

Accessibility in Calix[8]arene-Bound Gold Nanoparticles: Role of Ligand Flexibility

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NMR Spectra of Calix[8]arenes

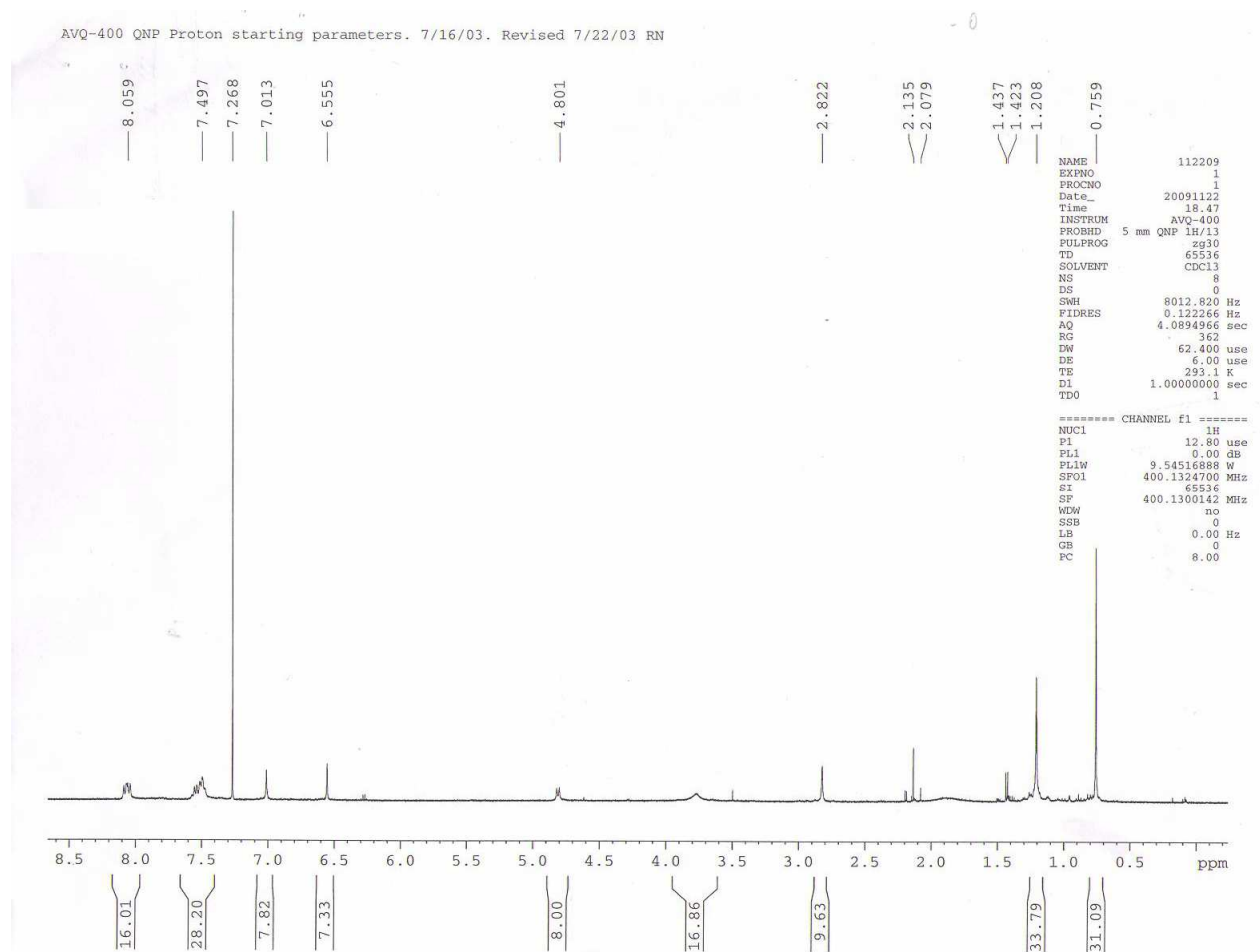


Figure S1. ^1H NMR spectra of **2a** (CDCl_3 , room temperature).

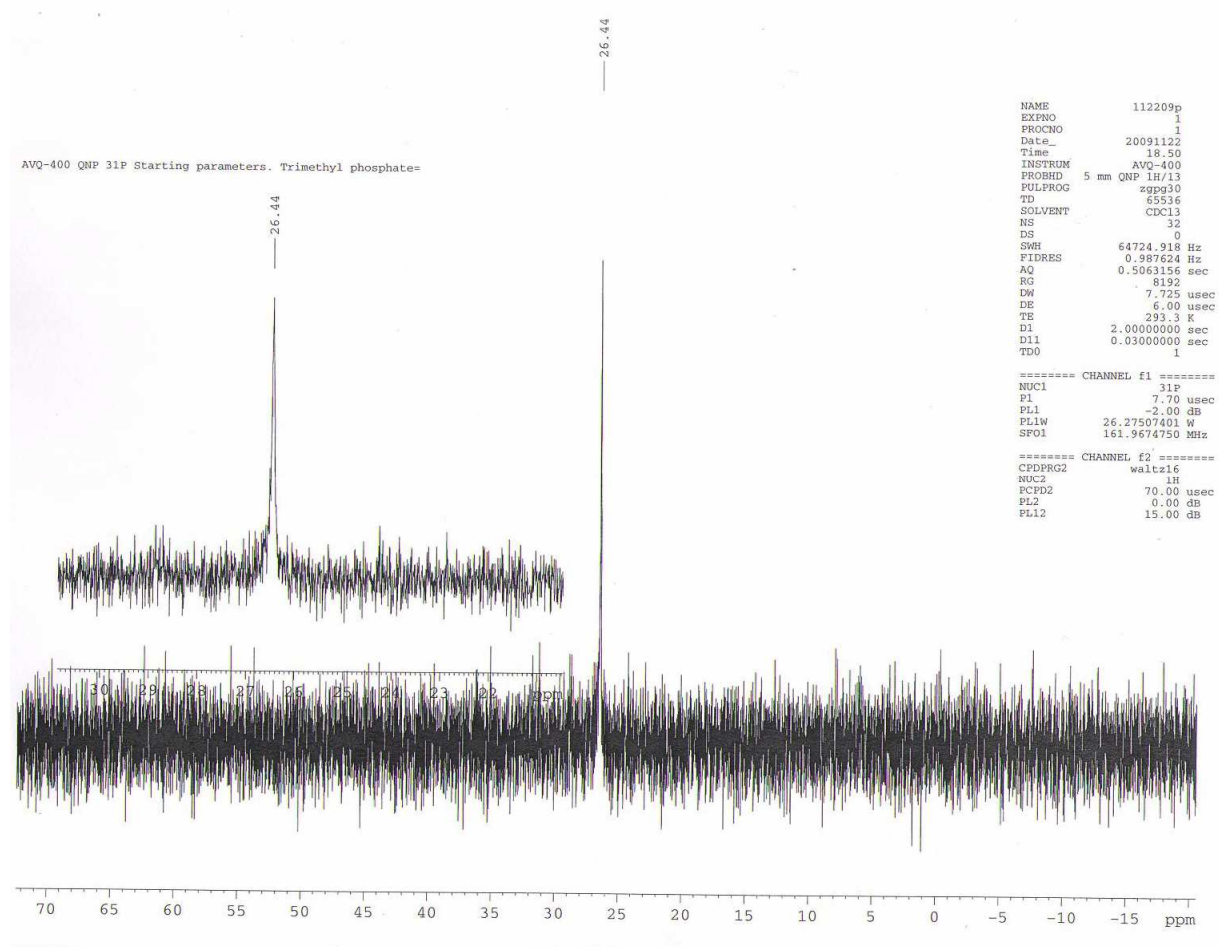


Figure S2. ^{31}P NMR spectra of **2a** (CDCl_3 , room temperature).

