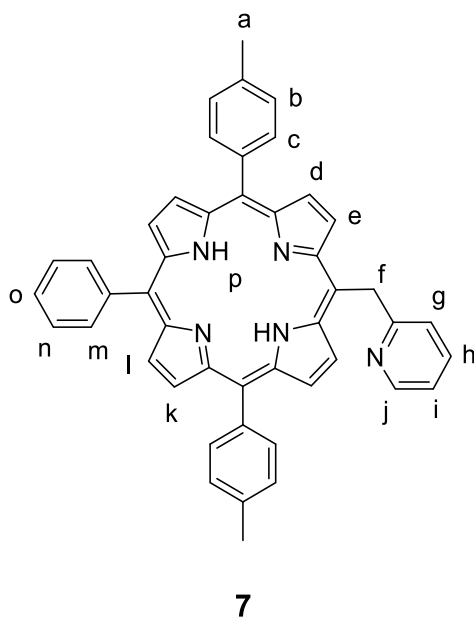


(Pyridin-2-ylmethyl)porphyrins: synthesis, characterization and C–N oxidative fusion attempts

Mathieu Berthelot^{Ⓢ, a}, Julie Echaubard^a, Asmae Bousfiha^a and Charles H. Devillers^{Ⓢ, *, a}

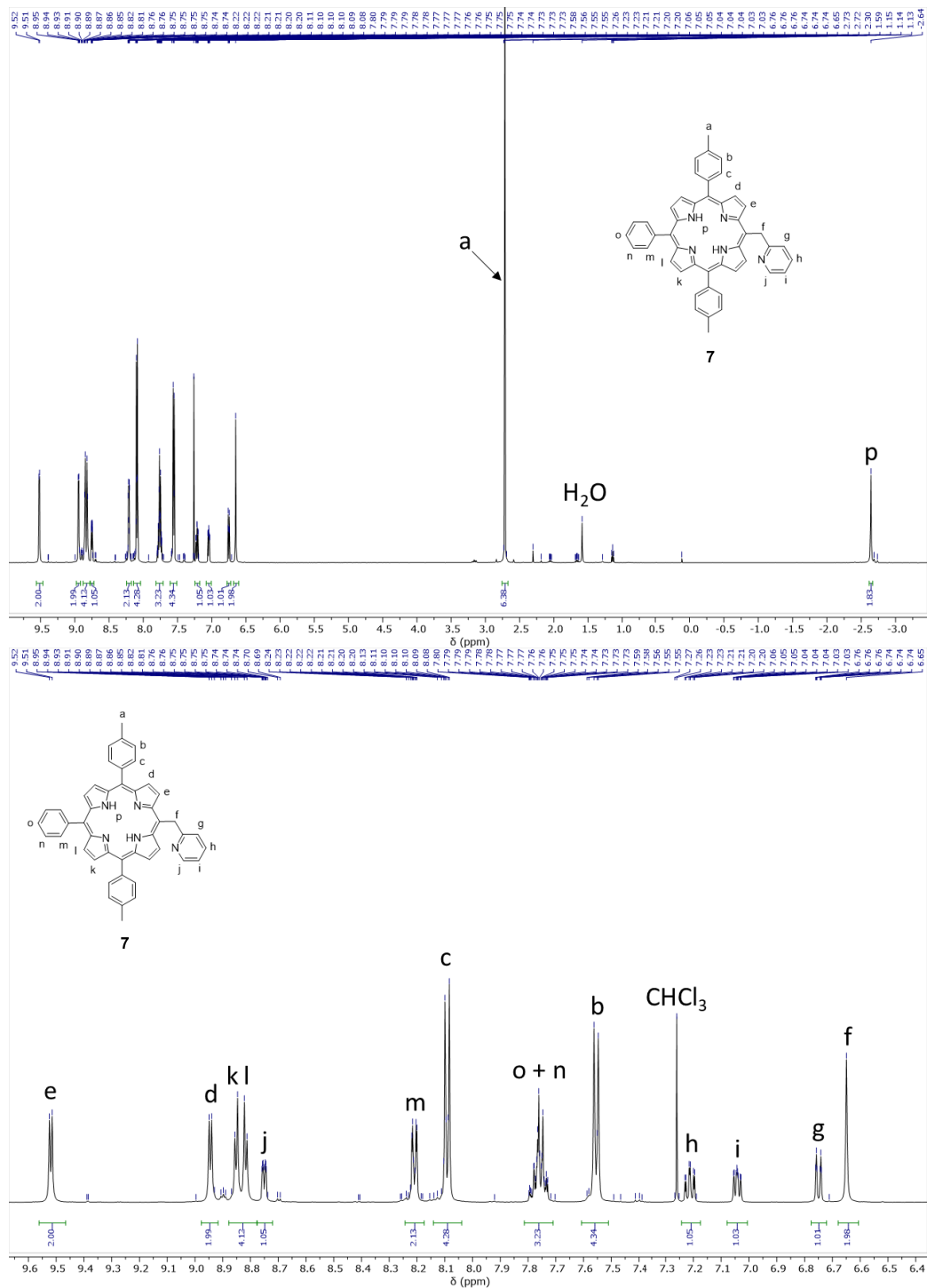
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Savary - BP 47870, 21078 DIJON Cedex, France
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1. Compound 7

