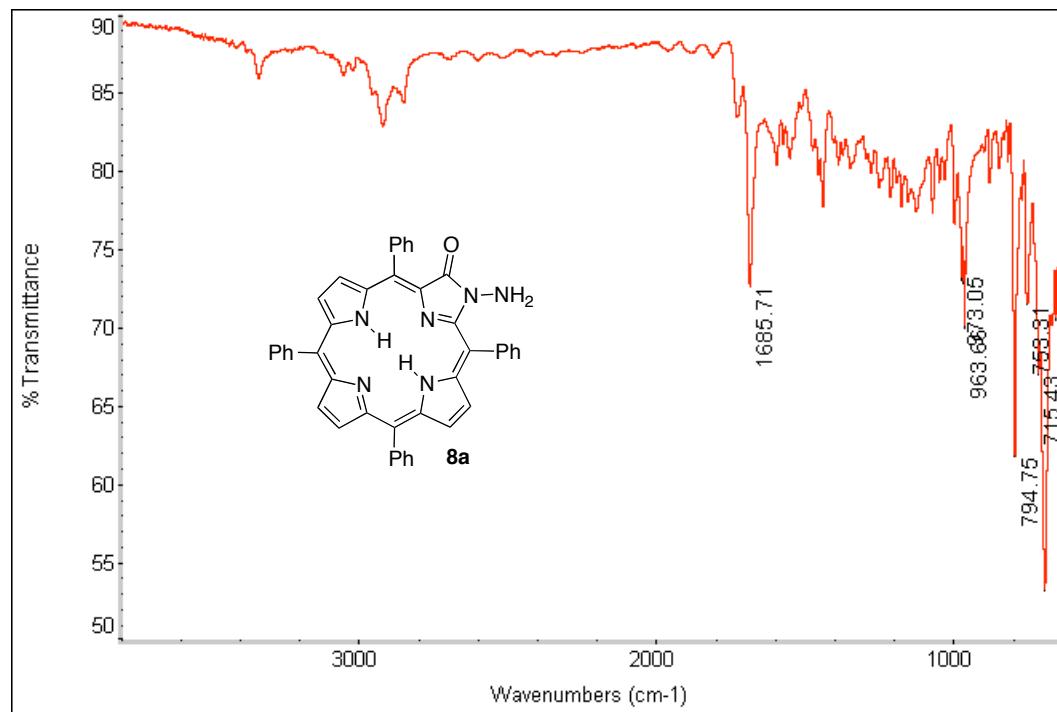
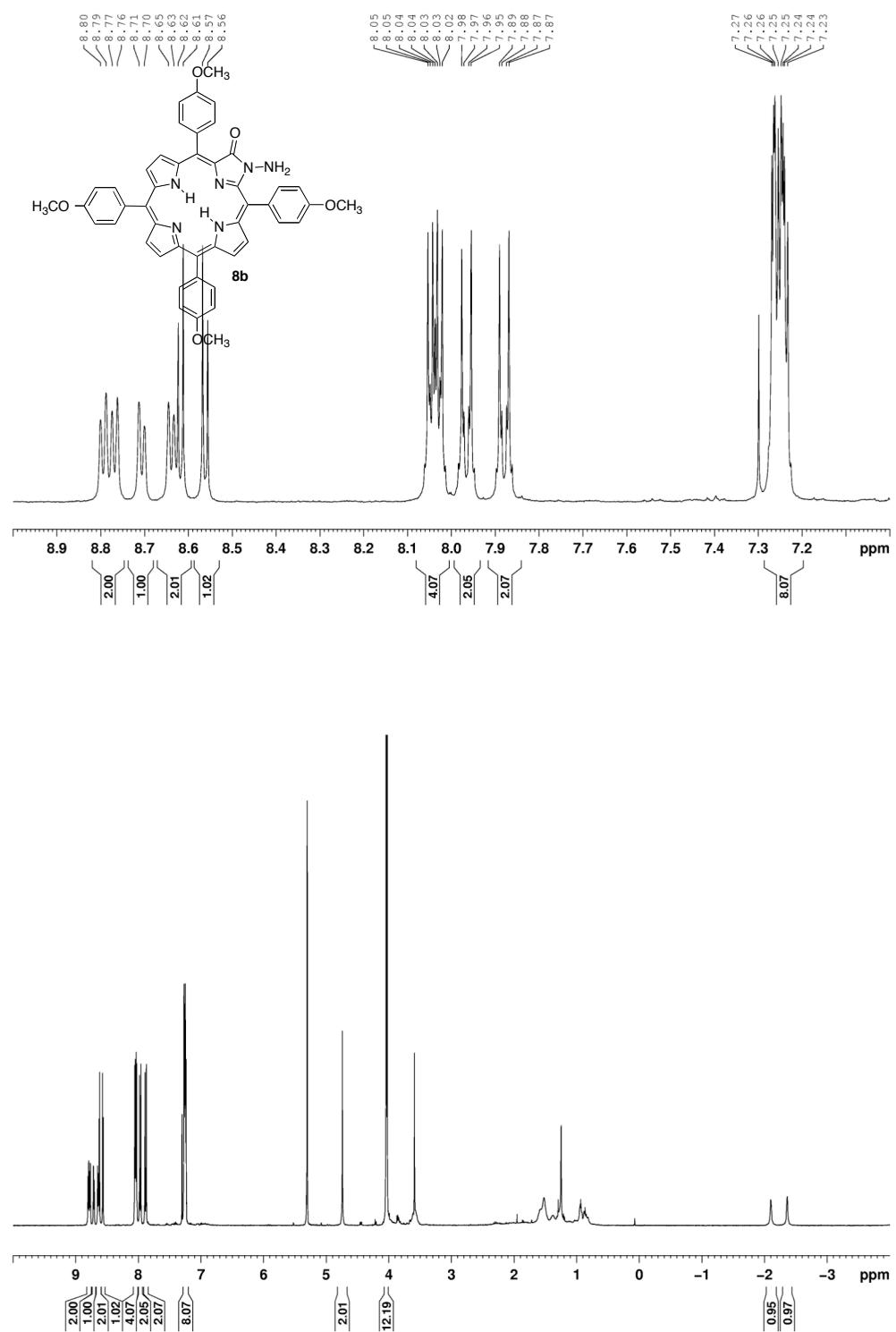


