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Assignment of the ^{13}C - and ^{15}N -NMR signals of 1 and 2.

2-Sulfonato-5,15-bis(4-sulfonatophenyl)porphyrin trisodium salt (1). ^{13}C NMR (DMSO- d_6 , 100 MHz) δ : 106.2 (C20), 106.7 (C10), 118.9 (C1''), 119.5 (C1'), 125.1 and 125.2 (C_{ar}), 130.0 and 130.2 (C7, C17), 131.0 (C3), 131.9 (C8), 132.4 (C18), 132.8 (C13), 134.6 and 134.8 (C_{ar} , C12), 141.2 (C4', C4''), 141.9 and 142.2 (C9, C19), 143.4 and 143.8 (C6, C16), 145.3 and 146.6 (C2, C4), 148.4 and 148.5 (C5, C15), 149.2 (C11), 150.8 (C-14), 152.5 (C1); ^{13}C NMR (DMF- d_7 , 100 MHz) δ : 106.0 (C10), 106.3 (C20), 118.9 and 119.6 (C1', C1''), 125.0 and 125.1 (C_{ar}), 130.0 and 130.1 (C7, C17), 130.5 (C3), 131.4 (C8), 132.1 (C18), 132.3 (C13), 133.9 (C12), 134.3 and 134.5 (C_{ar}), 141.2 and 141.3 (C4', C4''), 142.6 and 142.8 (C9, C19), 144.2 and 144.6 (C6, C16), 145.3 and 146.5 (C2, C4), 148.7 (C11), 149.0 and 149.1 (C5, C15), 150.4 (C14), 152.9 (C1); ^{15}N NMR (DMSO- d_6 , 60 MHz) δ : 165.1 (N_{24}), 165.4 (N_{22}), 212.2 (N_{23}), 212.9 (N_{21}); ^{15}N NMR (DMF- d_7 , 60 MHz) δ : 167.9 (N_{24}), 168.2 (N_{22}), 203.4 (N_{23}), 204.1 (N_{21}).

10-Bromo-2-sulfonato-5,15-bis(4-sulfonatophenyl)porphyrin trisodium salt (2). ^{13}C NMR (DMSO- d_6 , 100 MHz) δ : 103.4 (C10), 106.9 (C20), 120.4 (C1''), 121.0 (C1'), 124.9 and 125.1 (C_{ar}), 131.1 (C7, C17), 131.5 (C3), 132.0 (C8), 132.6 (C18), 134.4 and 134.7 (C12, C13, C_{ar}), 141.1 (C4', C4''), 148.6 and 148.7 (C5, C15), 152.7 (C1). [at 323 K in addition to the former signals, the following were detected: 141.4 (C9 or C19), 143.4 (C6 or C16), 146.0 (C2 or C4), 149.8 (C14)]; ^{13}C NMR (DMF- d_7 , 100 MHz) δ : 102.7 (C10), 106.7 (C20), 120.1 and 120.8 (C1', C1''), 124.6 and 124.7 (C_{ar}), 130.9 (C7, C17), 131.5 (C8), 131.9 (C18), 133.6 (C12, C13), 133.9 and 134.1 (C_{ar}), 141.0 (C4', C4''), 148.8 (C5, C15), 152.9 (C1).

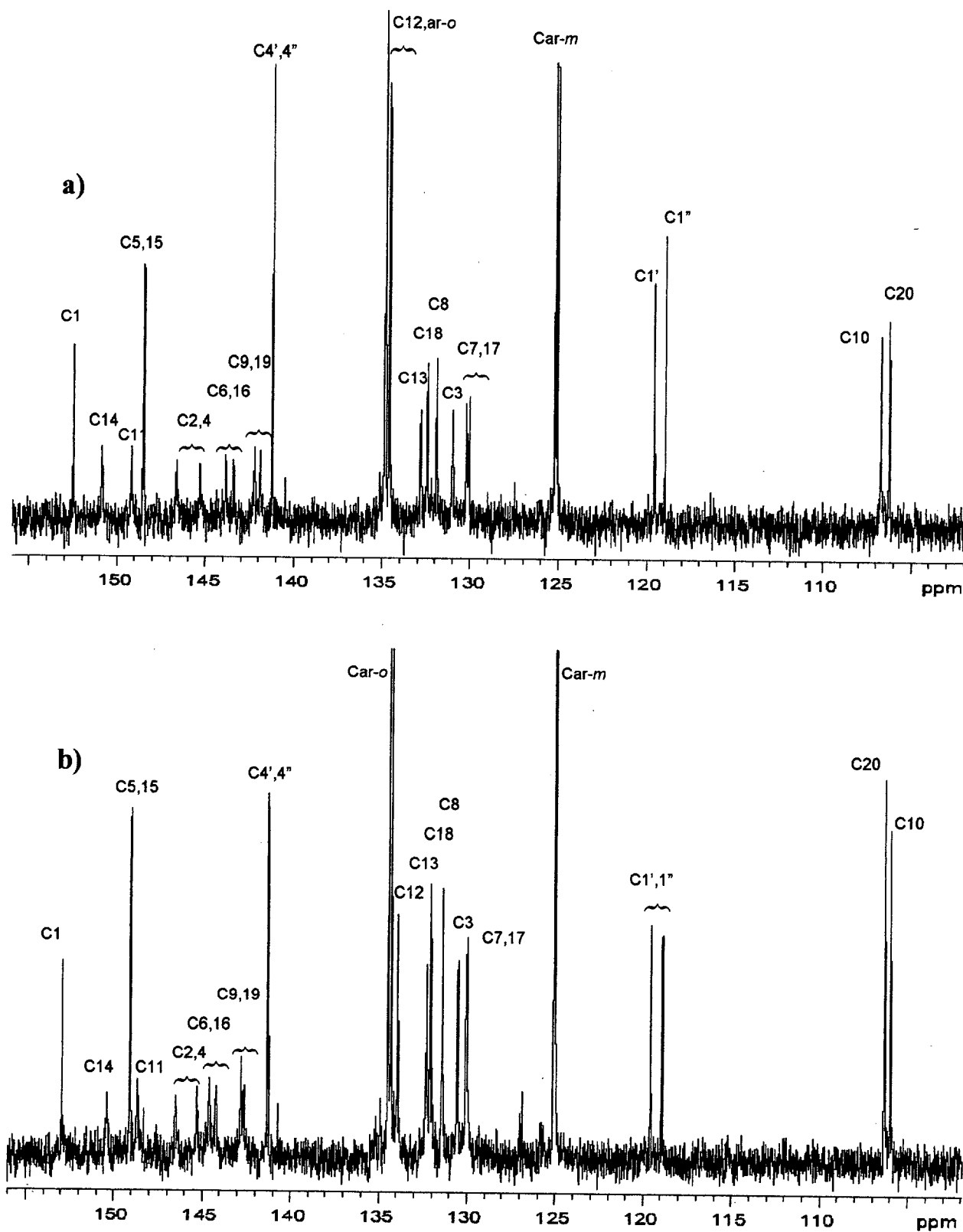


Figure S1. ^{13}C NMR (100 MHz) spectra of 1 at 298 K (a) in $\text{DMSO}-d_6$ and (b) in $\text{DMF}-d_7$.

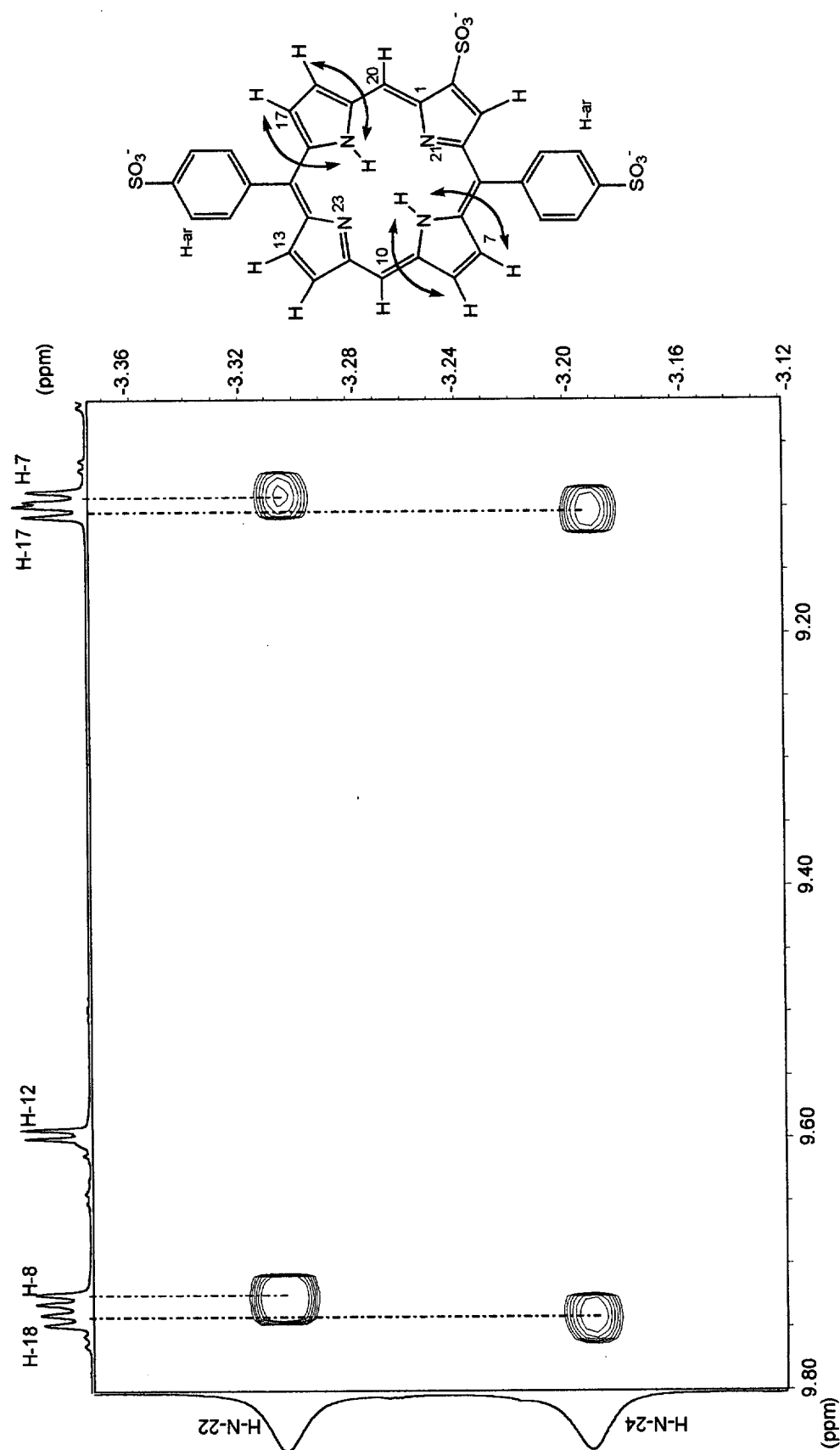


Figure S2. ¹H NMR COSY (600 MHz) spectrum of **1** in DMSO-*d*₆ at 298 K (N-H zone).

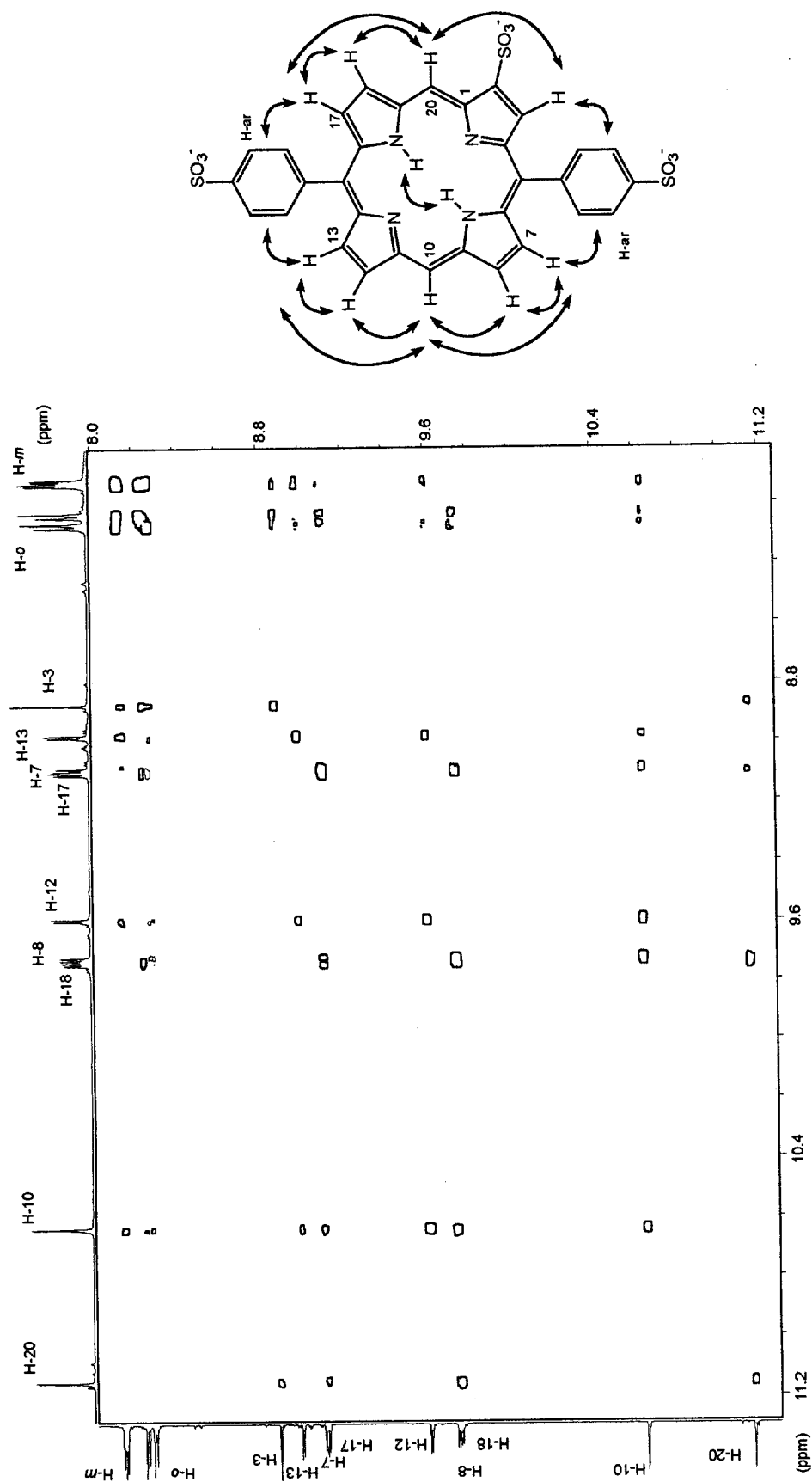


Figure S3. ¹H NMR COSY (600 MHz) spectrum of 1 in DMSO-*d*₆ at 298 K.