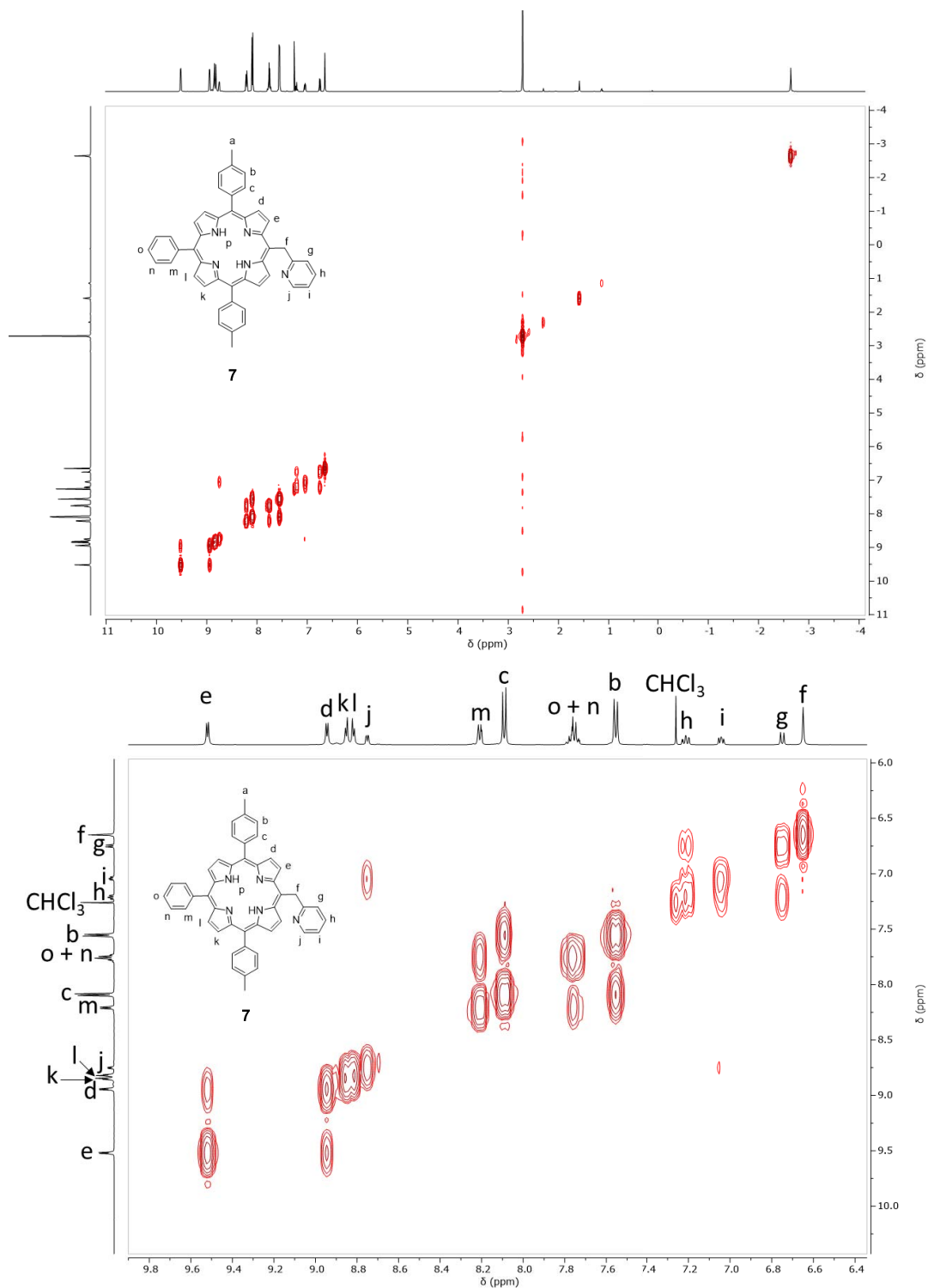


Chemical Formula: C₄₆H₃₅N₅
Exact Mass: 657.2892
Molecular Weight: 657.8210

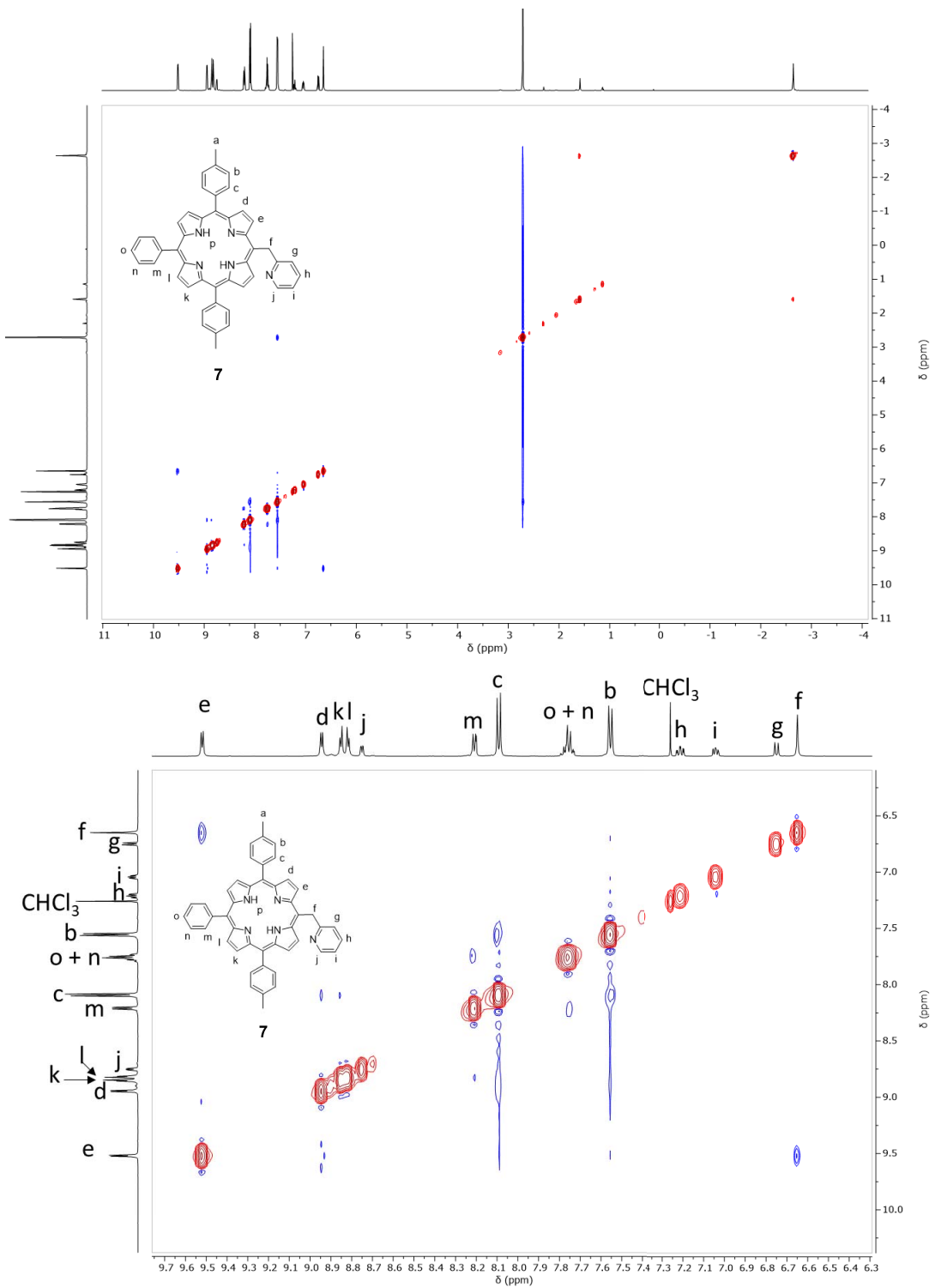
* Corresponding author.

1.1. NMR characterization of **7**

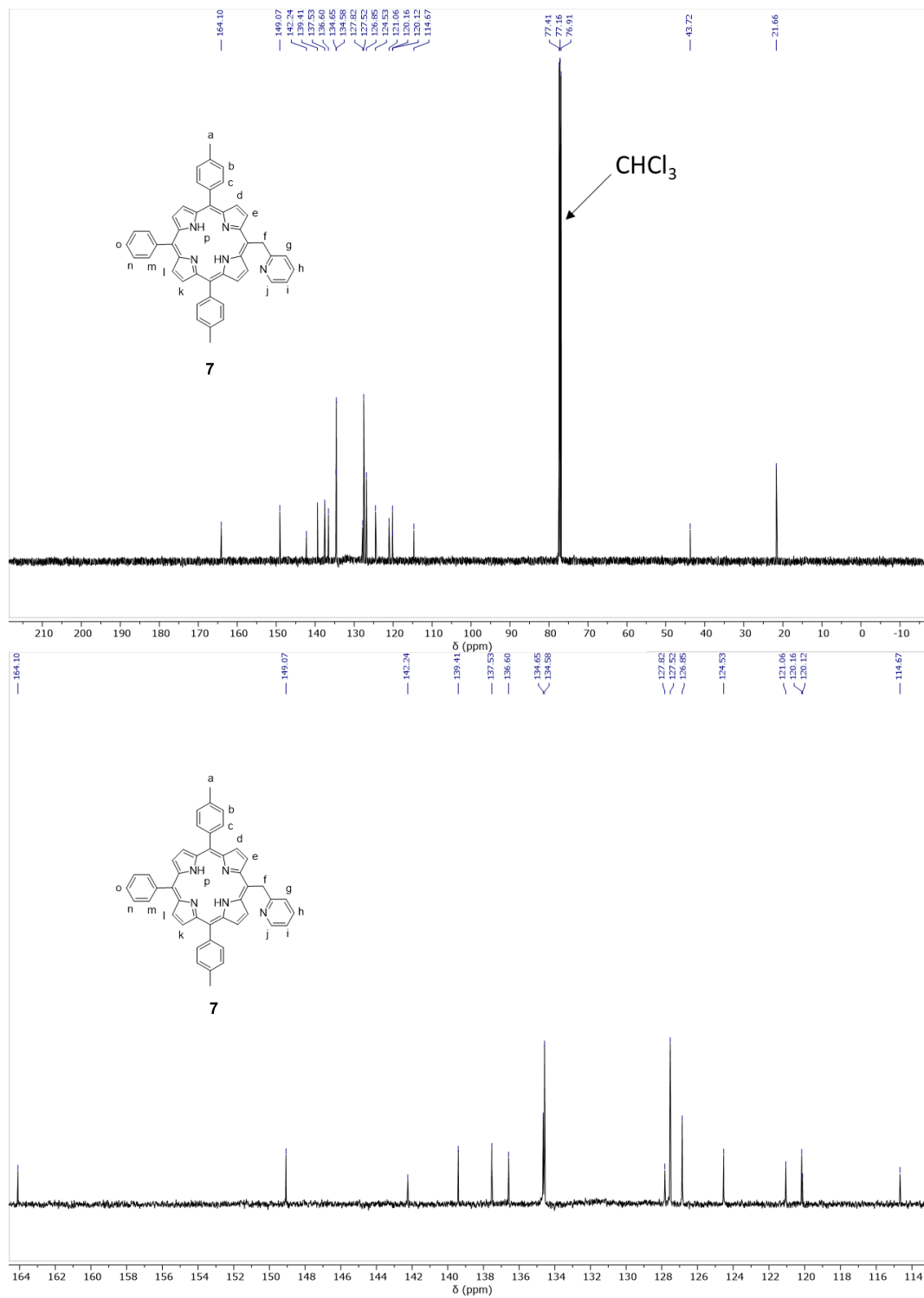
Supplementary Figure S1. Full range (top) and partial (bottom) ^1H NMR spectra of **7** in CDCl_3 , 500 MHz, 298 K.



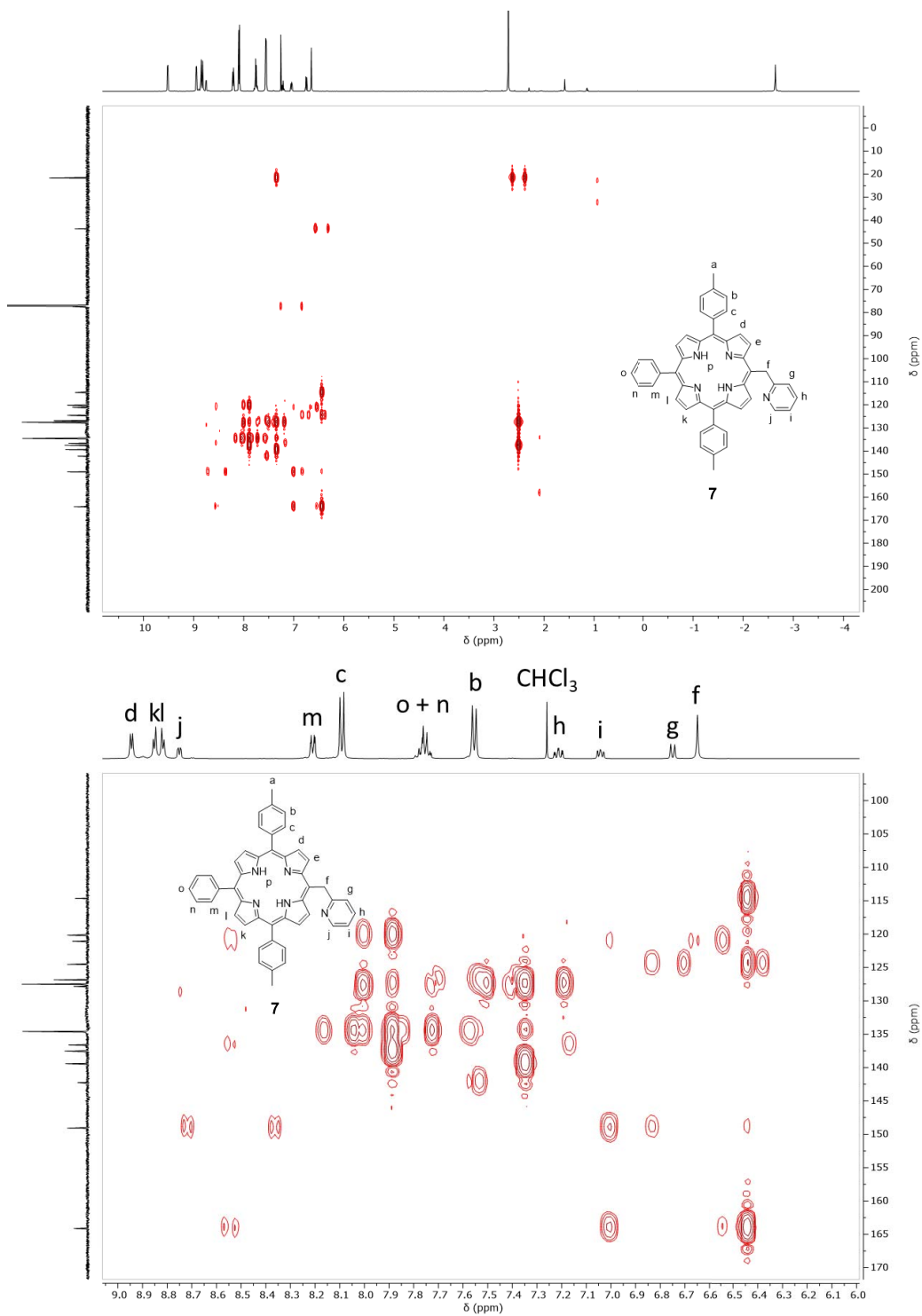
Supplementary Figure S2. Full range (top) and partial (bottom) ^1H - ^1H COSY NMR spectra of **7** in CDCl_3 500 MHz, 298 K.



