Electronic Supplementary Information for Dalton Transactions

OCHTAHEDRAL IRON (II) PHTHALOCYANINE COMPLEXES: MULTINUCLEAR NMR AND RELEVANCE AS NO_2 CHEMICAL SENSORS

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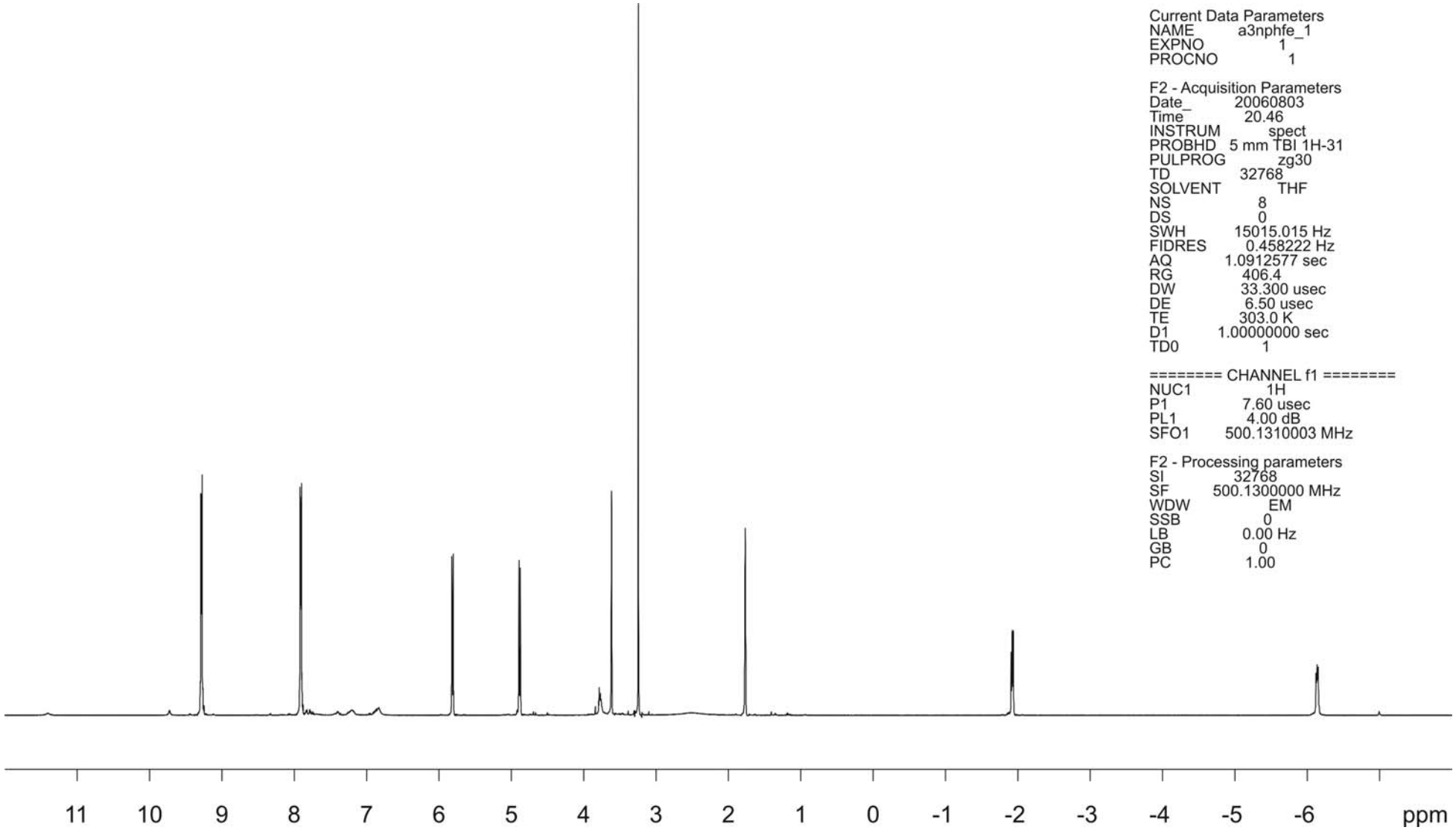

Figure 1. ^{1}H NMR (500.13 MHz) spectrum of **4** in THF-d_8.

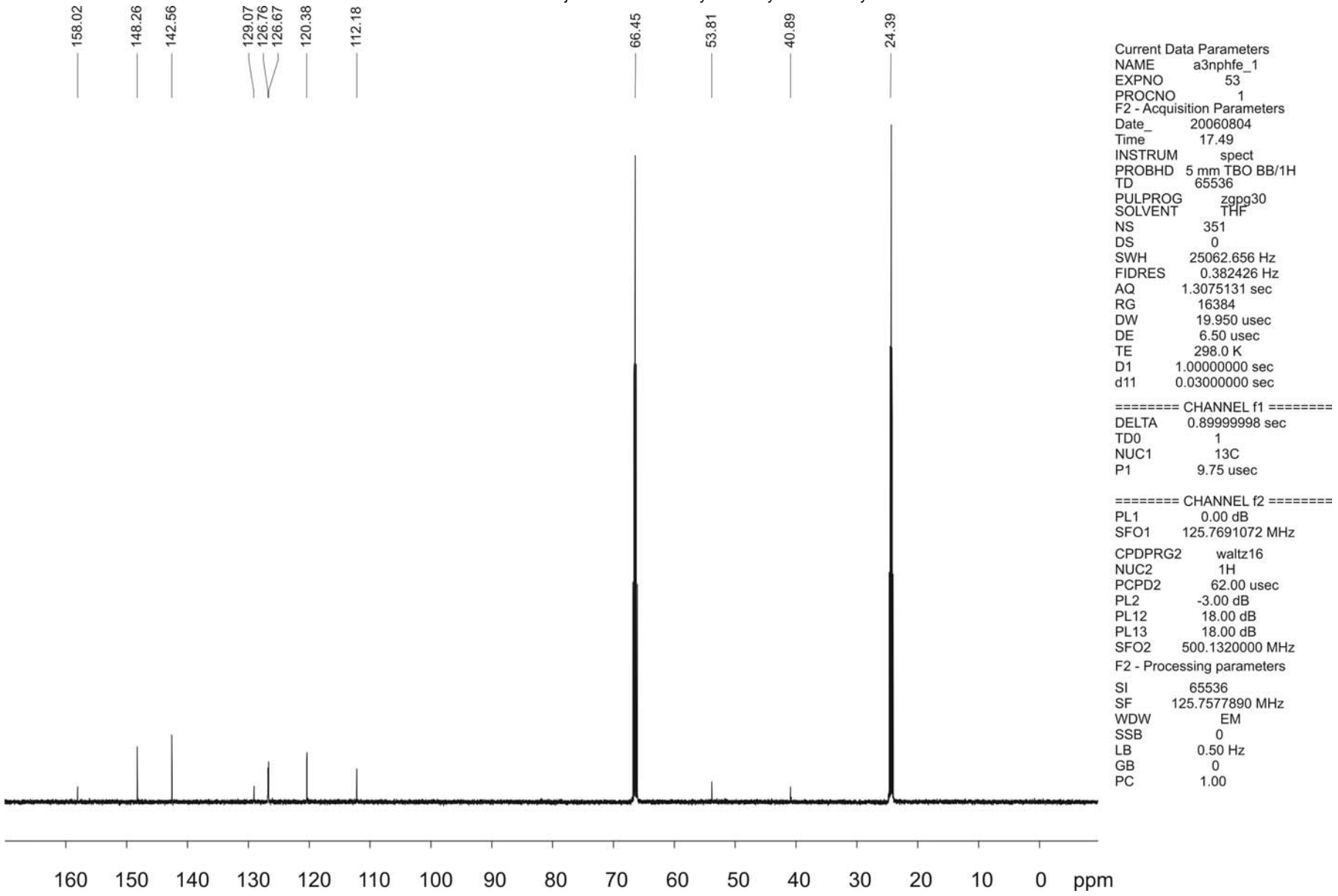

Figure 2. ^{13}C NMR (125.7 MHz) spectrum of **4** in THF-d_8.