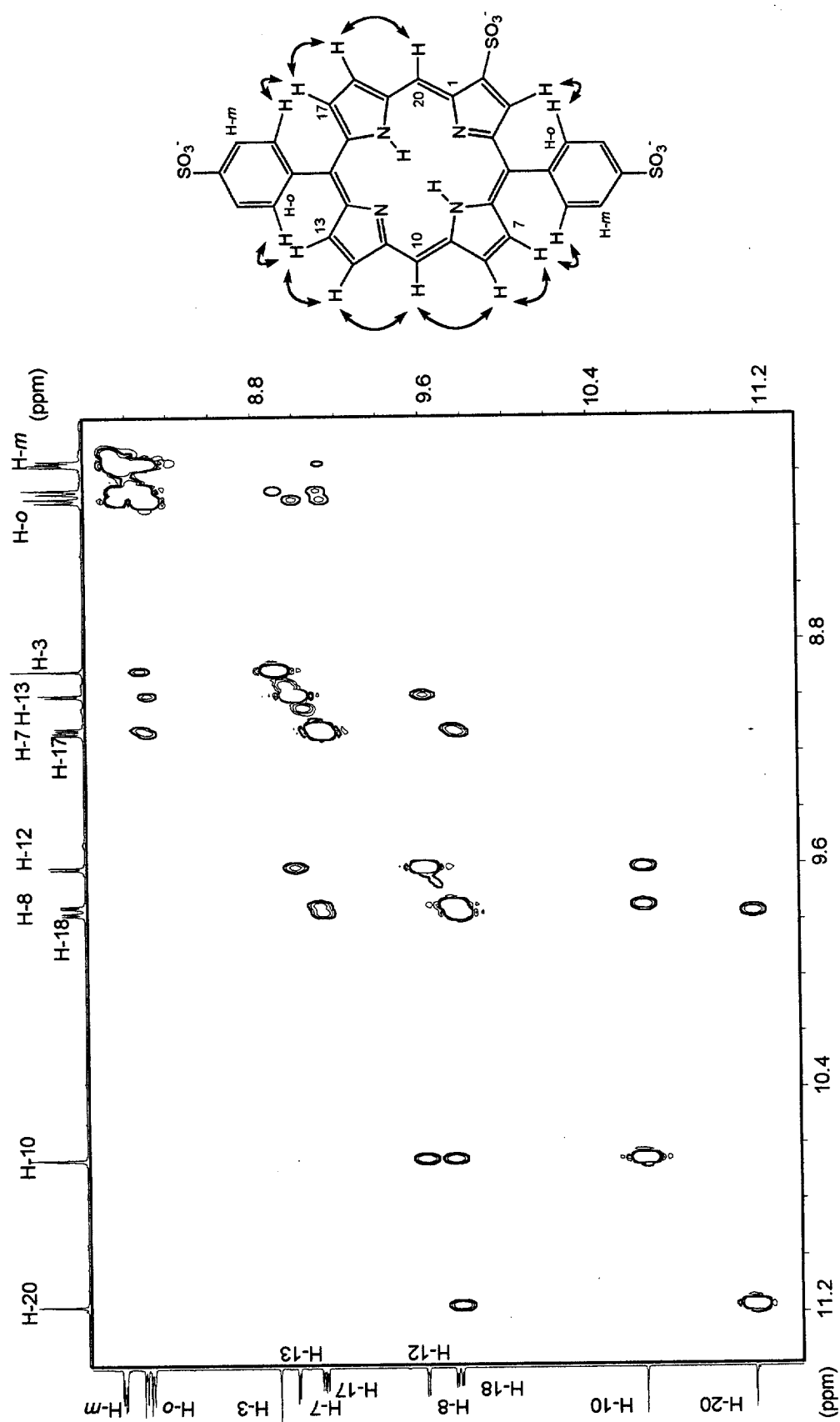


Figure S4. ^1H NMR NOESY (600 MHz) spectrum of **1** in $\text{DMSO}-d_6$ at 298 K.

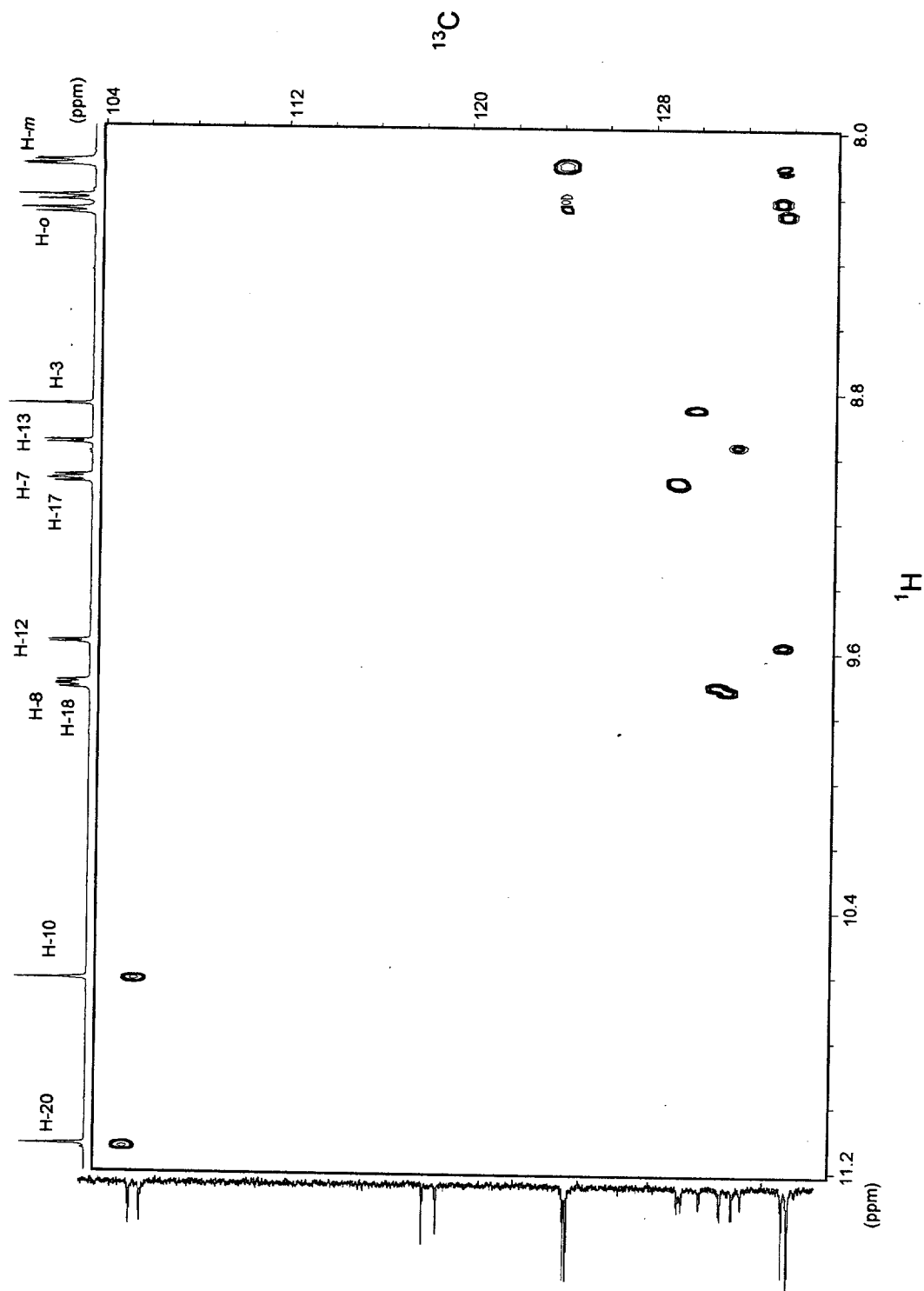


Figure S5. ^1H - ^{13}C HSQC (600 MHz) spectrum of **1** in $\text{DMSO}-d_6$ at 298 K.

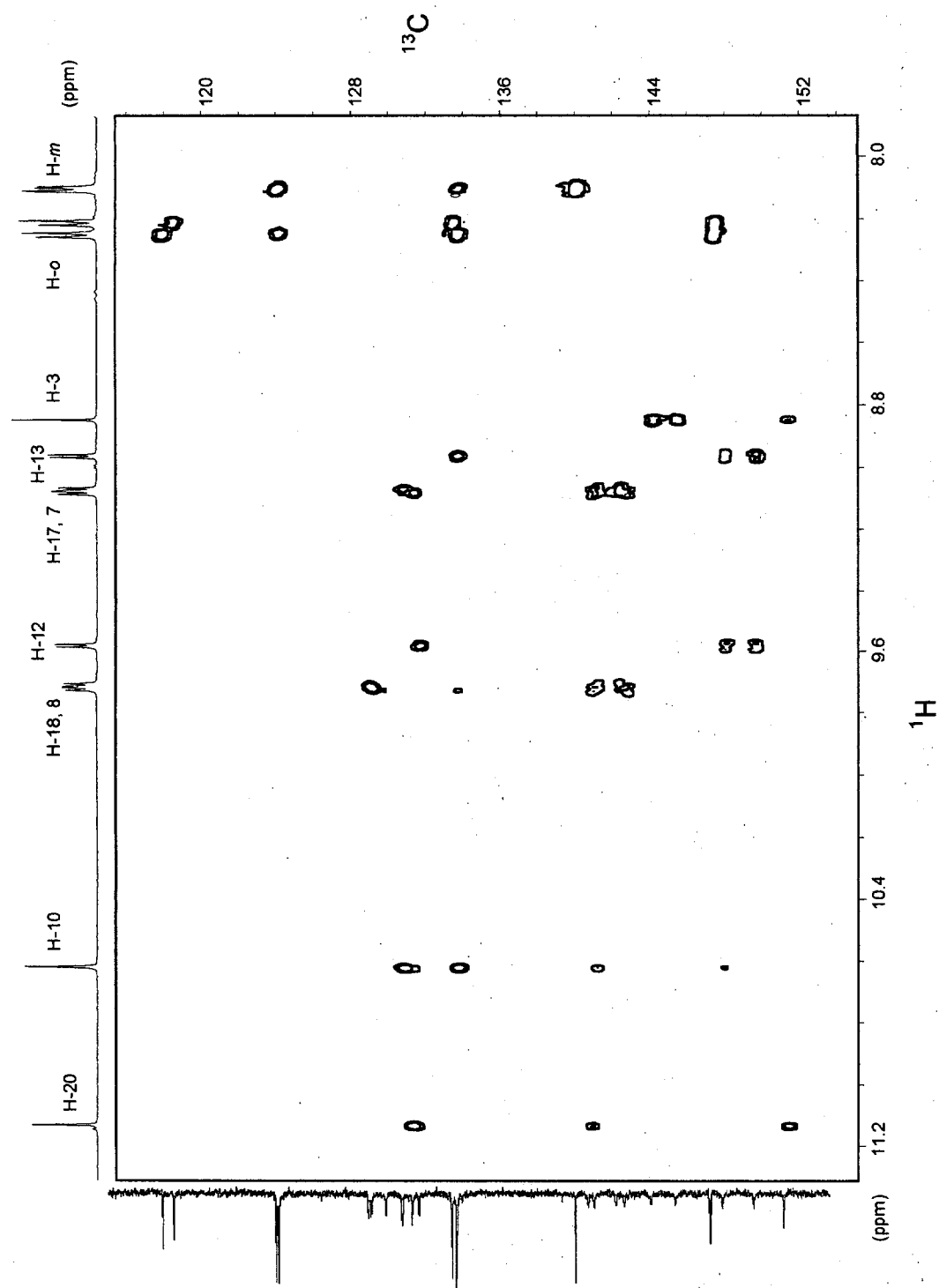


Figure S6. ^1H - ^{13}C HMBC (600 MHz) spectrum of **1** in $\text{DMSO}-d_6$ at 298 K.