Figure 9. FT-IR Spectrum (neat, diffuse reflectance) of **8a**



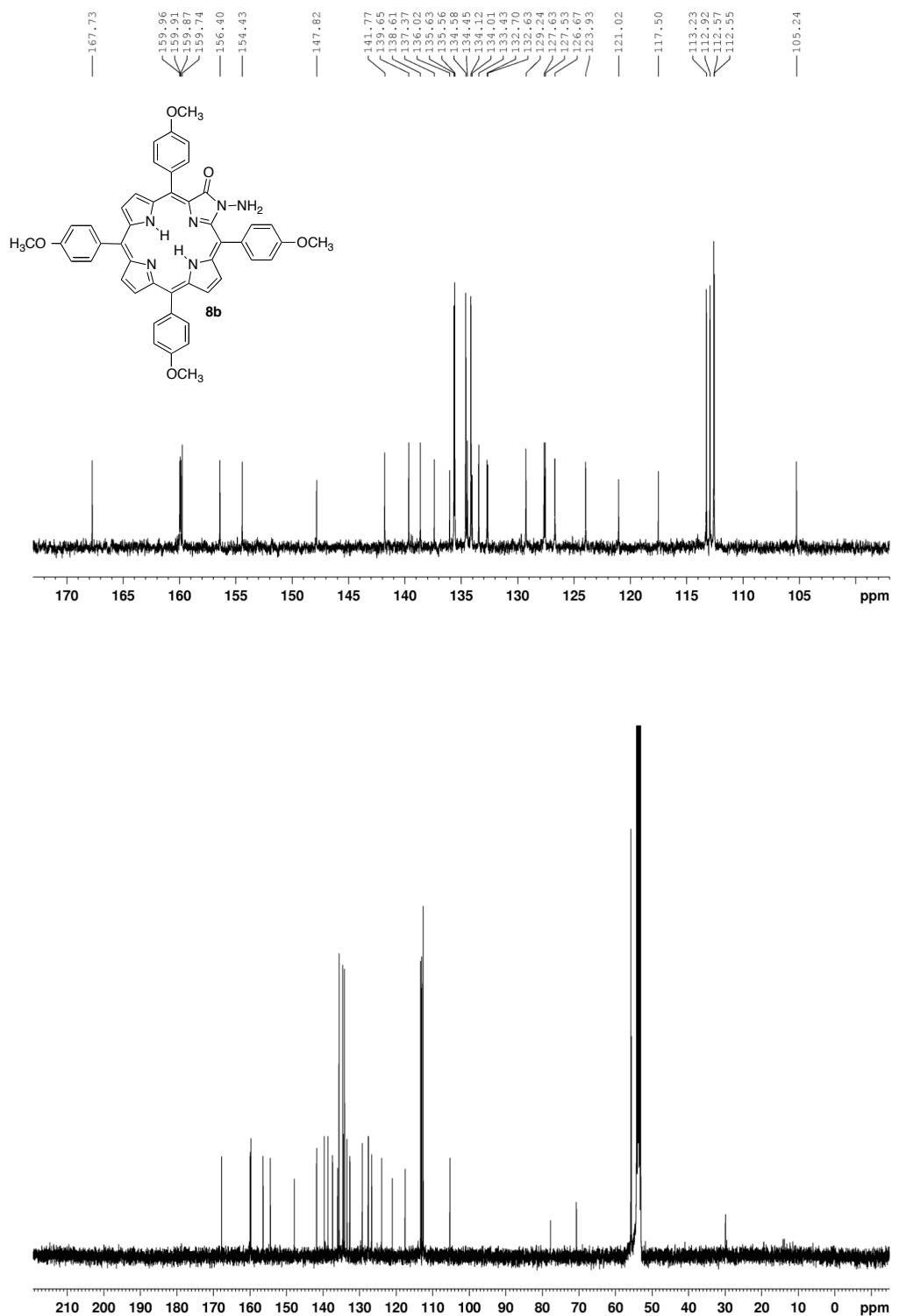


Figure 11. ^{13}C NMR Spectrum (100 MHz, CD₂Cl₂, D1 = 5s) of **8b**

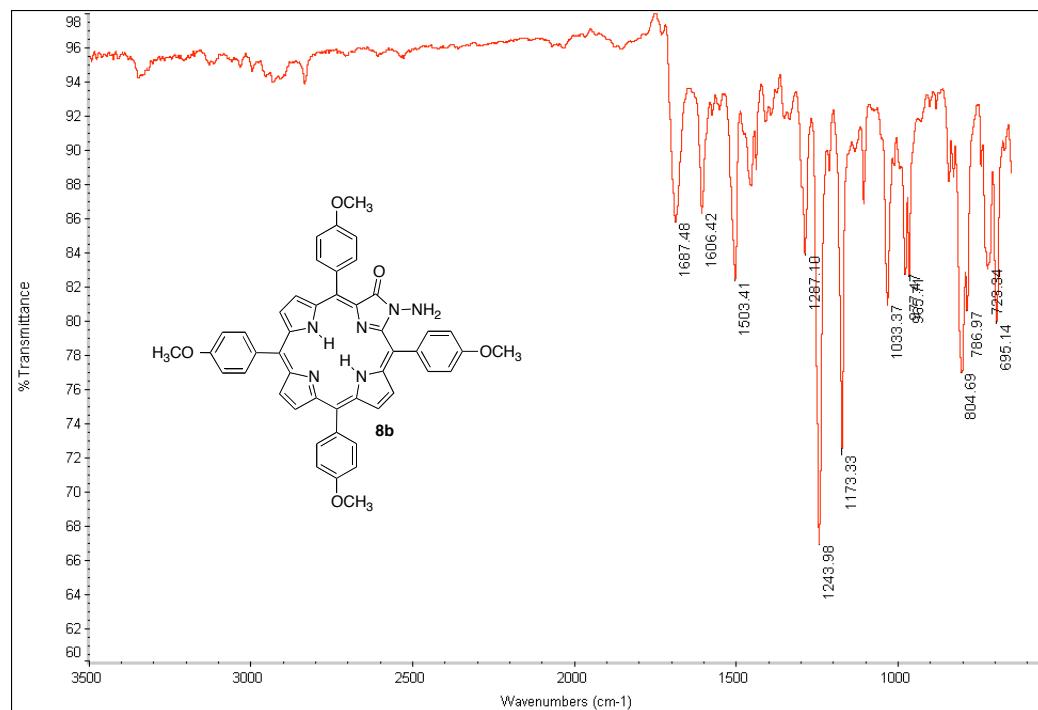


Figure 12. FT-IR Spectrum (neat, diffuse reflectance) of **8b**

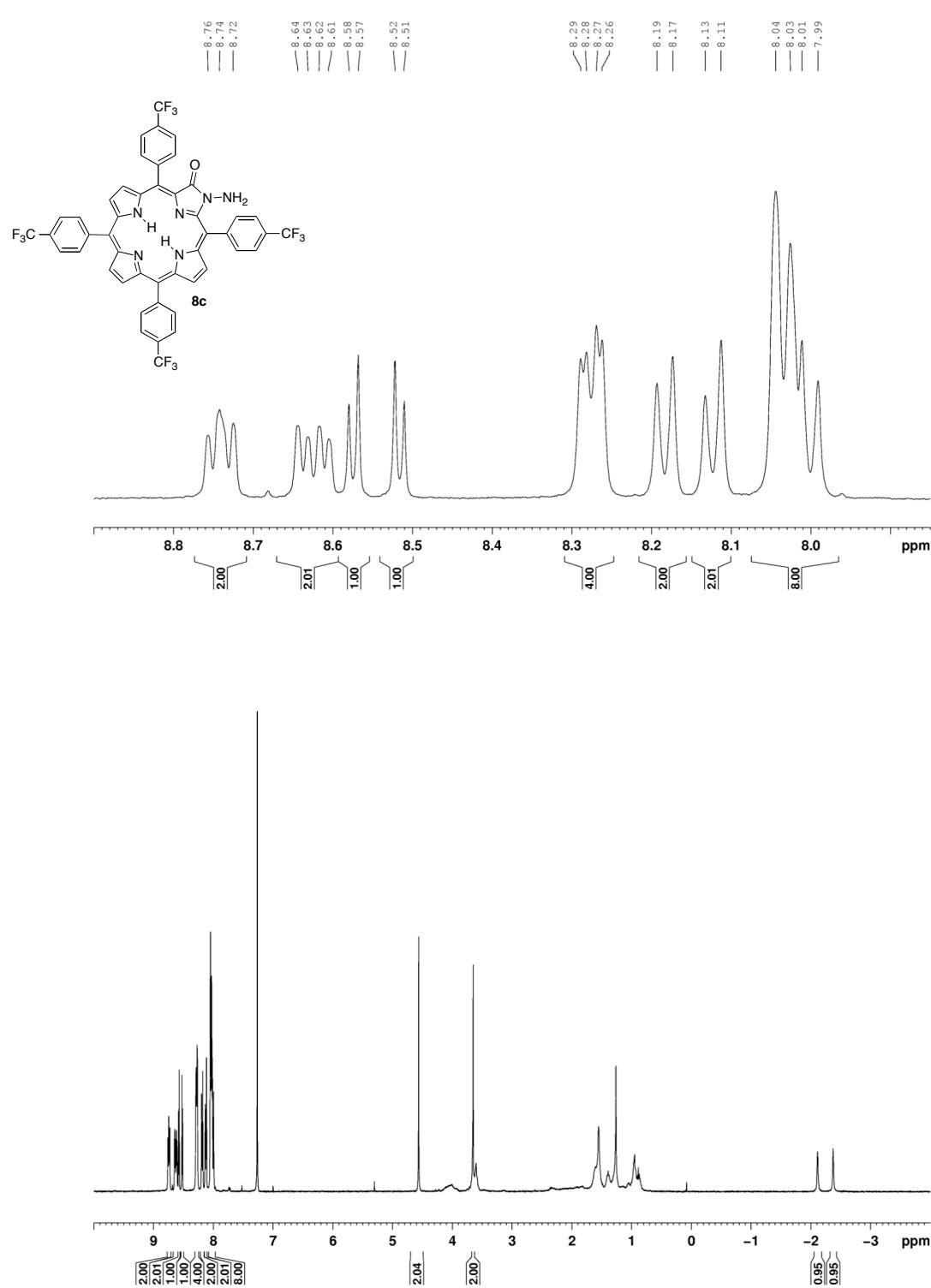


Figure 13. ¹H NMR Spectrum (400 MHz, CDCl₃) of **8c**

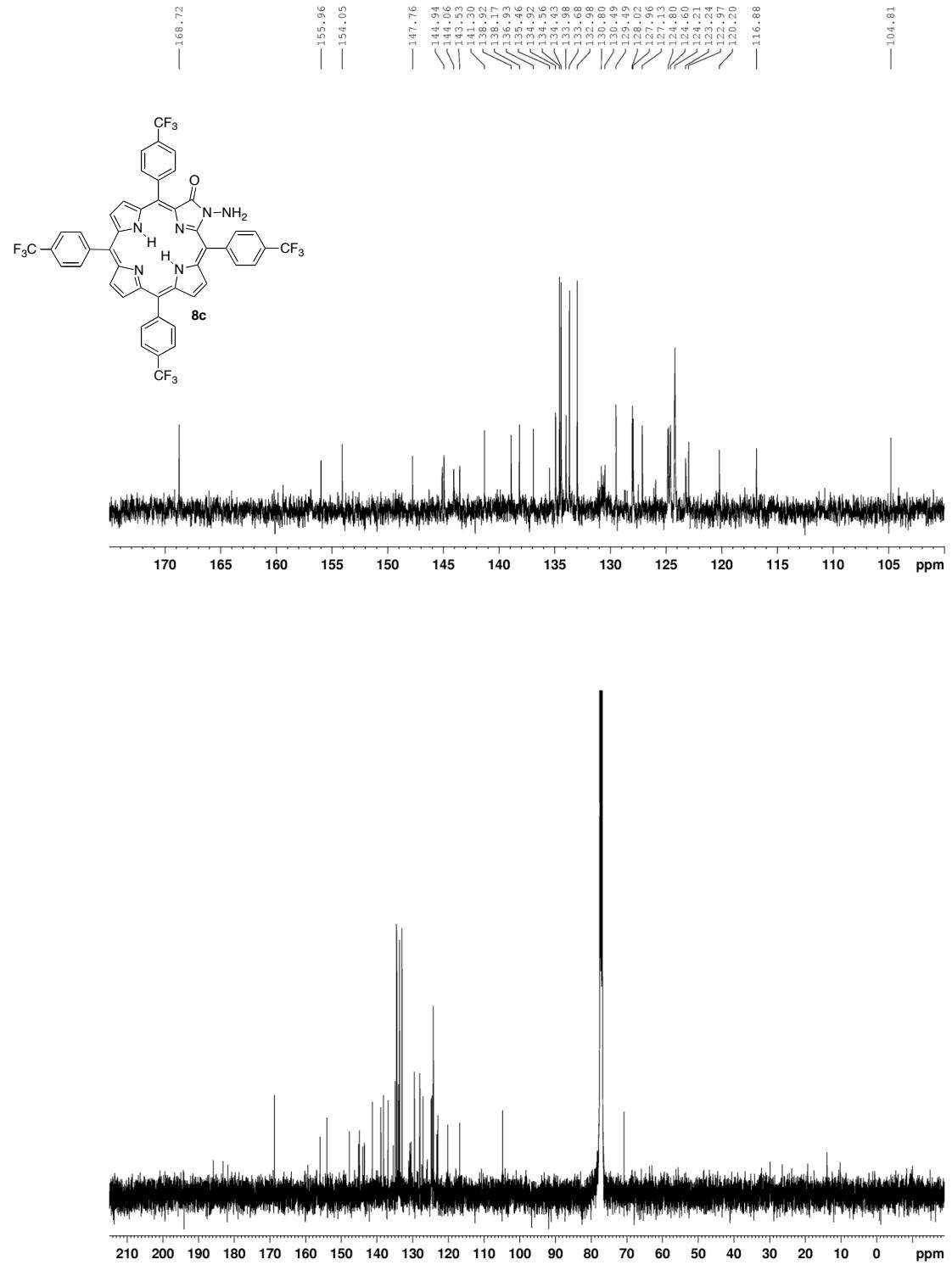