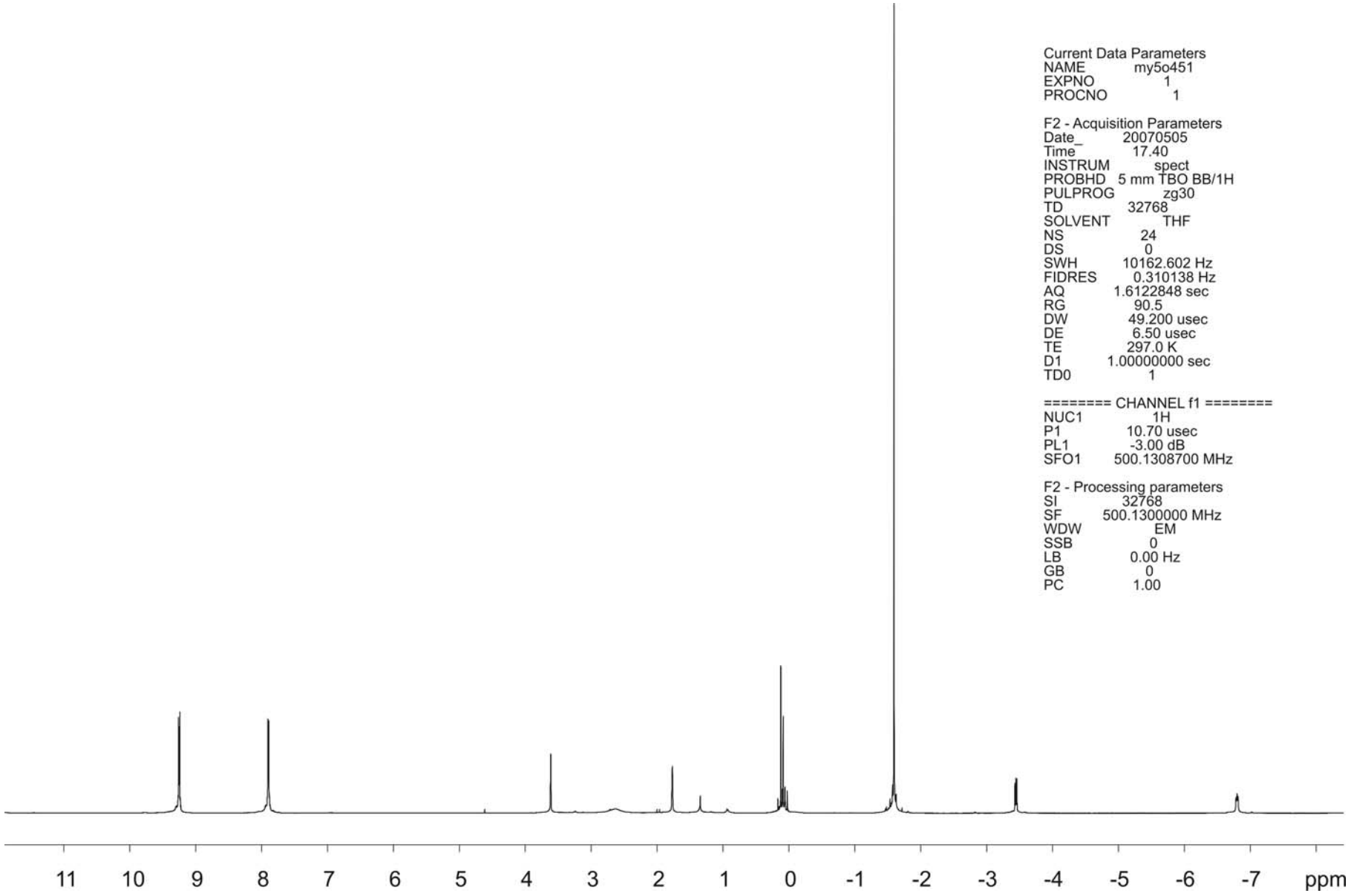

Figure 3. ^{1}H NMR (500.13 MHz) spectrum of **5** in THF-d_8.

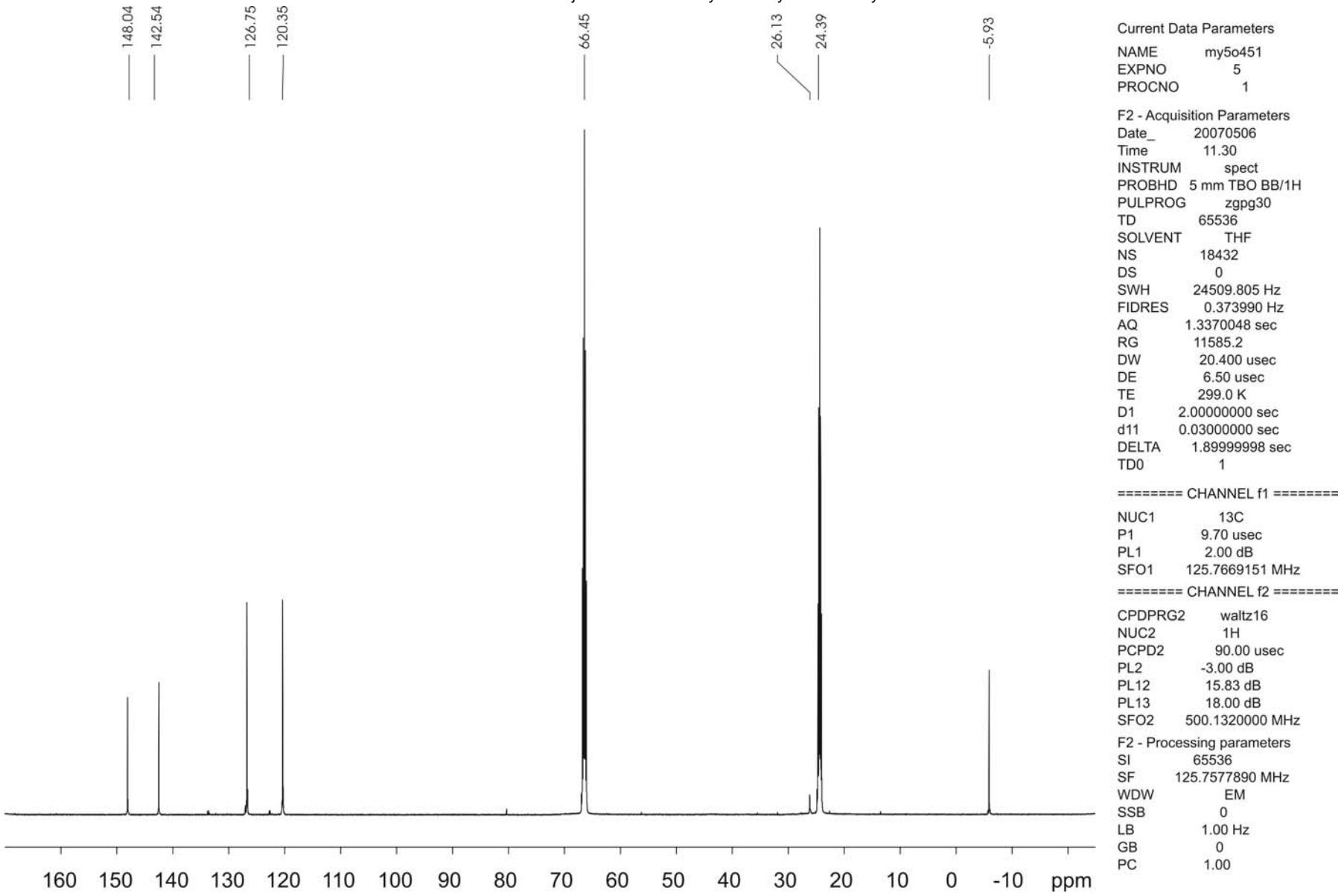

Figure 4. ^{13}C NMR (125.7 MHz) spectrum of **5** in THF-d_8.