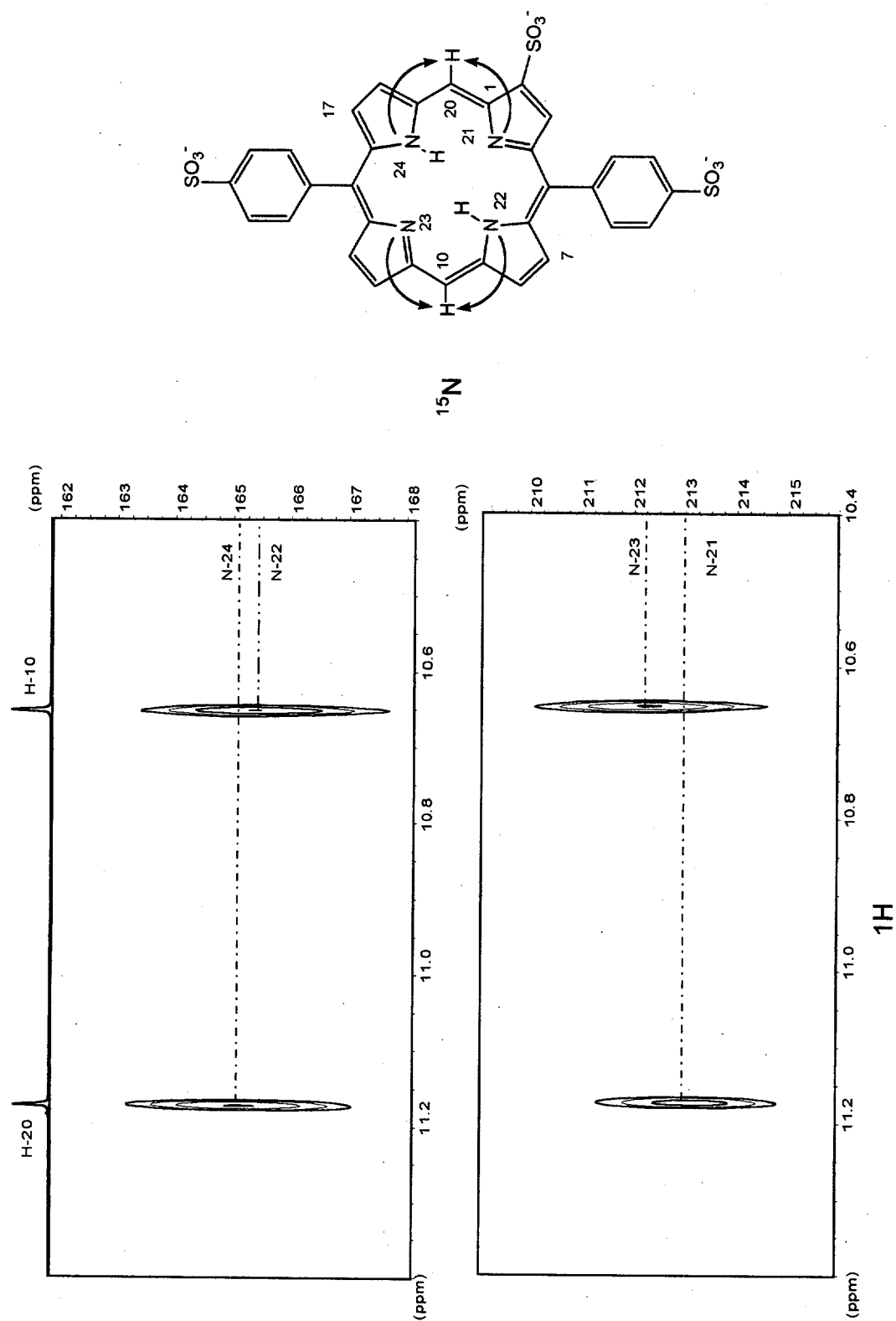


Figure S7. H-C partial section of the ^1H - ^{15}N HMBC (600 MHz) spectrum of **1** in $\text{DMSO}-d_6$ at 298 K.

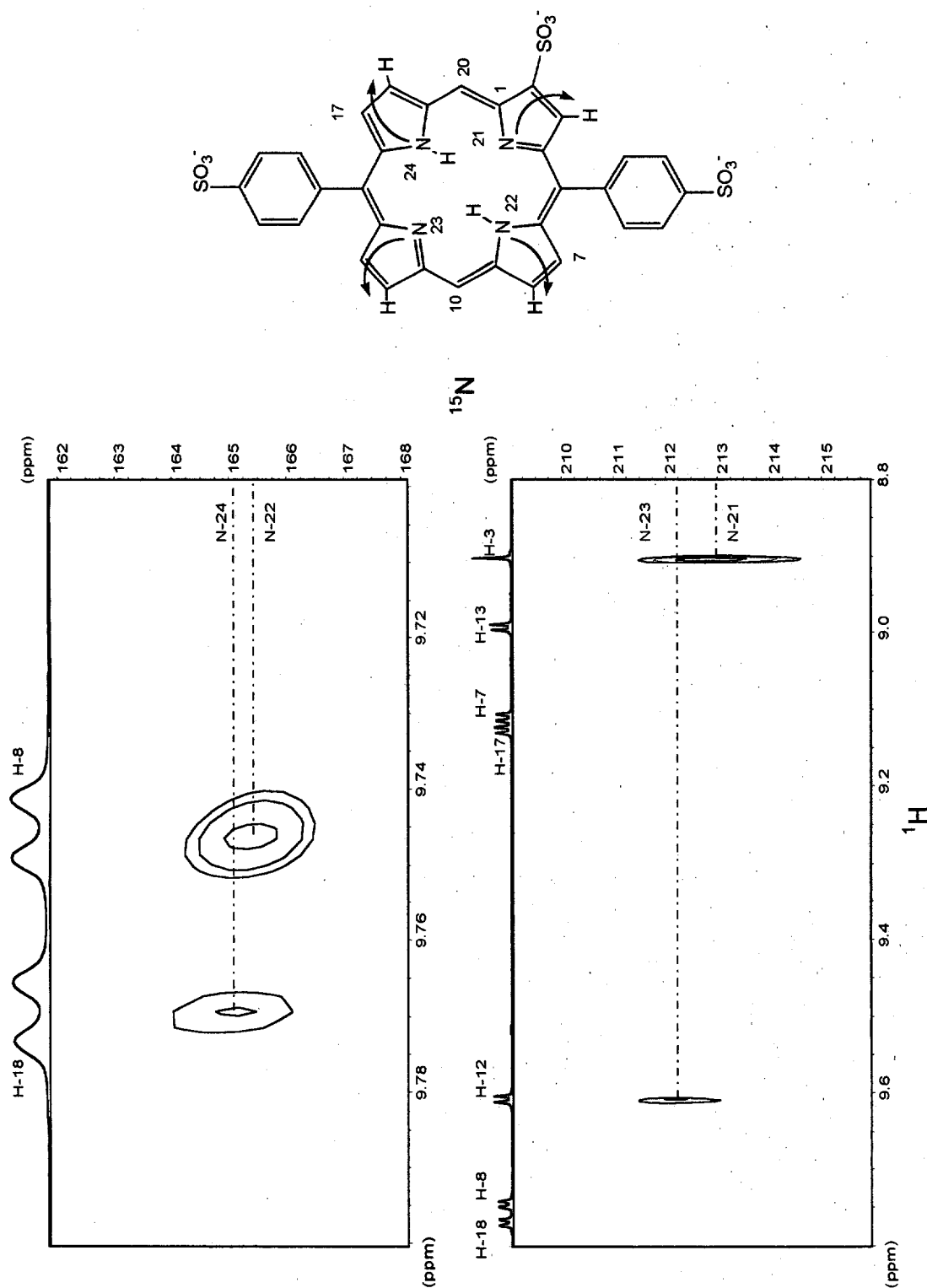


Figure S8. H-C partial section of the ^1H - ^{15}N HMBC (600 MHz) spectrum of **1** in DMSO- d_6 at 298 K.

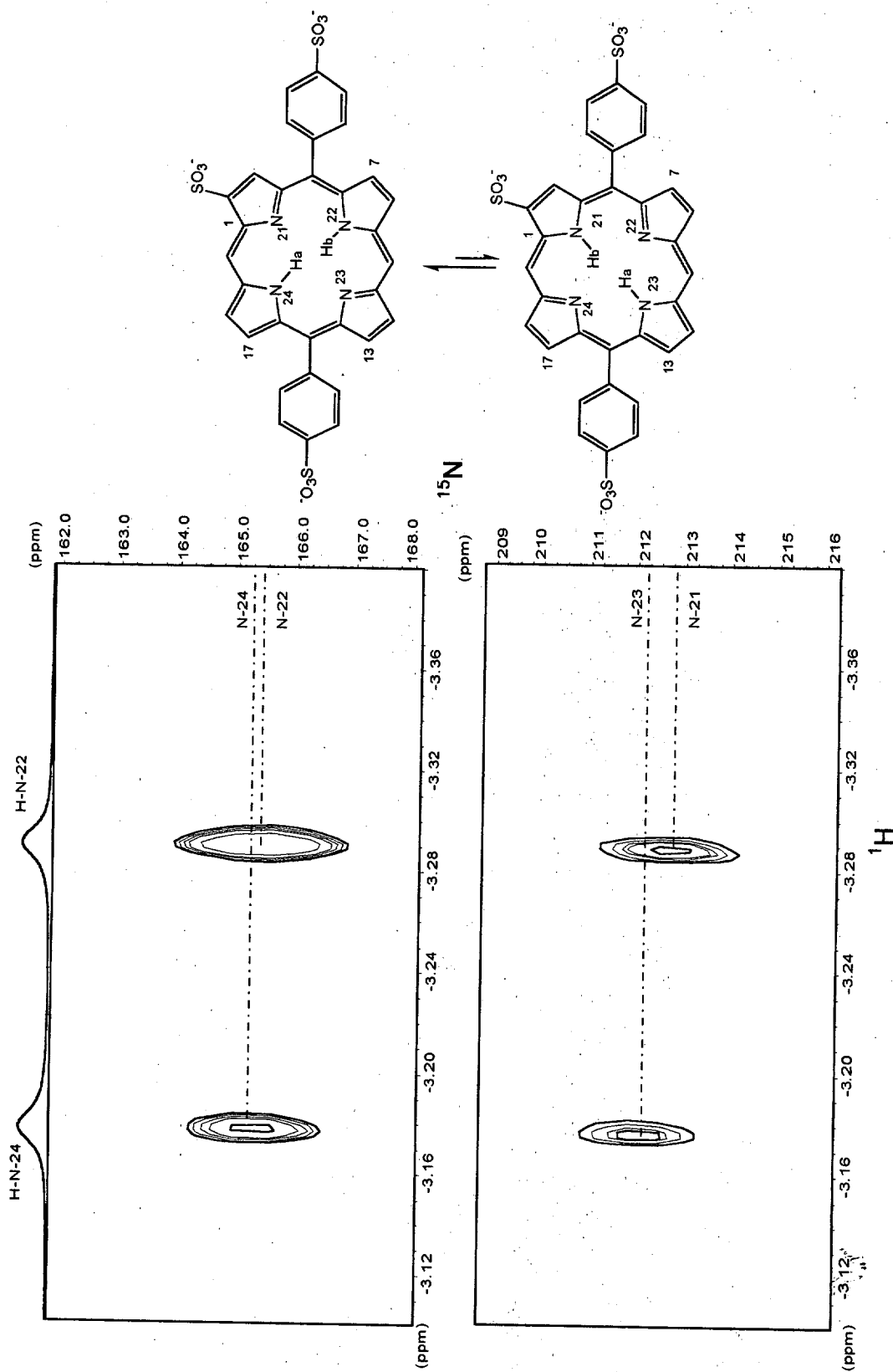


Figure S9. H-N section of the ^1H - ^{15}N HSQC (600 MHz) spectrum of 1 in $\text{DMSO}-d_6$ at 298 K.

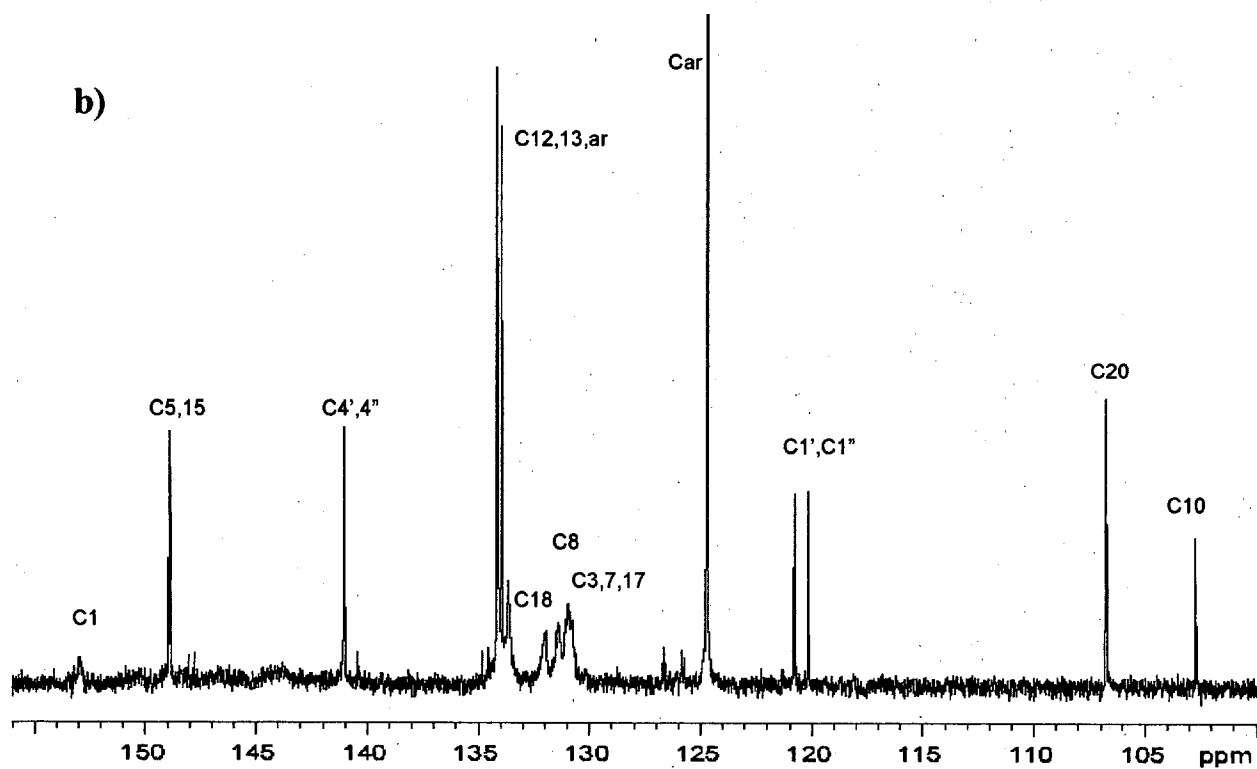
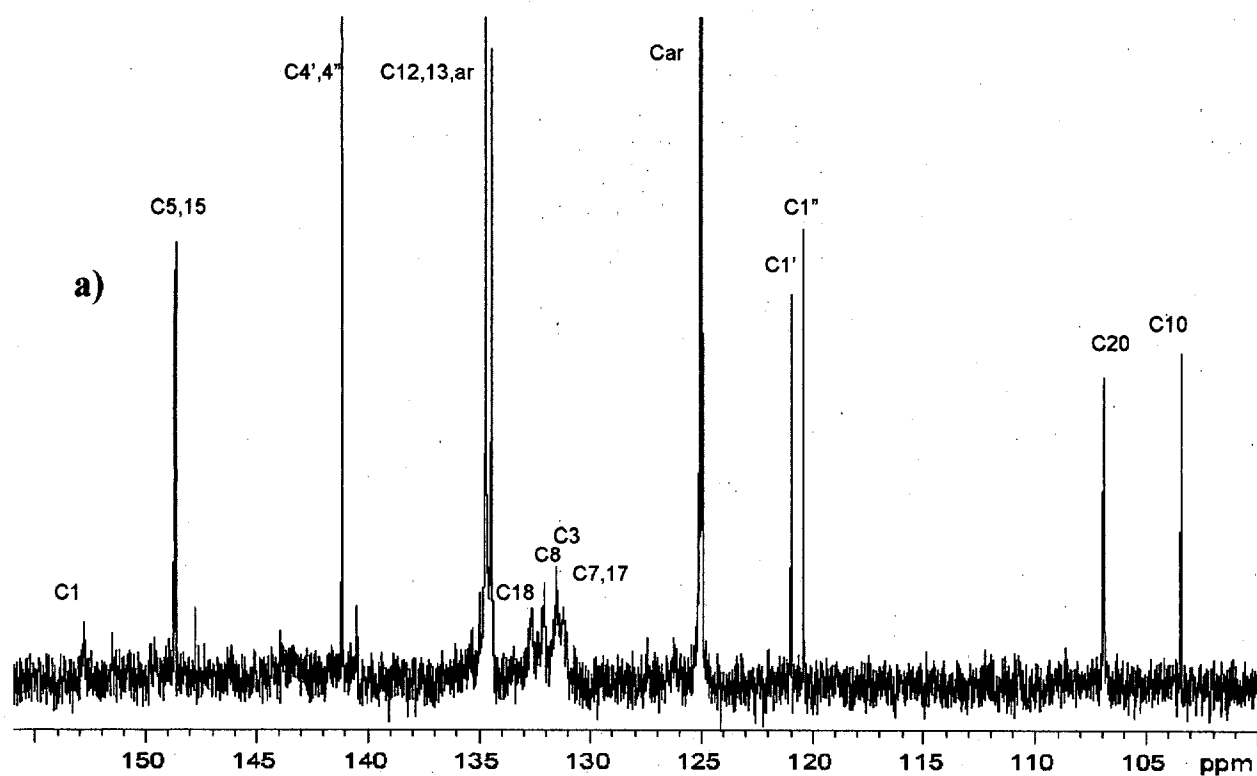