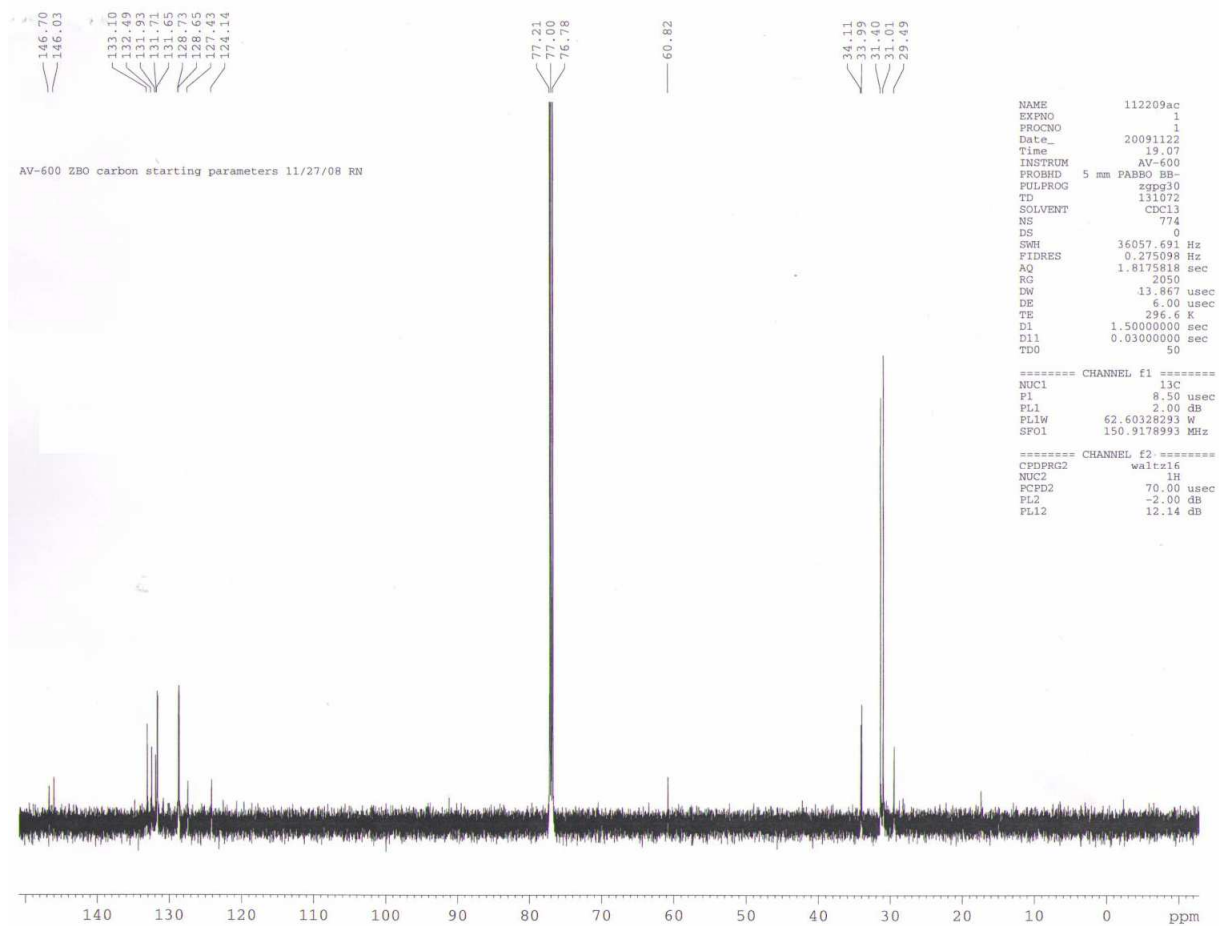


Figure S3. ^{13}C NMR spectra of **2a** (CDCl_3 , room temperature).

1H starting parameters (zg30)
 DRX-500 zBBO probe

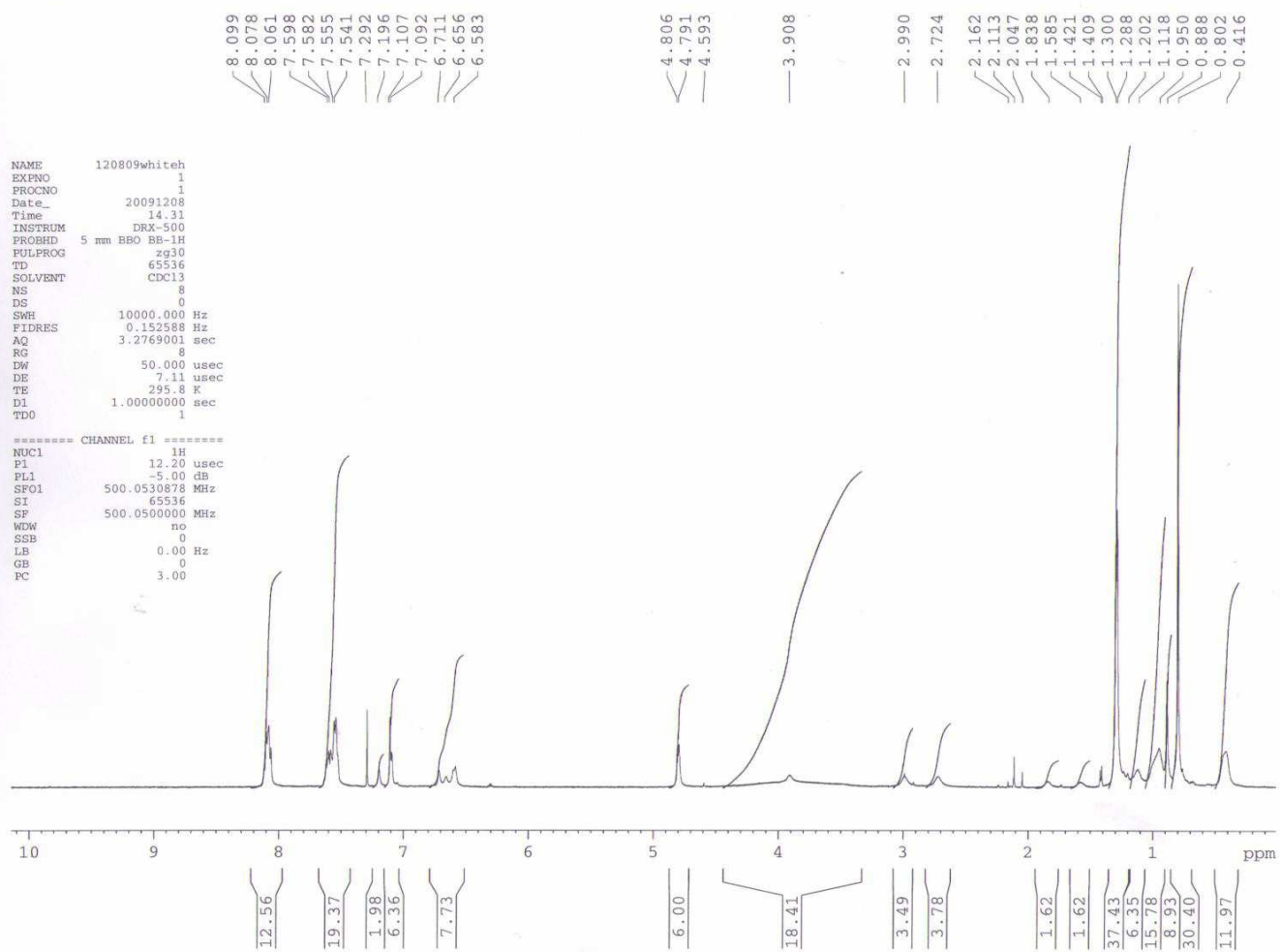


Figure S4. ^1H NMR spectra of **2b** (CDCl_3 , room temperature).

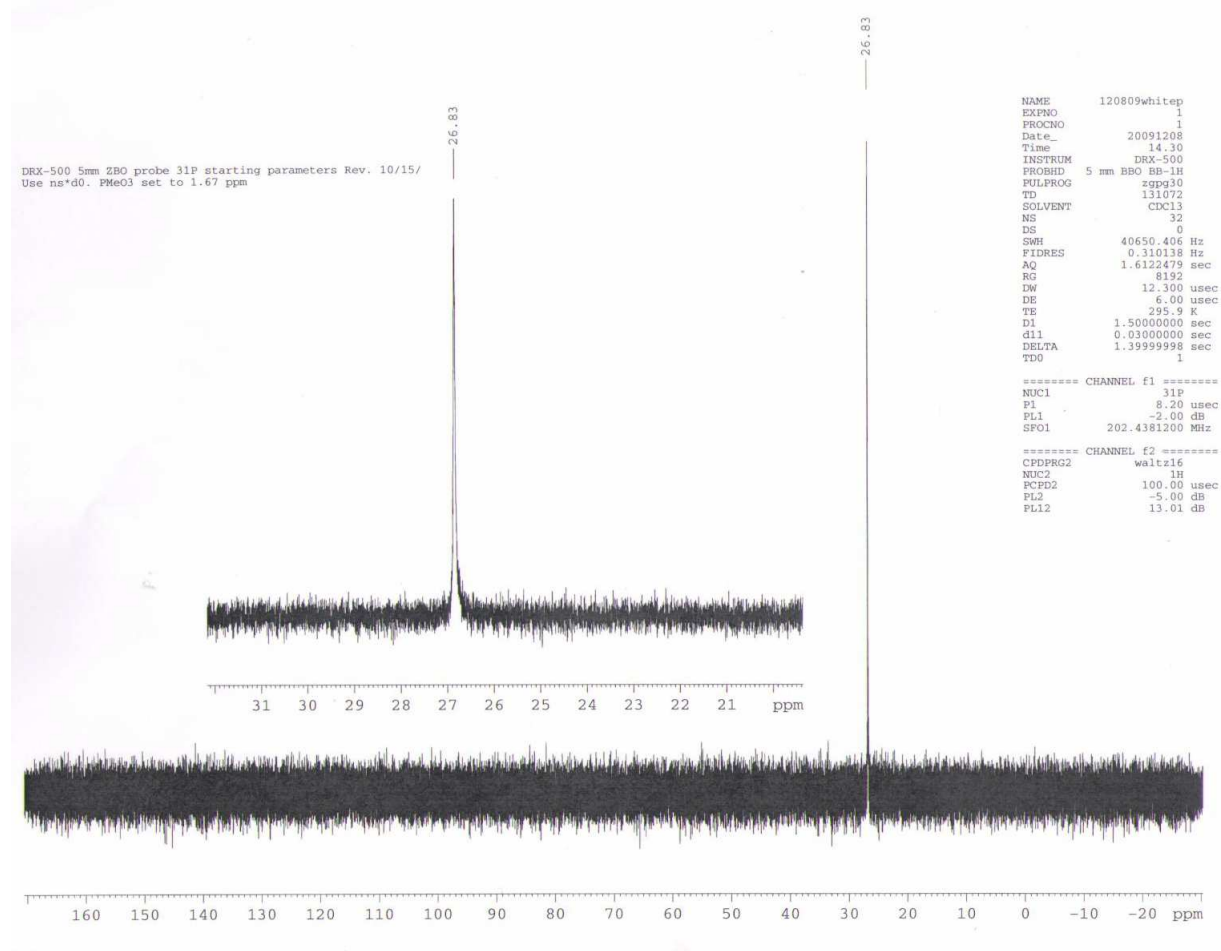


Figure S5. ^{31}P NMR spectra of **2b** (CDCl_3 , room temperature).