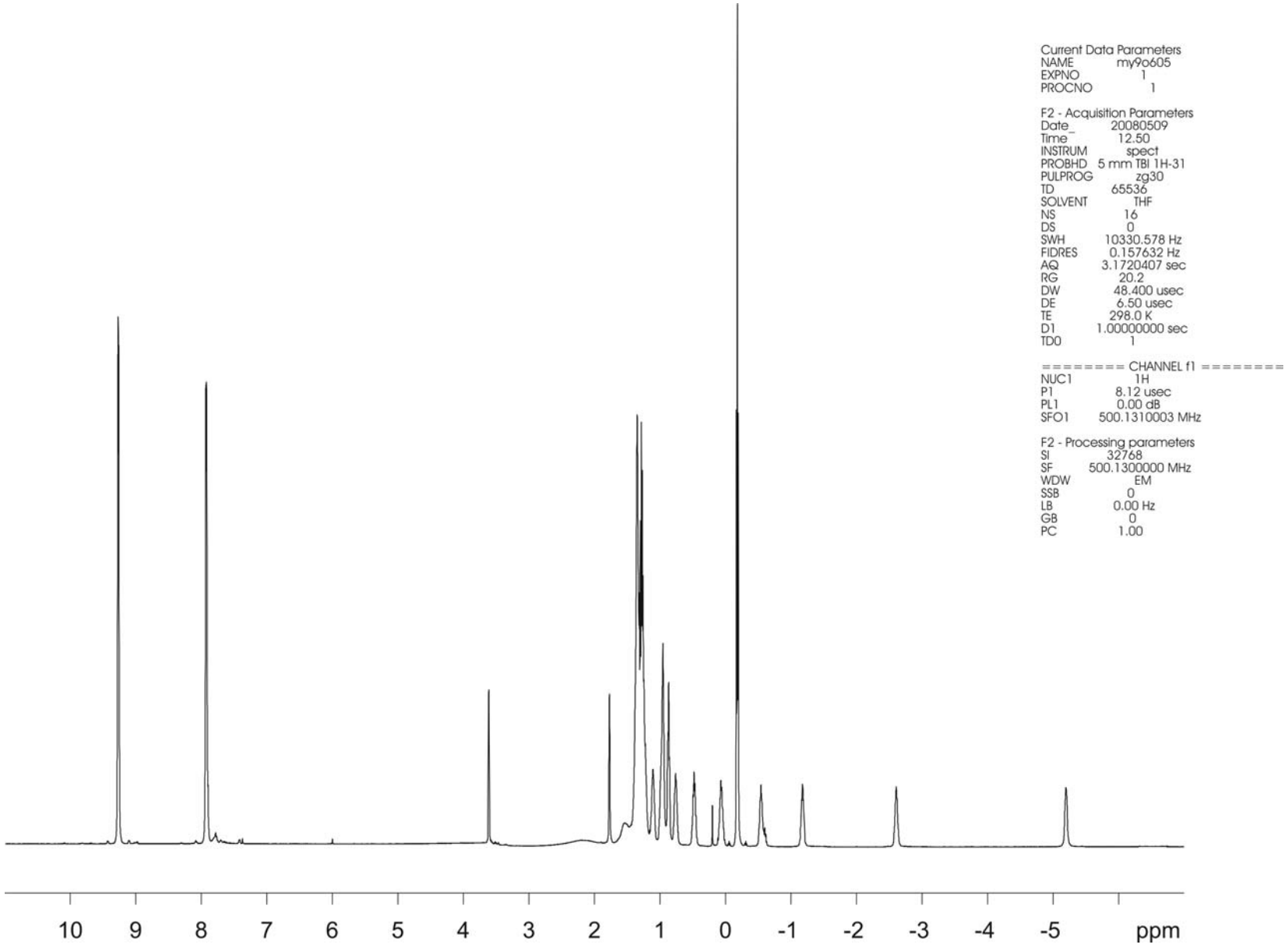

Figure 5. ^{1}H NMR (500.13 MHz) spectrum of **6** in THF-d_8.

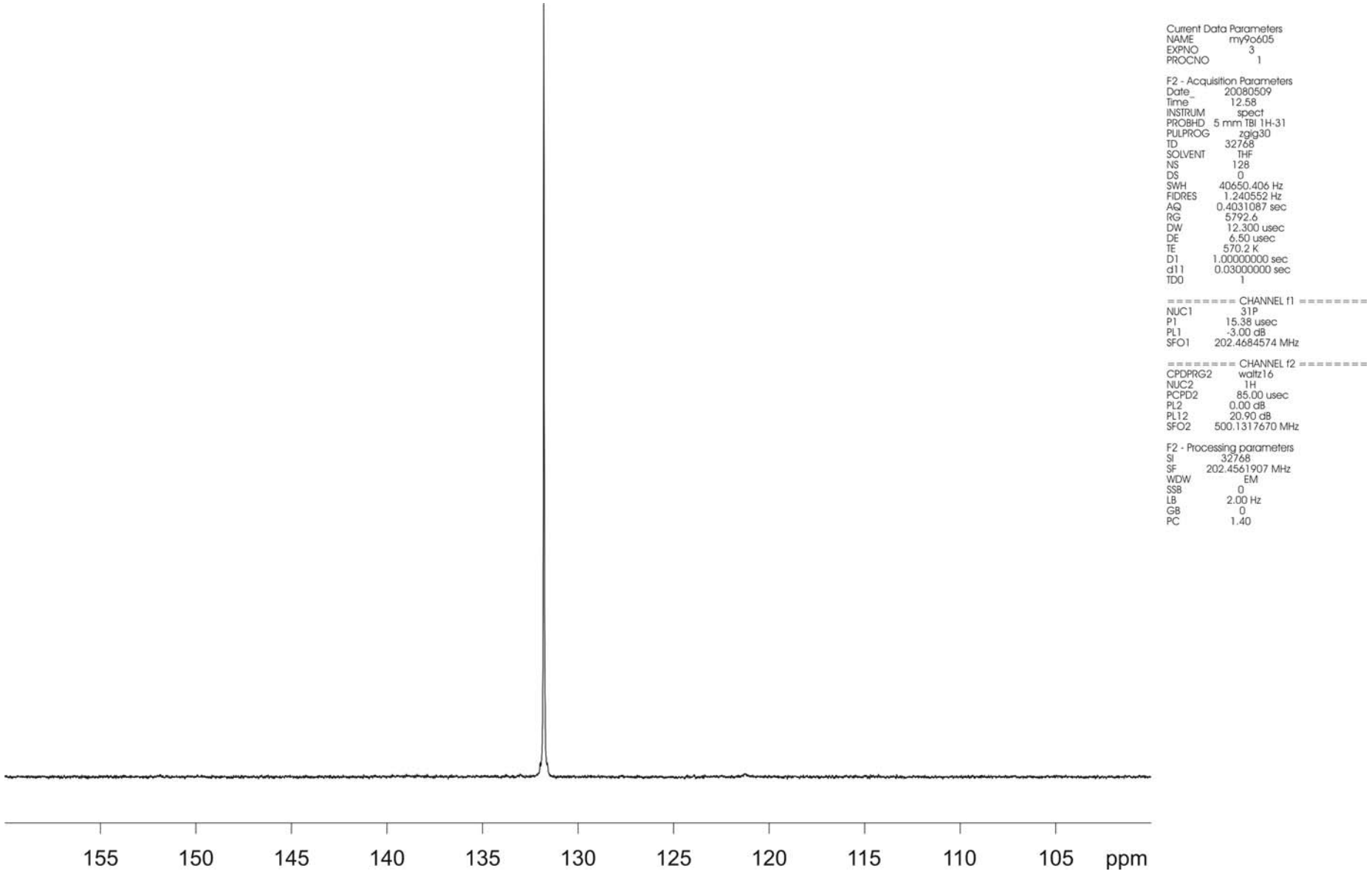

Figure 6. ^{31}P NMR (202.4 MHz) spectrum of **6** in THF-d_8.

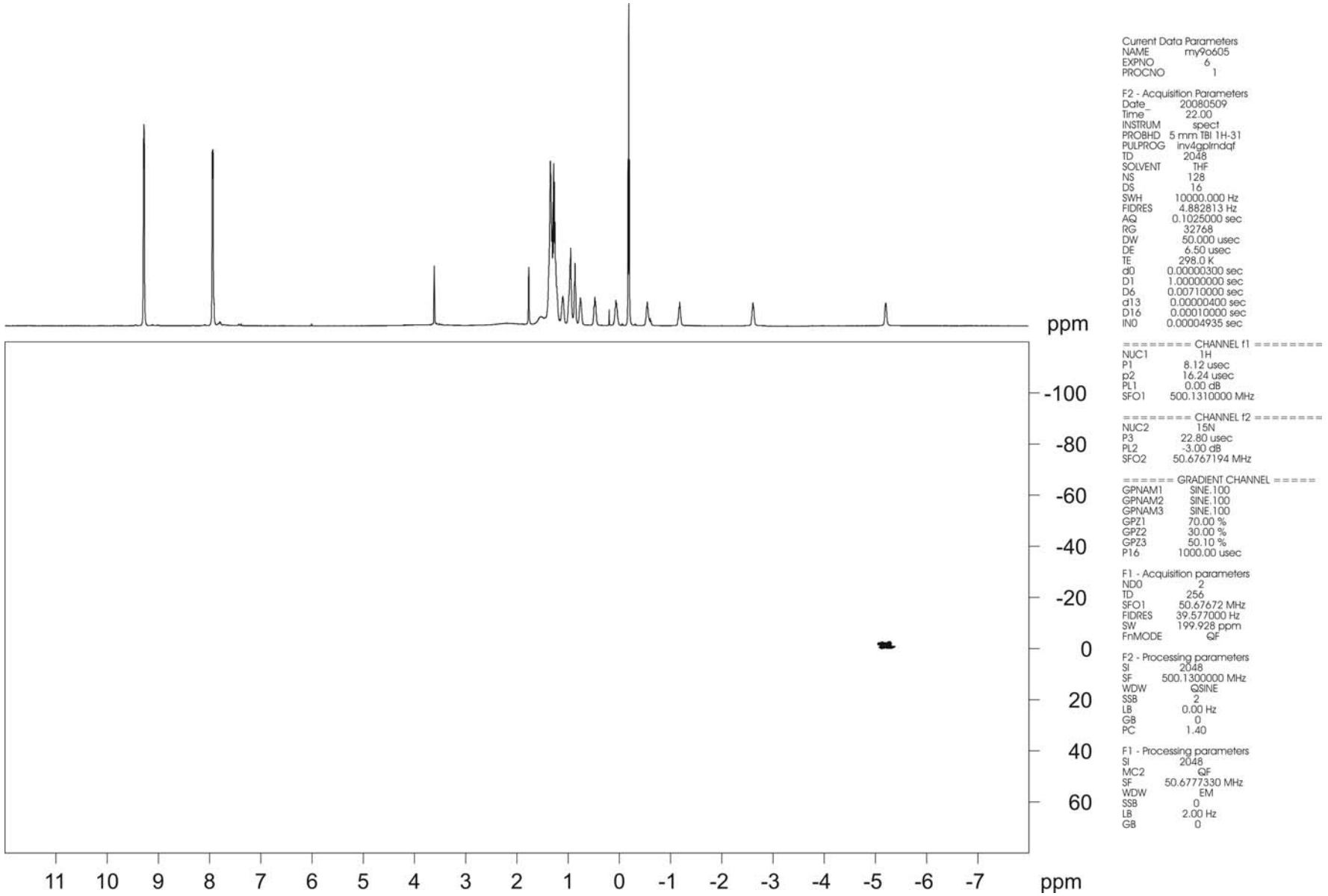

Figure 7. ^{1}H, ^{15}N gHMQC NMR spectrum of **6** in THF-d_8.