Figure 14. ^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 5s) of **8c**

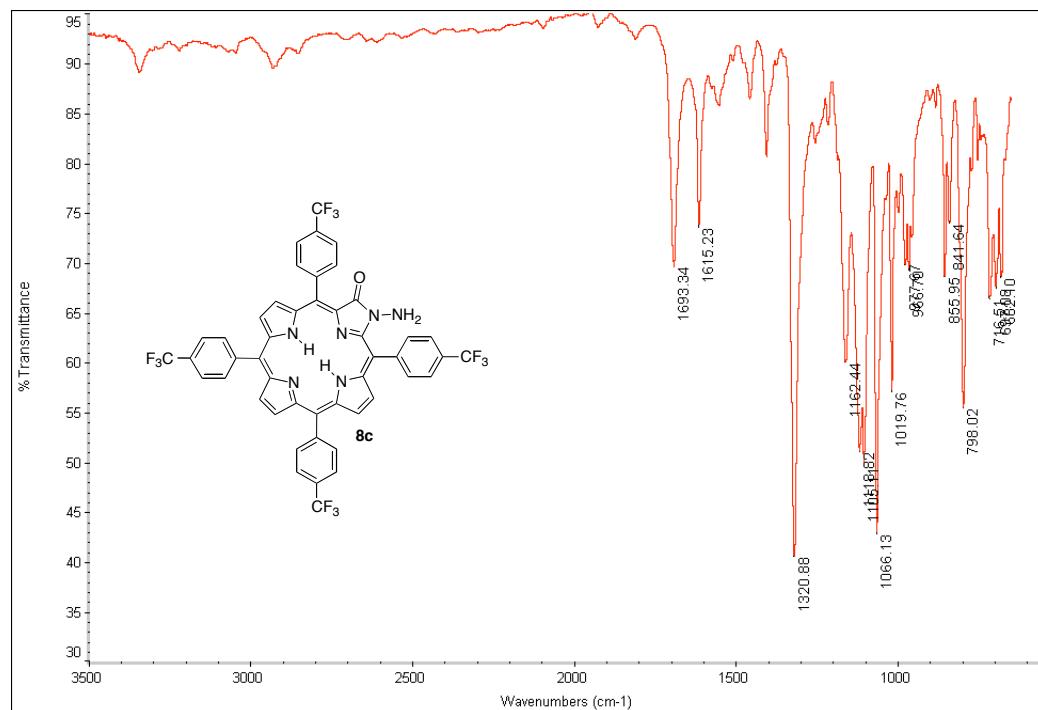


Figure 15. FT-IR Spectrum (neat, diffuse reflectance) of **8c**

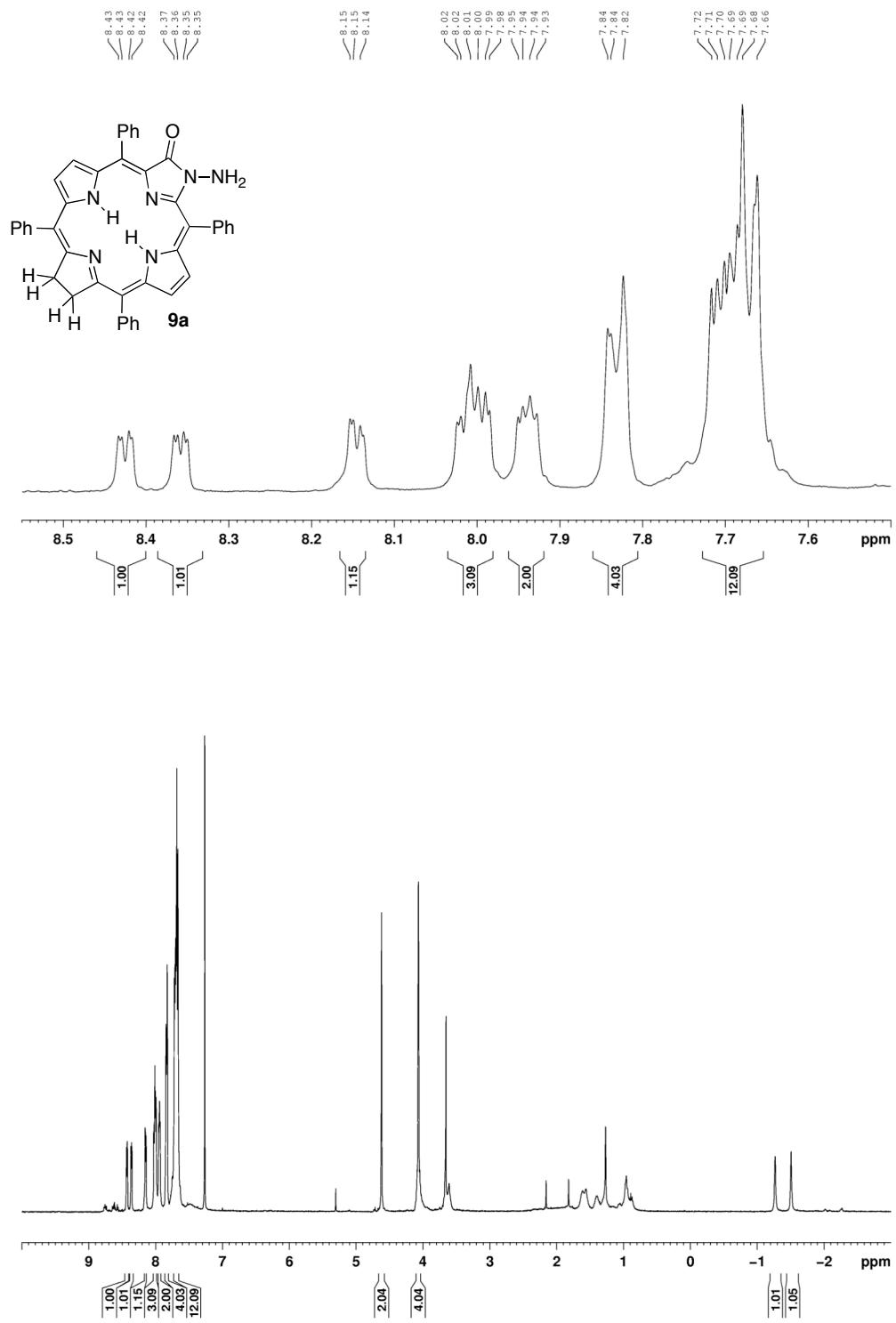


Figure 16. ¹H NMR Spectrum (400 MHz, CDCl₃) of **9a**

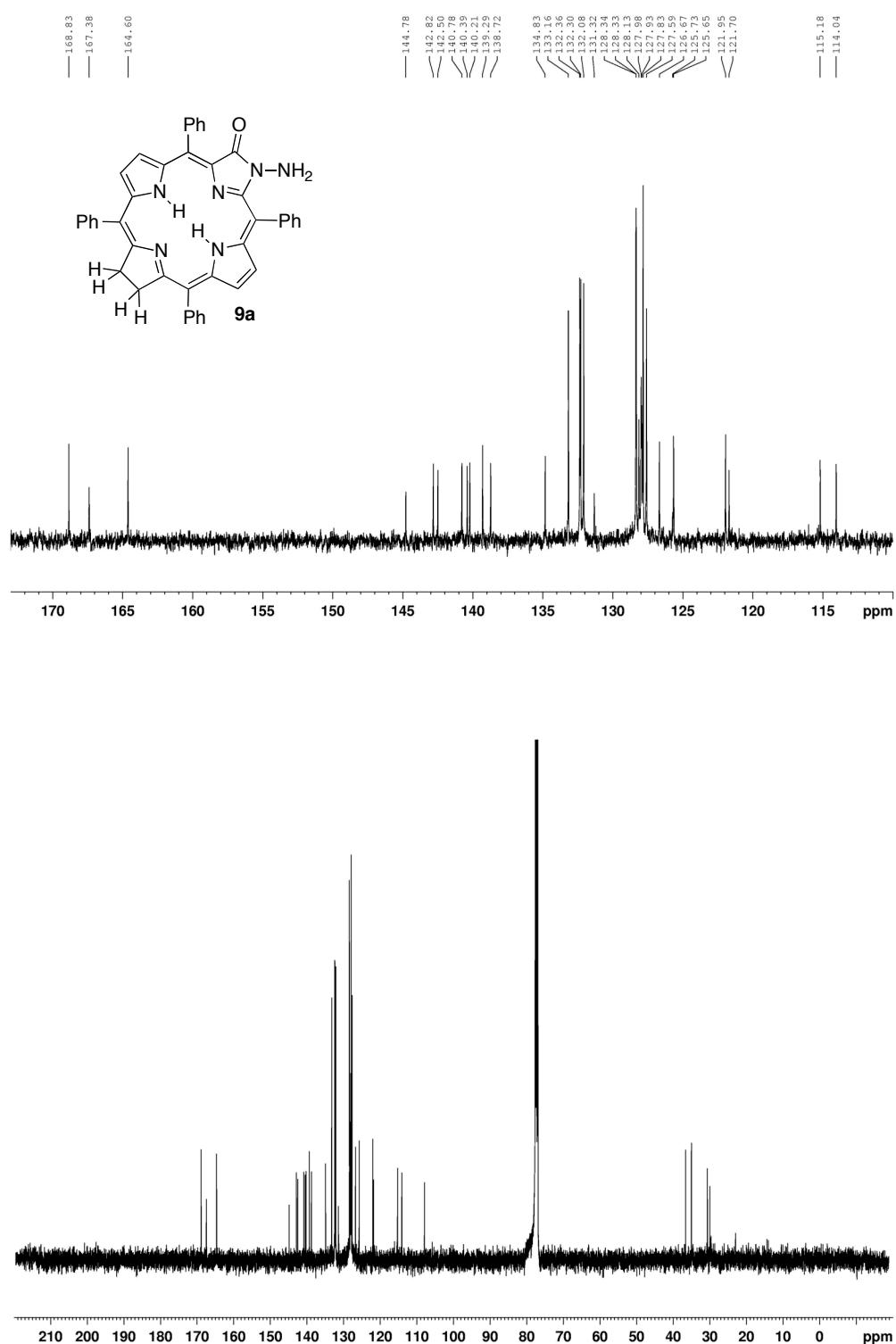


Figure 17. ¹³C NMR Spectrum (100 MHz, CDCl₃, D1 = 3s) of **9a**

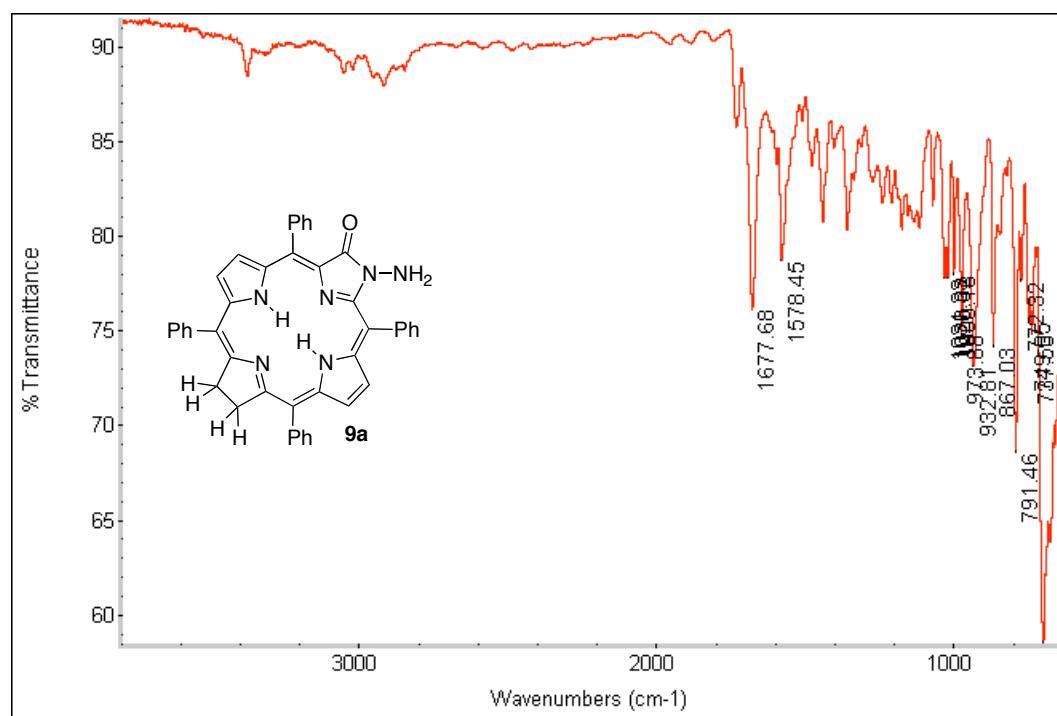


Figure 18. FT-IR Spectrum (neat, diffuse reflectance) of **9a**