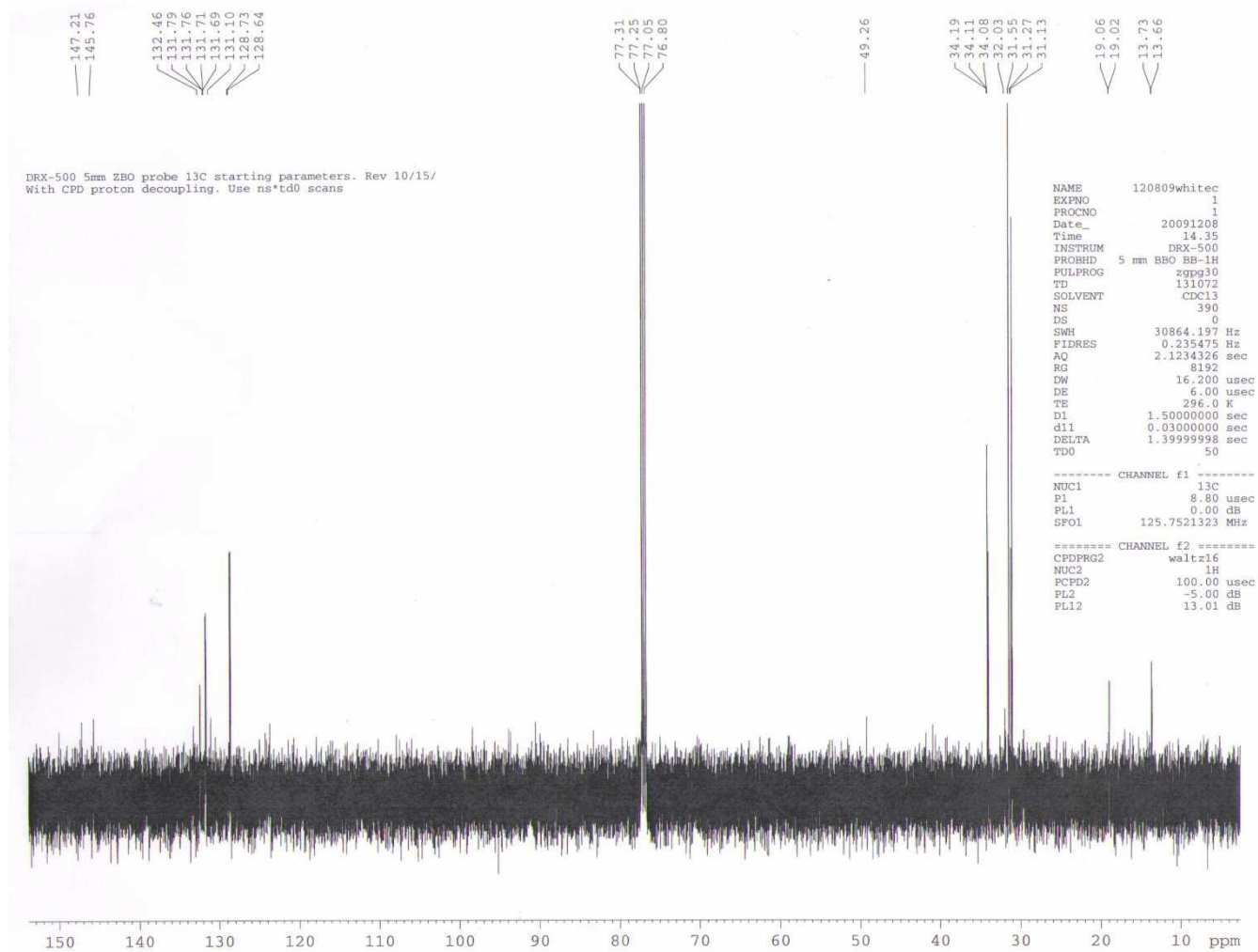


Figure S6. ^{13}C NMR spectra of **2b** (CDCl_3 , room temperature).

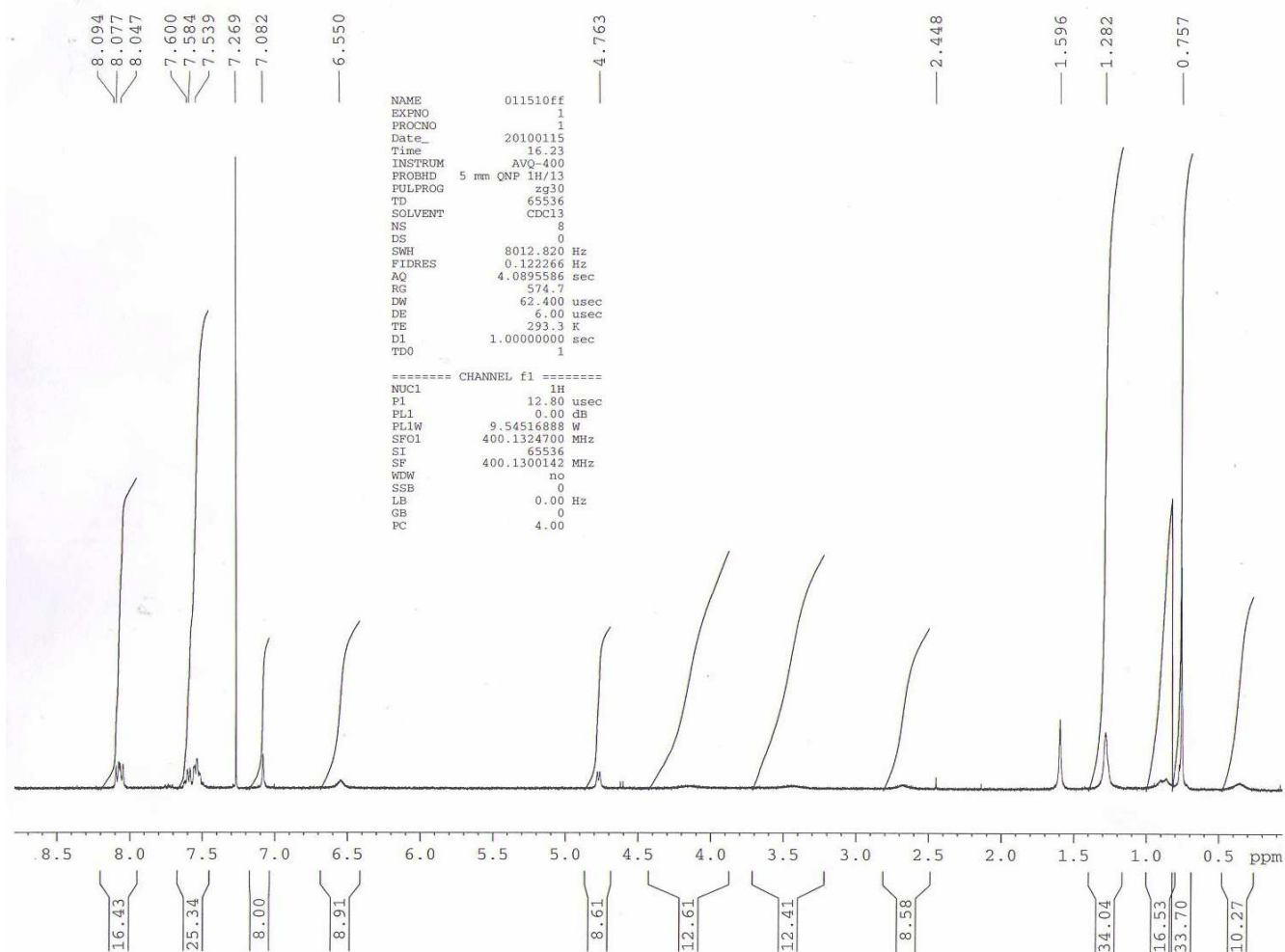


Figure S7. ^1H NMR spectra of **2c** (CDCl_3 , room temperature).

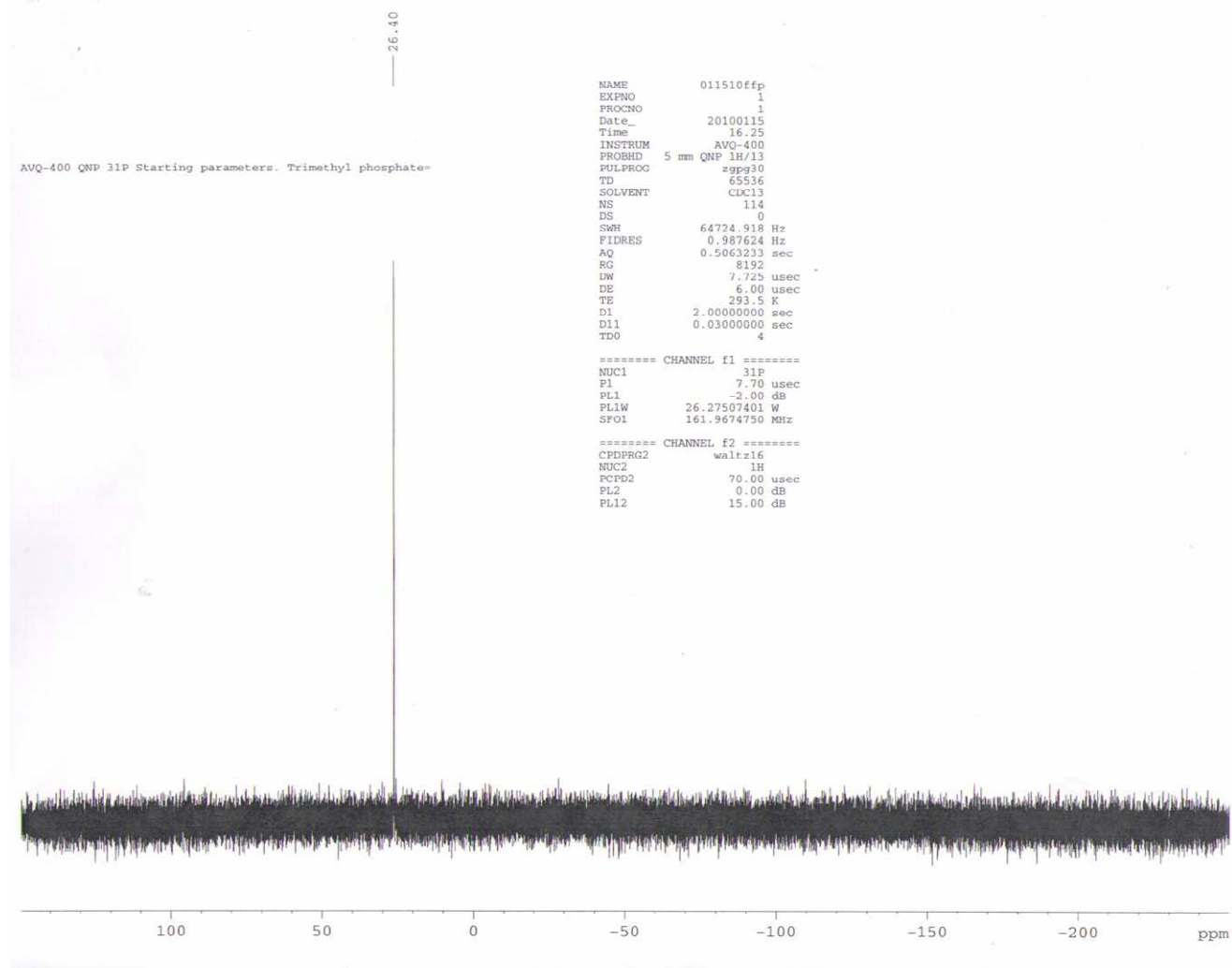


Figure S8. ^{31}P NMR spectra of **2c** (CDCl_3 , room temperature).