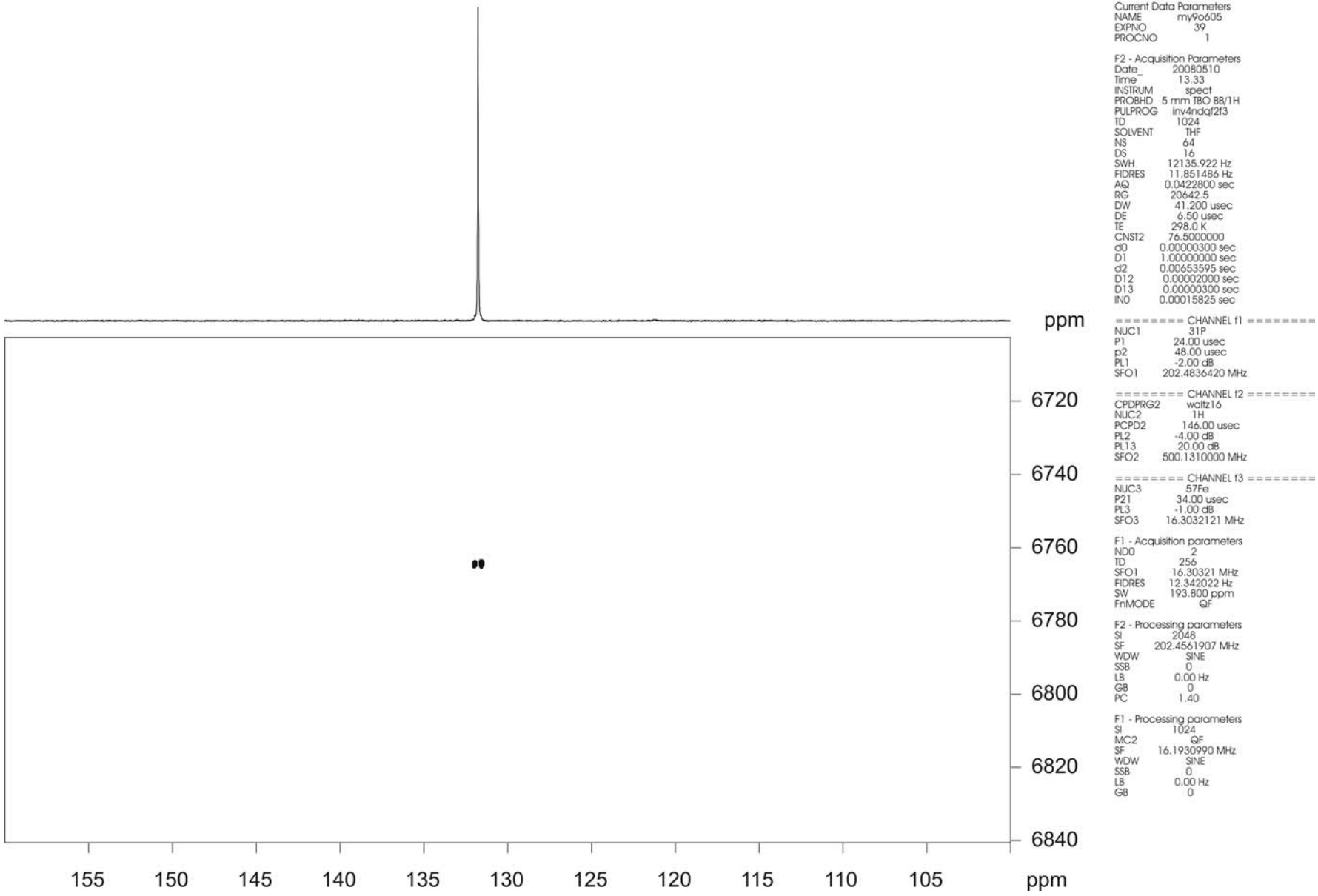

Figure 8. $^{31}P,^{57}Fe$ HMQC NMR spectrum of **6** in THF-d_8.

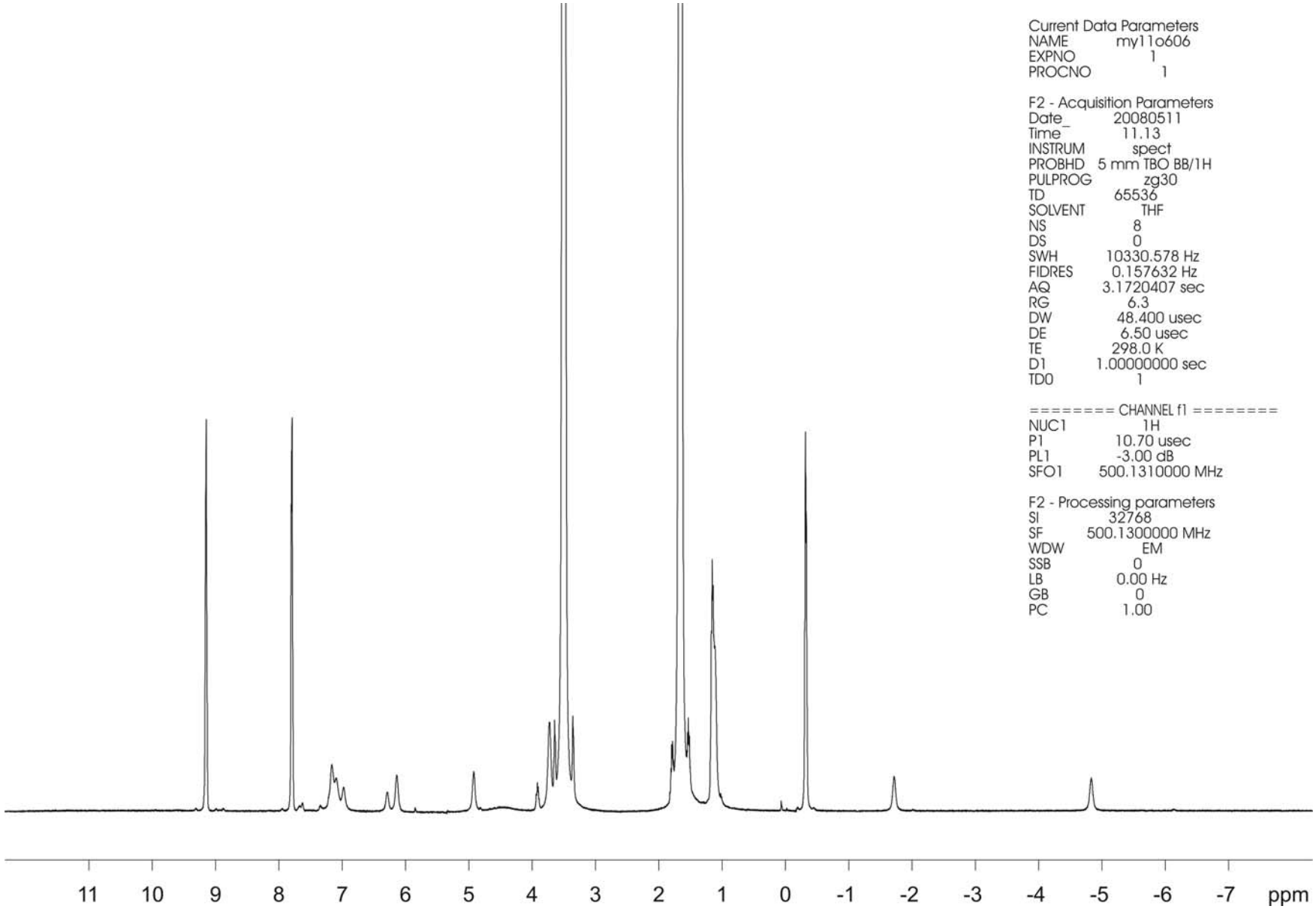

Figure 9. ^{1}H NMR (500.13 MHz) spectrum of **7** in THF.