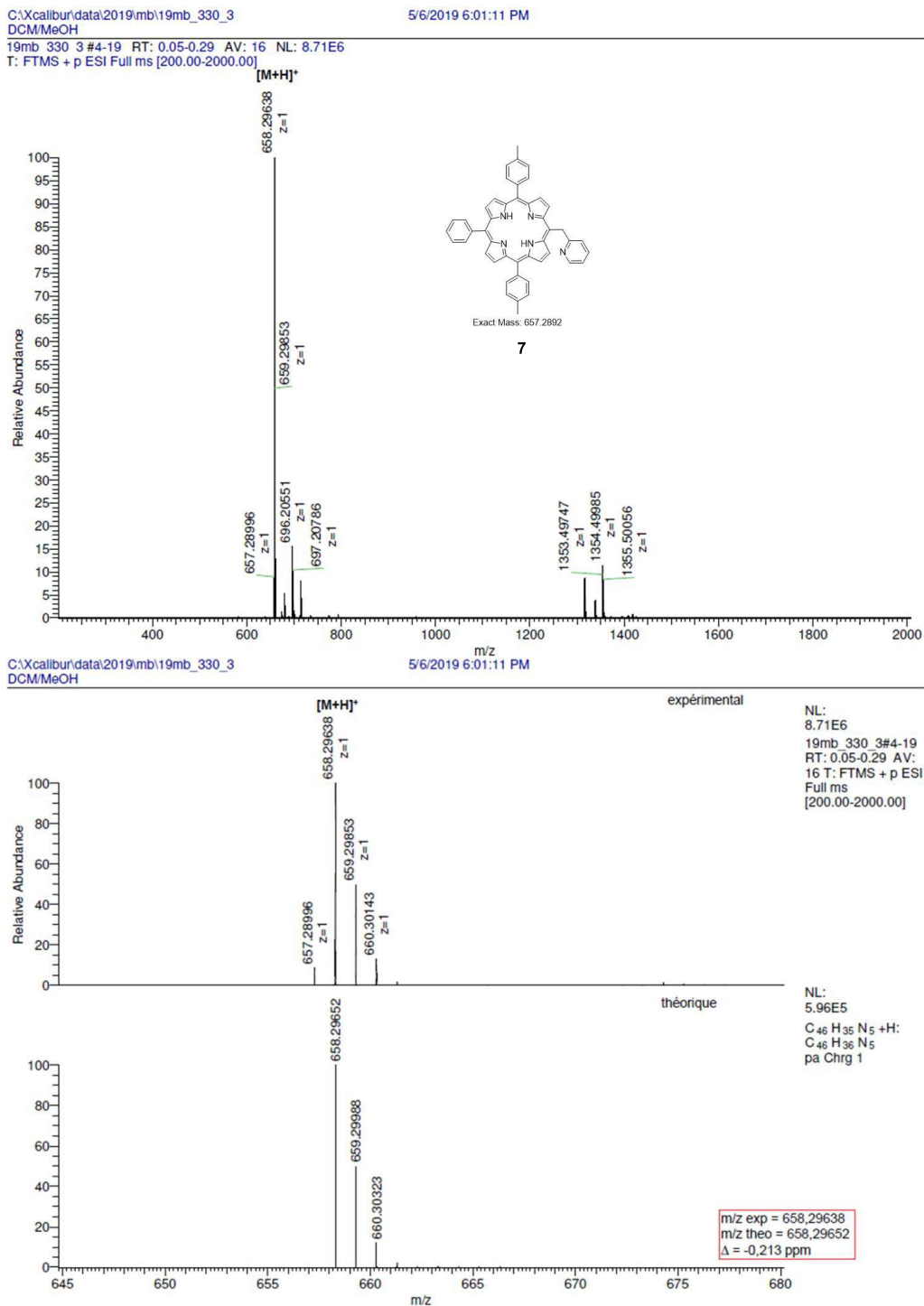
Supplementary Figure S3. Full range (top) and partial (bottom) ^1H - ^1H NOESY NMR spectra of **7** in CDCl_3 , 500 MHz, 298 K.

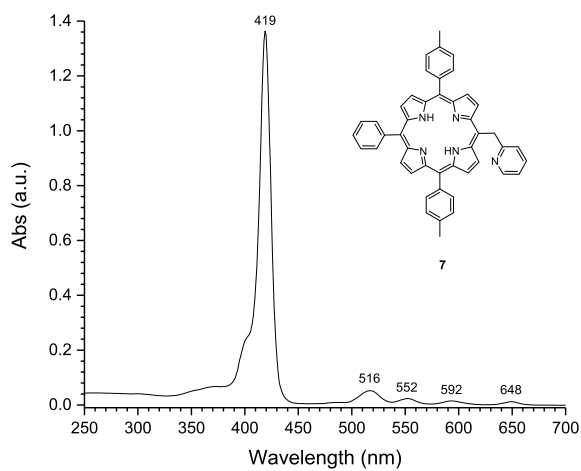


Supplementary Figure S4. Full range (top) and partial (bottom) $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of **7** in CDCl_3 , 126 MHz, 298 K.

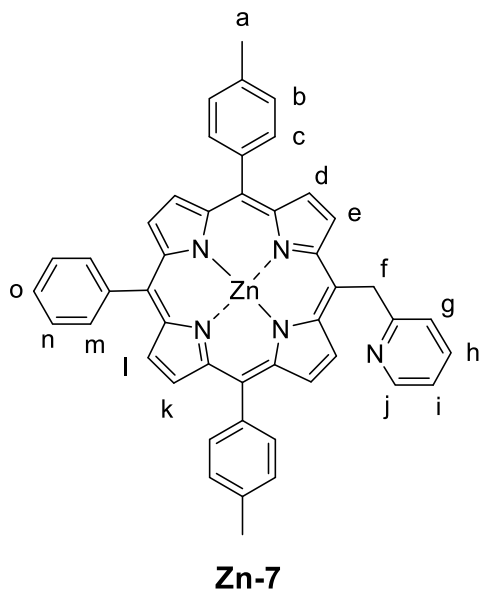


Supplementary Figure S5. Full range (top) and partial (bottom) ^1H - ^{13}C HMBC NMR spectra of **7** in CDCl_3 , 500 MHz, 298 K.

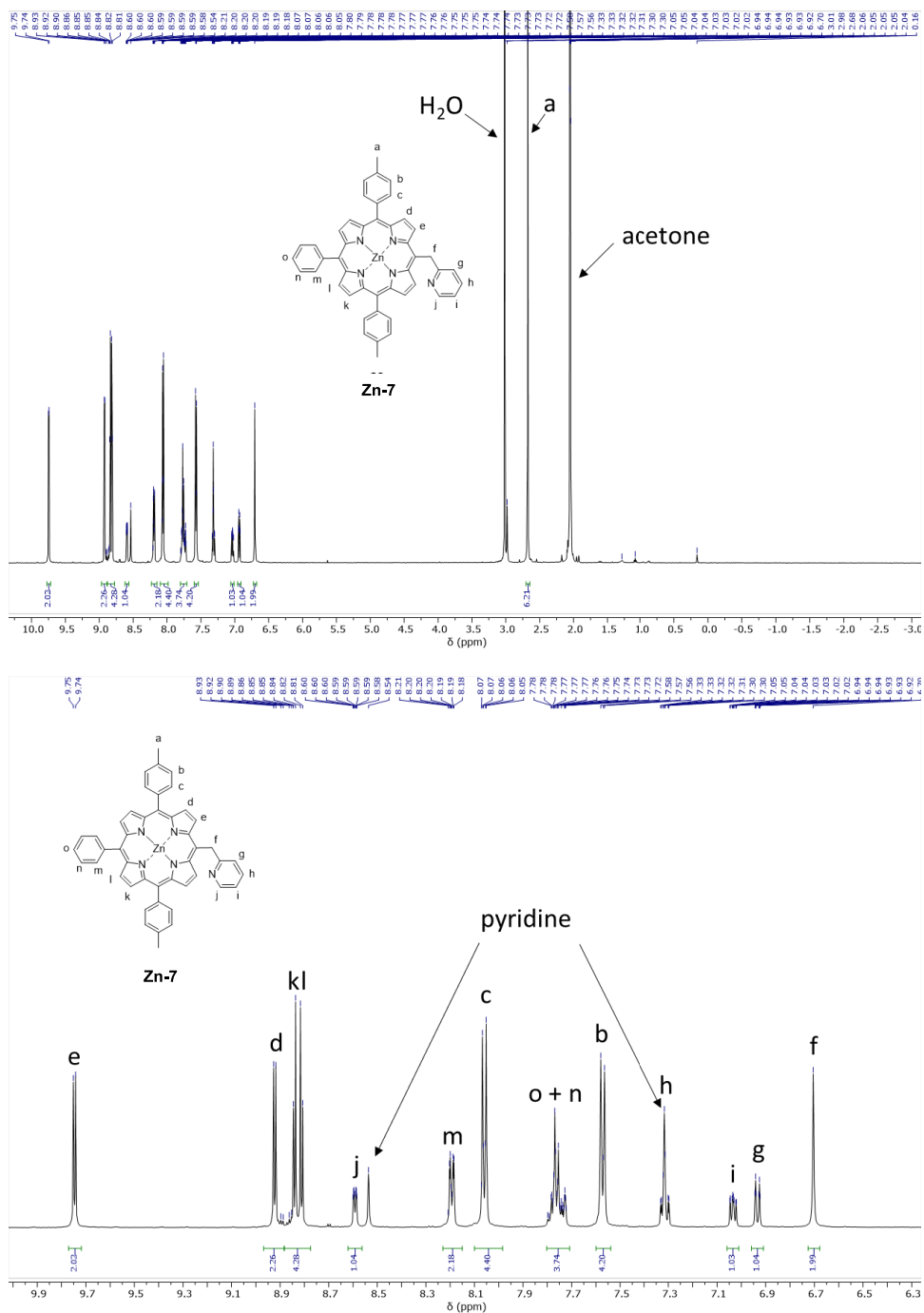
1.2. Mass spectrometry characterization of **7**Supplementary Figure S6. High resolution ESI mass spectrum of **7** and simulation of its isotopic pattern.