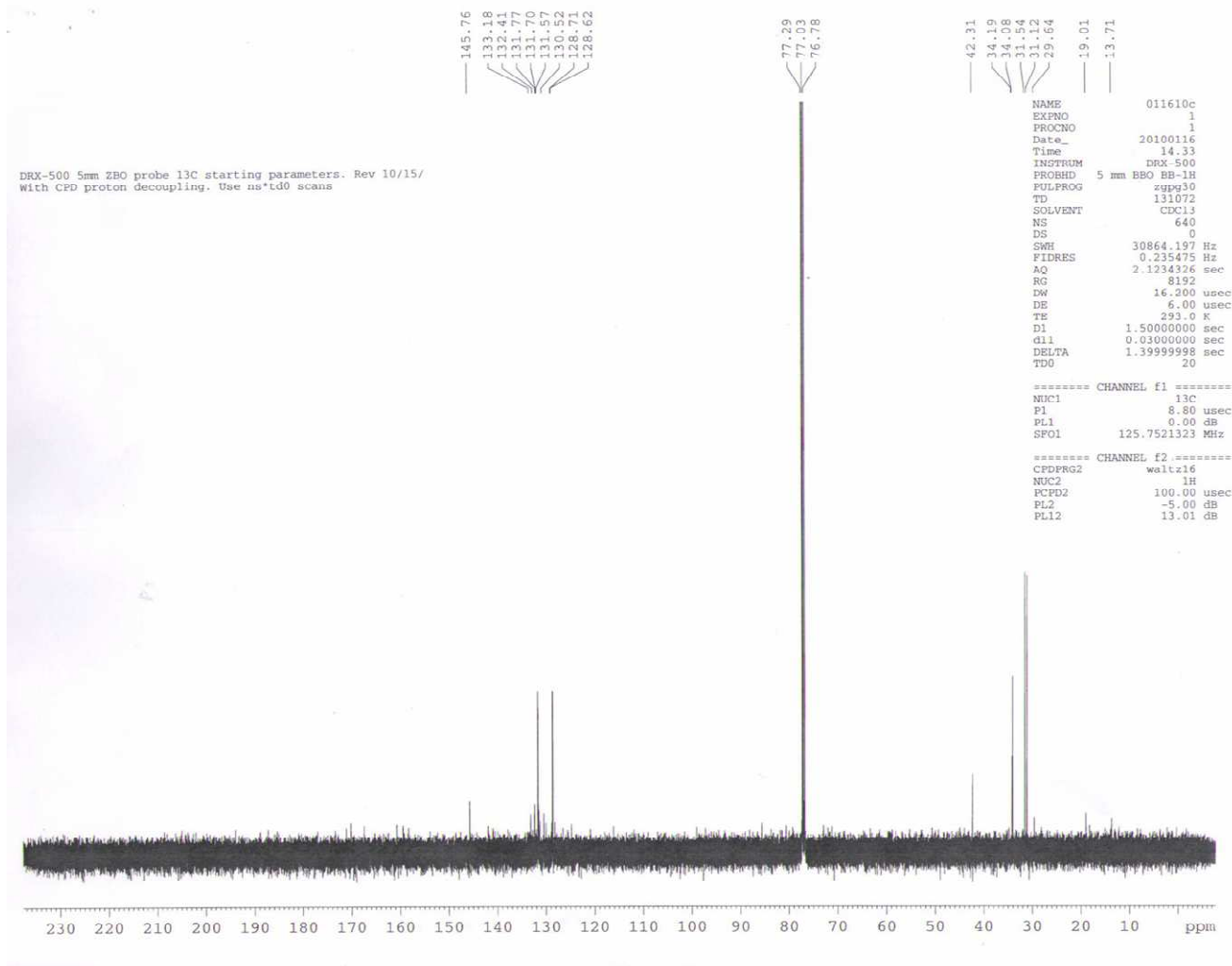


Figure S9. ^{13}C NMR spectra of **2c** (CDCl_3 , room temperature).

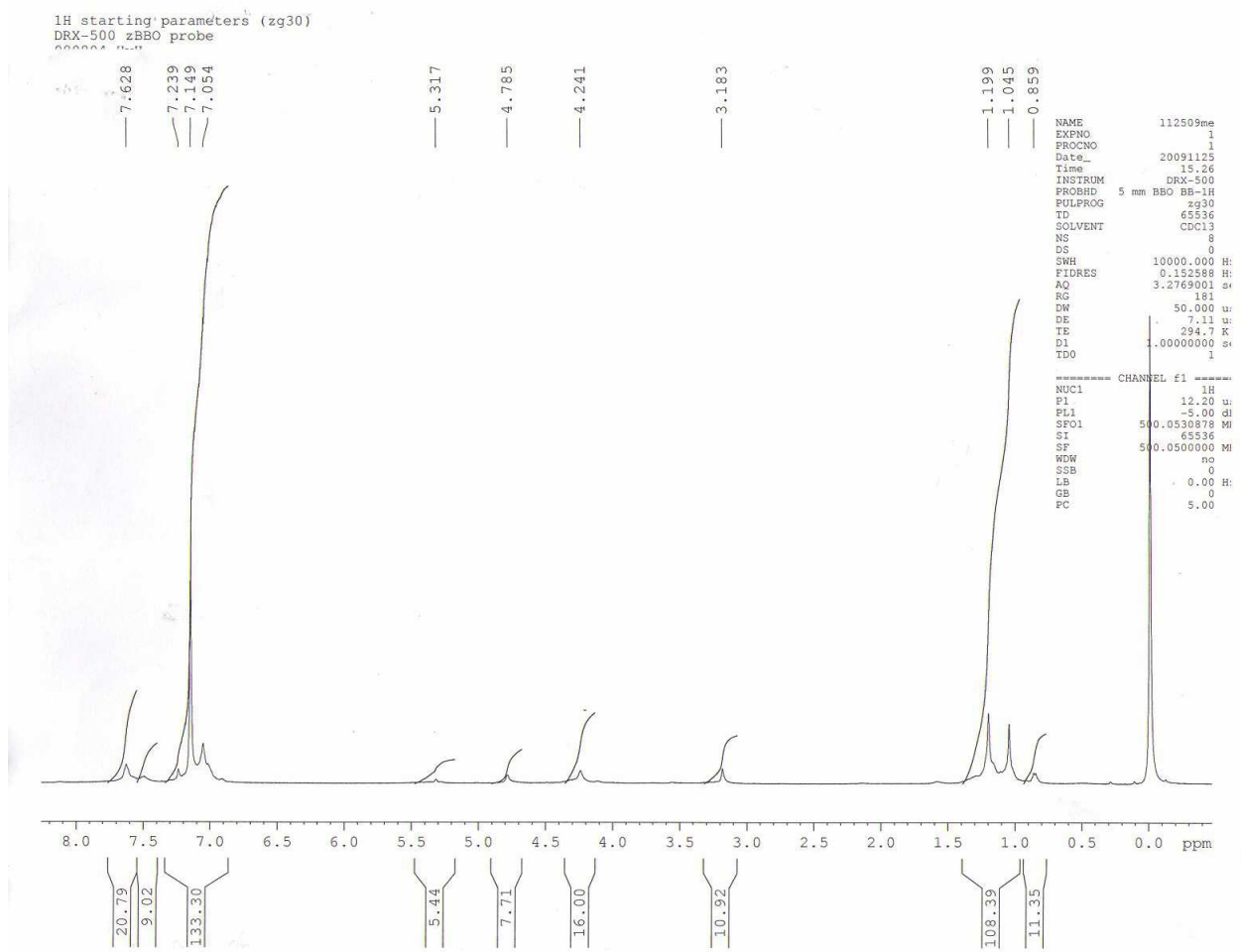


Figure S10. ^1H NMR spectra of **3a** (C_6D_6 , room temperature).