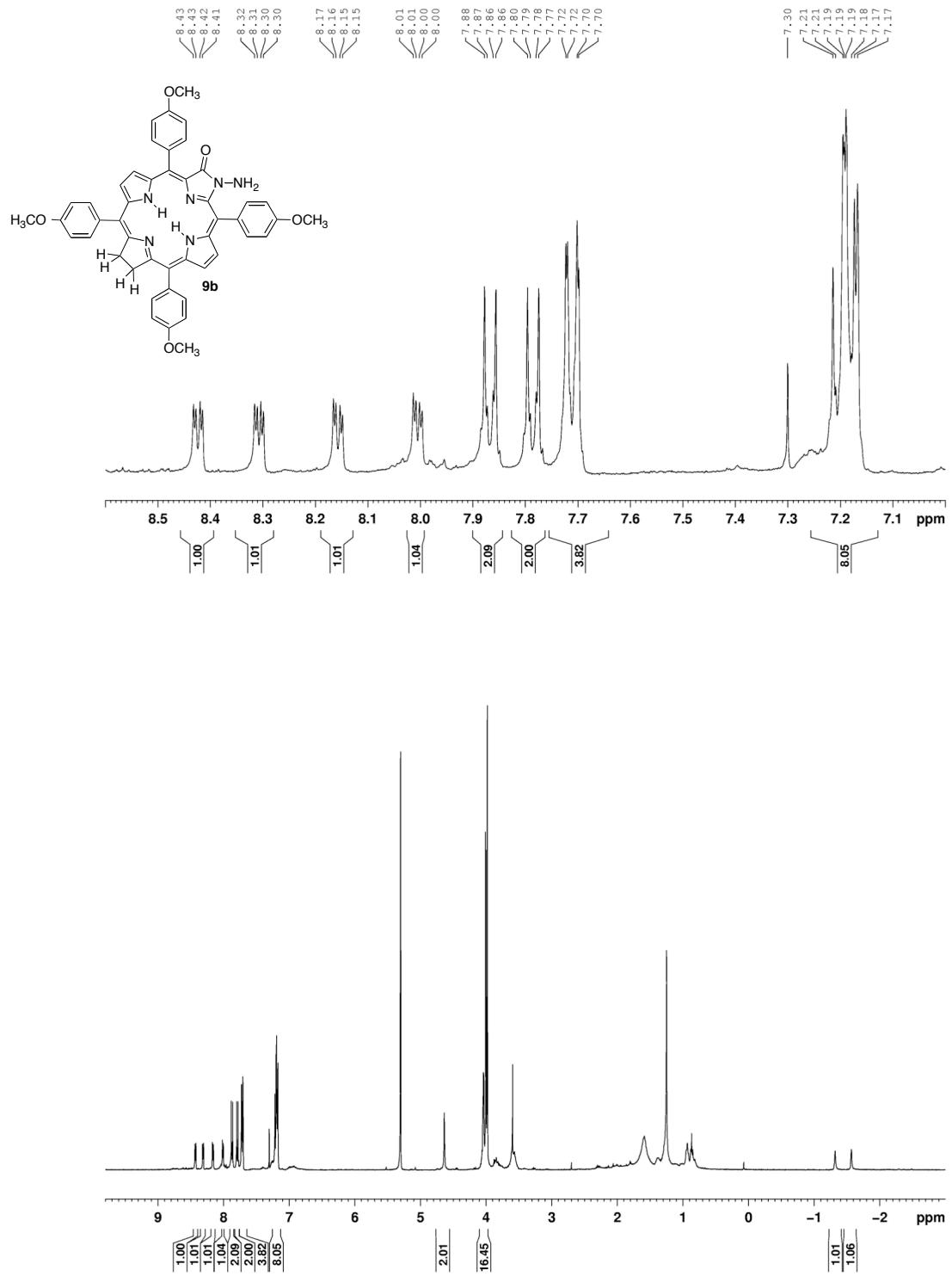


Figure 19. ¹H NMR Spectrum (400 MHz, CD₂Cl₂) of **9b**

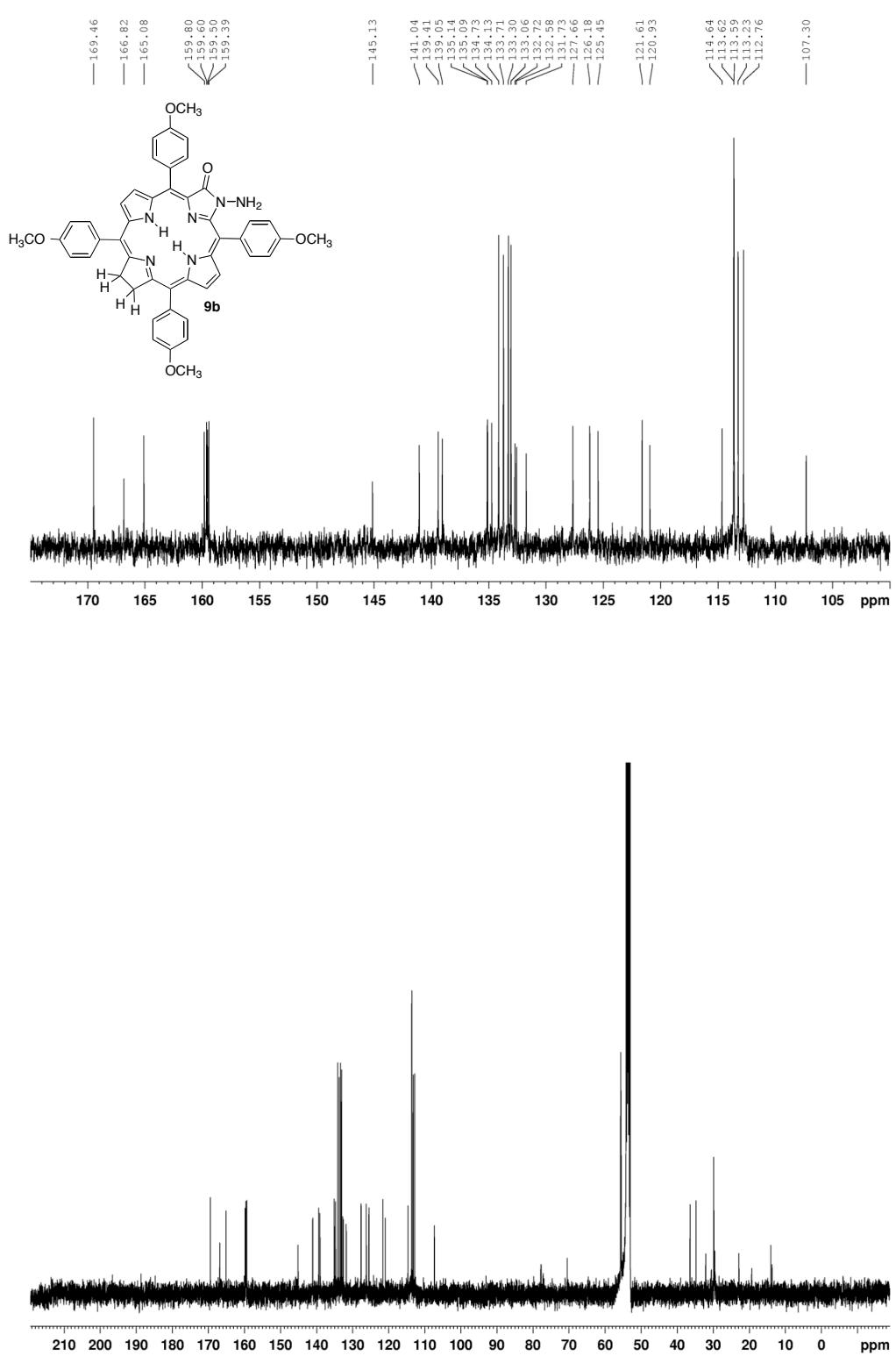


Figure 20. ^{13}C NMR Spectrum (100 MHz, CD₂Cl₂, D1 = 5s) of **9b**

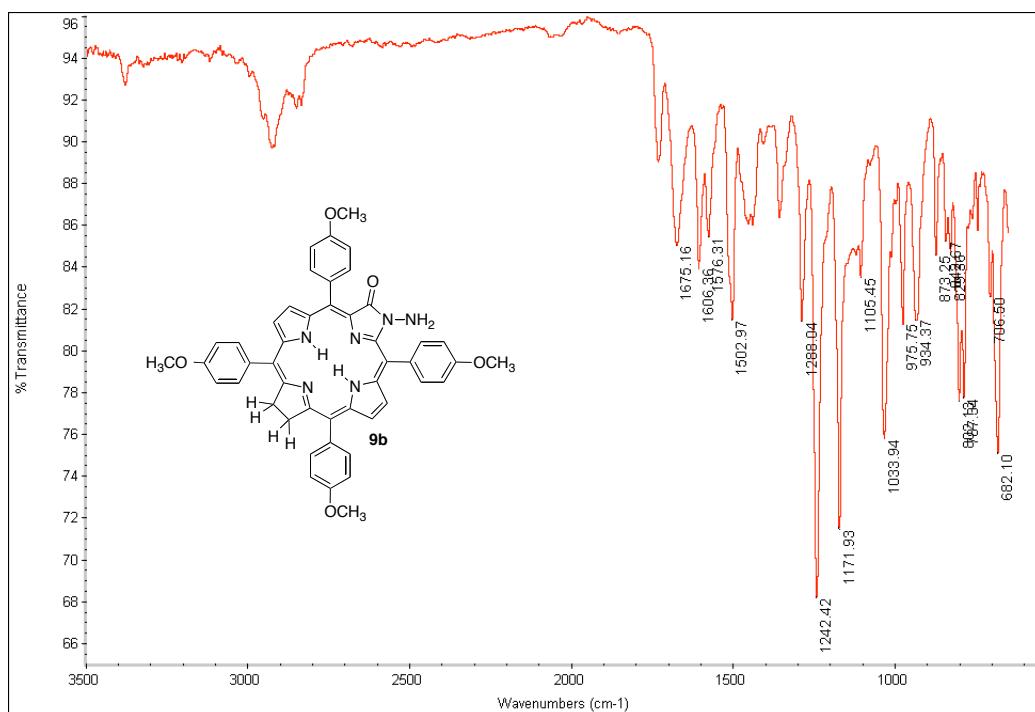


Figure 21. FT-IR Spectrum (neat, diffuse reflectance) of **9b**

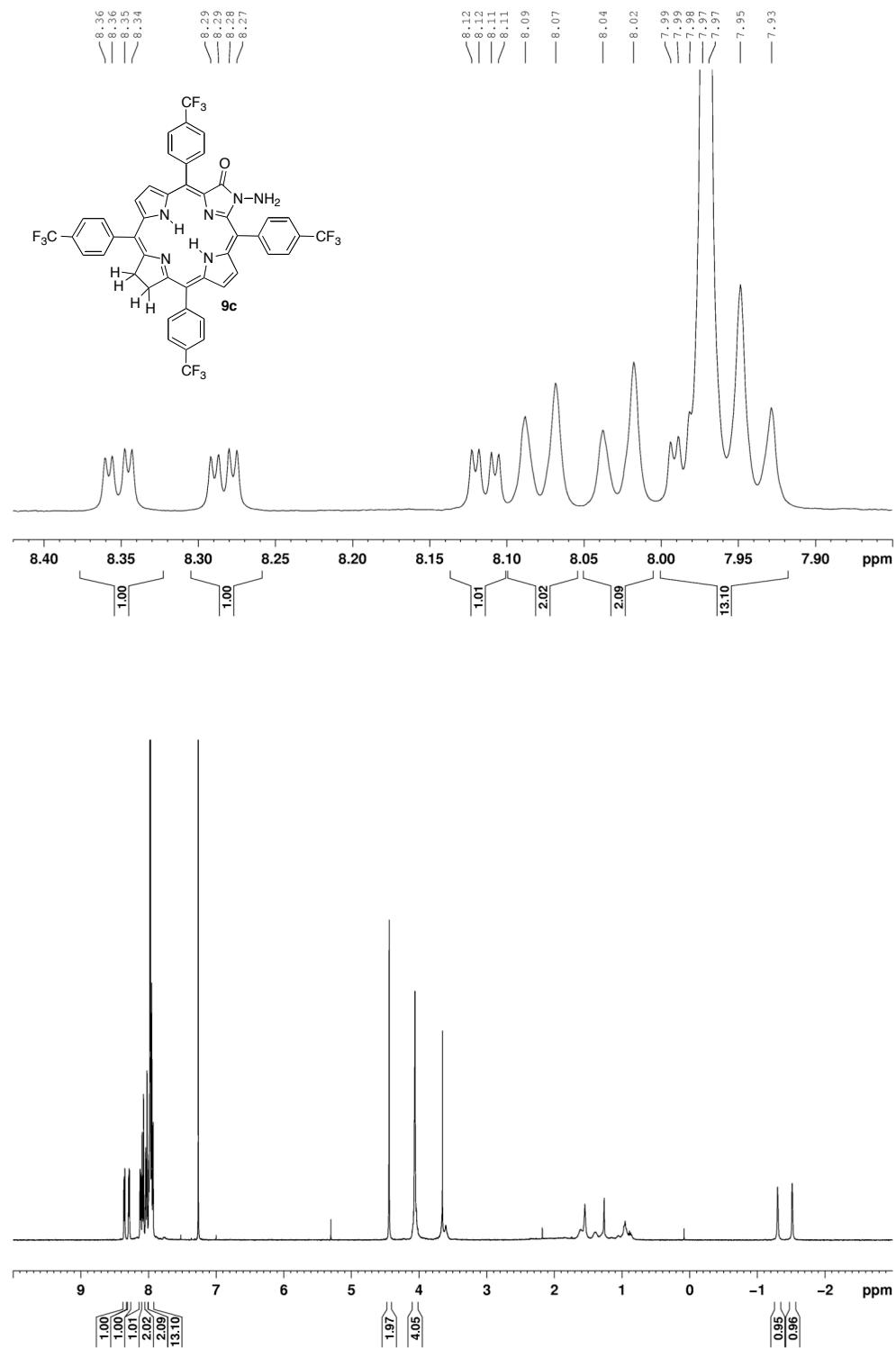


Figure 22. ¹H NMR Spectrum (400 MHz, CDCl₃) of **9c**

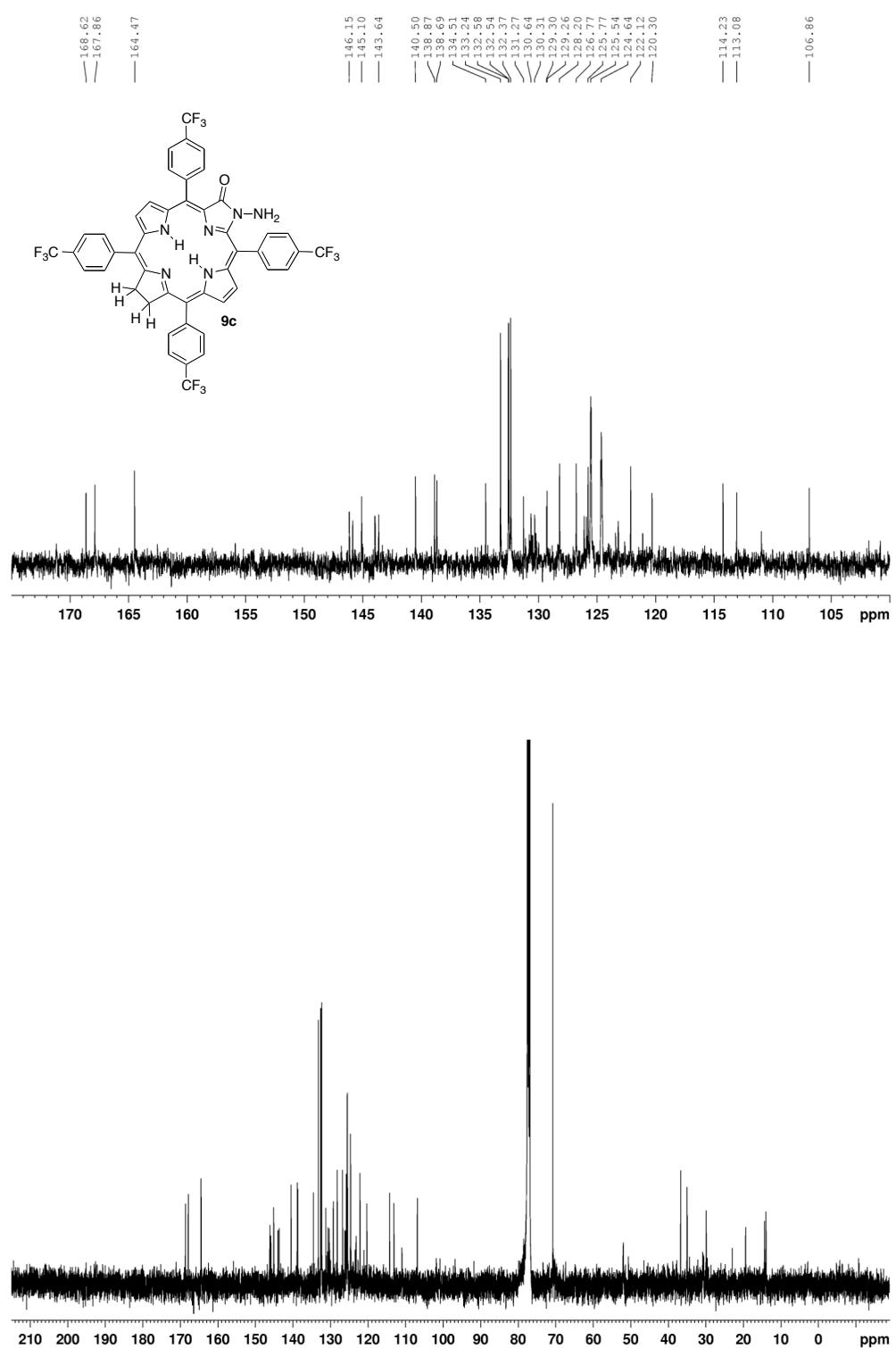