1.3. UV-visible absorption spectrum of **7****Supplementary Figure S7.** UV-Vis. absorption spectrum of **7** in CH_2Cl_2 .

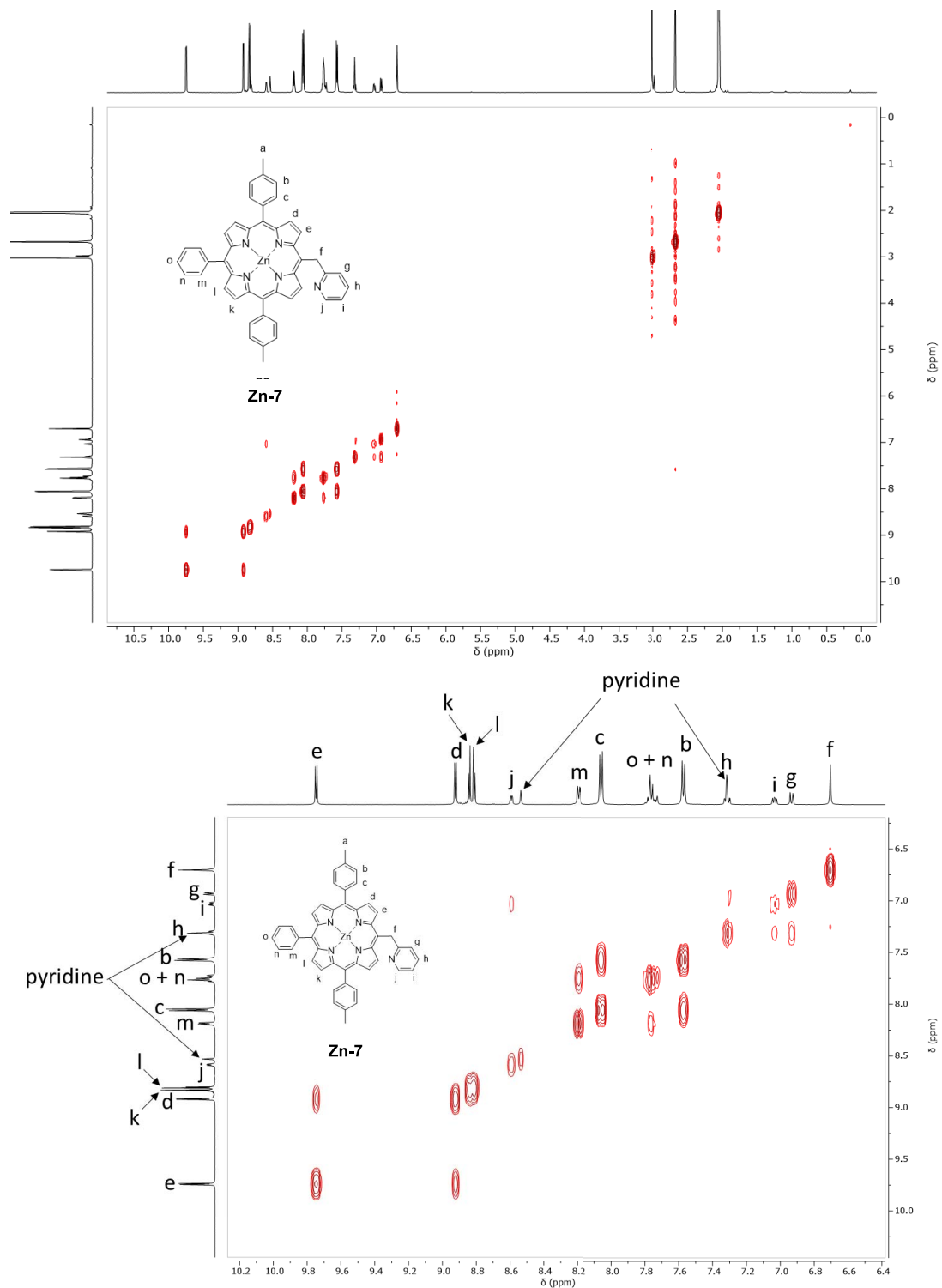
2. Compound Zn-7



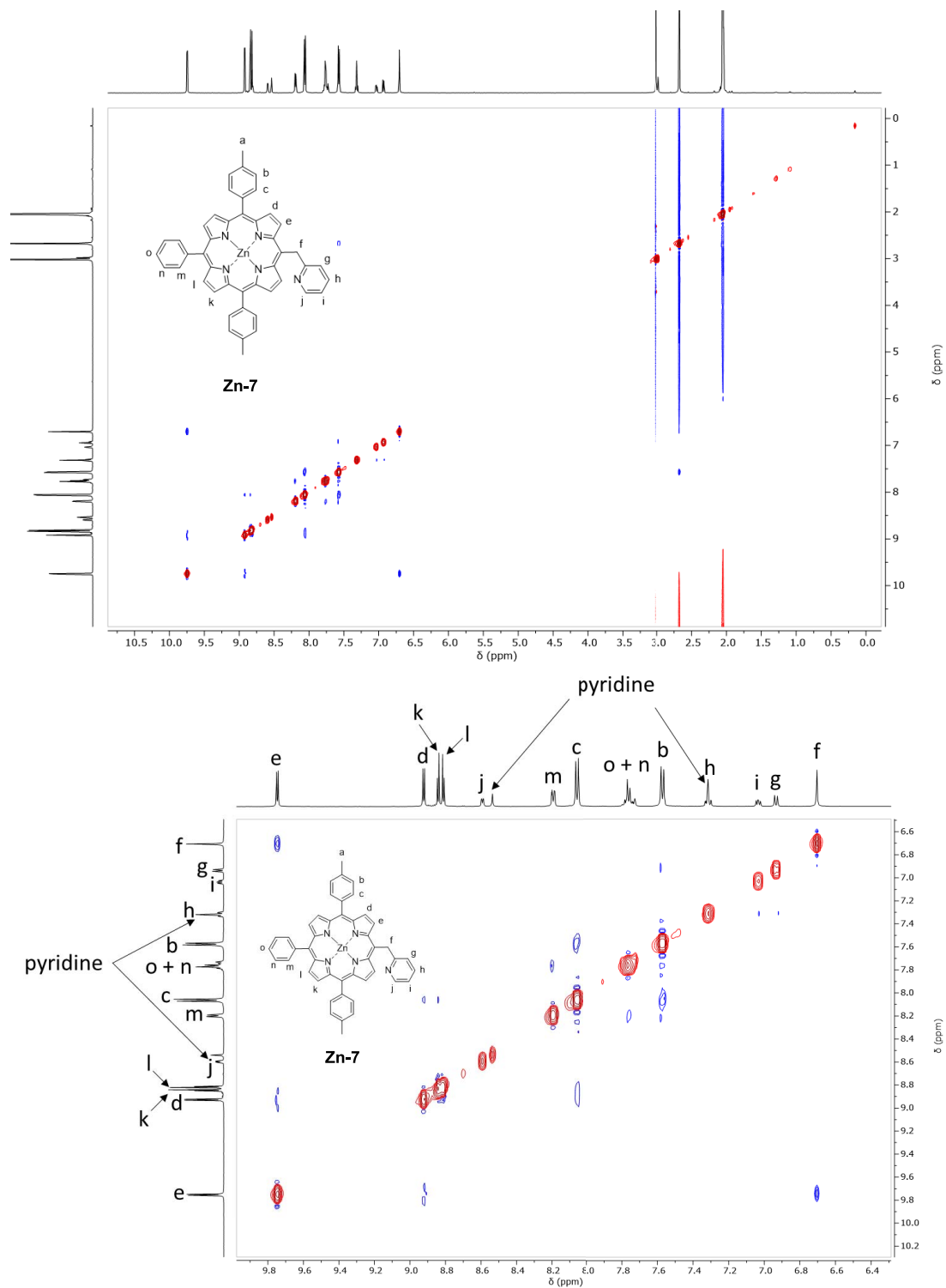
Chemical Formula: $\text{C}_{46}\text{H}_{33}\text{N}_5\text{Zn}$
Exact Mass: 719.2027
Molecular Weight: 721.1850

2.1. NMR characterization of **Zn-7**

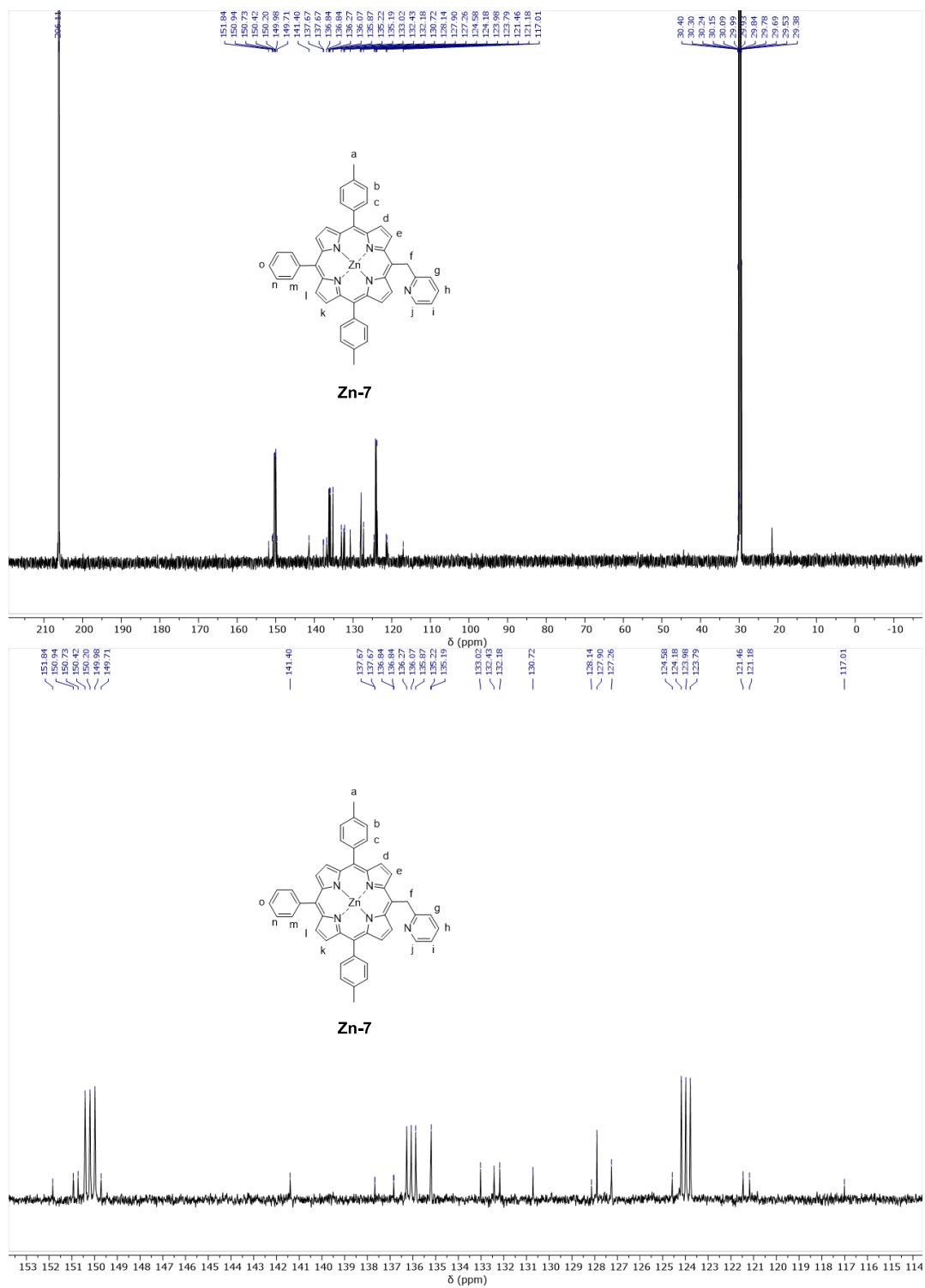
Supplementary Figure S8. Full range (top) and partial (bottom) ^1H NMR spectra of **Zn-7** in CD_3COCD_3 -pyridine- d_5 , 500 MHz, 298 K.