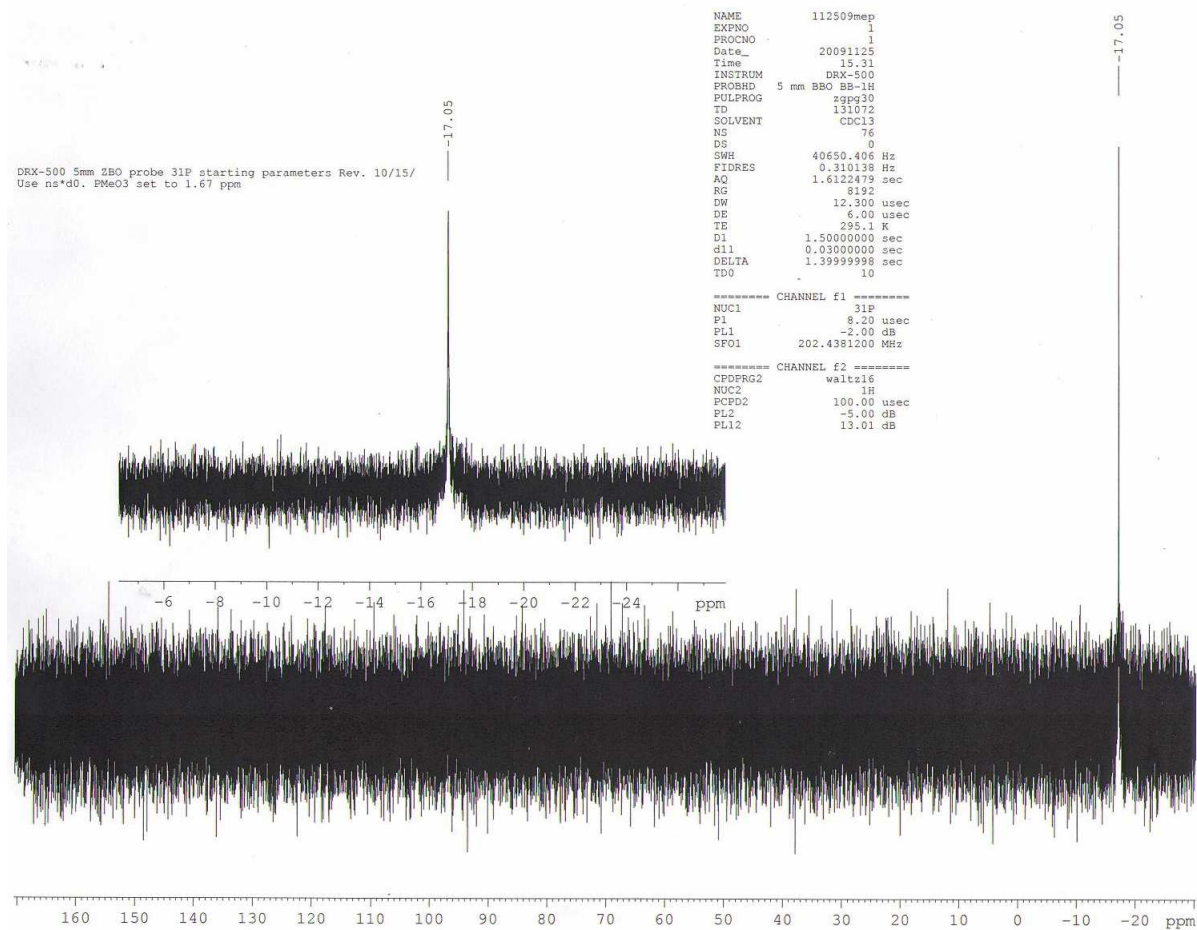


Figure S11. ^{31}P NMR spectra of **3a** (C_6D_6 , room temperature).

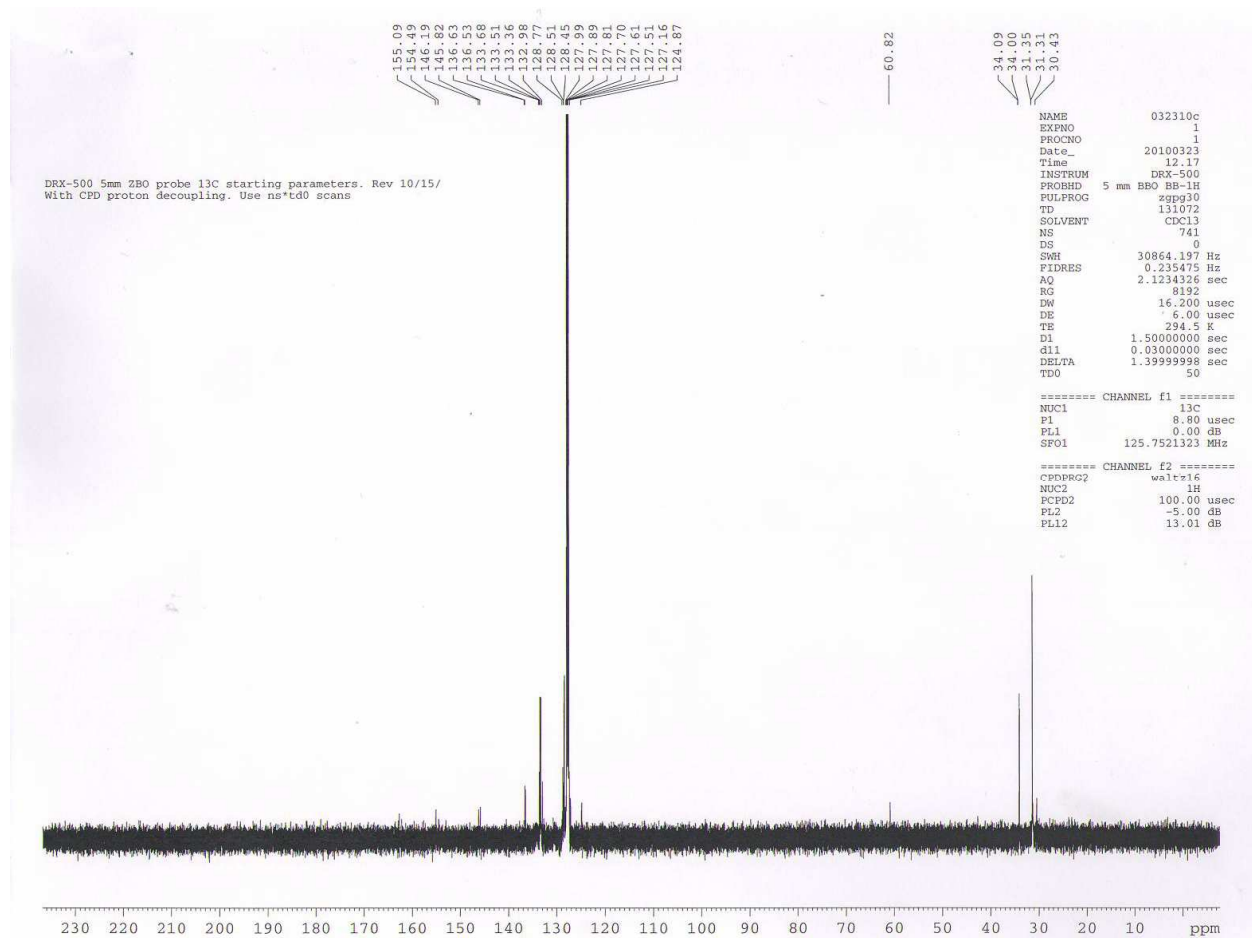


Figure S12. ^{13}C NMR spectra of **3a** (C_6D_6 , room temperature).

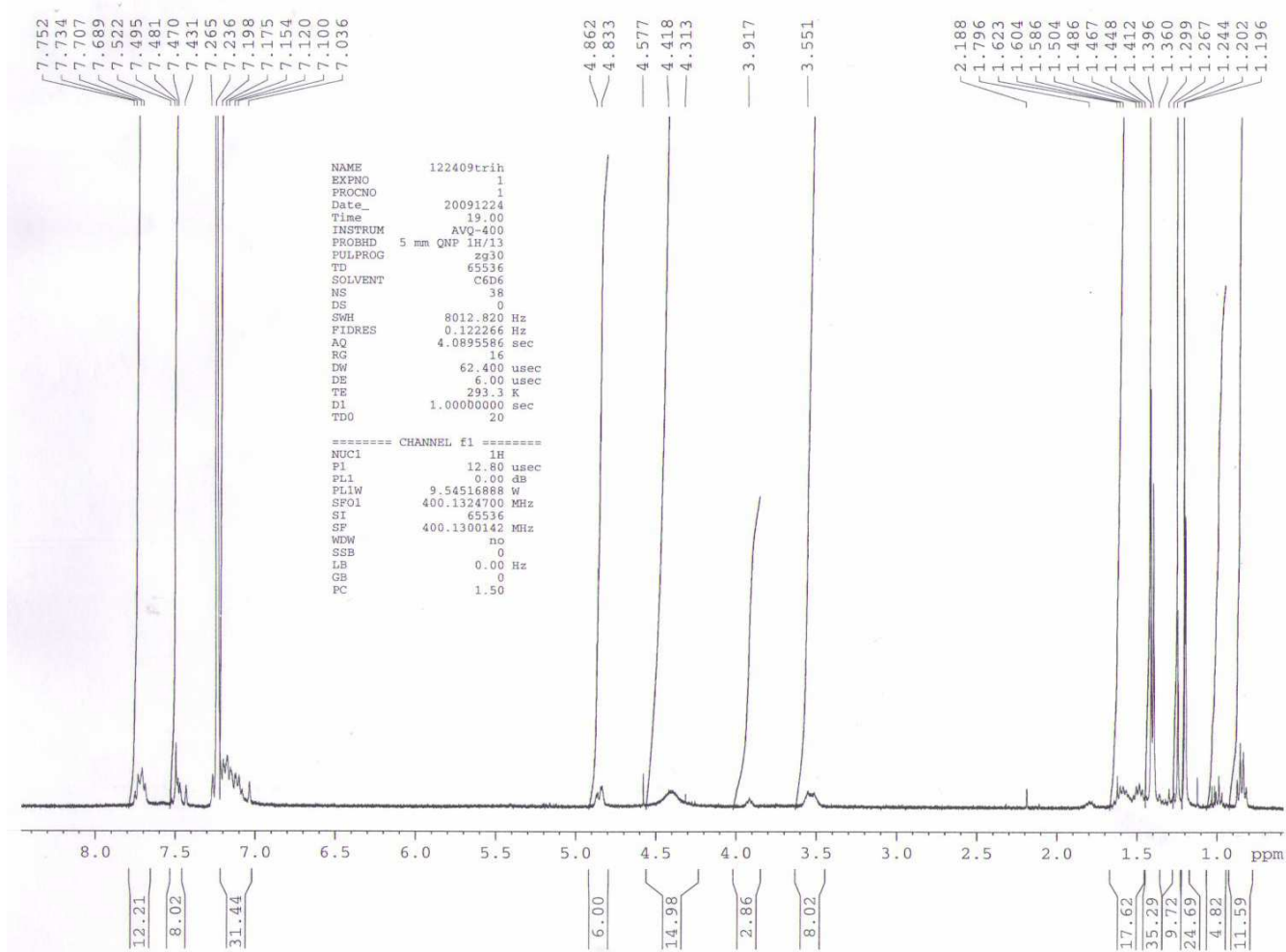


Figure S13. ^1H NMR spectra of **3b** (C_6D_6 , room temperature).