Figure 23. ^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 5s) of **9c**

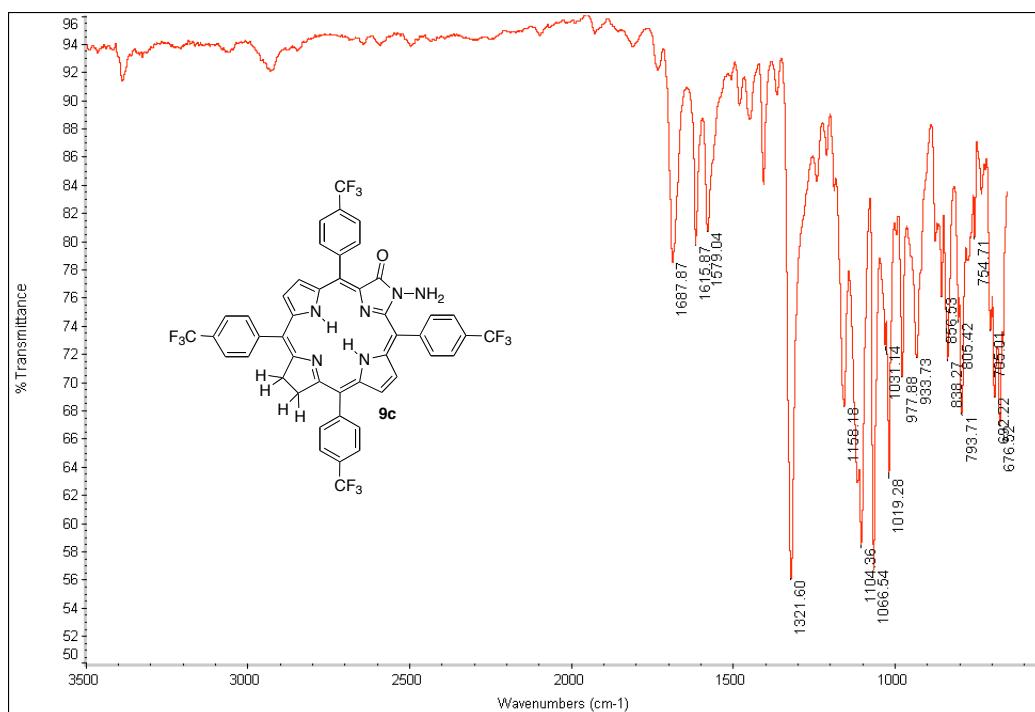


Figure 24. FT-IR Spectrum (neat, diffuse reflectance) of **9c**

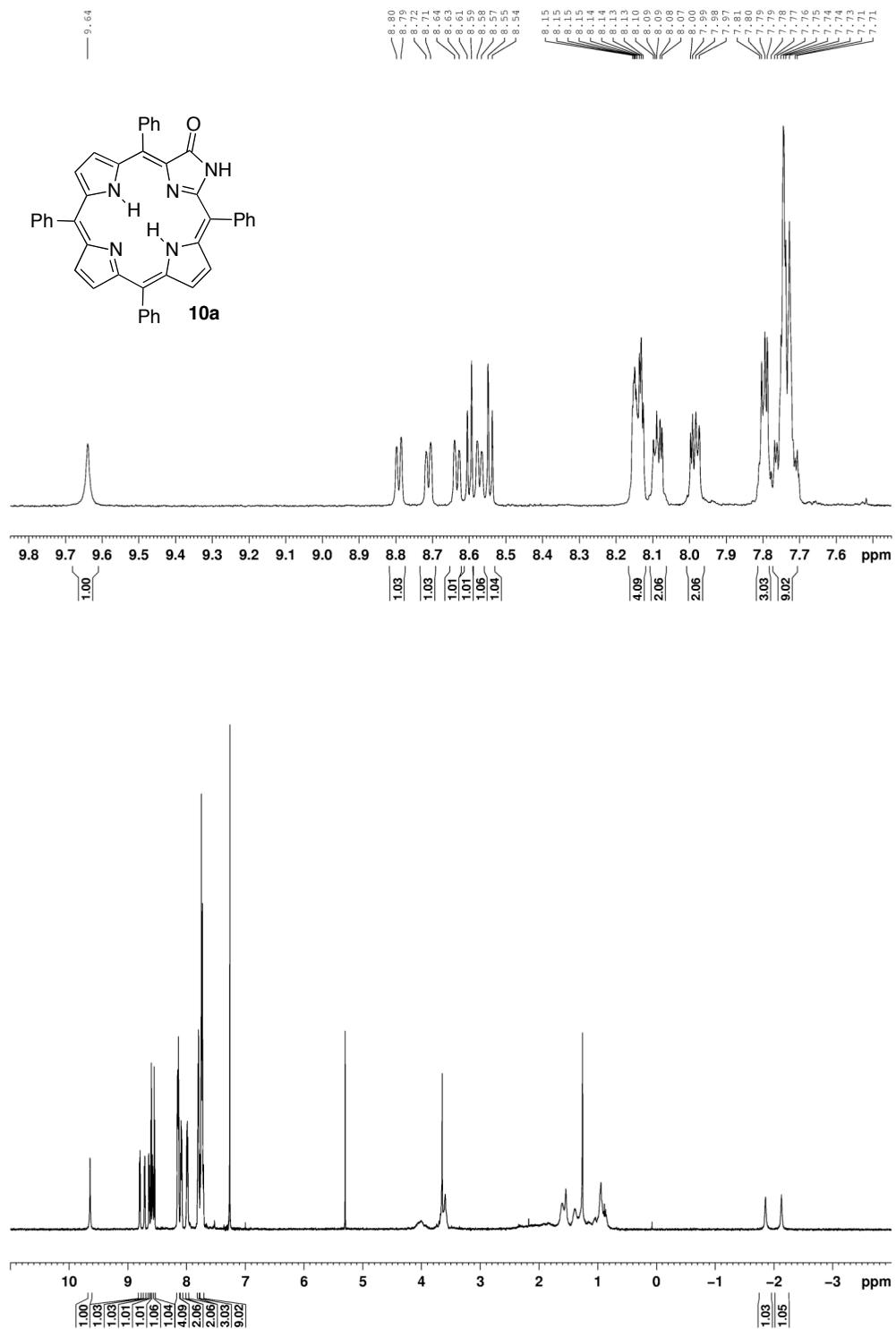


Figure 25. ^1H NMR Spectrum (400 MHz, CDCl_3) of **10a**

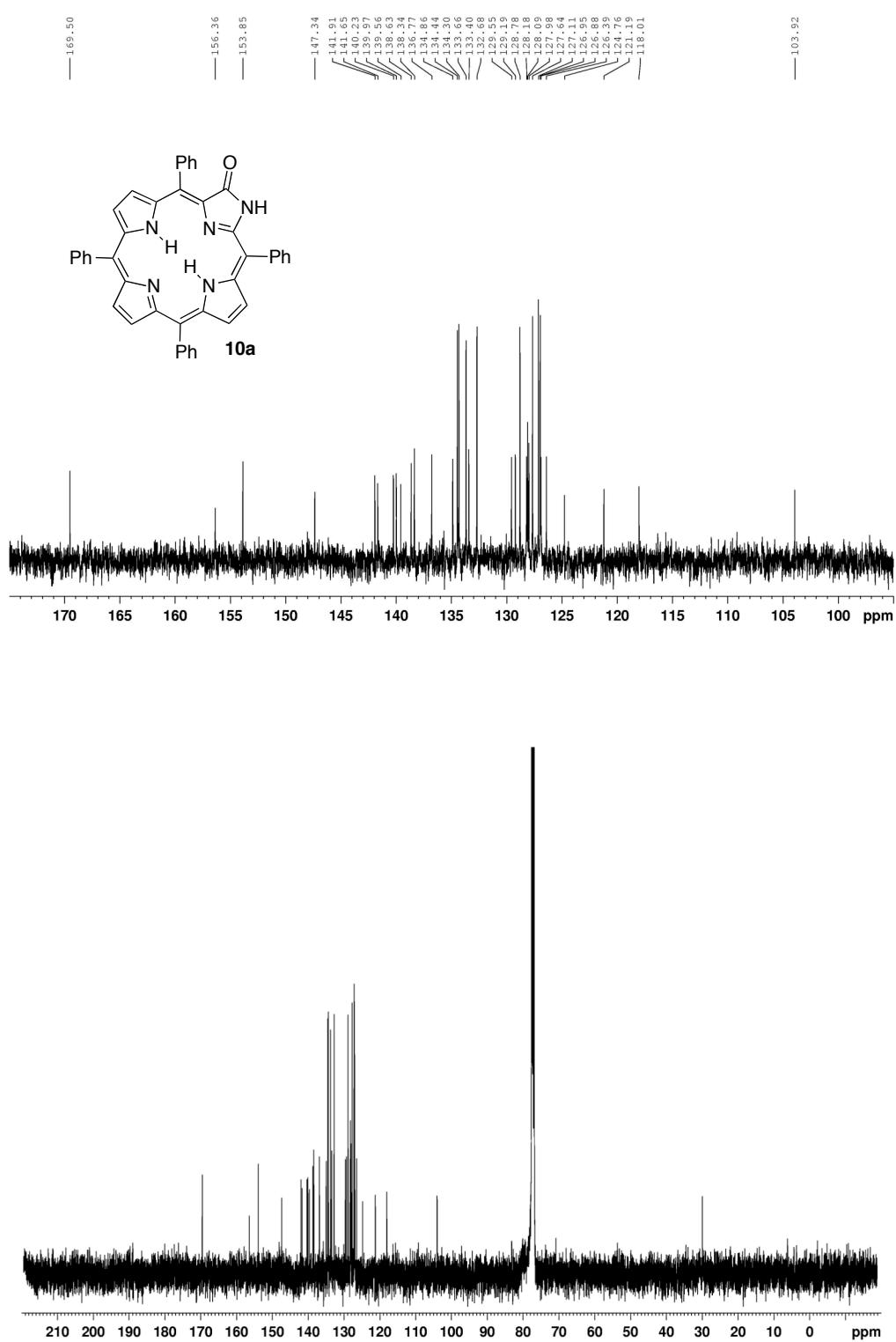


Figure 26. ^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 3s) of **10a**

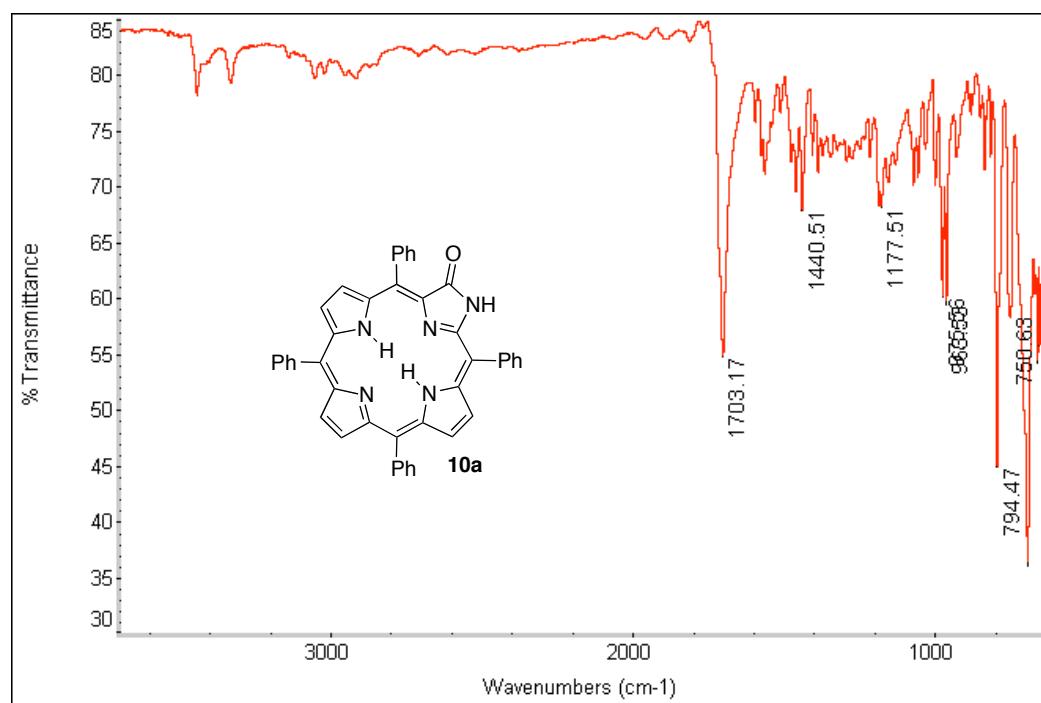