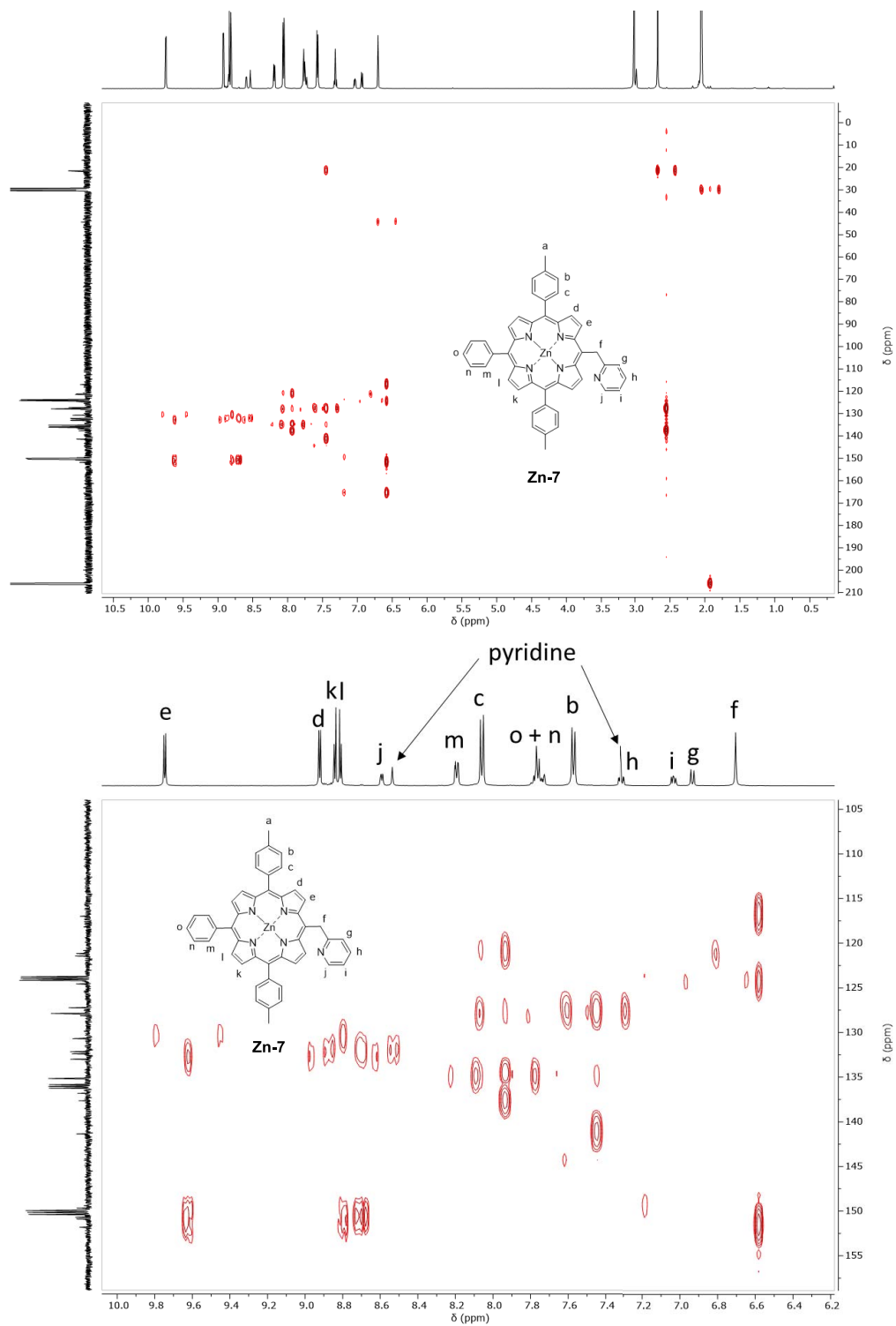
Supplementary Figure S9. Full range (top) and partial (bottom) ^1H - ^1H COSY NMR spectra of **Zn-7** in CD_3COCD_3 -pyridine- d_5 , 500 MHz, 298 K.



Supplementary Figure S10. Full range (top) and partial (bottom) ^1H - ^1H NOESY NMR spectra of **Zn-7** in CD_3COCD_3 -pyridine- d_5 , 500 MHz, 298 K.

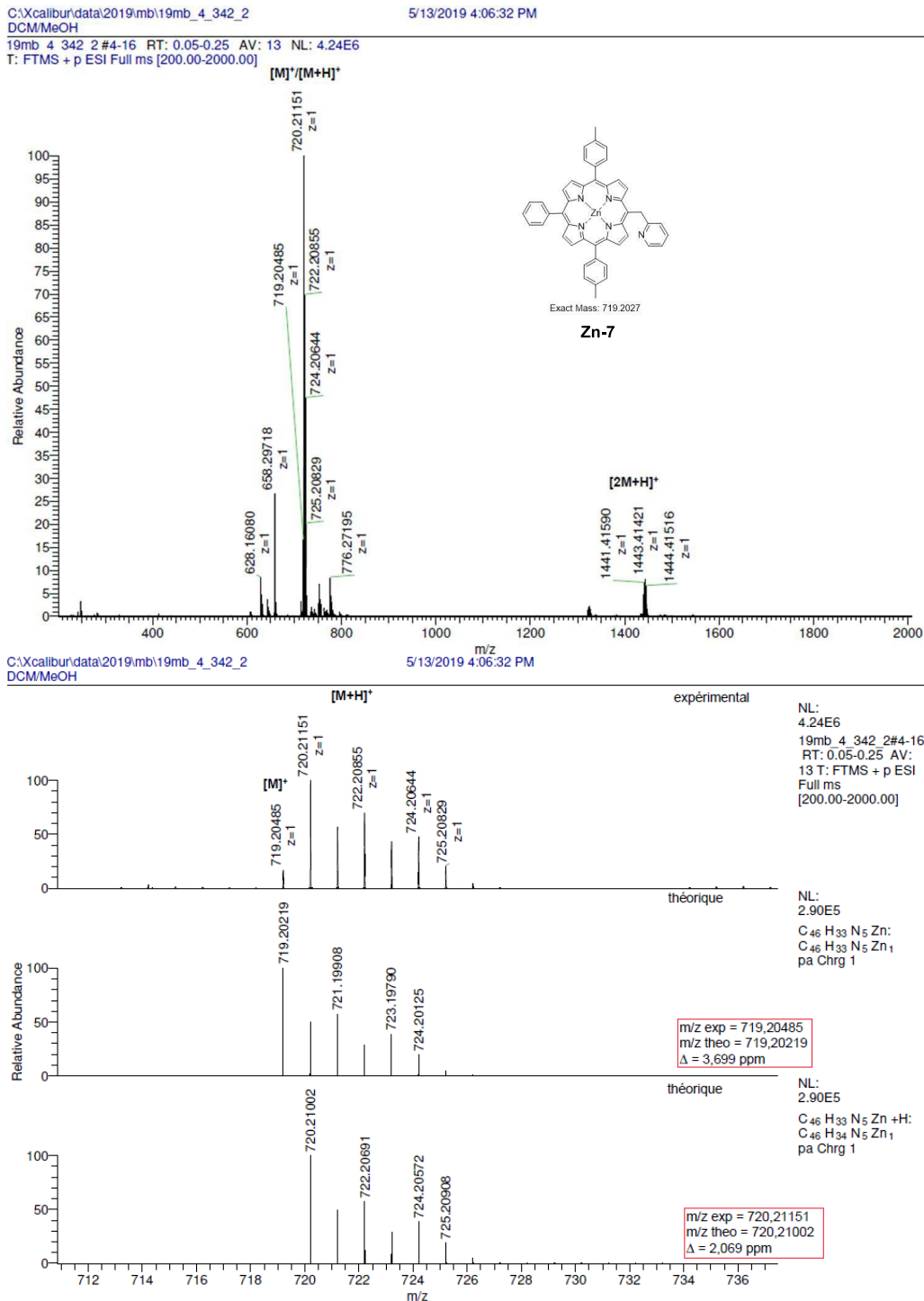


Supplementary Figure S11. Full range (top) and partial (bottom) $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of Zn-7 in CD_3COCD_3 -pyridine- d_5 , 126 MHz, 298 K.