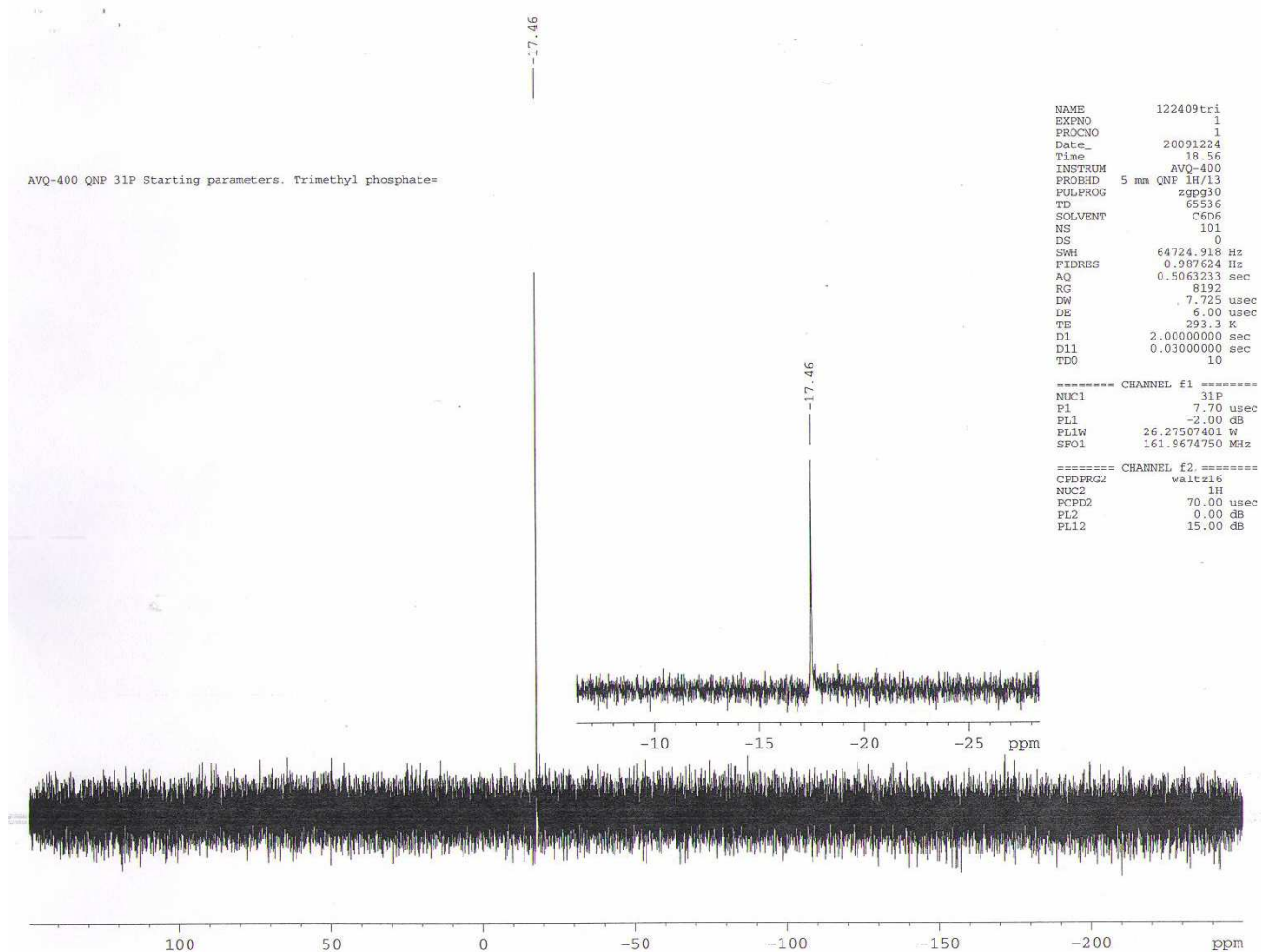


Figure S14. ^{31}P NMR spectra of **3b** (C_6D_6 , room temperature).

DRX-500 5mm ZBQ probe 13C starting parameters. Rev 10/15/07 RN
With CPD proton decoupling. Use ns*td0

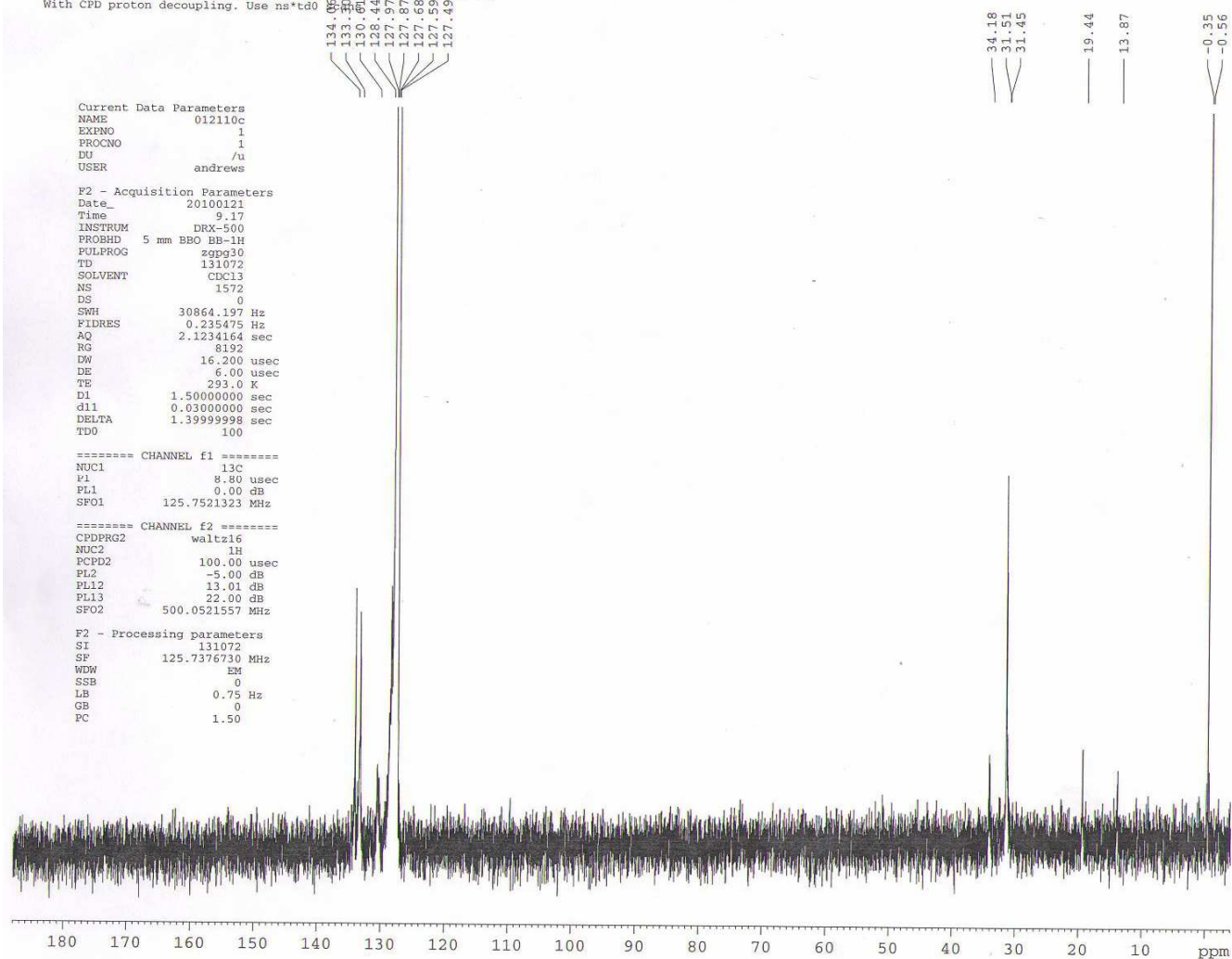


Figure S15. ^{13}C NMR spectra of **3b** (C_6D_6 , room temperature).