Figure 27. FT-IR Spectrum (neat, diffuse reflectance) of **10a**

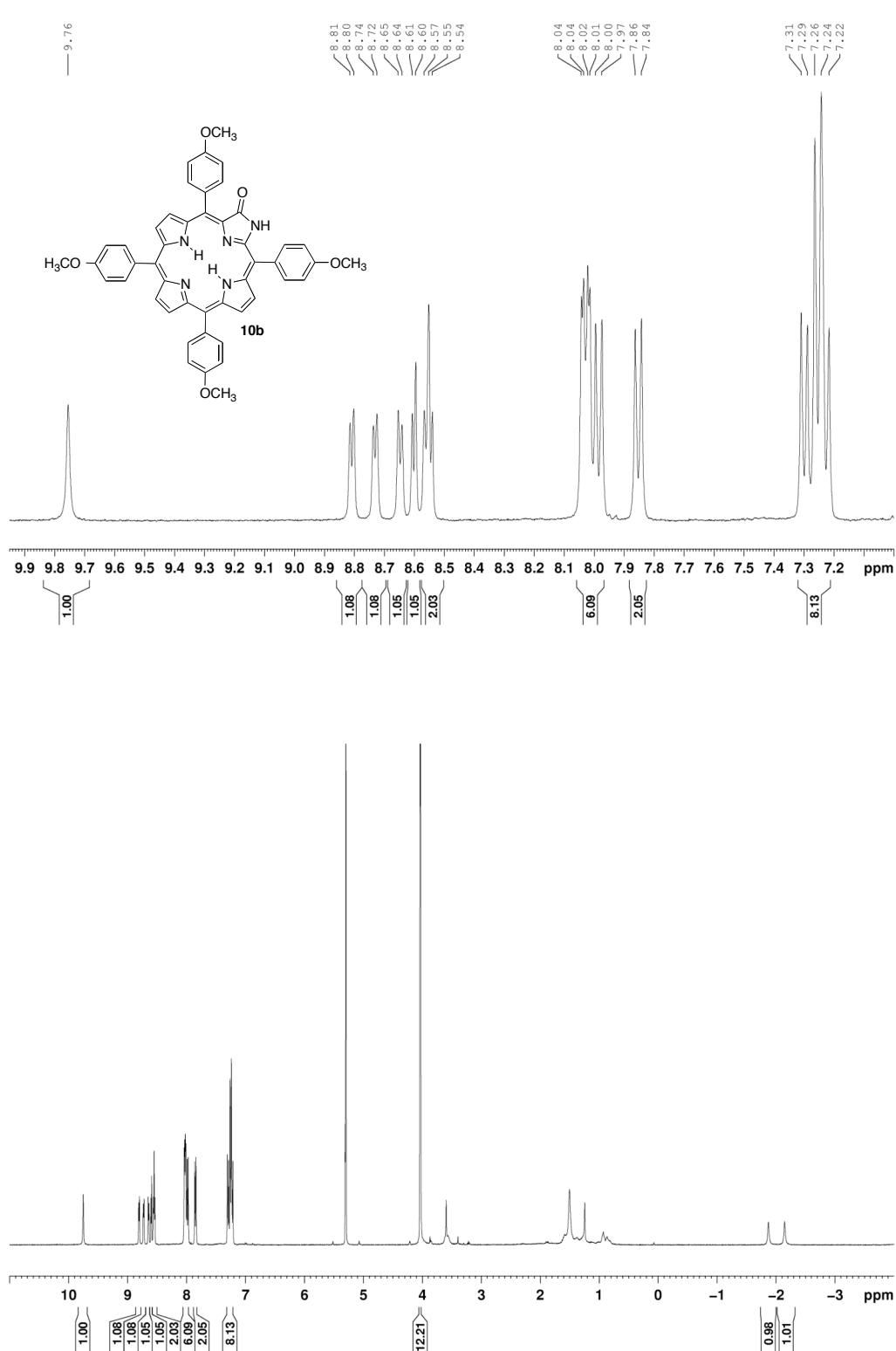


Figure 28. ¹H NMR Spectrum (400 MHz, CD_2Cl_2) of **10a**

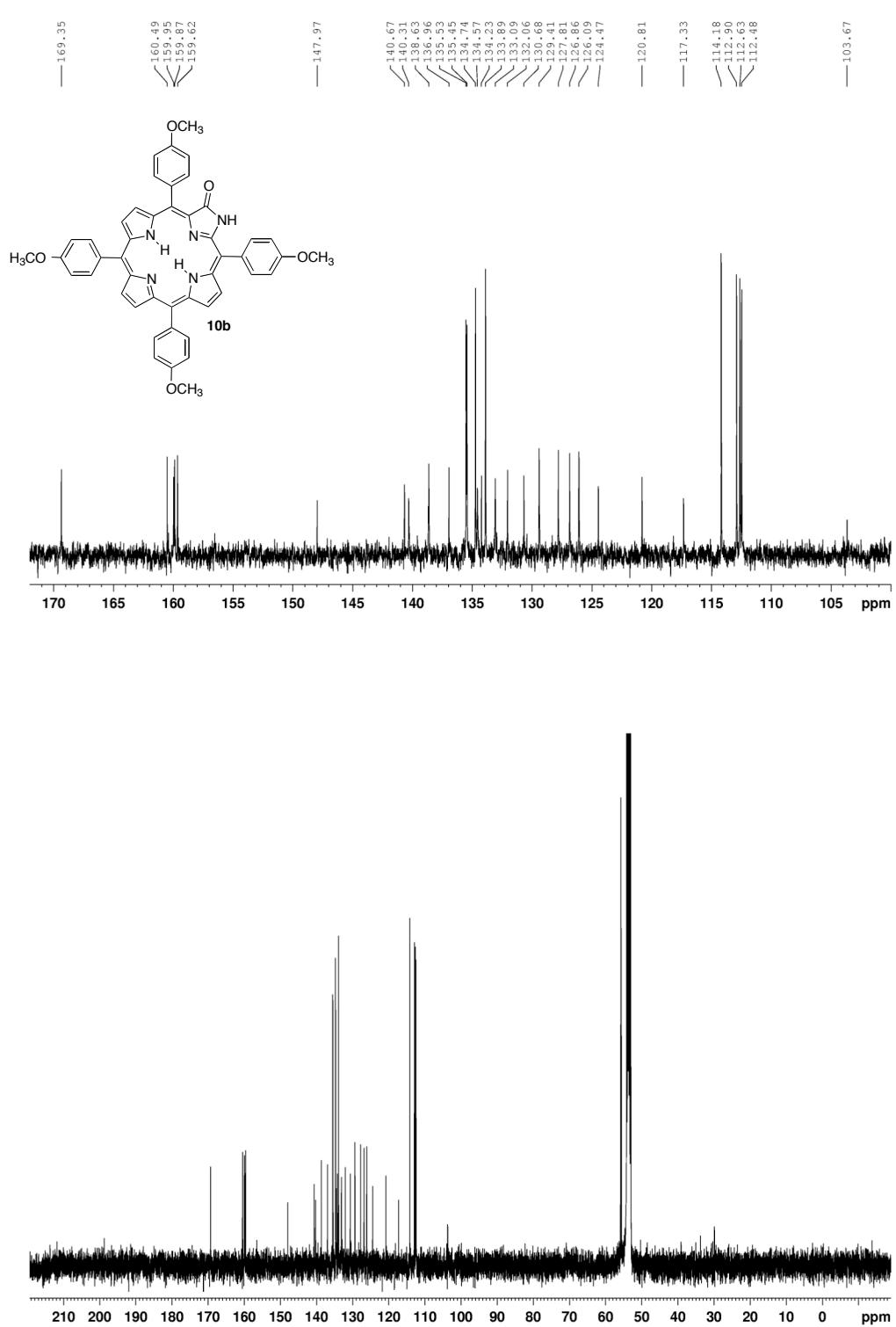


Figure 29. ^{13}C NMR Spectrum (100 MHz, CD_2Cl_2) of **10b**

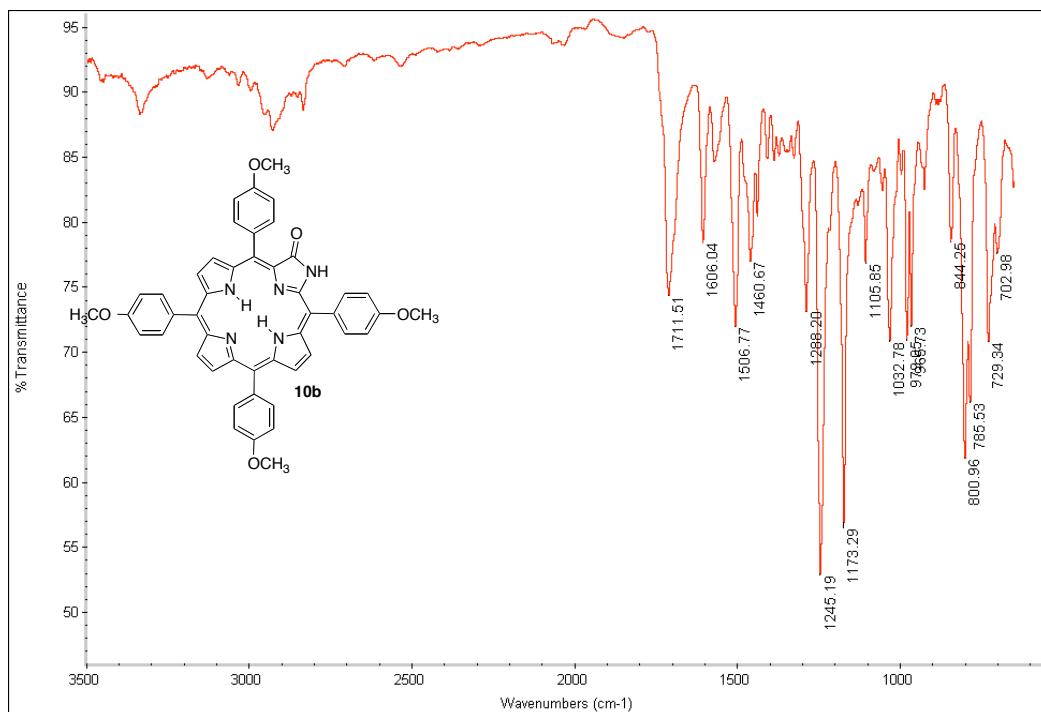


Figure 30. FT-IR Spectrum (neat, diffuse reflectance) of **10b**

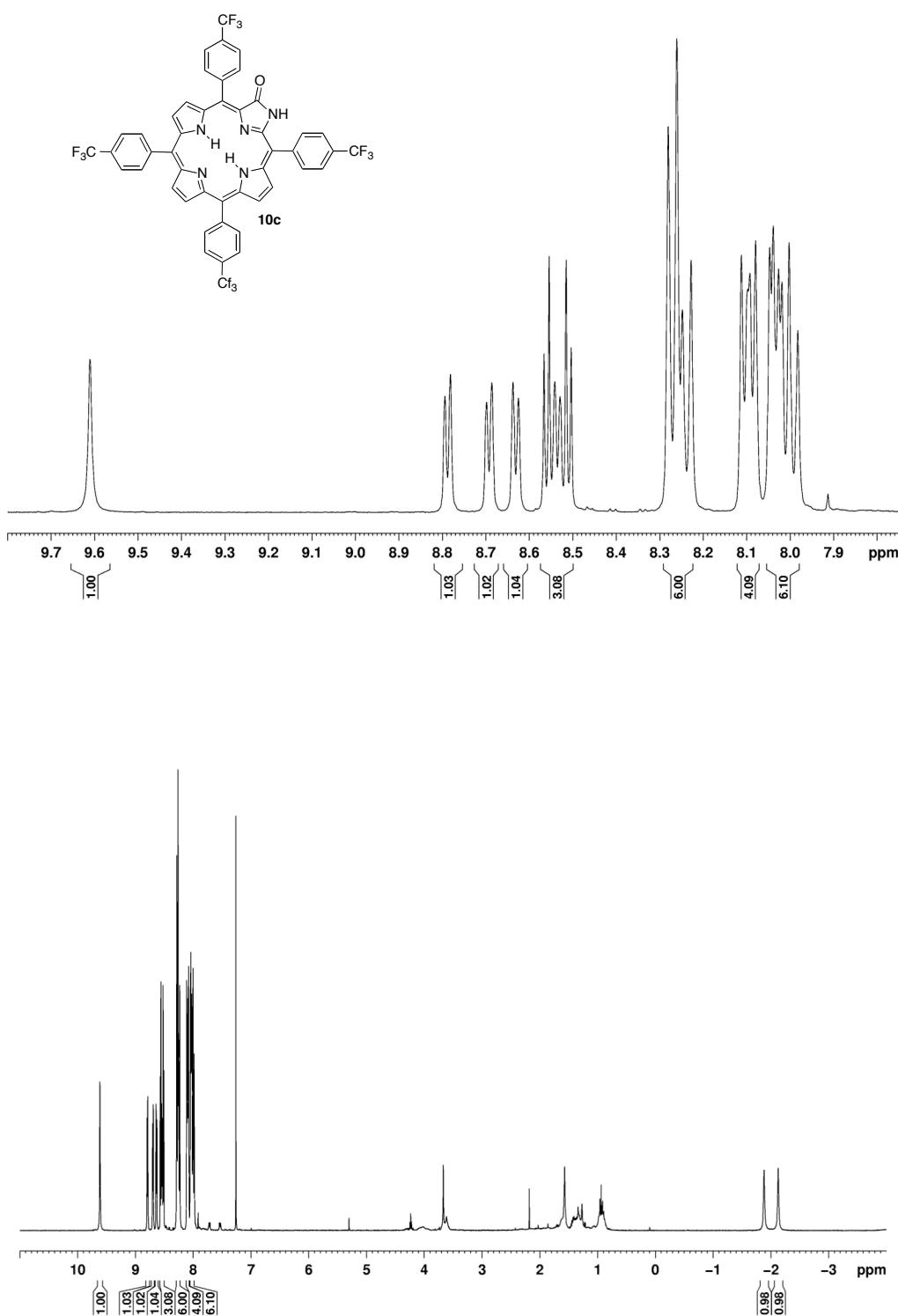