Figure S10. ^{13}C NMR (100 MHz) spectra of **2** at 298 K (a) in $\text{DMSO}-d_6$ and (b) in $\text{DMF}-d_7$.

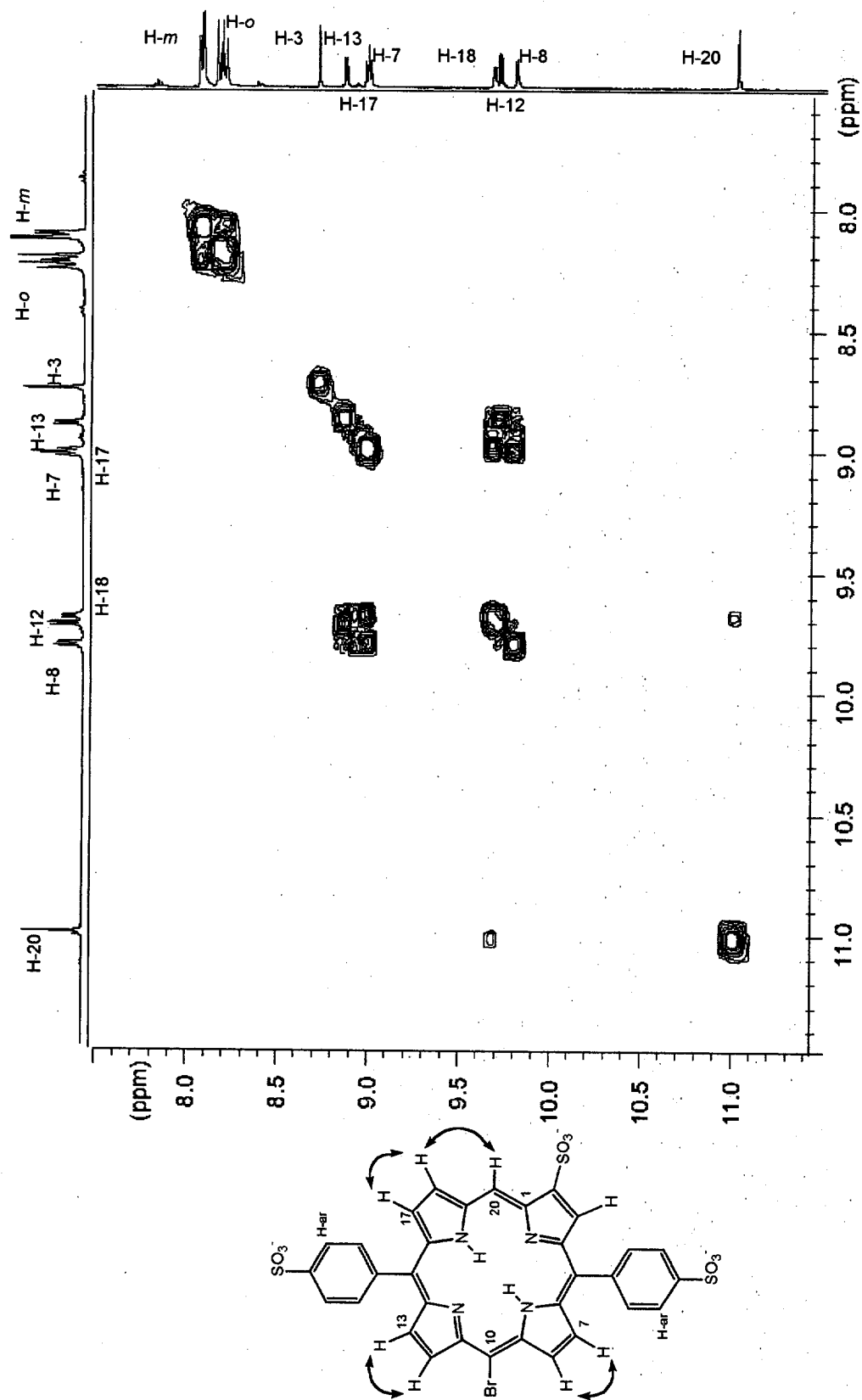


Figure S11. ^1H NMR COSY (400 MHz) spectrum of **2** in $\text{DMSO}-d_6$ at 298 K.

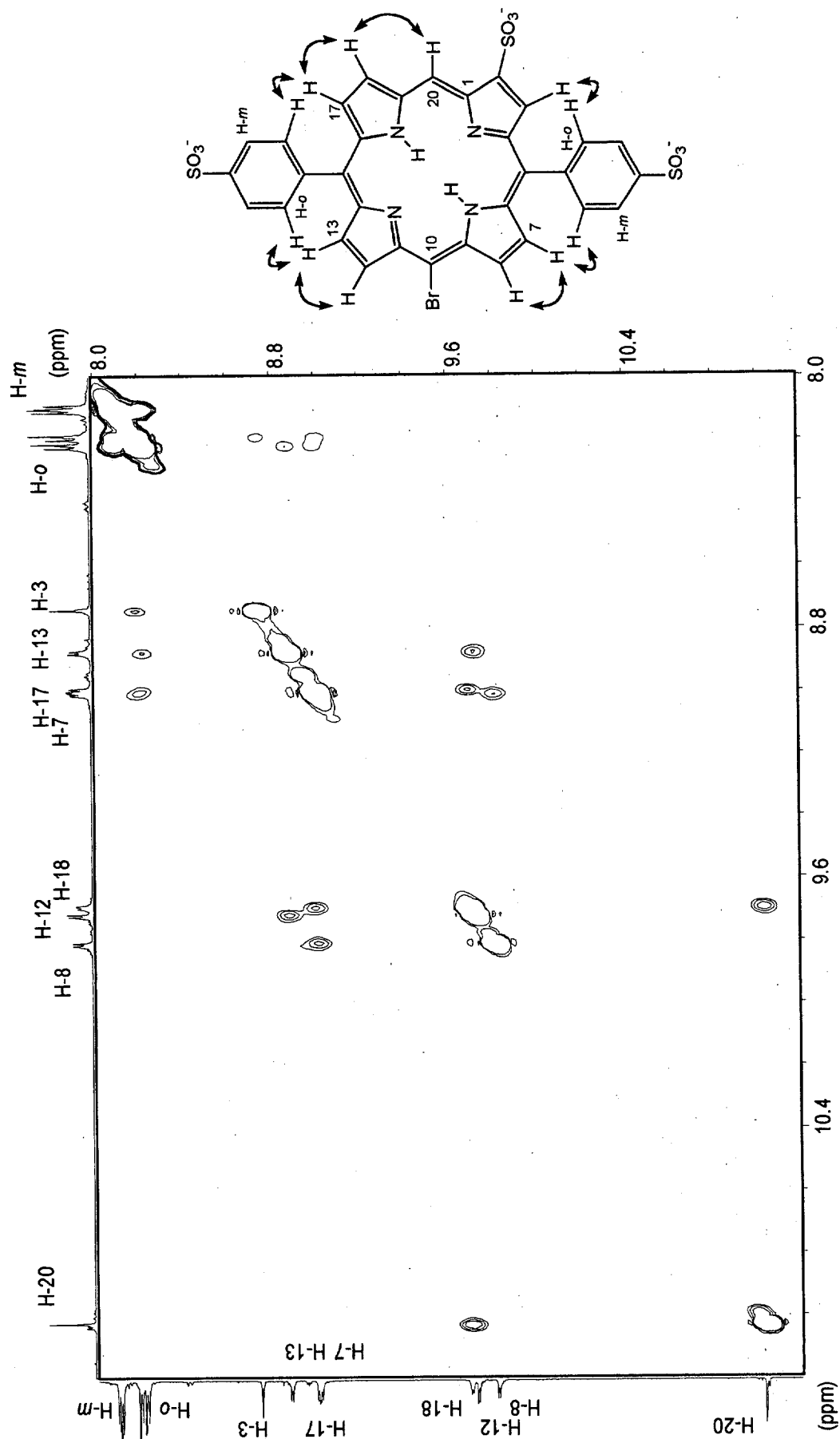


Figure S12. ¹H NMR NOESY (600 MHz) spectrum of **2** in DMSO-*d*₆ at 298 K.

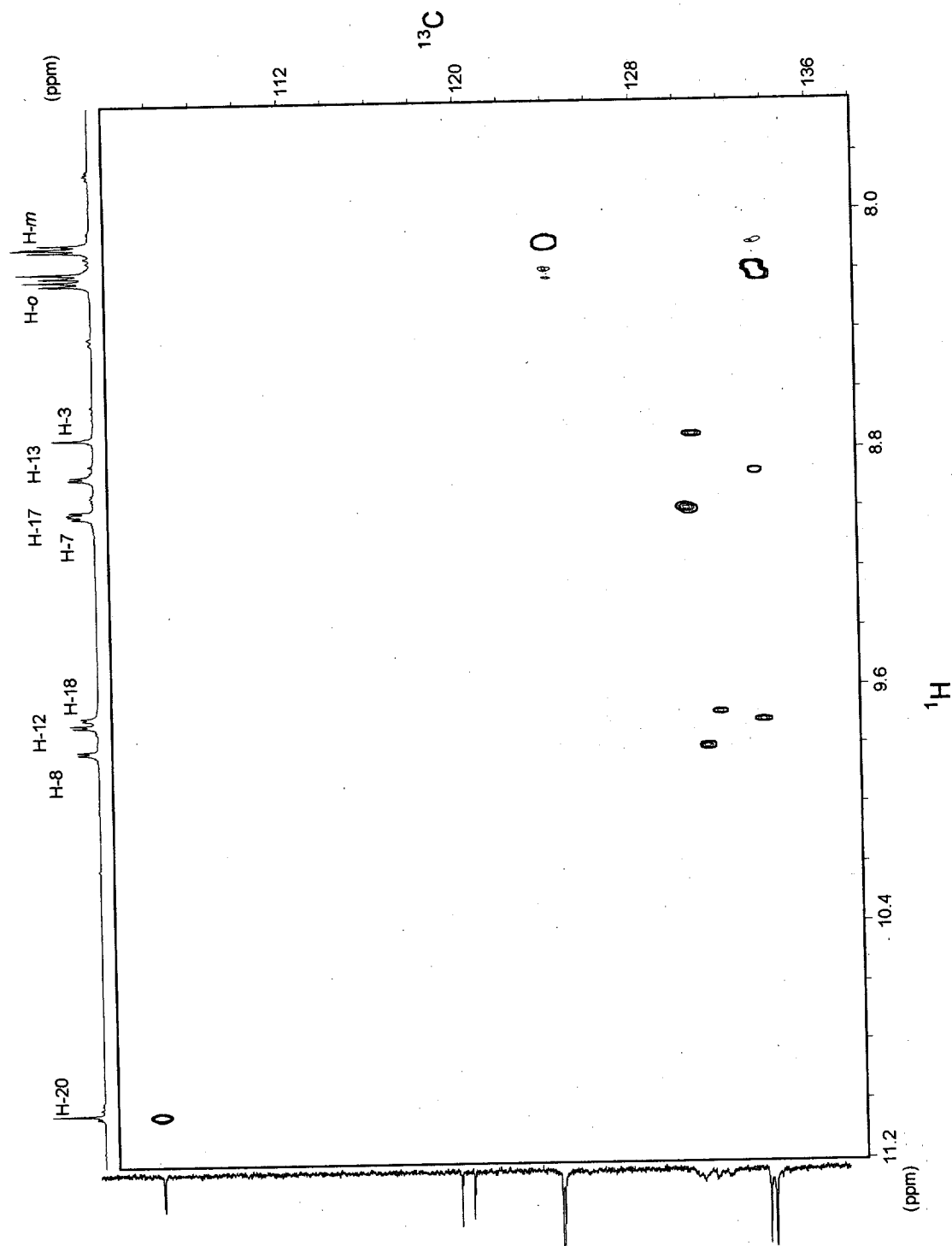


Figure S13. ^1H - ^{13}C HSQC (600 MHz) spectrum of **2** in $\text{DMSO}-d_6$ at 298 K.