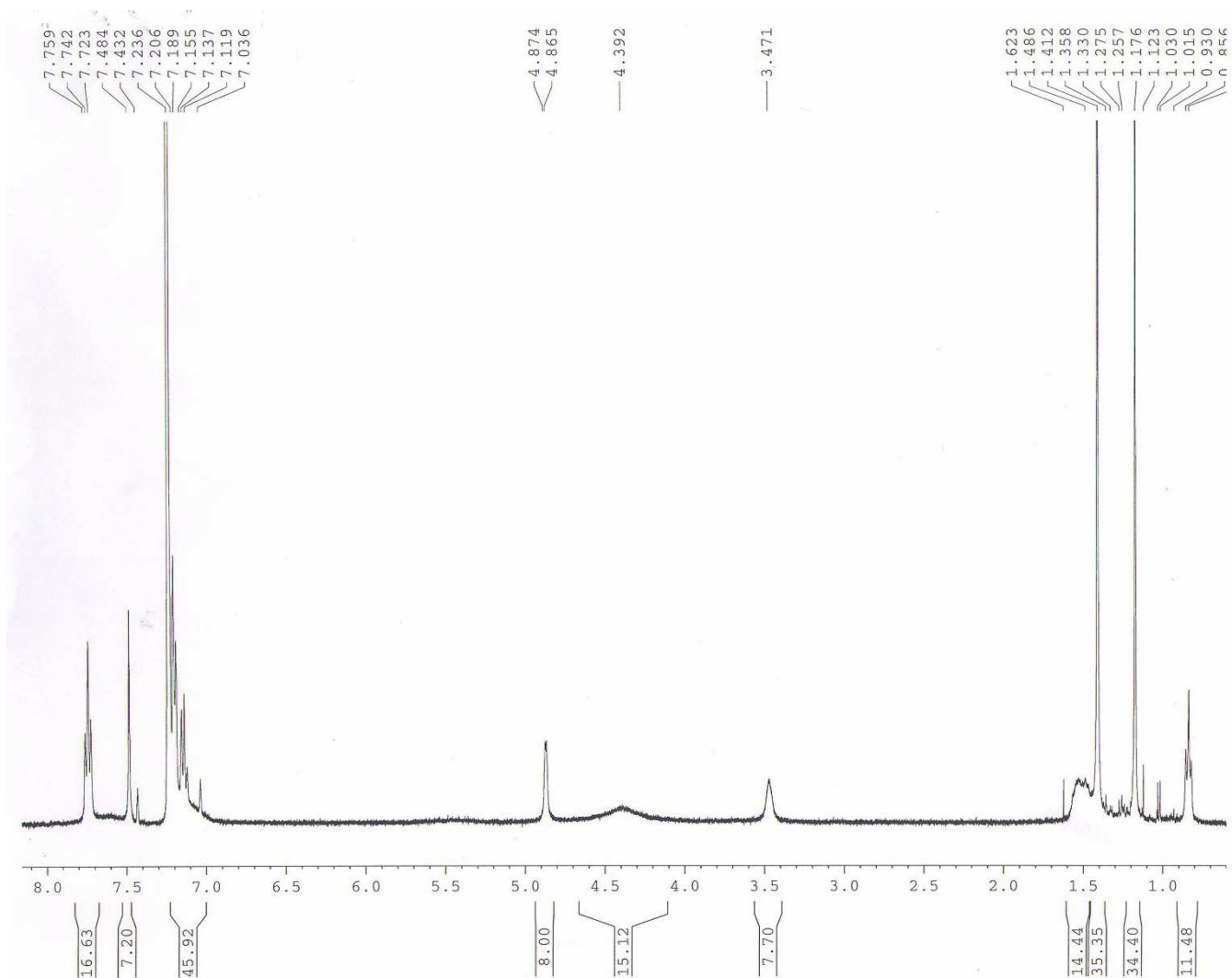


Figure S16. ¹H NMR spectra of **3c** (C₆D₆, room temperature).

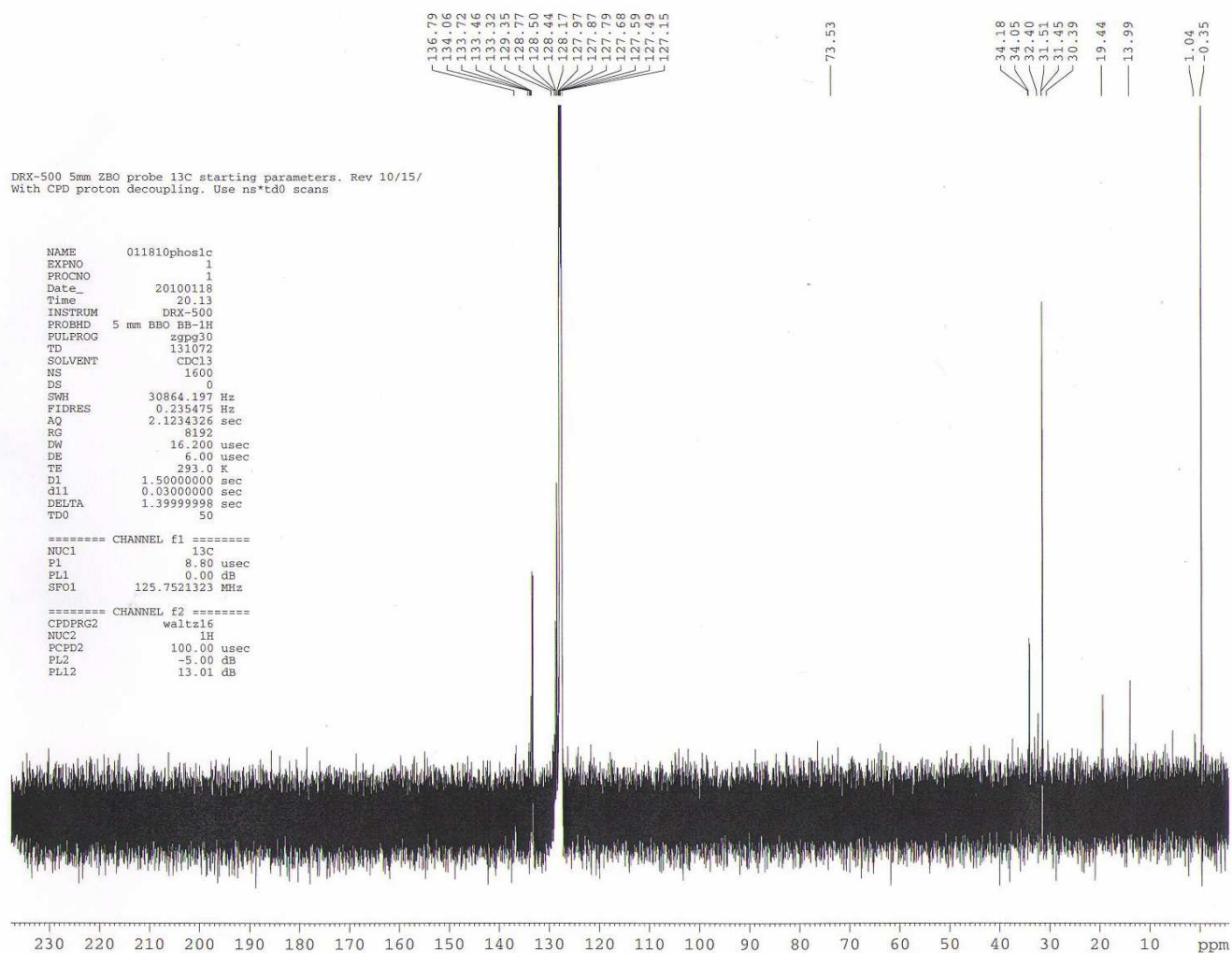


Figure S18. ^{13}C NMR spectra of **3c** (C_6D_6 , room temperature).

TEM Images of Gold Nanoparticles

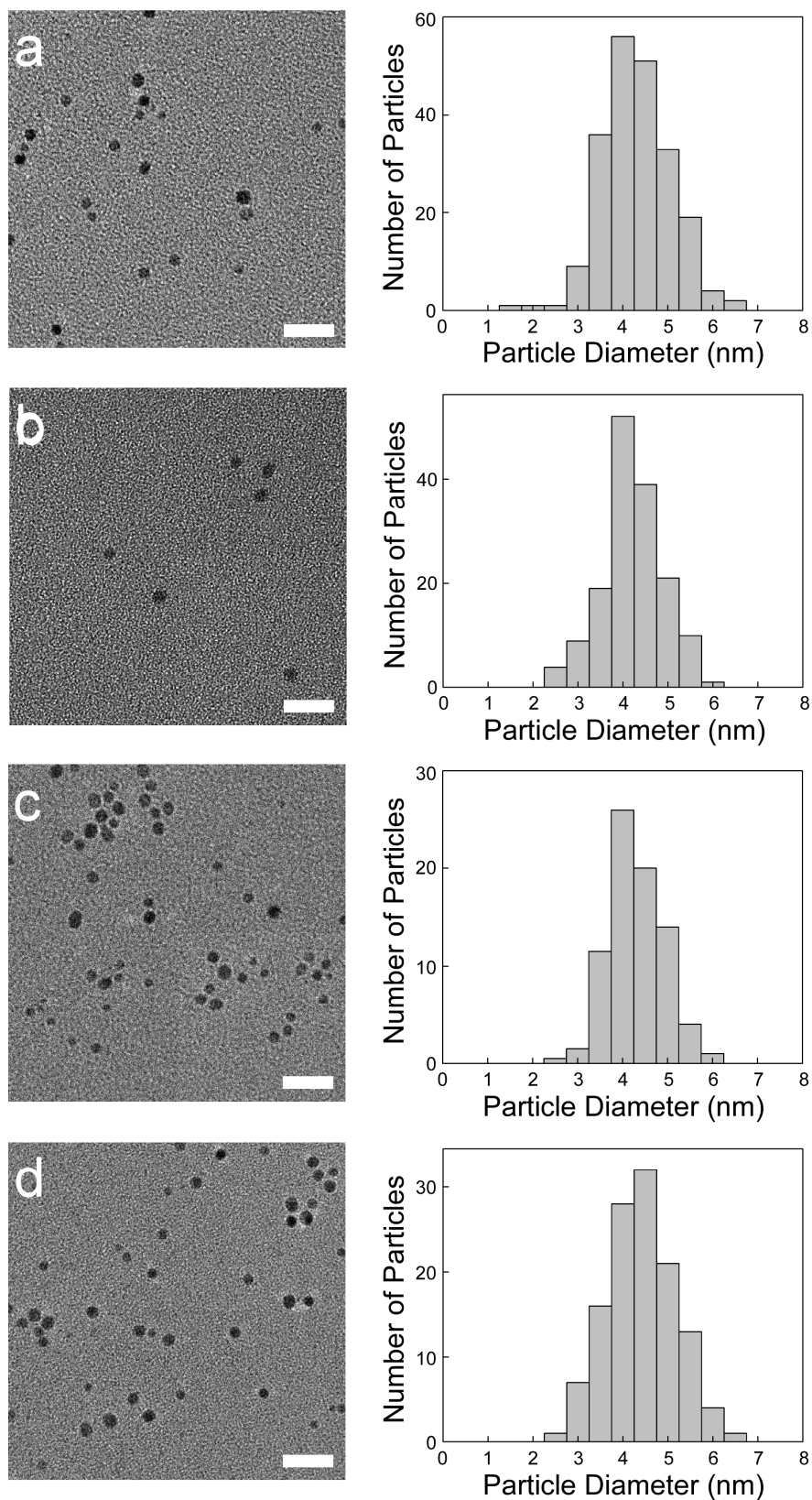


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Fluorescence of 2NT Bound to Gold Nanoparticles