Figure 31. ¹H NMR Spectrum (400 MHz, CDCl₃) of **10c**

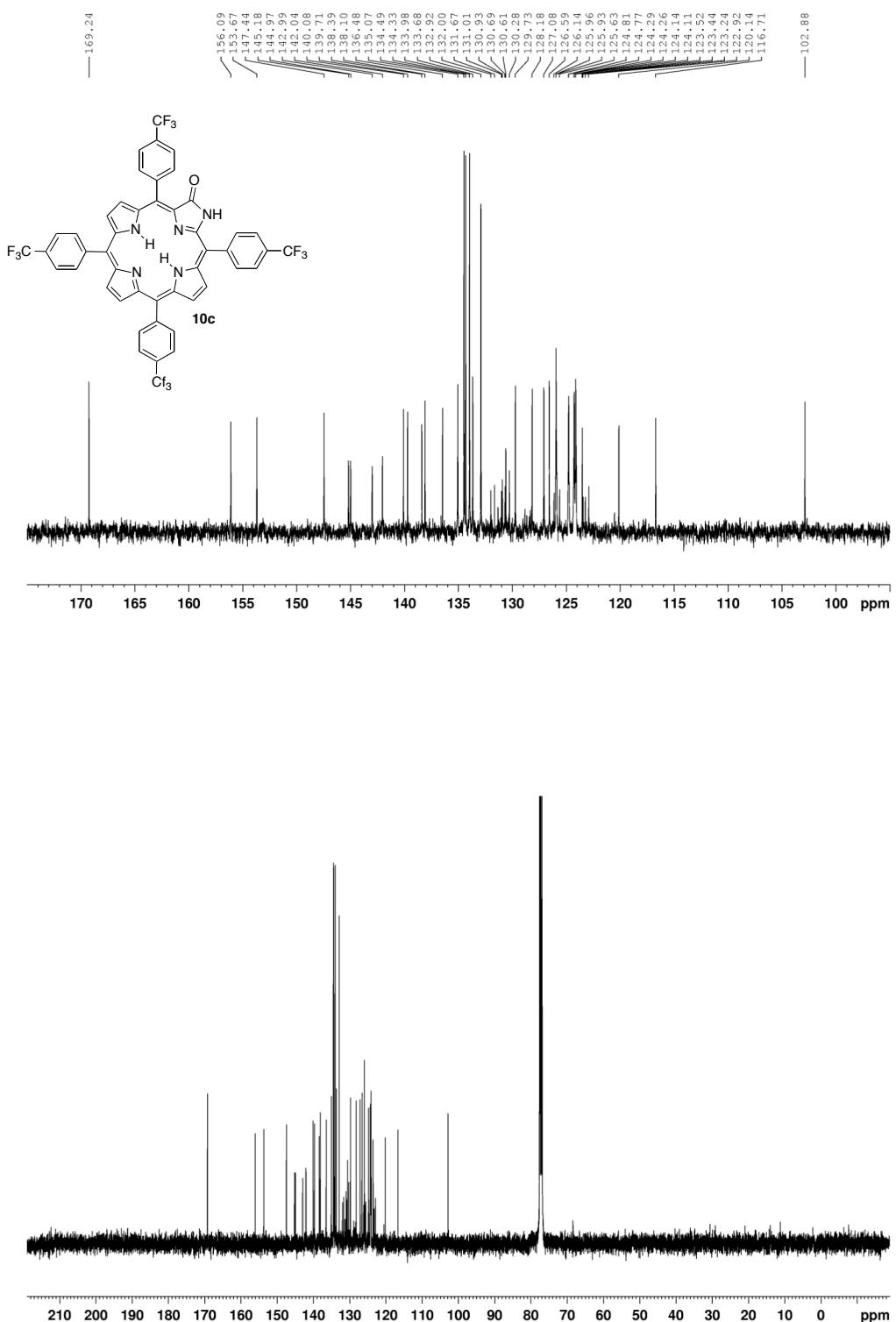


Figure 32. ^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 3s) of **10c**

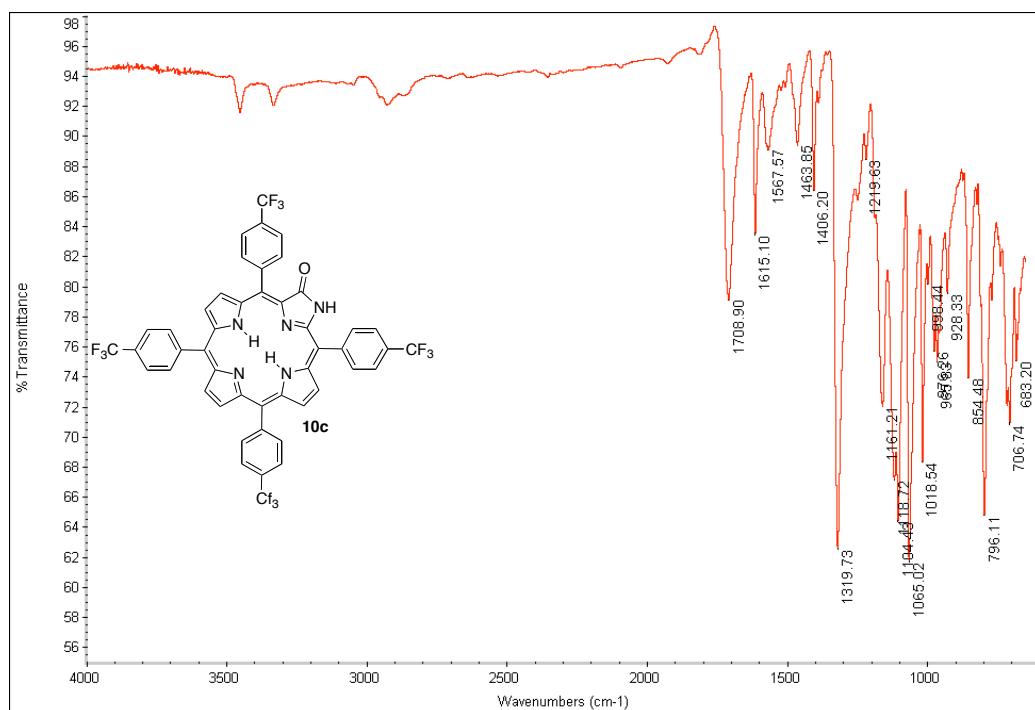


Figure 33. FT-IR Spectrum (neat, diffuse reflectance) of **10c**

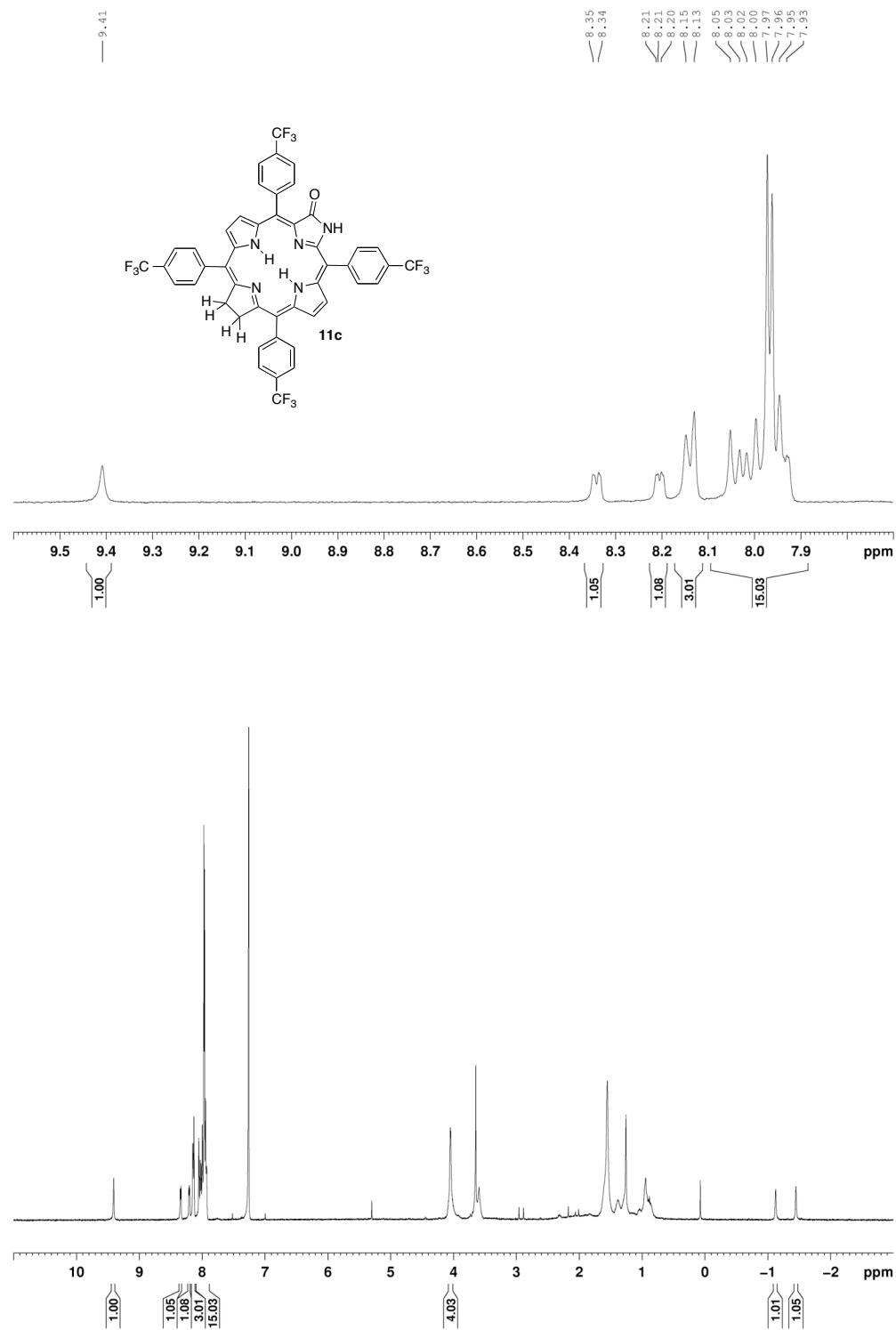


Figure 34. ¹H NMR Spectrum (400 MHz, CDCl₃) of **11c**

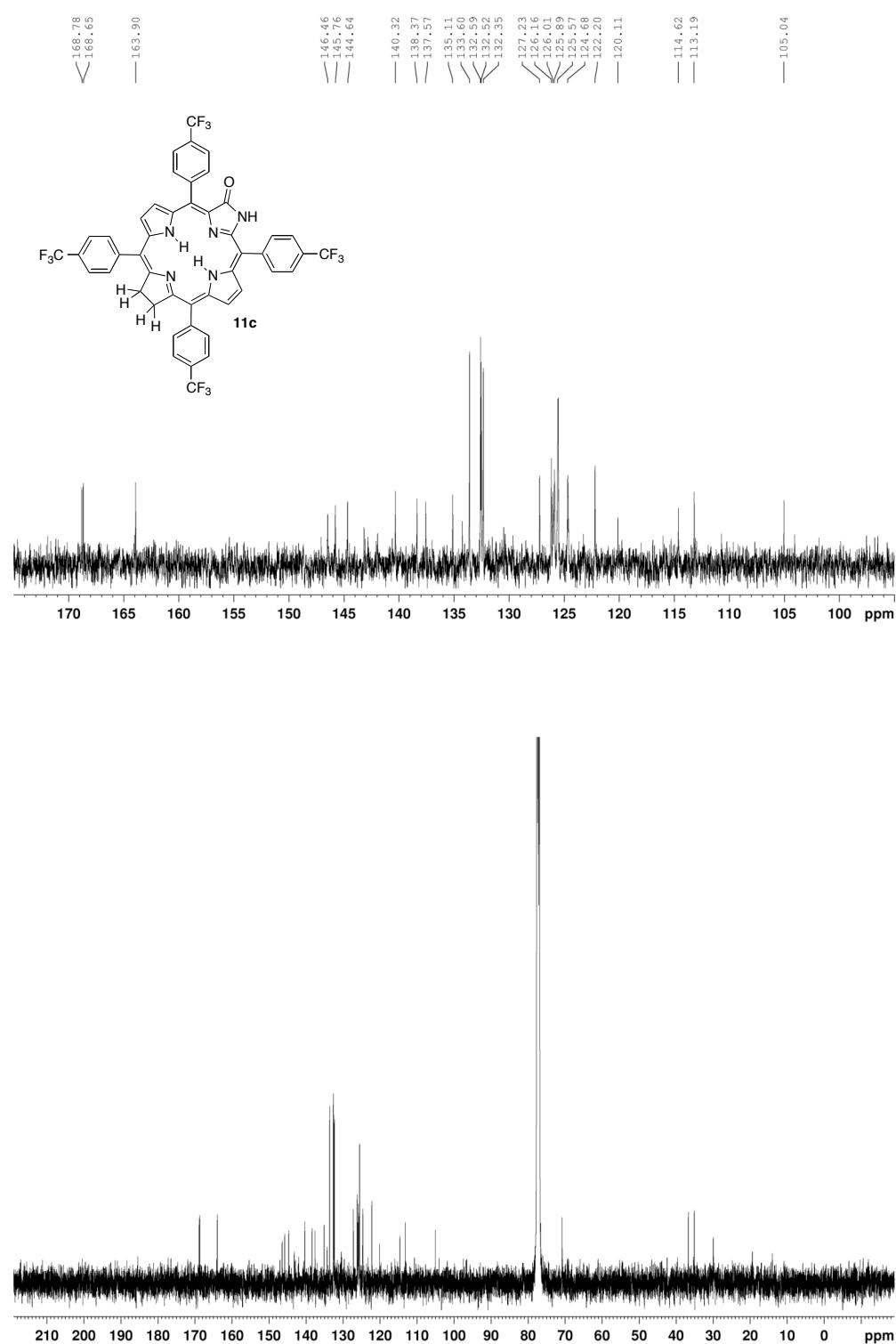


Figure 35. ^{13}C NMR Spectrum (100 MHz, CDCl_3 , D1 = 3s) of **11c**