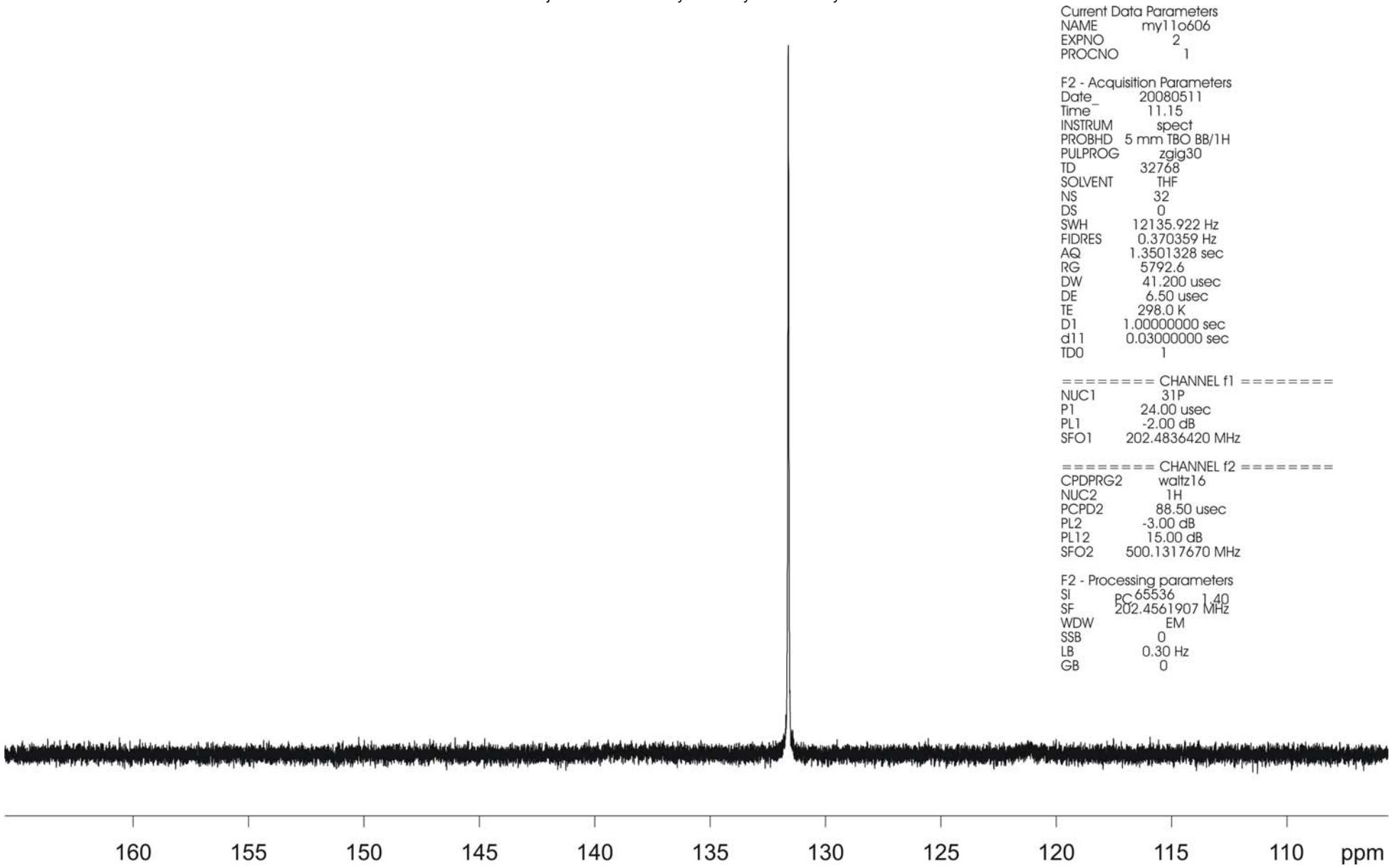

Figure 10. ^{31}P NMR (202.4 MHz) spectrum of **7** in THF.

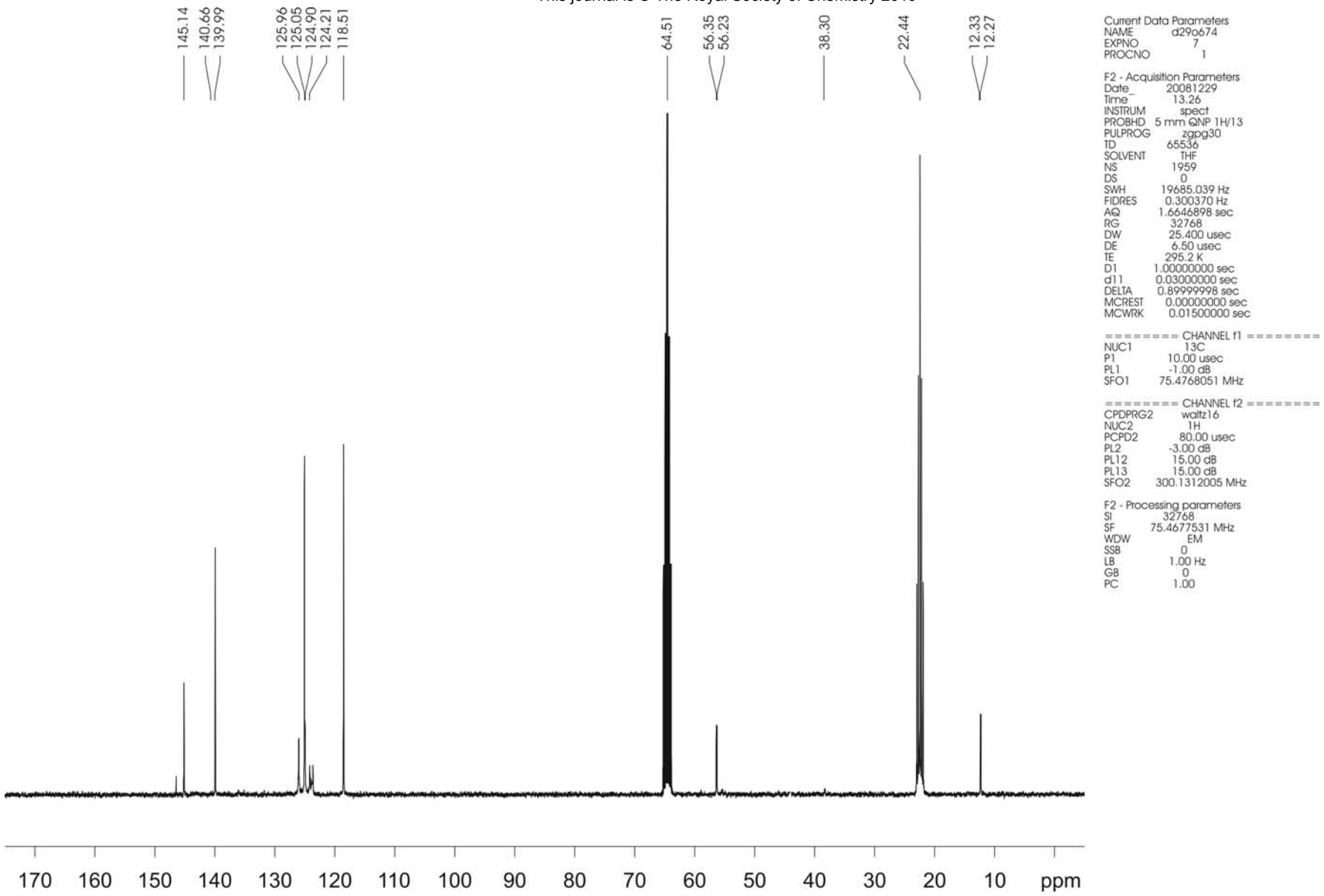

Figure 11. ^{13}C NMR (75.5 MHz) spectrum of **7** in THF-d_8.

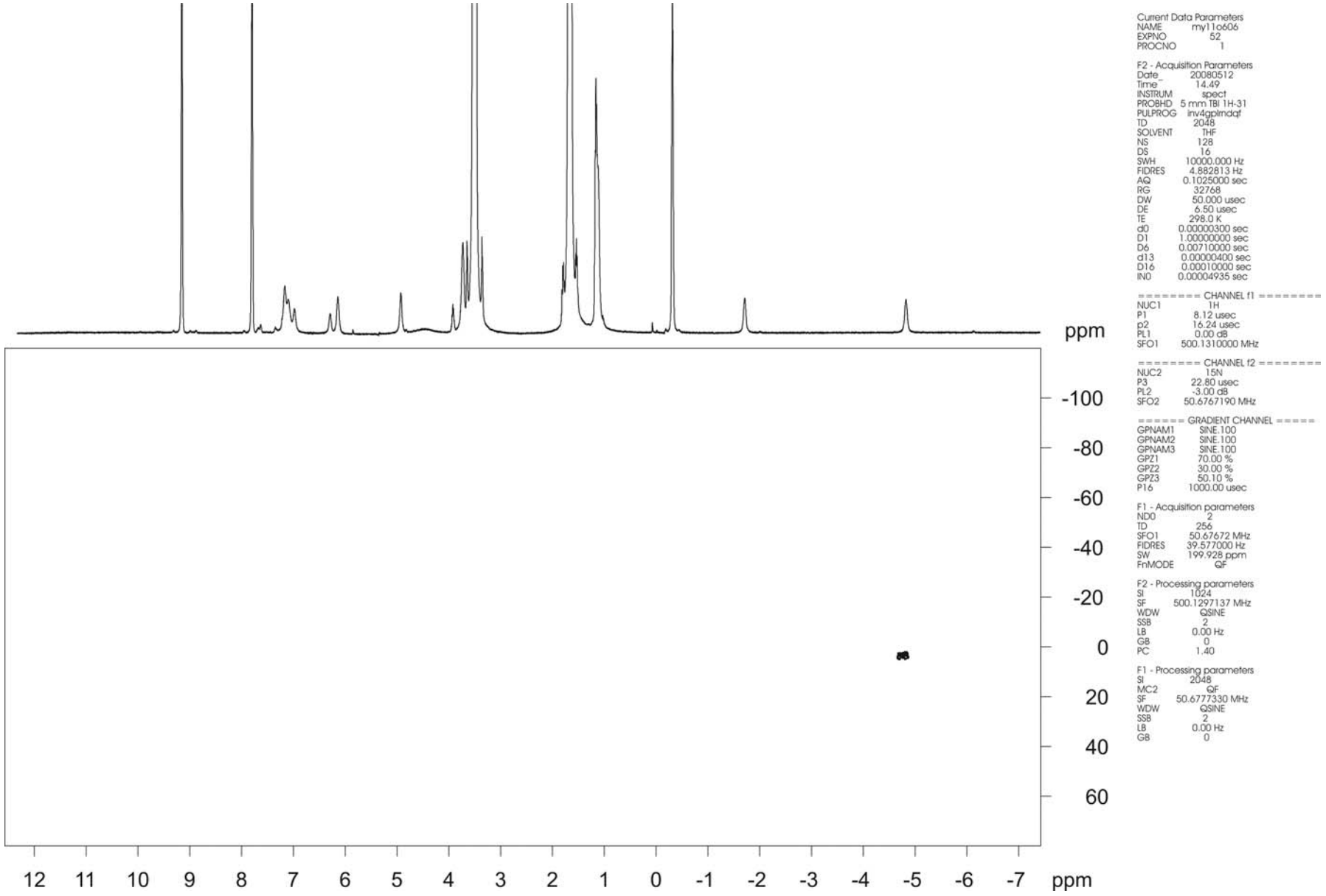

Figure 12. ^{1}H, ^{15}N gHMQC NMR spectrum of **7** in THF.