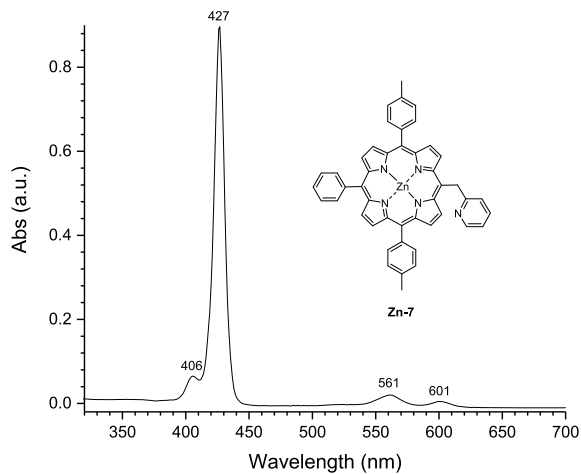
Supplementary Figure S12. Full range (top) and partial (bottom) ^1H - ^{13}C HMBC NMR spectra of **Zn-7** in CD_3COCD_3 -pyridine- d_5 , 500 MHz, 298 K.

2.2. Mass spectrometry characterization



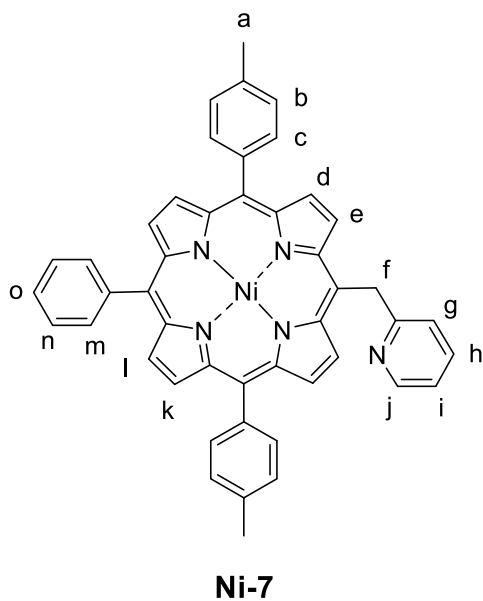
Supplementary Figure S13. High resolution ESI mass spectrum of **Zn-7** and simulation of its isotopic pattern.

2.3. UV-visible absorption spectra of **Zn-7**



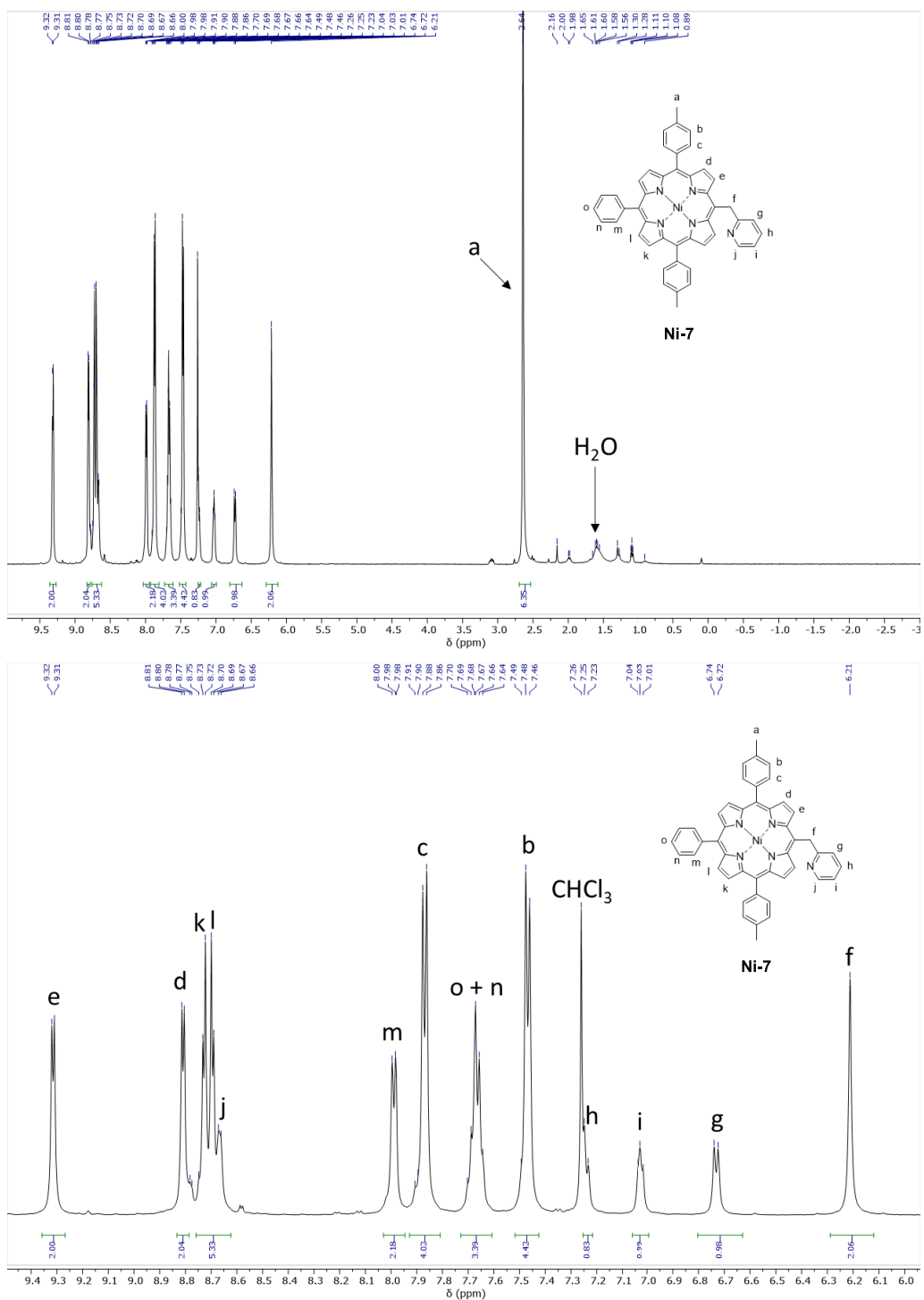
Supplementary Figure S14. UV-Vis. absorption spectrum of **Zn-7** in DME.

3. Compound **Ni-7**

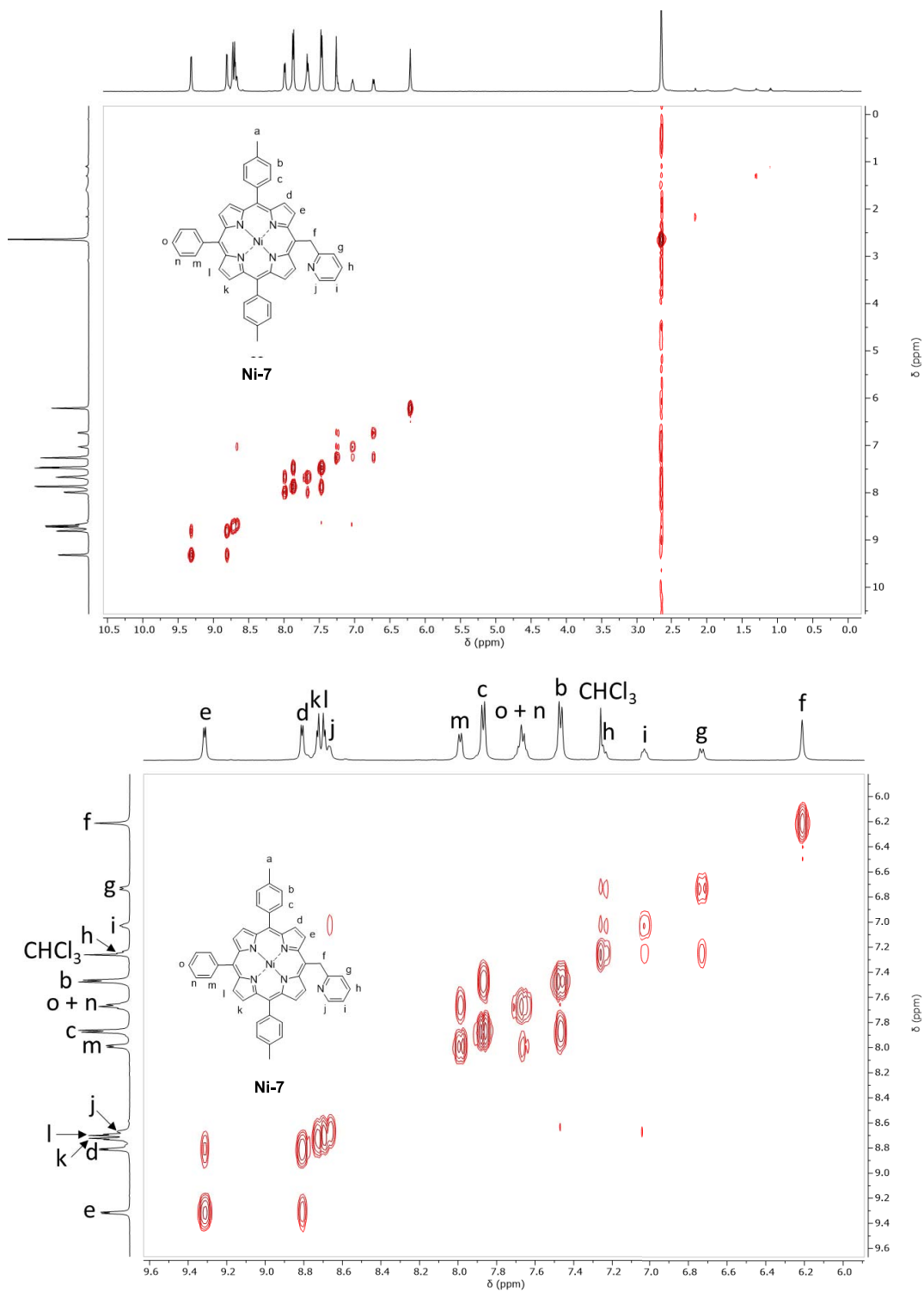


Chemical Formula: $C_{46}H_{33}N_5Ni$
Exact Mass: 713.2089
Molecular Weight: 714.4984