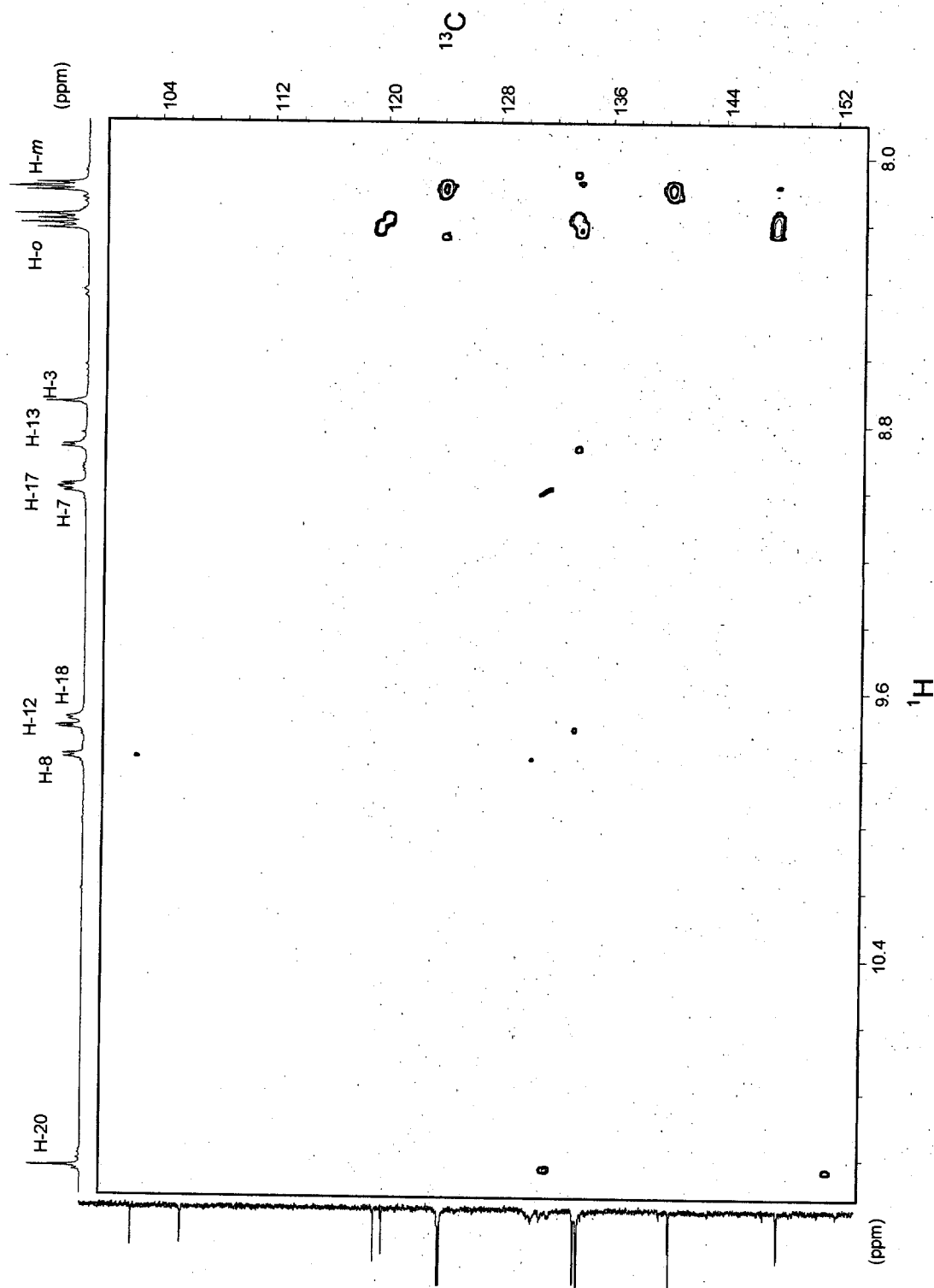


Figure S14. ^1H - ^{13}C HMBC (600 MHz) spectrum of **2** in $\text{DMSO}-d_6$ at 296 K.

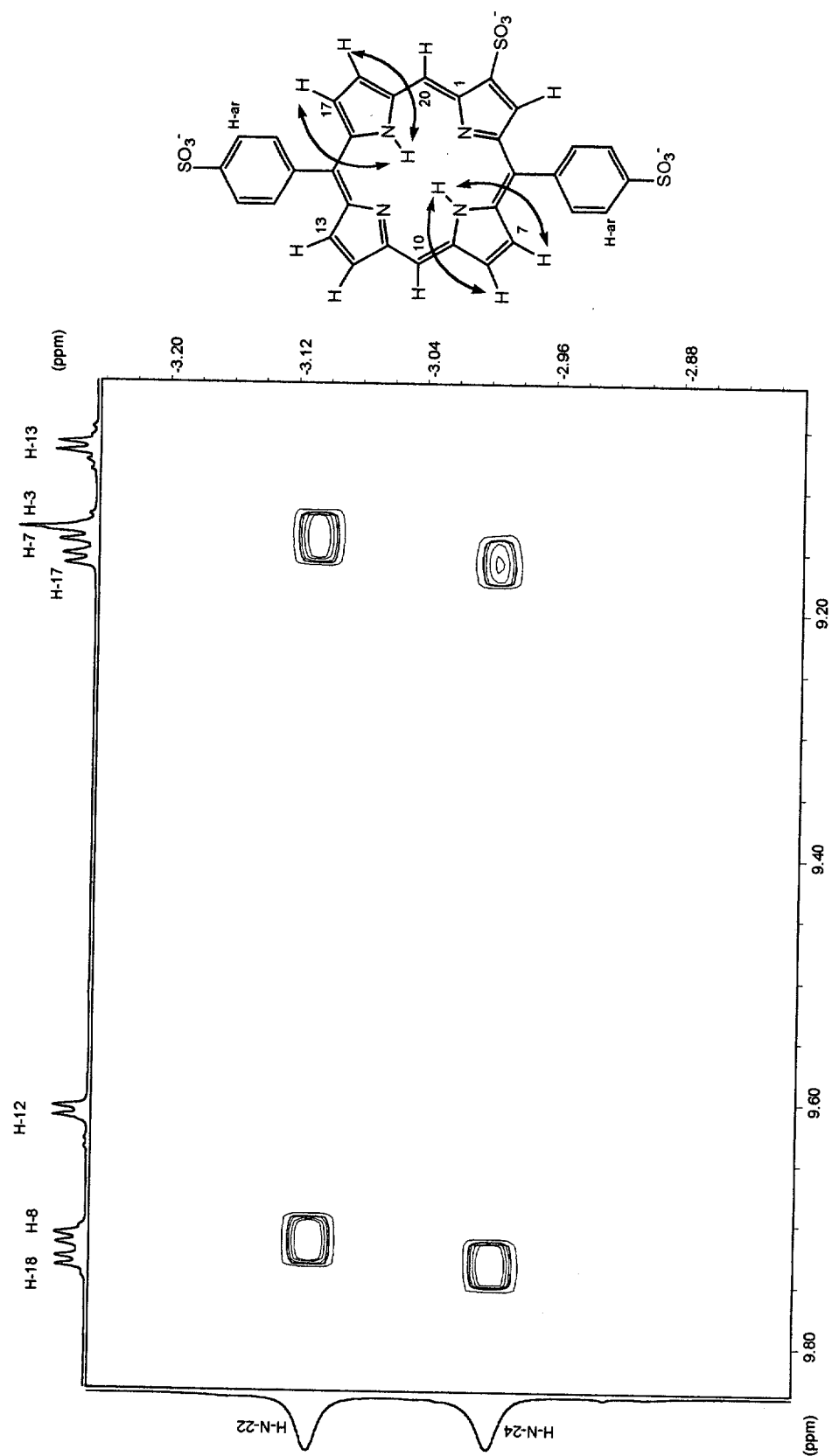


Figure S15. ^1H NMR COSY (600 MHz) spectrum of **1** in $\text{DMF-}d_7$ at 298 K (N-H zone).

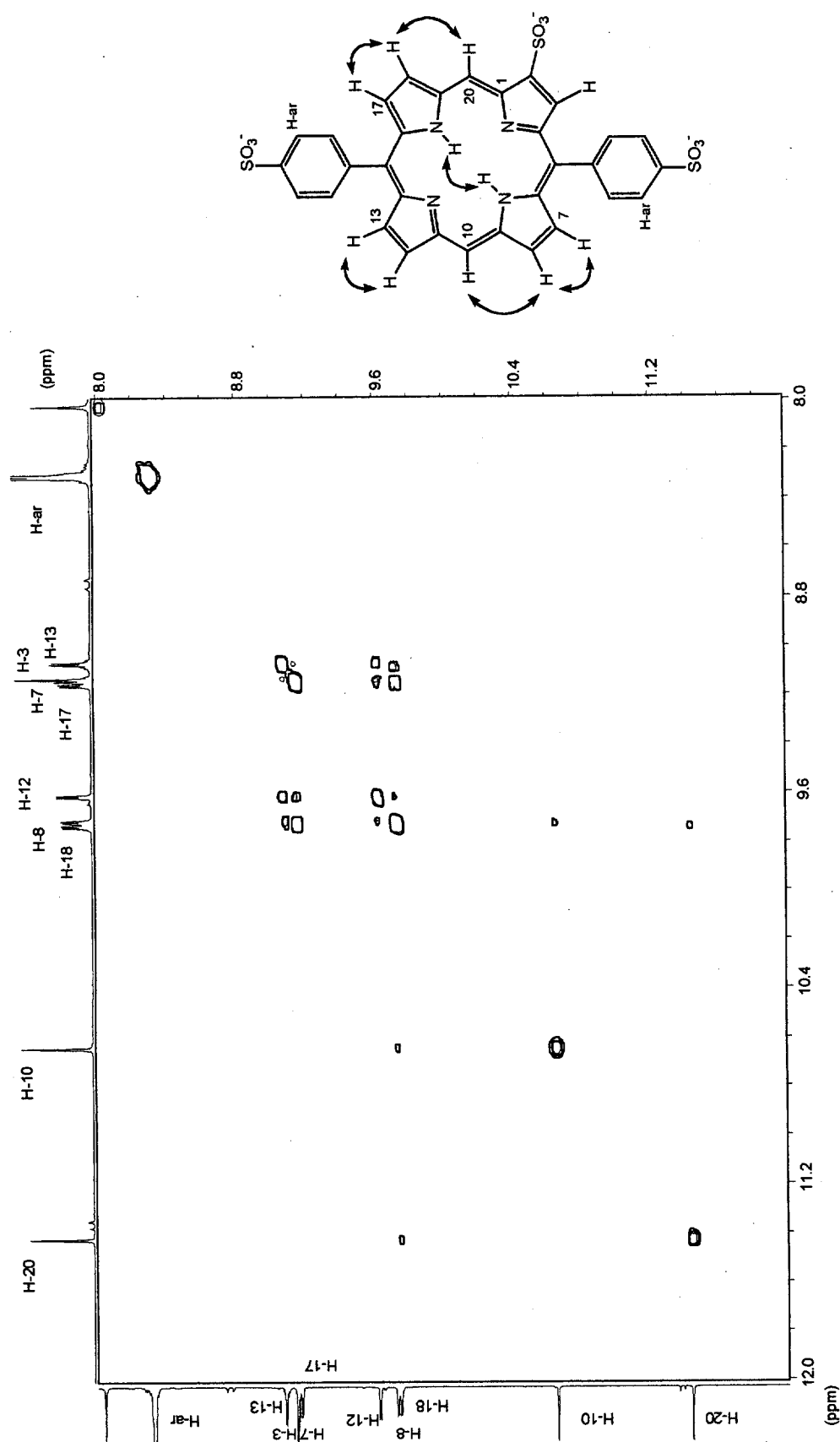


Figure S16. ¹H NMR COSY (600 MHz) spectrum of **1** in DMF-*d*₇ at 298 K.