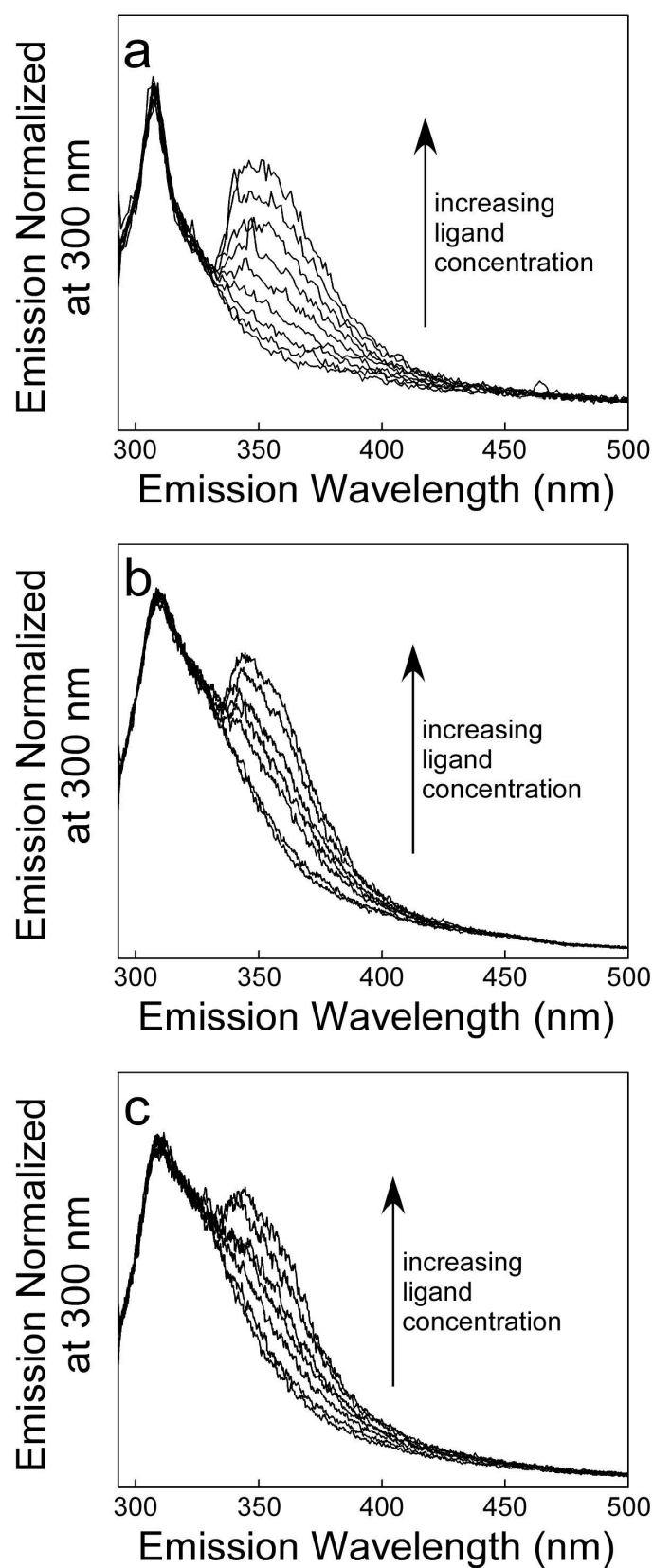


Figure S20. Representative fluorescence emission spectra of 2NT bound to gold nanoparticles modified with 2.5 μM of (a) **3a**, (b) **3b**, and (c) **3c**, respectively. 2NT concentration for each scan increases by 0.25 μM . All the spectra were excited at 283 nm and normalized at 300 nm. Each solution contains 200 μM of gold atoms.

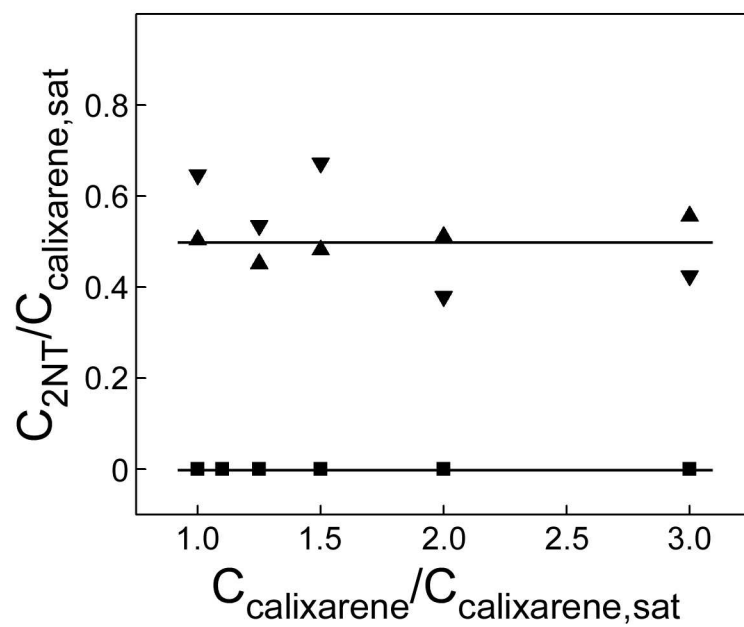
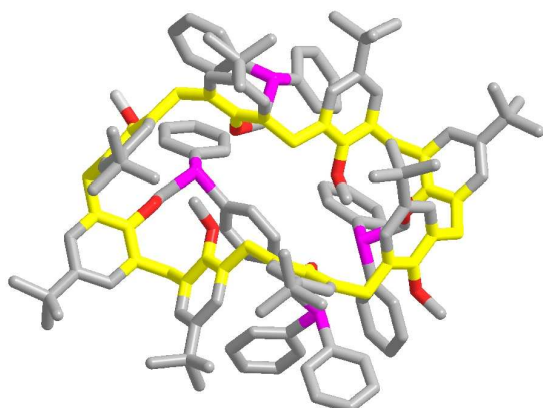


Figure S21 Accessible surface of gold nanoparticles modified with (a) **3a** (■), (b) **3b** (▲), and (c) **3c** (▼) depending on the concentration of calix[8]arene ligands..

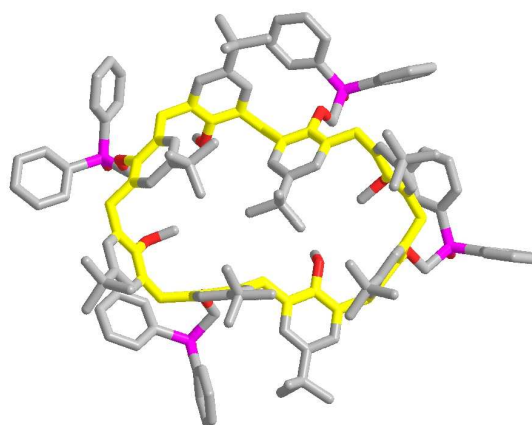
Calculated Energy-Minimized Molecular Structures of Calix[8]arenes

Unbound ligand

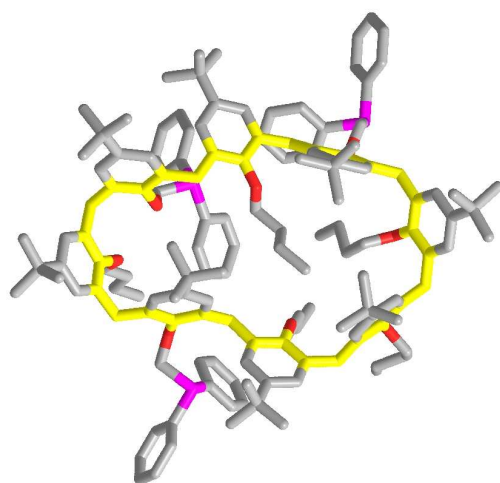
Model bound ligand



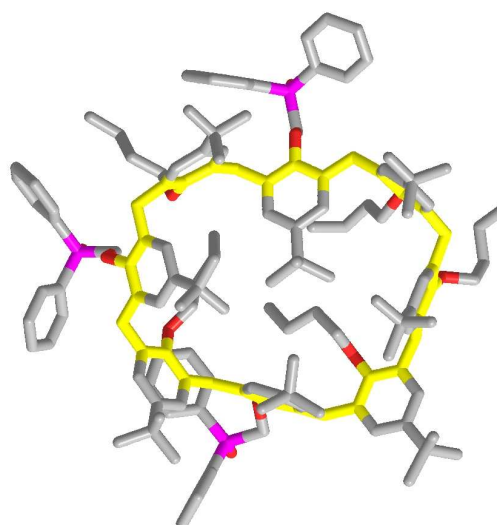
3a



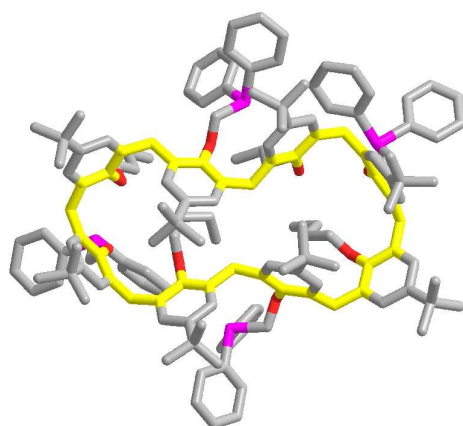
2a as model for 3a



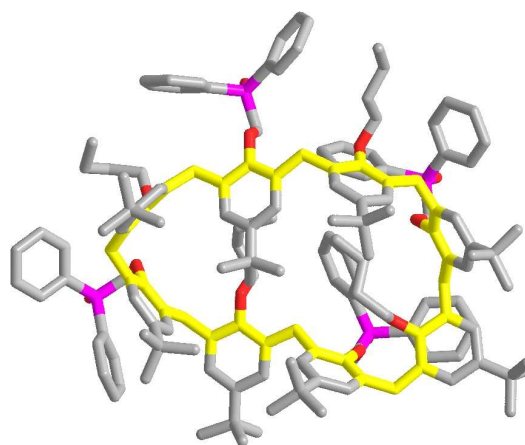
3b



2b as model for 3b



3c



2c as model for 3c

Figure S22 Representative calculated energy-minimized molecular structures of calix[8]arenes. Yellow color highlights the shape of a calixarene cavity.