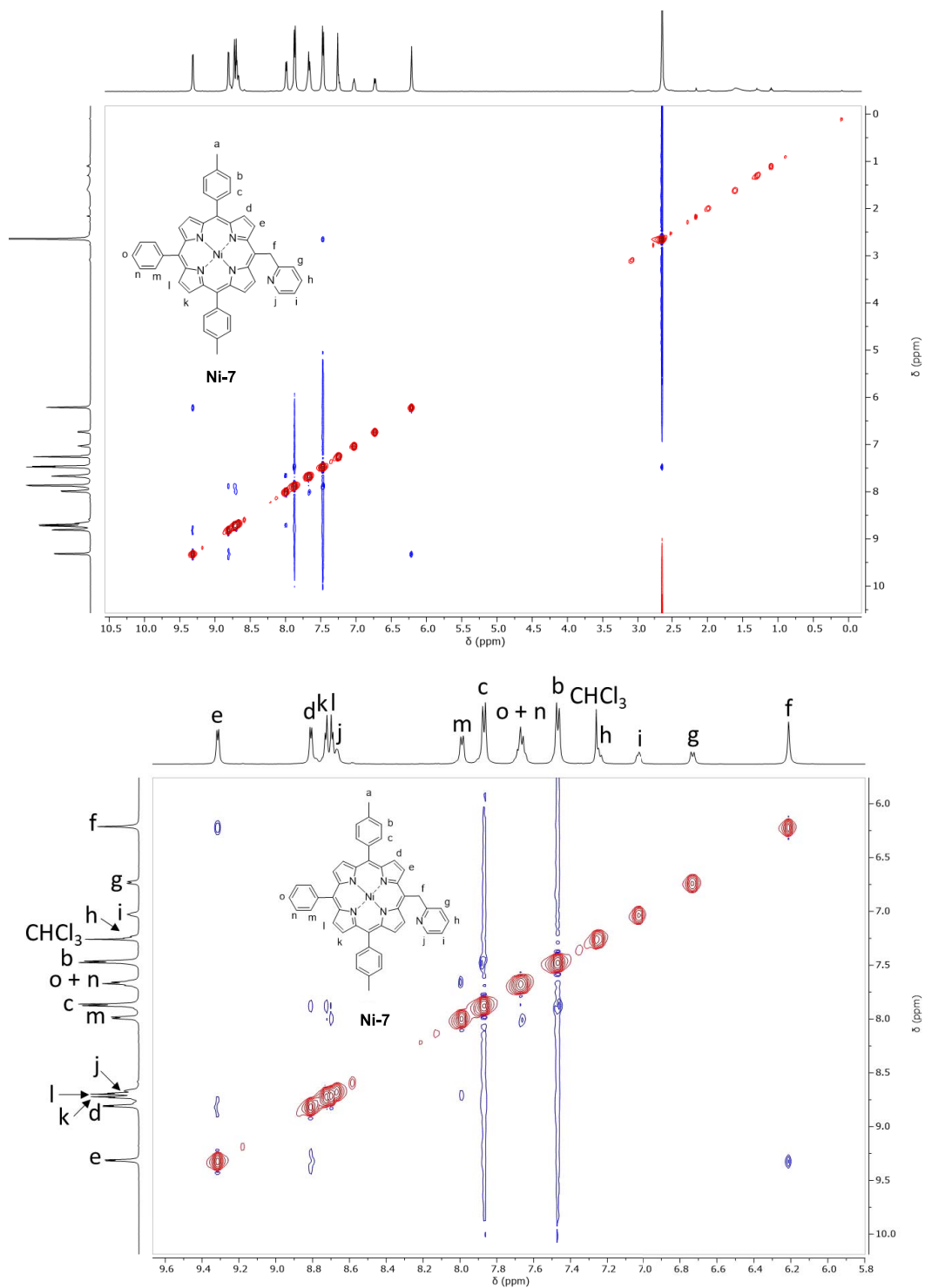
3.1. NMR characterization of Ni-7



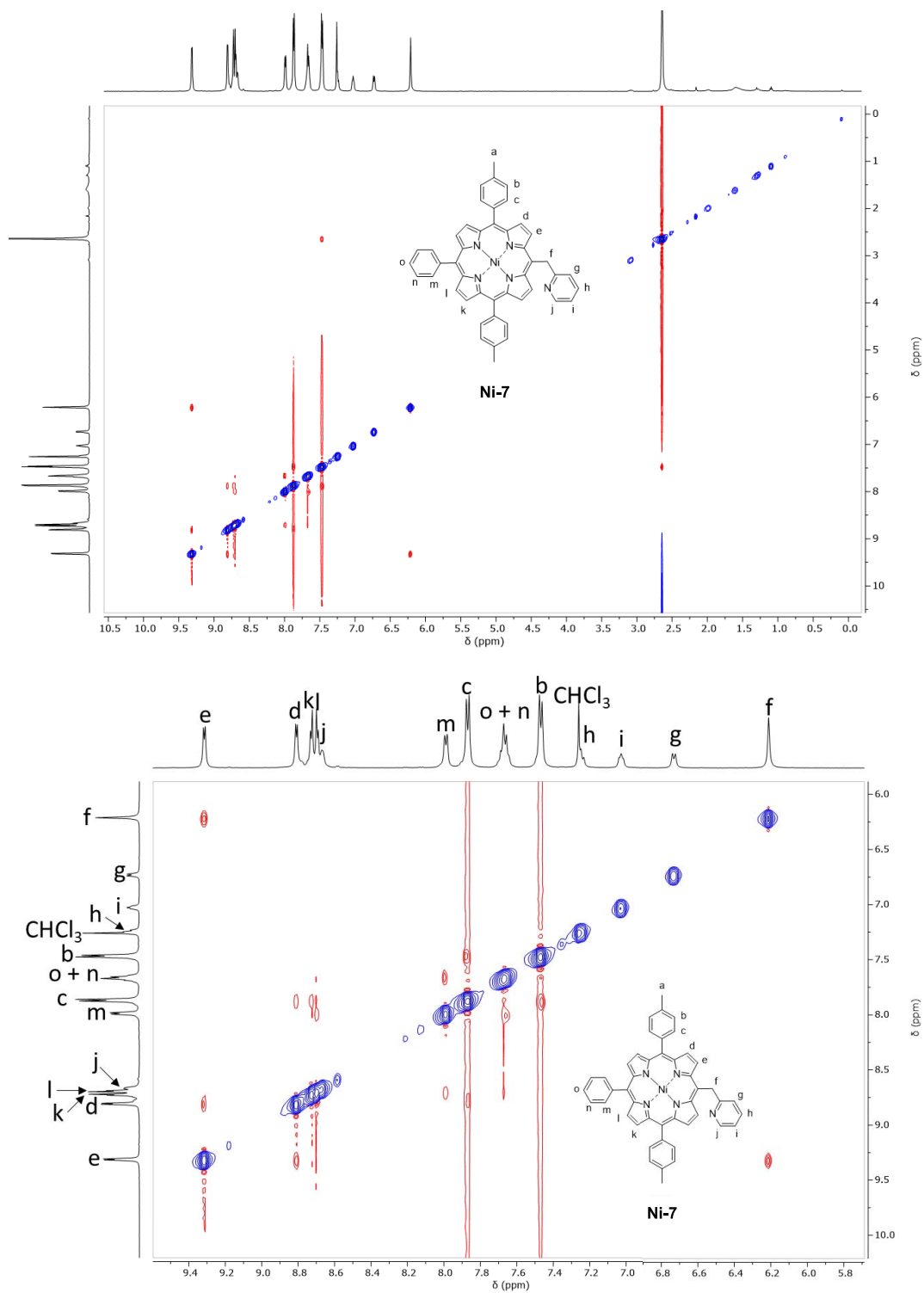
Supplementary Figure S15. Full range (top) and partial (bottom) ¹H NMR spectra of Ni-7 in CDCl₃, 500 MHz, 298 K.



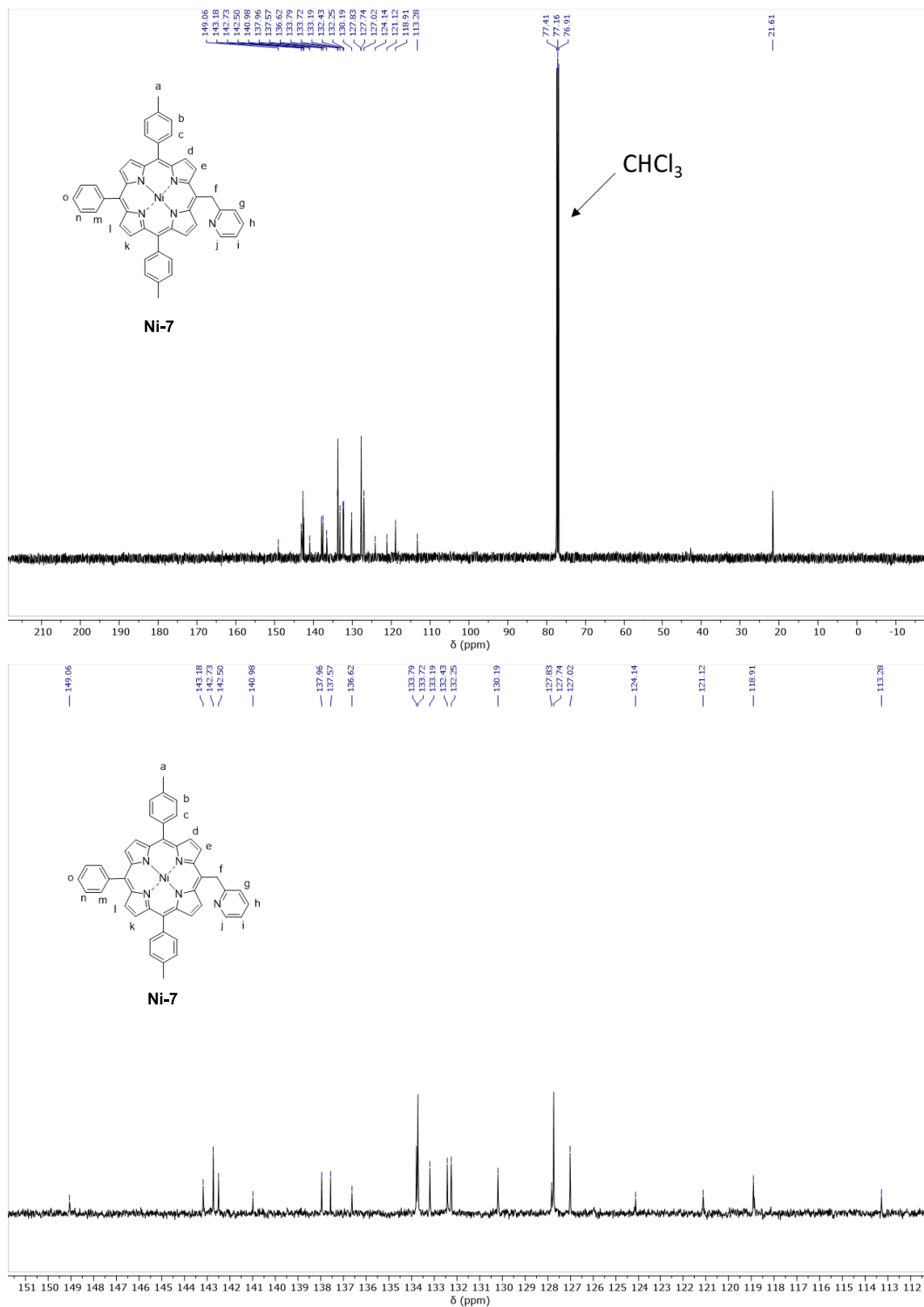
Supplementary Figure S16. Full range (top) and partial (bottom) ^1H - ^1H COSY NMR spectra of **Ni-7** in CDCl_3 , 500 MHz, 298 K.