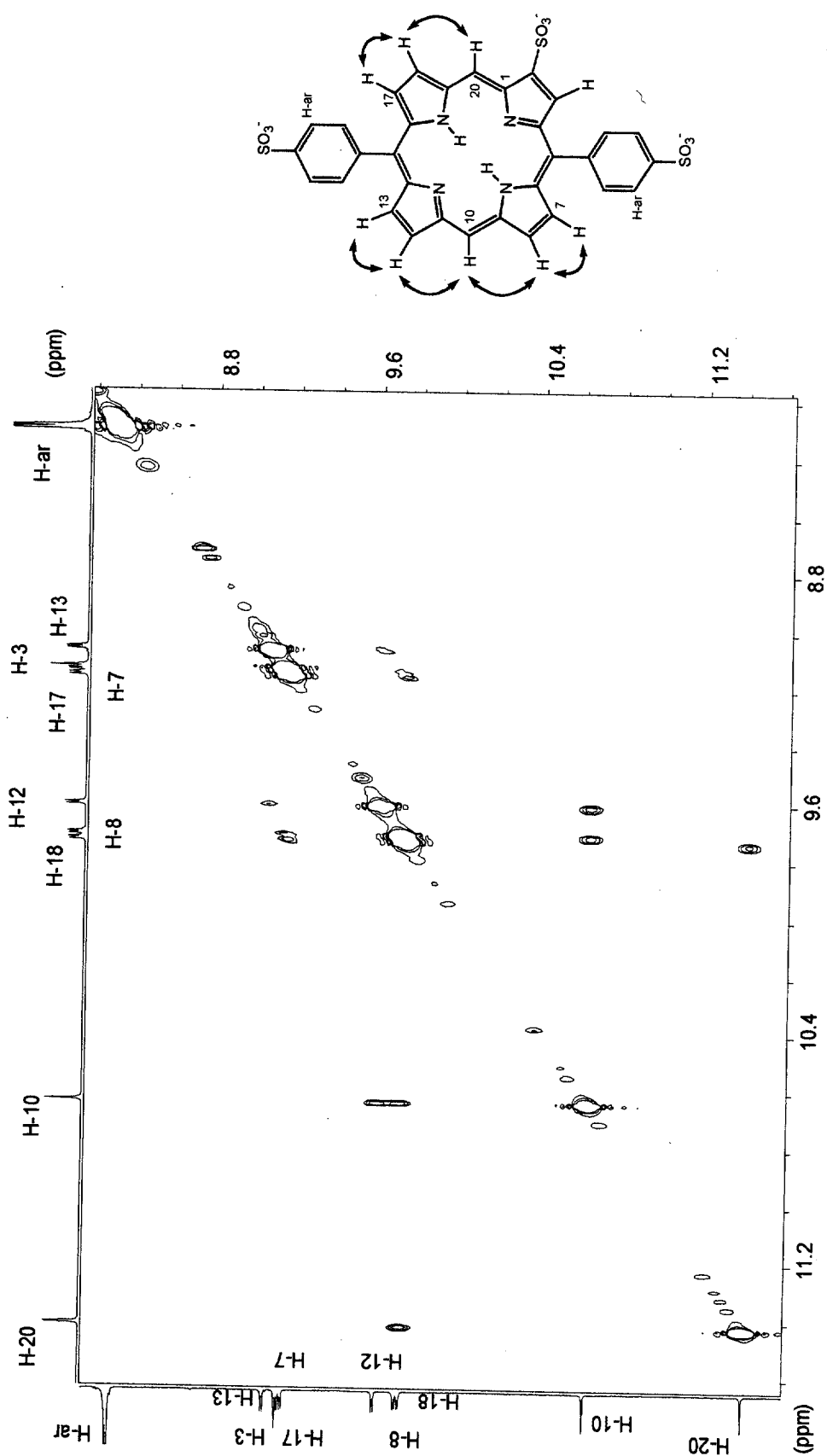


Figure S17. ^1H NMR NOESY (600 MHz) spectrum of **1** in $\text{DMF-}d_7$ at 298 K.

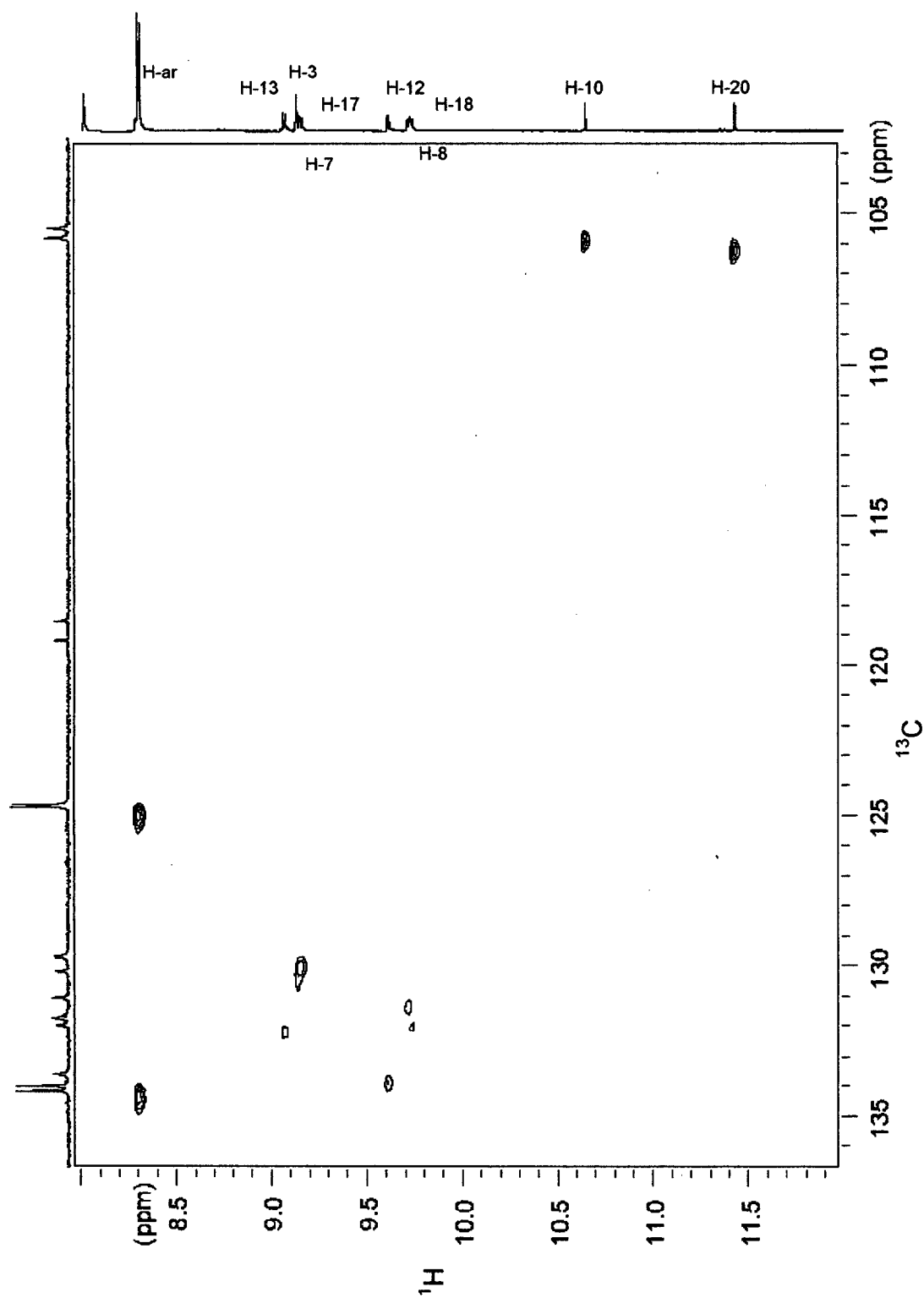


Figure S18. ^1H - ^{13}C HSQC (400 MHz) spectrum of **1** in $\text{DMF-}d_7$ at 298 K.

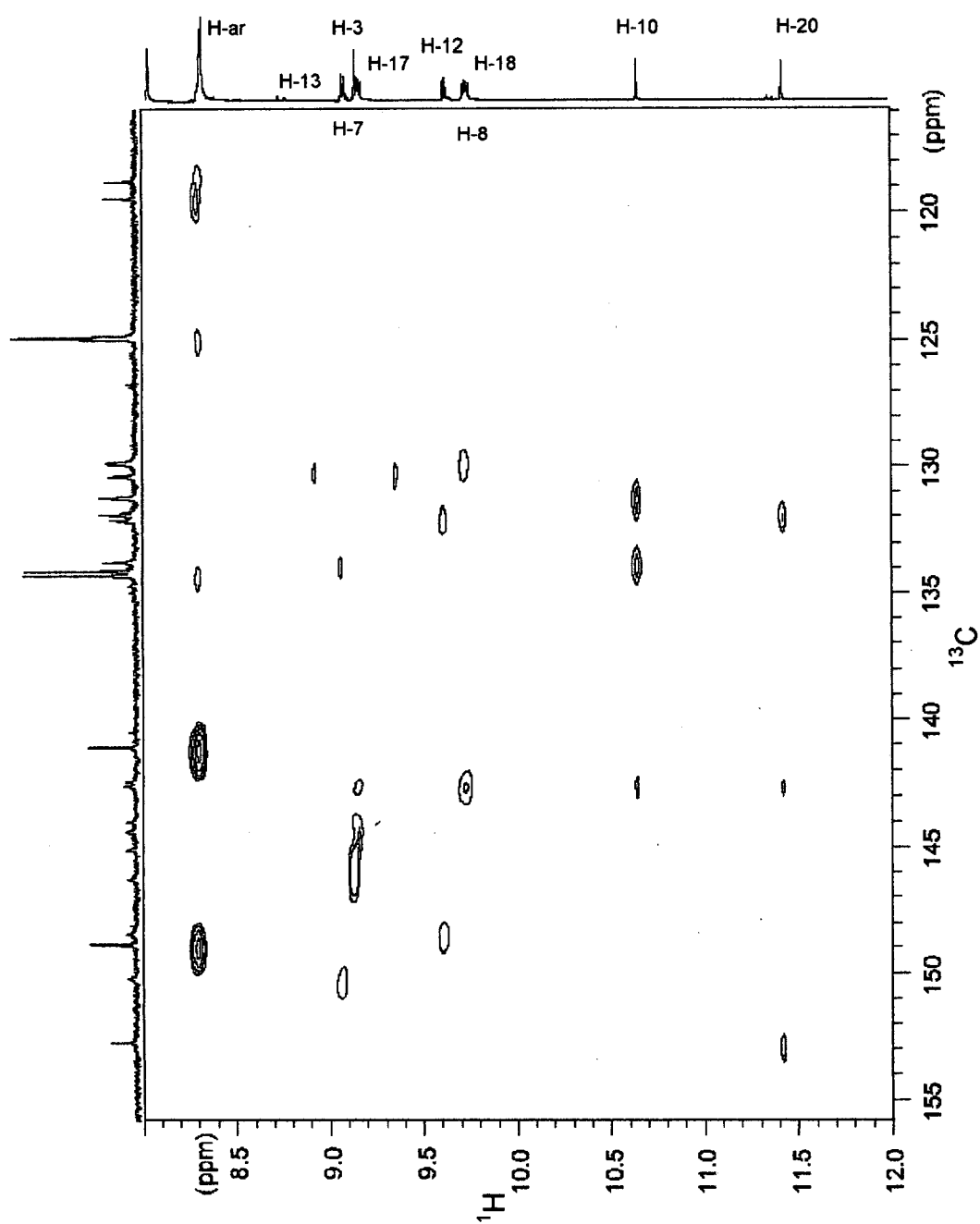


Figure S19. ^1H - ^{13}C HMBC (400 MHz) spectrum of **1** in $\text{DMF-}d_7$ at 298 K.

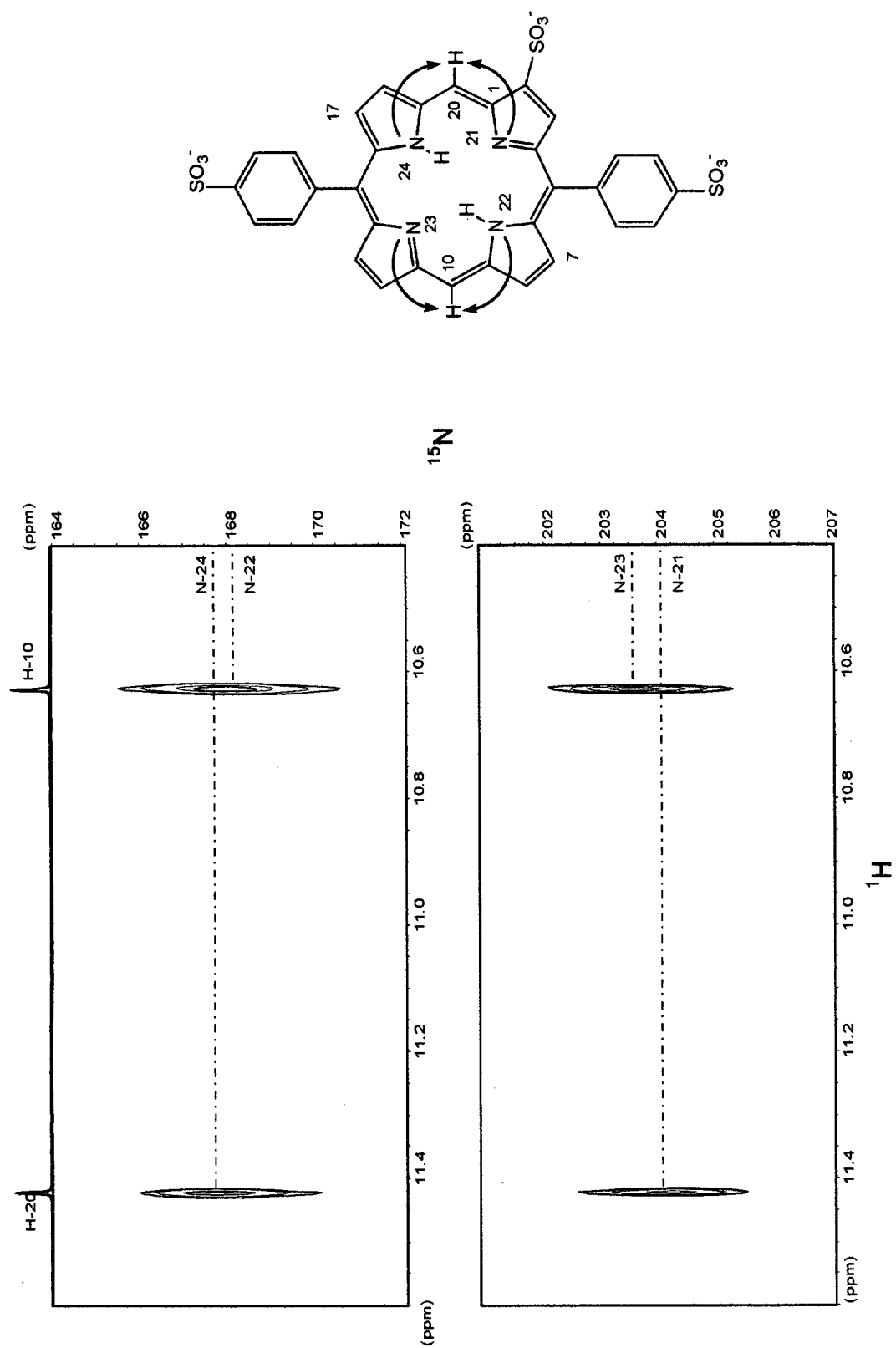


Figure S20. H-C partial section of the ^1H - ^{15}N HMBC (600 MHz) spectrum of **1** in $\text{DMF-}d_7$ at 298 K.