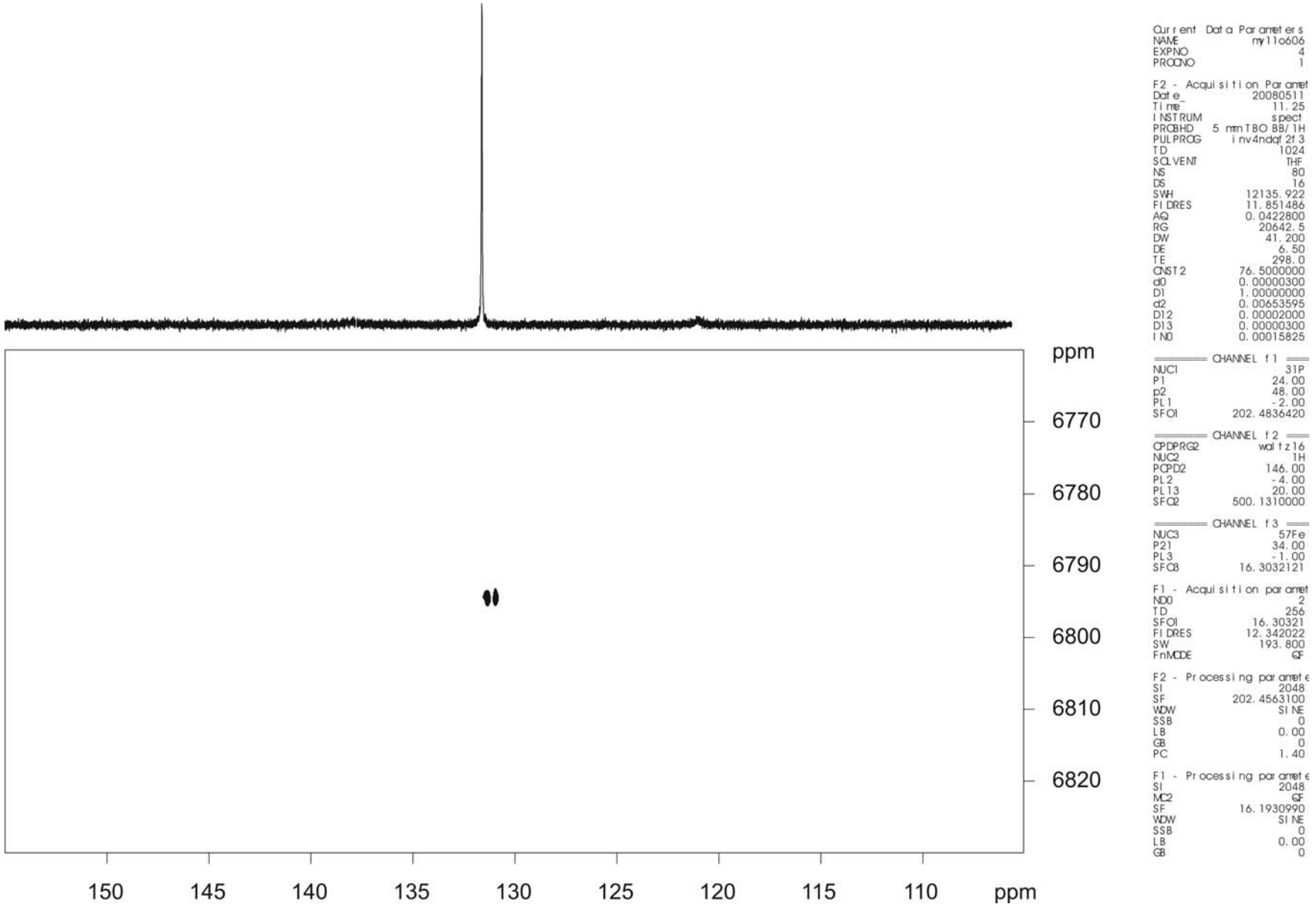

Figure 13. $^{31}P,^{57}Fe$ HMQC NMR spectrum of **7** in THF.

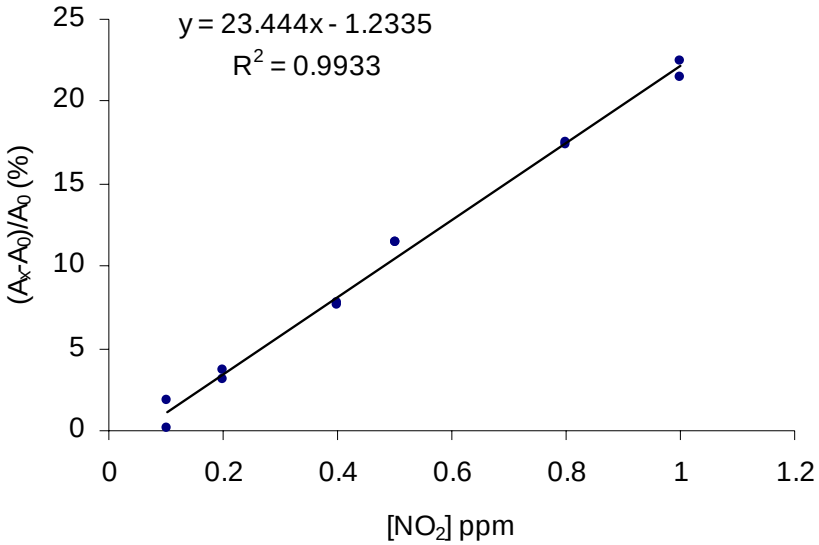

Figure 14. Calibration curve of complex 7 immobilized into AP200/19 for NO_2; the calculated LOD is 1.2 ppb. A_0 is the absorbance before exposure to NO_2 and A_x is the absorbance upon exposure to NO_2 for 300 s in air with 50% RH at a flow rate of 200 mL min^{-1}.

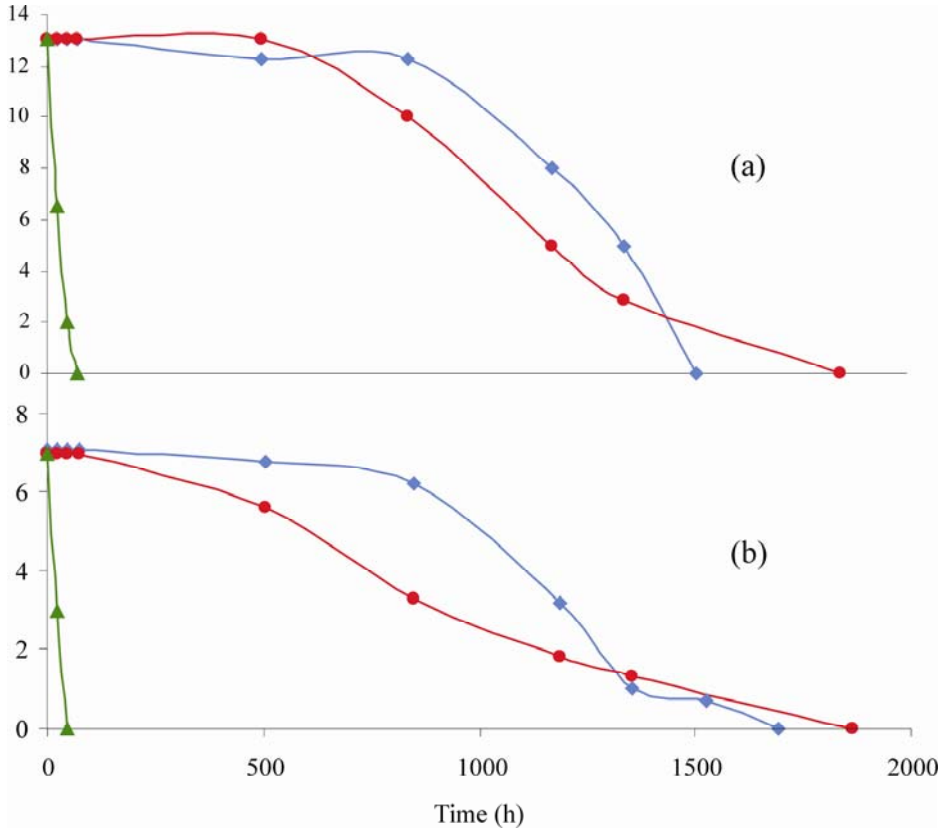

Figure 15. Stability studies at (♦) 4ºC, (●) 25ºC and (▲) 60ºC for sensing layers containing a) complex **4**, and b) complex **5**, incorporated into AP200/19. A_0 is the absorbance before exposure to NO_2 and A_x is the absorbance upon exposure to NO_2 for 300 s in air with 50% RH.