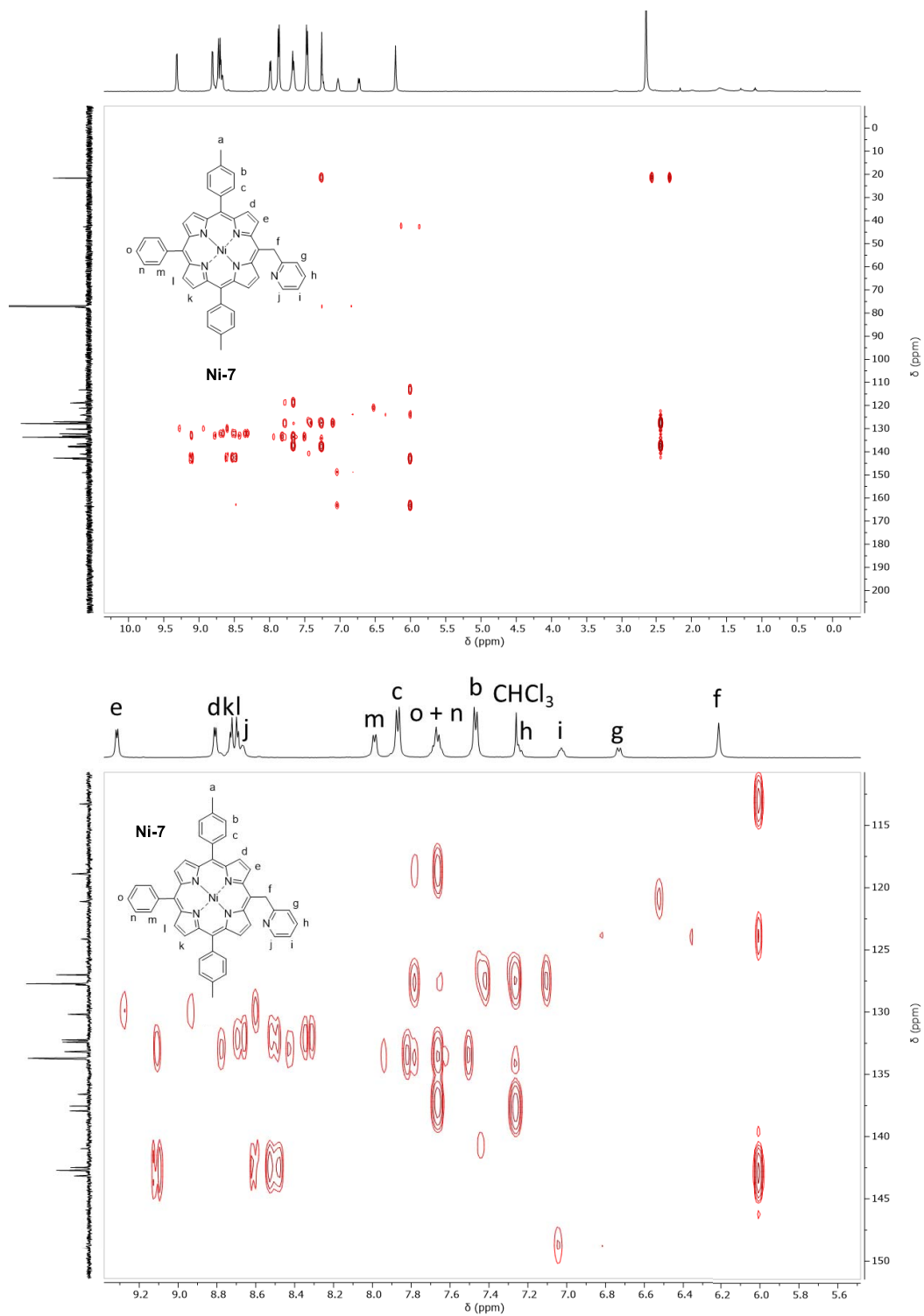
Supplementary Figure S17. Full range (top) and partial (bottom) ^1H - ^1H NOESY NMR spectra of Ni-7 in CDCl_3 , 500 MHz, 298 K.



Supplementary Figure S18. Full range (top) and partial (bottom) ^1H - ^1H ROESY NMR spectra of **Ni-7** in CDCl_3 , 500 MHz, 298 K.

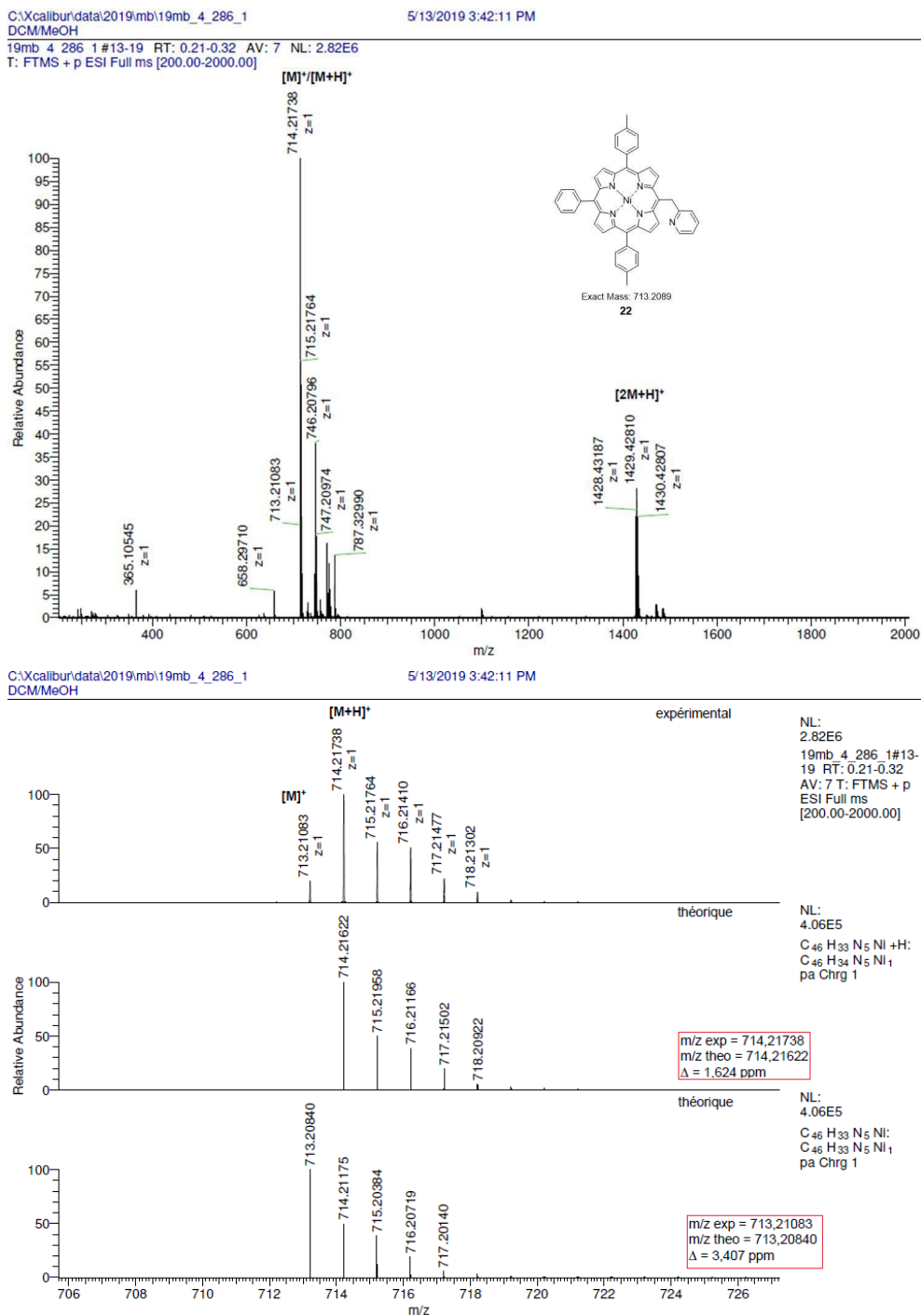


Supplementary Figure S19. Full range (top) and partial (bottom) $^{13}\text{C}\{^1\text{H}\}$ NMR spectra of Ni-7 in CDCl_3 , 126 MHz, 298 K.



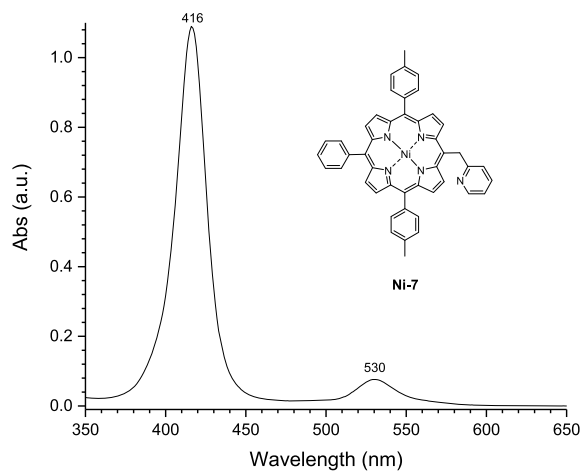
Supplementary Figure S20. Full range (top) and partial (bottom) ¹H-¹³C HMBC NMR spectra of Ni-7 in CDCl₃, 500 MHz, 298 K.

3.2. Mass spectrometry characterization of Ni-7



Supplementary Figure S21. High resolution ESI mass spectrum of Ni-7 and simulation of its isotopic pattern.

3.3. UV-vis absorption spectrum of Ni-7



Supplementary Figure S22. UV-Vis. absorption spectrum of Ni-7 in CH_2Cl_2 .