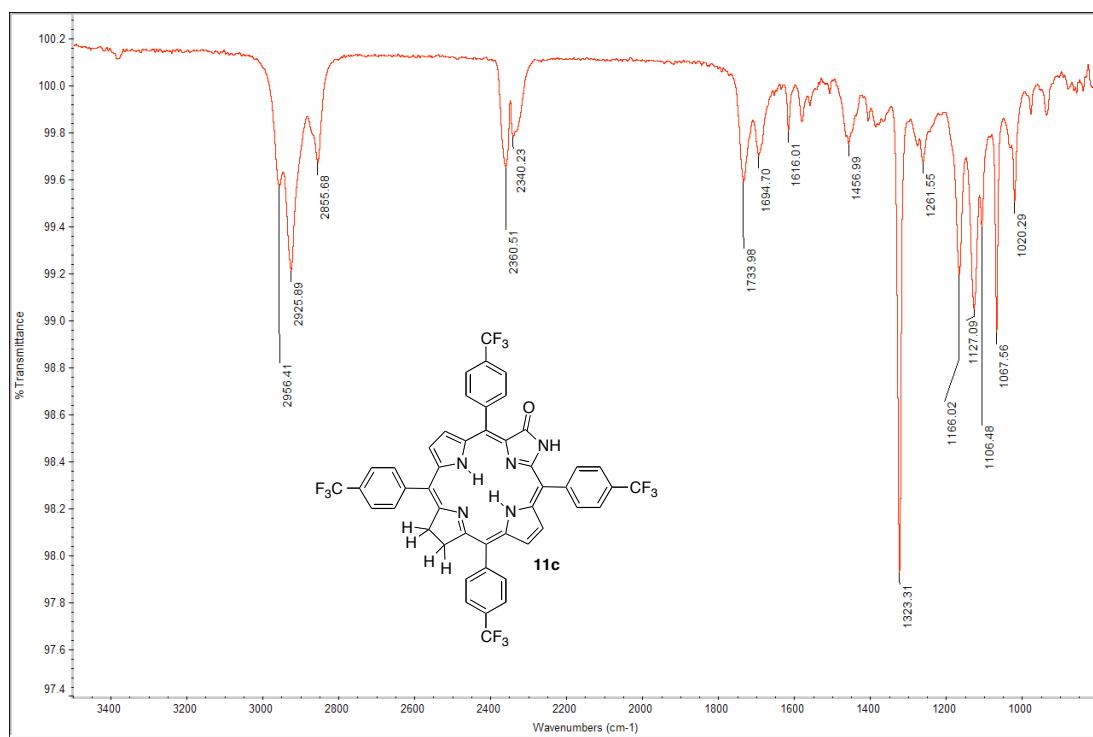


Figure 36 FT-IR Spectrum (neat, diffuse reflectance) of **11c**

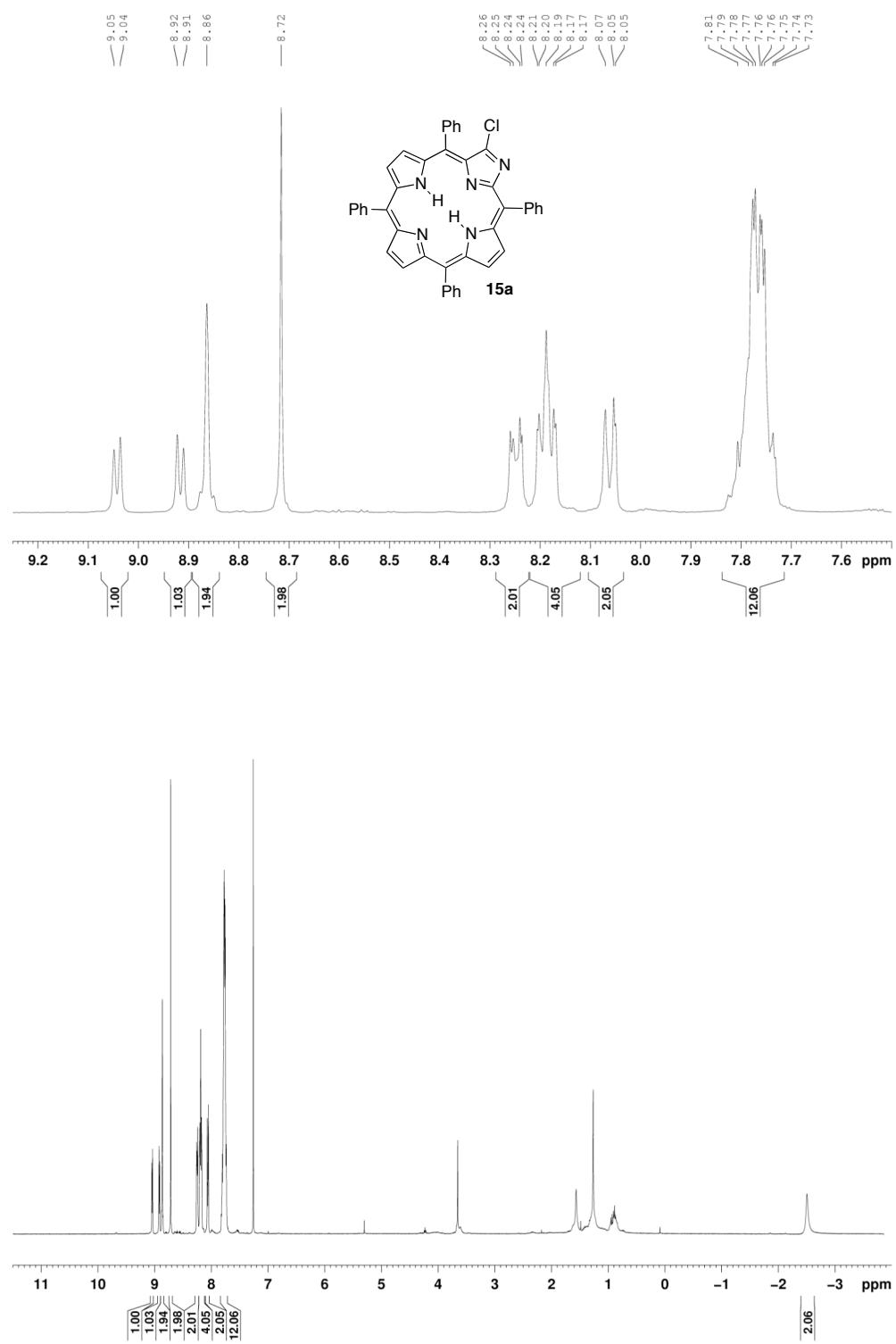


Figure 37. ^1H NMR Spectrum (400 MHz, CDCl_3) of **15a**

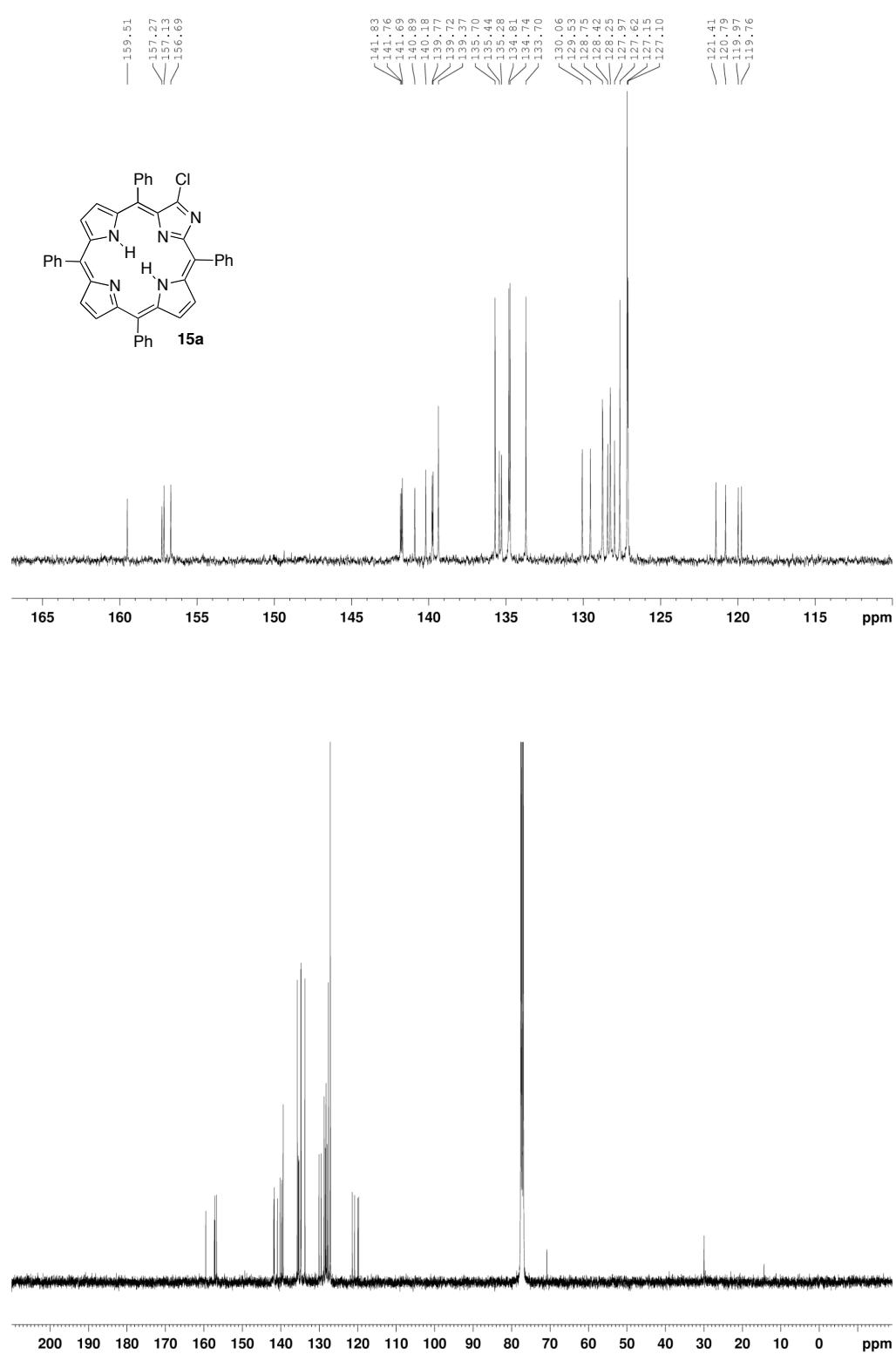


Figure 38. ¹³C NMR Spectrum (100 MHz, CDCl₃, D1 = 3s) of **15a**

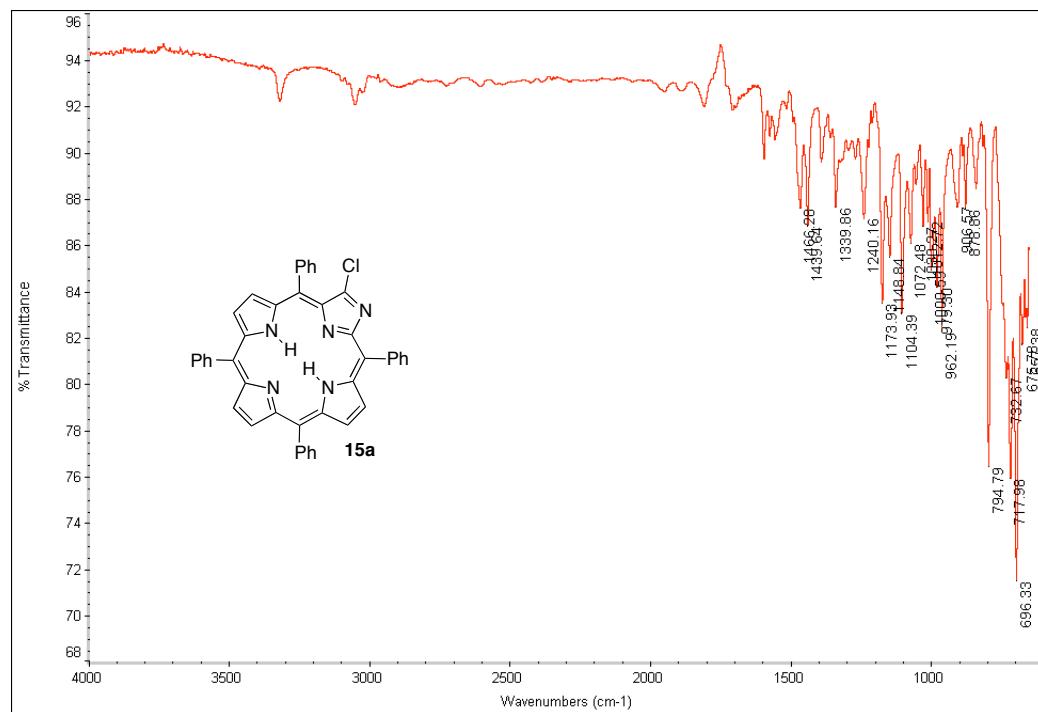


Figure 39. FT-IR Spectrum (neat, diffuse reflectance) of **15a**