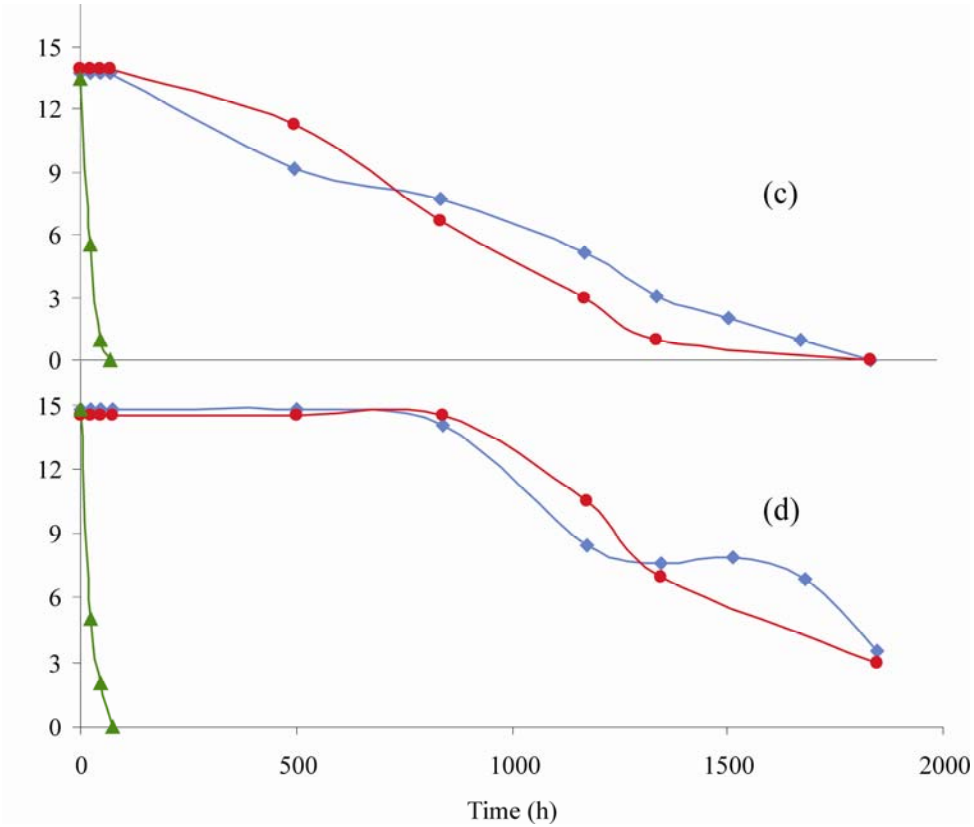

Figure 16. Stability studies at (♦) 4ºC, (●) 25ºC and (▲) 60ºC for sensing layers containing a) complex **6**, and b) complex **7**, incorporated into AP200/19. A_0 is the absorbance before exposure to NO_2 and A_x is the absorbance upon exposure to NO_2 for 300 s in air with 50% RH.

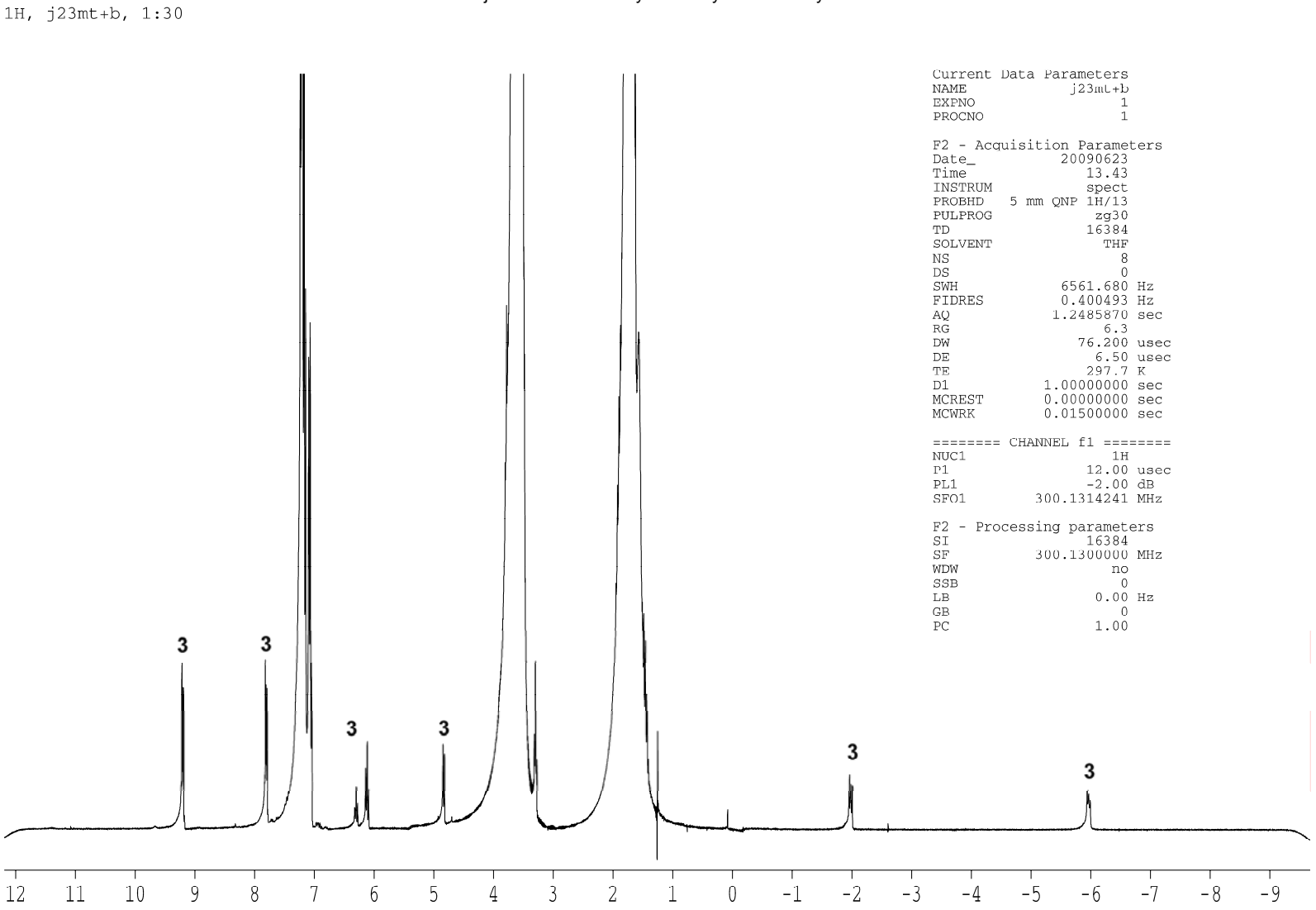

Figure 17. ^{1}H NMR of the THF cocktail based on **1**:benzylamine, in the ratio 1:30. Complex **3** can be clearly identified among THF and benzylamine signals.