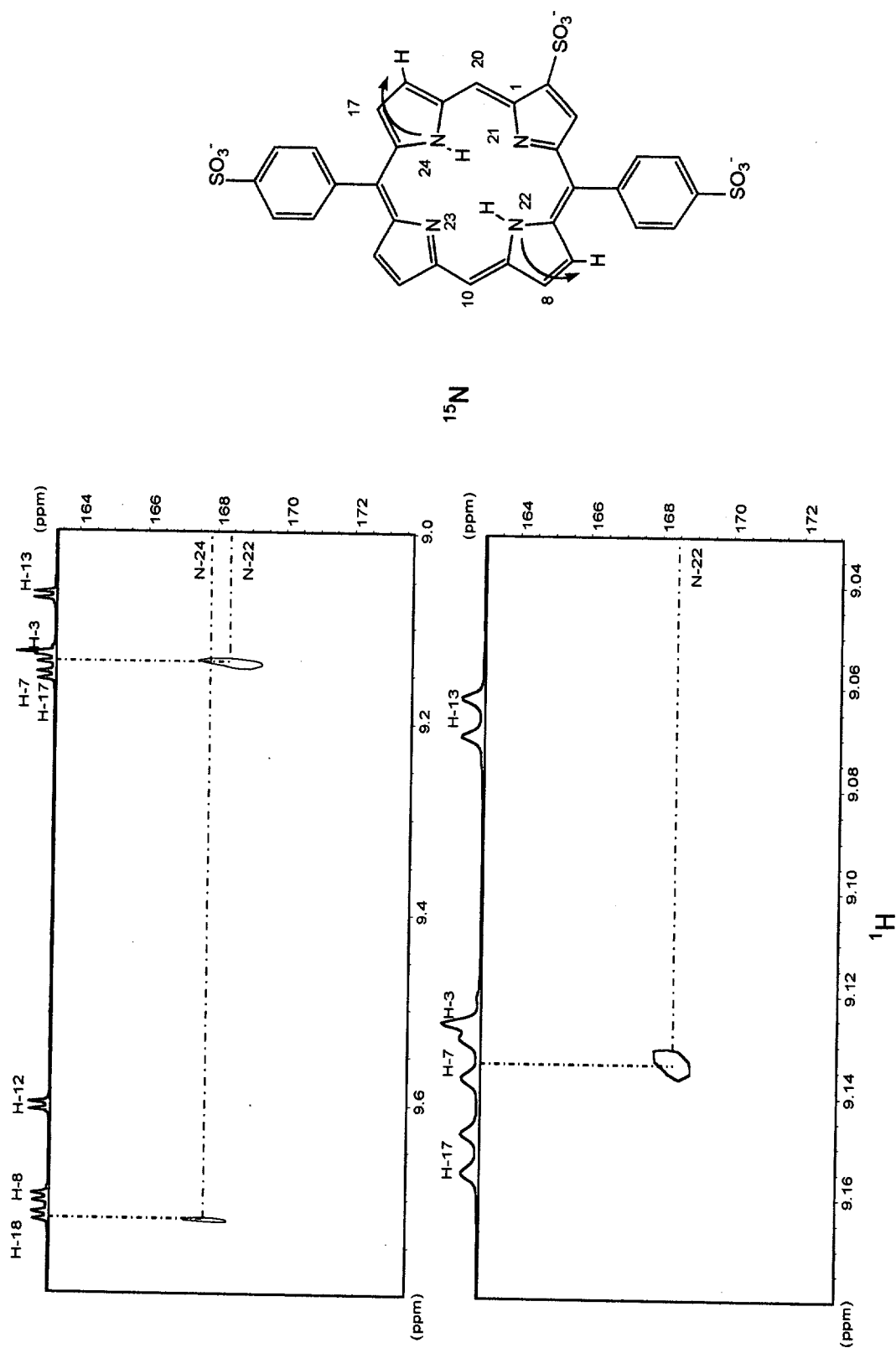


Figure S21. H-C partial section of the ¹H-¹⁵N HMBC (600 MHz) spectrum of 1 in DMF-*d*₇ at 298 K.

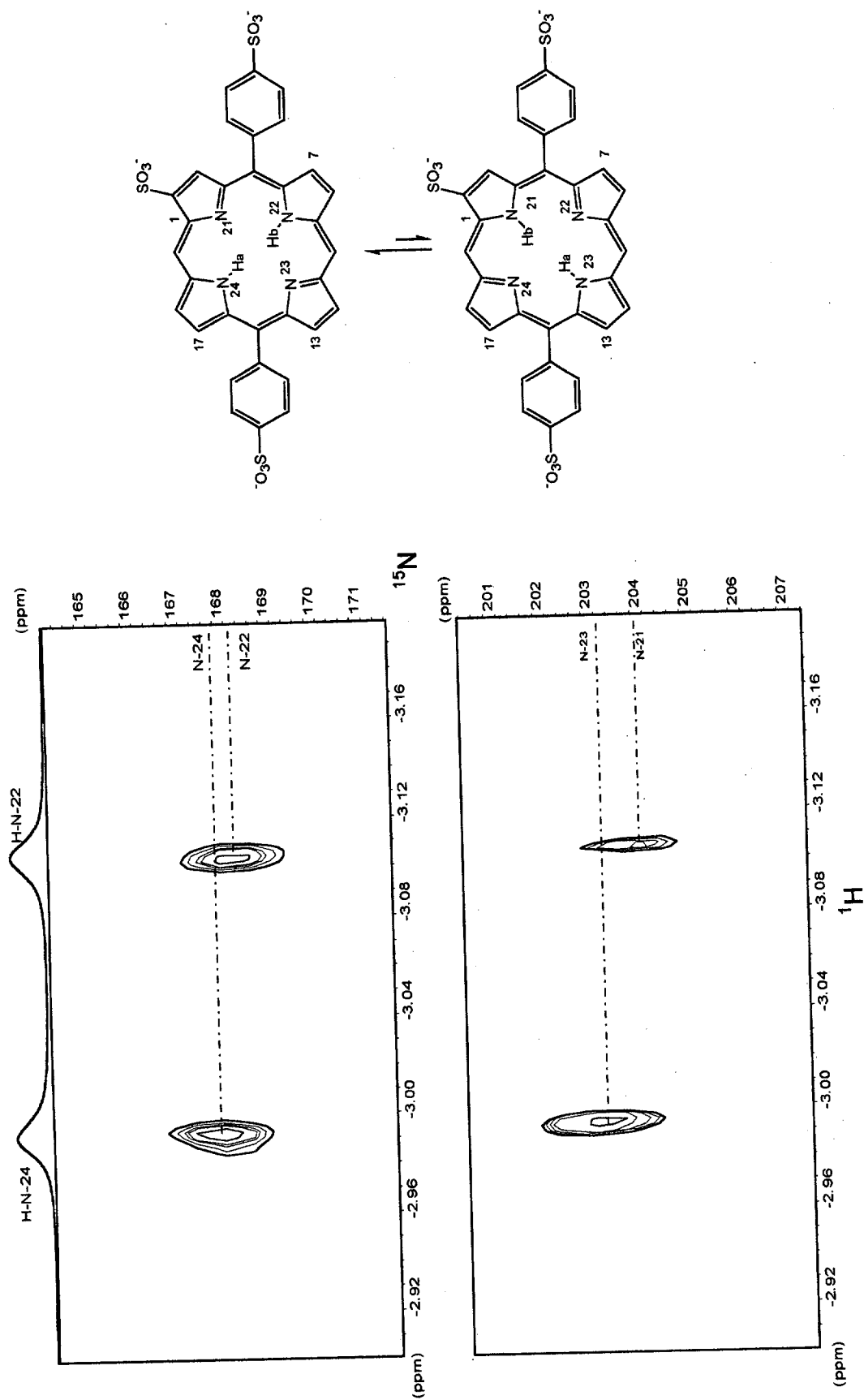


Figure S22. H-Nsection of the ^1H - ^{15}N HSQC (600 MHz) spectrum of **1** in $\text{DMF-}d_7$ at 298 K.

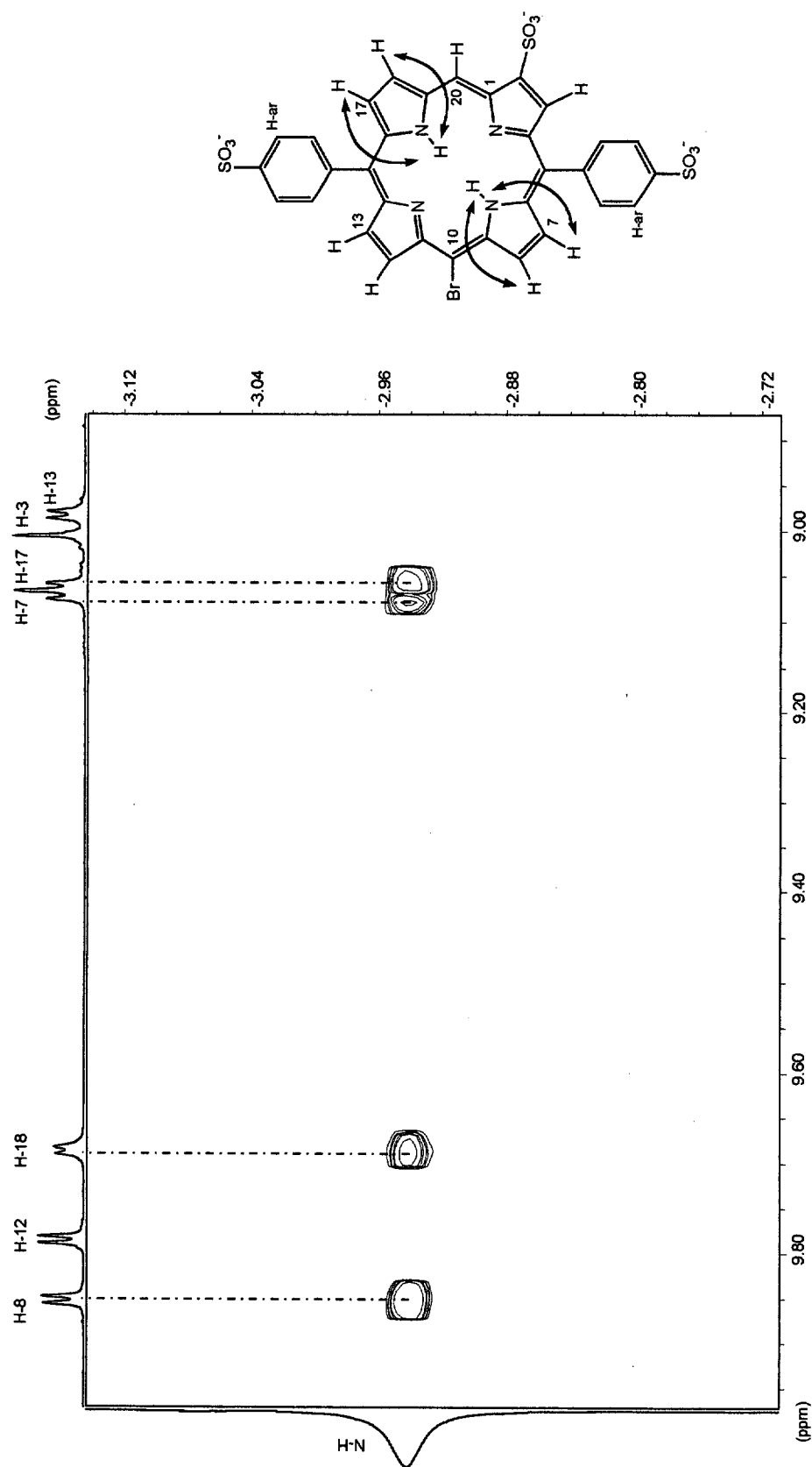


Figure S23. ¹H NMR COSY (600 MHz) spectrum of **2** in DMF-*d*₇ at 298 K (N-H zone).

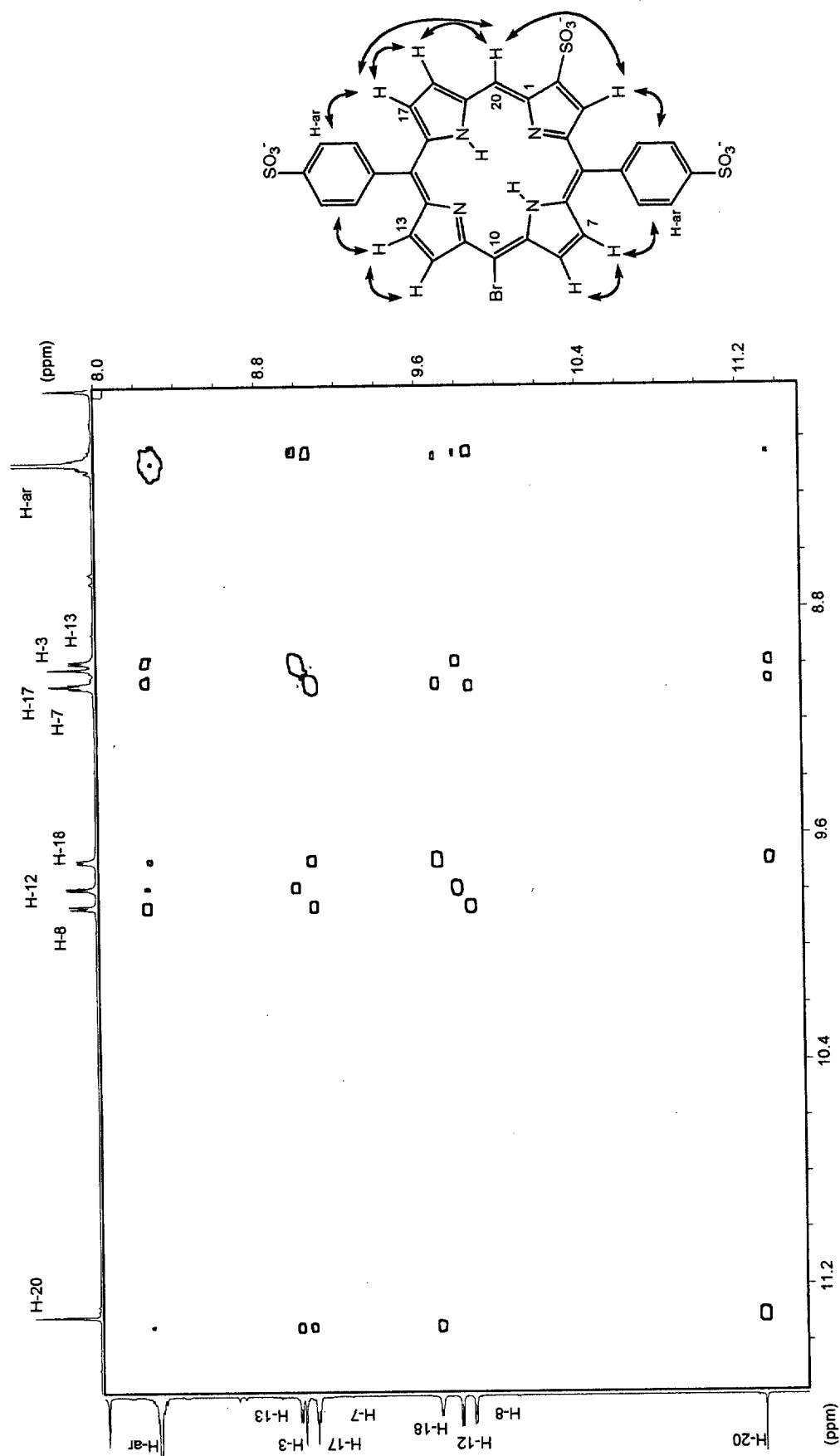


Figure S24. ^1H NMR COSY (600 MHz) spectrum of 2 in $\text{DMF-}d_7$ at 298 K.

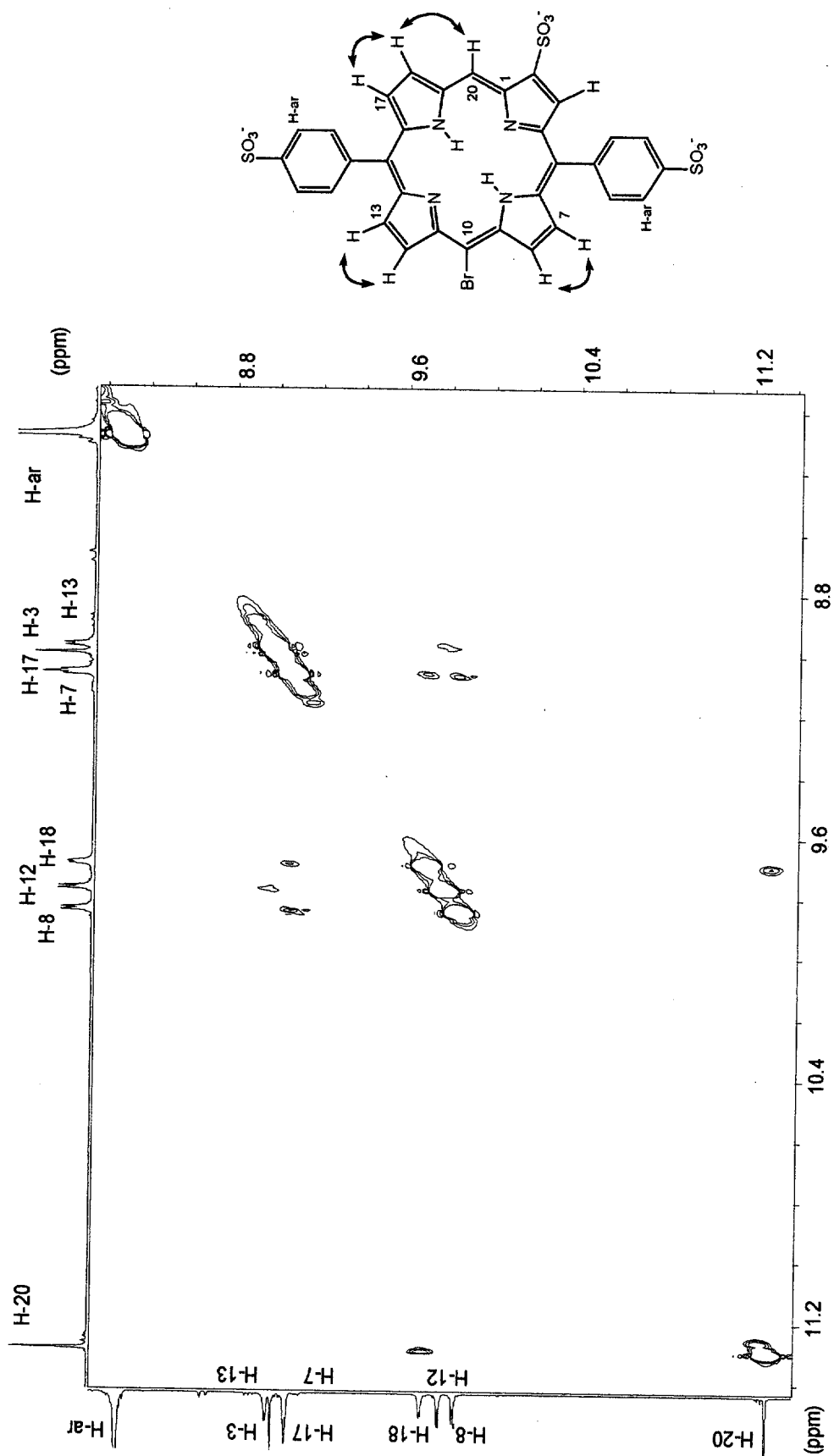


Figure S25. ^1H NMR NOESY (600 MHz) spectrum of **2** in $\text{DMF-}d_7$ at 298 K.

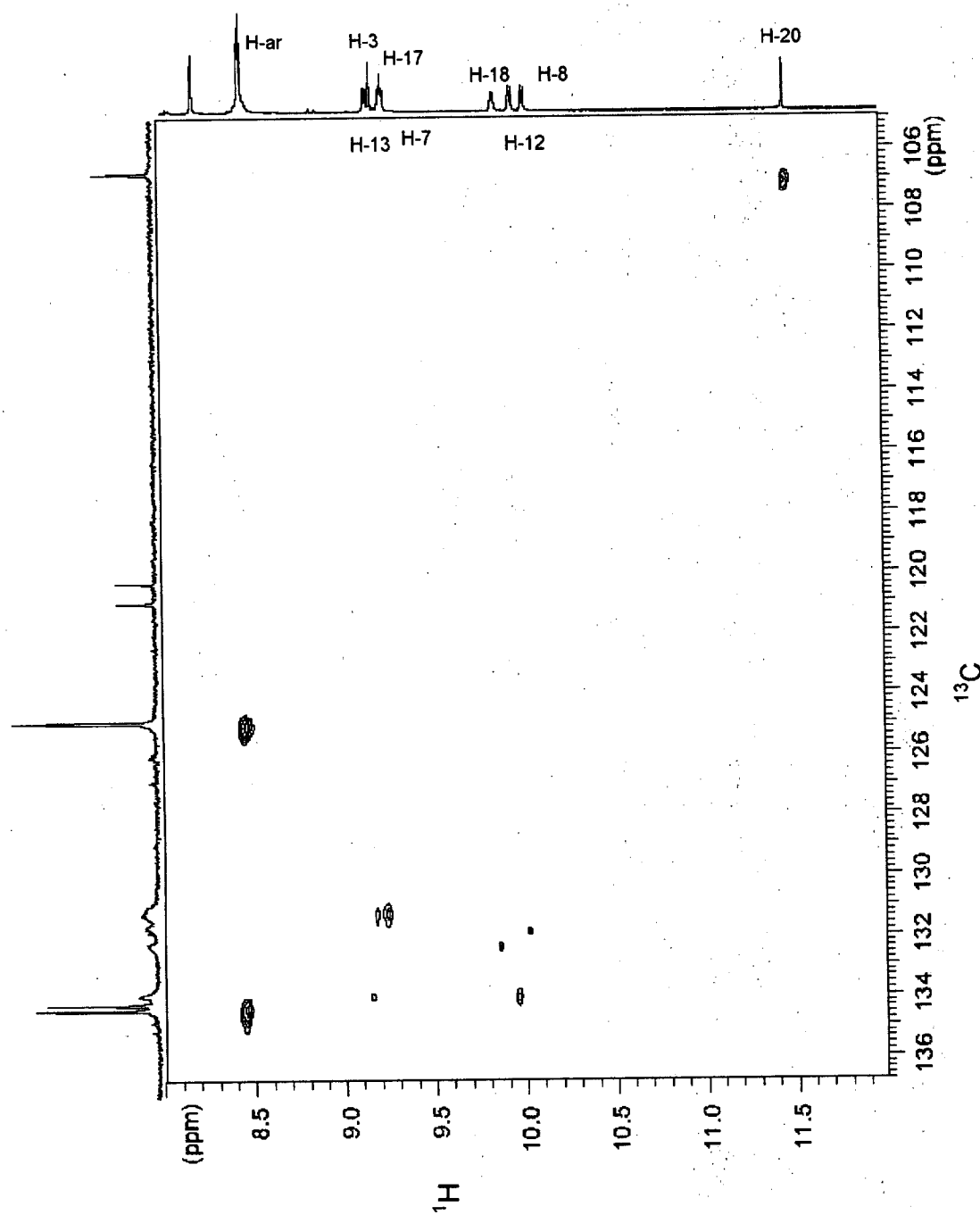


Figure S26. ^1H - ^{13}C HSQC (400 MHz) spectrum of **2** in $\text{DMF-}d_7$ at 298 K.

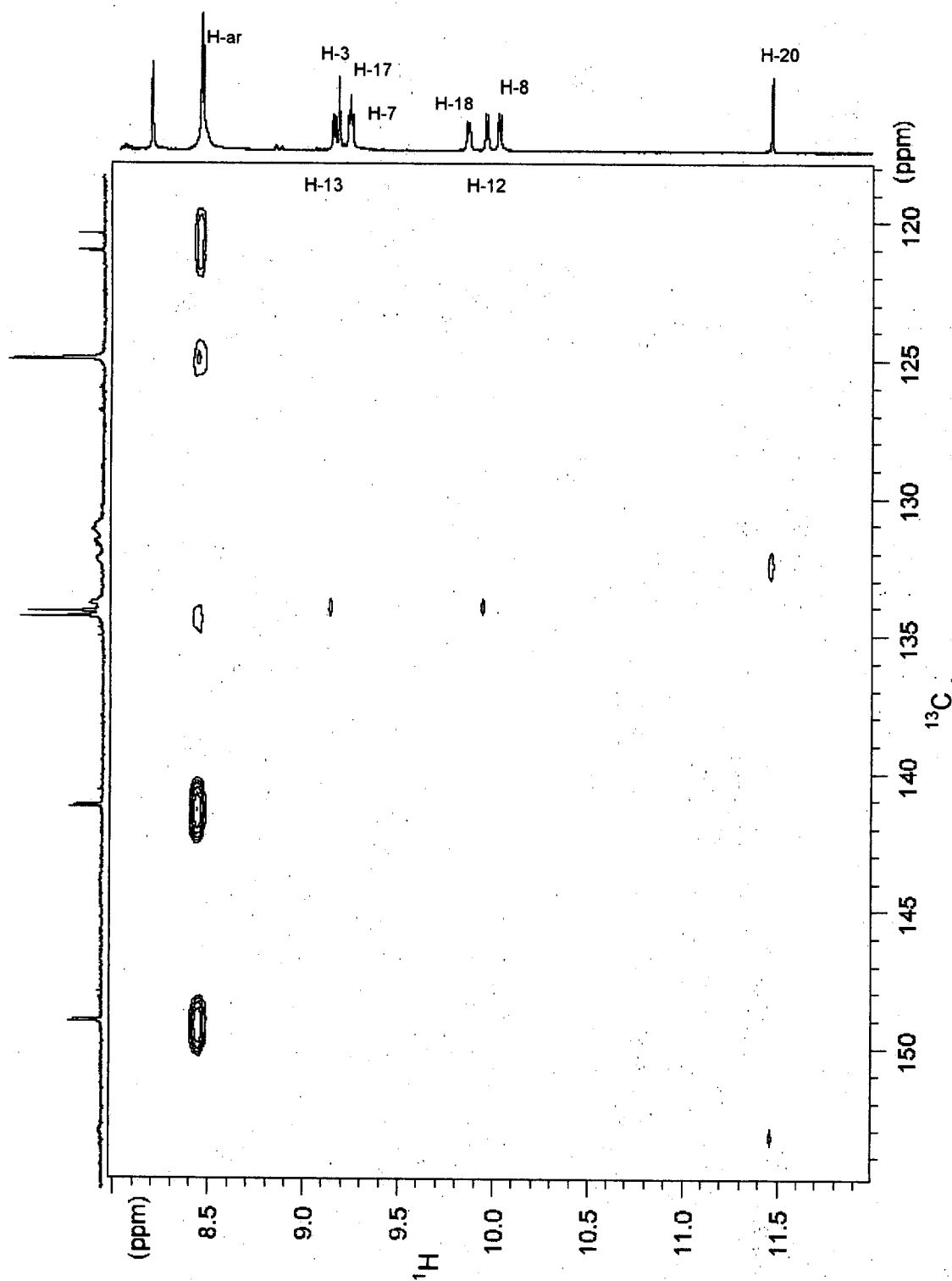


Figure S27. ^1H - ^{13}C HMBC (400 MHz) spectrum of **2** in DMF-d_7 at 298 K.