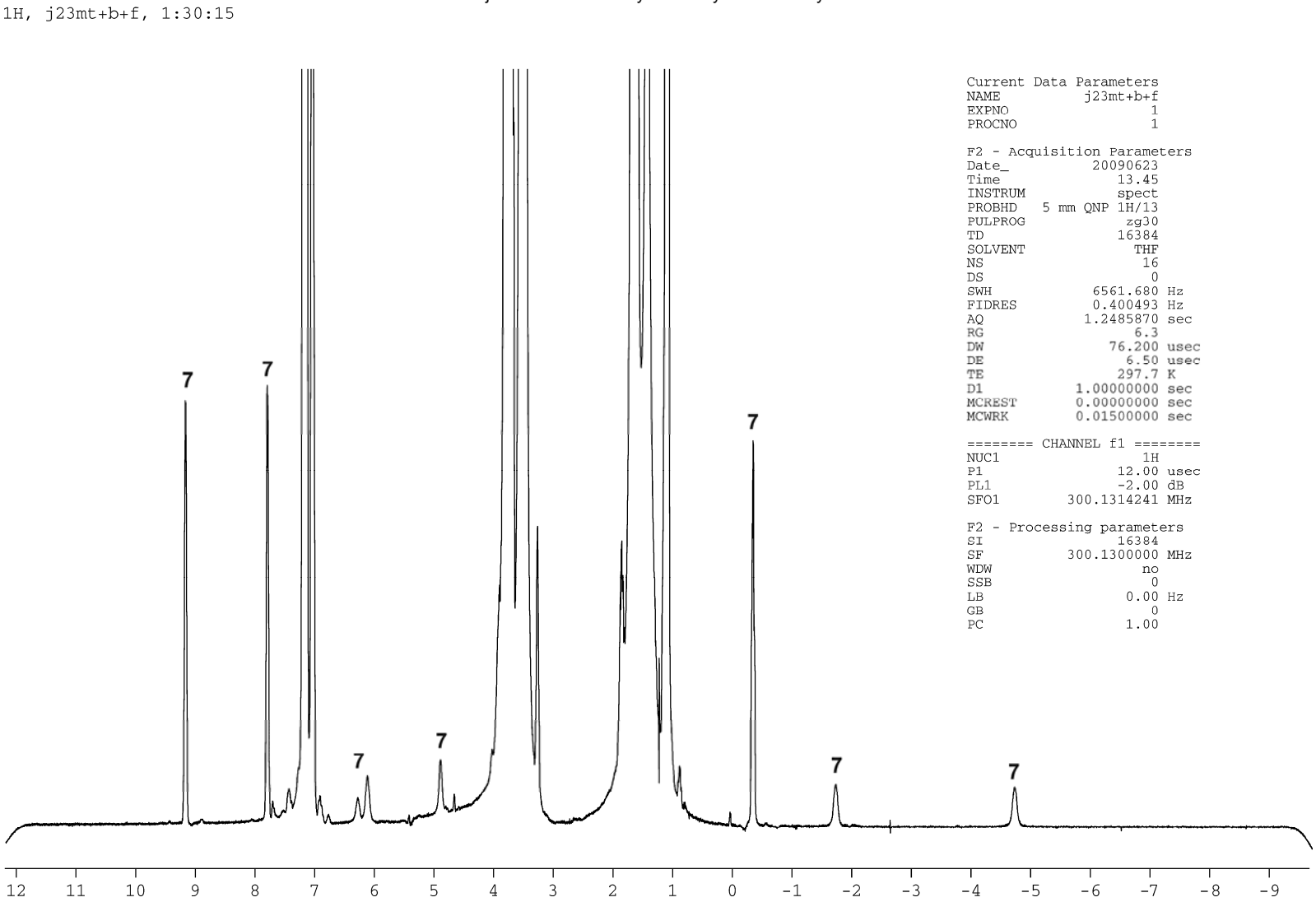

Figure 18. ^{1}H NMR of the THF cocktail based on **1**:benzylamine:P(EtO)$_3$), in the ratio 1:30:15. Complex **7** can be clearly identified among THF, benzylamine, and triethylphosphite signals.

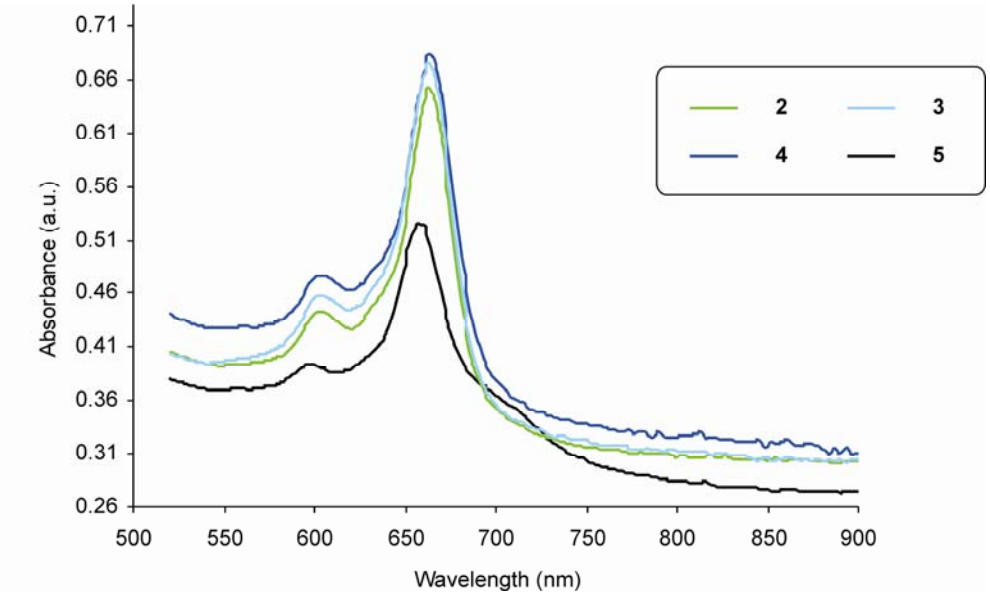

Figure 19. Absorption spectra of complexes **2-5** (FePc:amine molar ratio 1:30) immobilized into AP200/19 in air with 50% RH and at flow-rate of 200 mL min^{-1}.

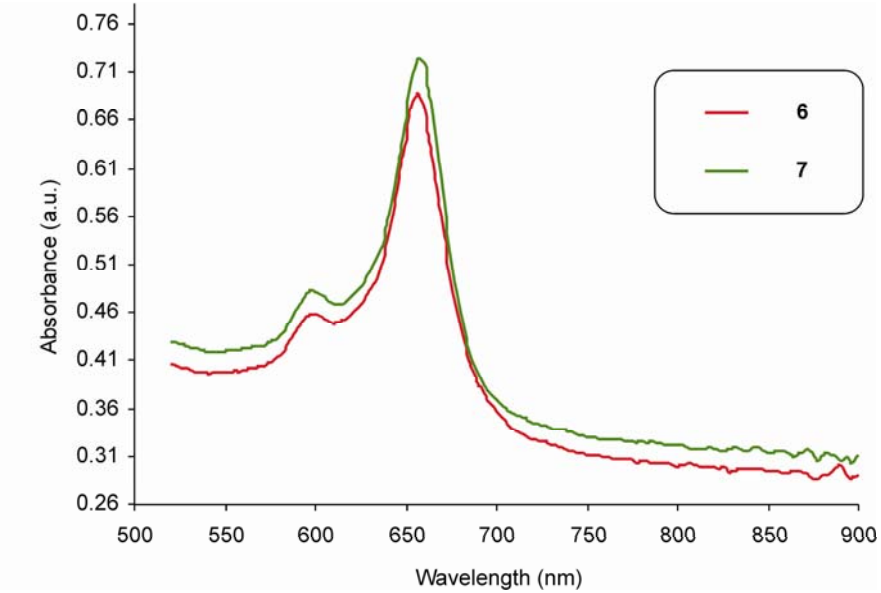

Figure 20. Absorption spectra of the cocktails for complexes **6** and **7** formation (FePc:amine:$P(OEt)_3$ molar ratio 1:30:15) immobilized into AP200/19 in air with 50% RH and at flow-rate of 200 mL min^{-1}.

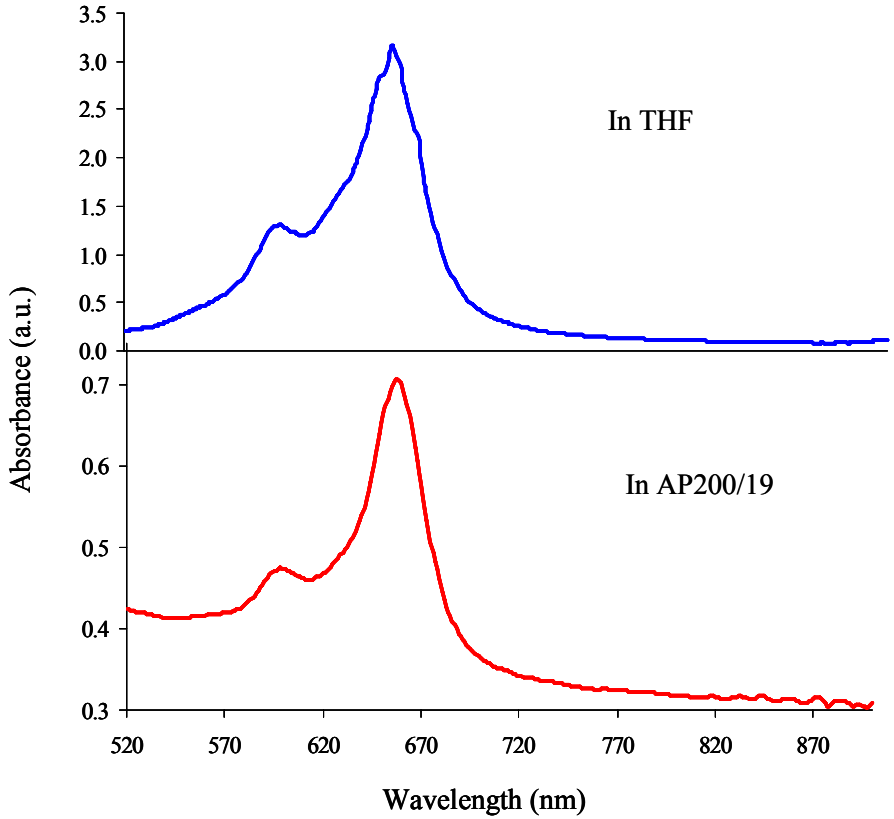

Figure 21. Absorption spectra of complex **7** in THF solution (top) and incorporated into AP200/19 (bottom).