SUPPORTING INFORMATION

Iterative Synthesis and Characterization of Cross-conjugated *iso*-Polydiacetylenes

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1. General experimental details.
2. ^{1}H and ^{13}C NMR spectra for compounds **9**-**16**, **18**,**19**, **20**-**24**, **27** and **29**; ^{1}H NMR spectra for compounds **17** and **19**.
3. X-ray crystallographic details for **12**.
4. Electronic absorption spectra for:
    a. TMS-end-capped *iso*-PDA oligomers: **13**, **15**, **17**, and **23**.
    b. Adamantylidene substituted *iso*-PDA oligomers: **27** and **28**.
    c. The comparison of pentamers **15**, **16** and **28**
    d. Compound **21** in various solvents.
    e. Compound **15** at various concentrations.
5. Approximated Band-gaps (E_g) for TMS and TIPS End-capped *iso*-PDAs.

General experimental details. Column chromatography: *silica gel-60* (230-400 mesh) from *General Intermediates of Canada*. Thin layer chromatography (TLC): aluminum sheet coated with *silica gel* F_{254} from *Whatman*; visualization by UV light or $KMnO_4$ stain. Melting point: *Fisher-Johns* or *Gallenkamp* apparatus; uncorrected. UV-Vis spectra: *Pharmacia Biotech Ultrospec 300* or *Varian Cary 400* at rt; λ in nm (ε in $L \cdot M^{-1} \cdot cm^{-1}$). IR spectra ($cm^{-1}$): *Nicolet Magna-IR 750* (neat) or *Nic-Plan IR Microscope* (solids). ^{1}H- and ^{13}C-NMR: *Varian Gemini-300* or *-500* and *Bruker AM-300* instruments, at rt in benzene-d_6 or $CDCl_3$; solvent peaks (7.15 and 7.24 ppm for ^{1}H and 127.9 and 77.0 ppm for ^{13}C) as reference. EI MS (*m/z*): *Kratos MS 50* instrument. ES MS (*m/z*): *Micromass Zabspec oaTOF* or *PE Biosystems Mariner TOF* instruments; solvent: CH_3NO_2. Elemental analyses were performed by the Microanalytical Service, Department of Chemistry-University of Alberta.

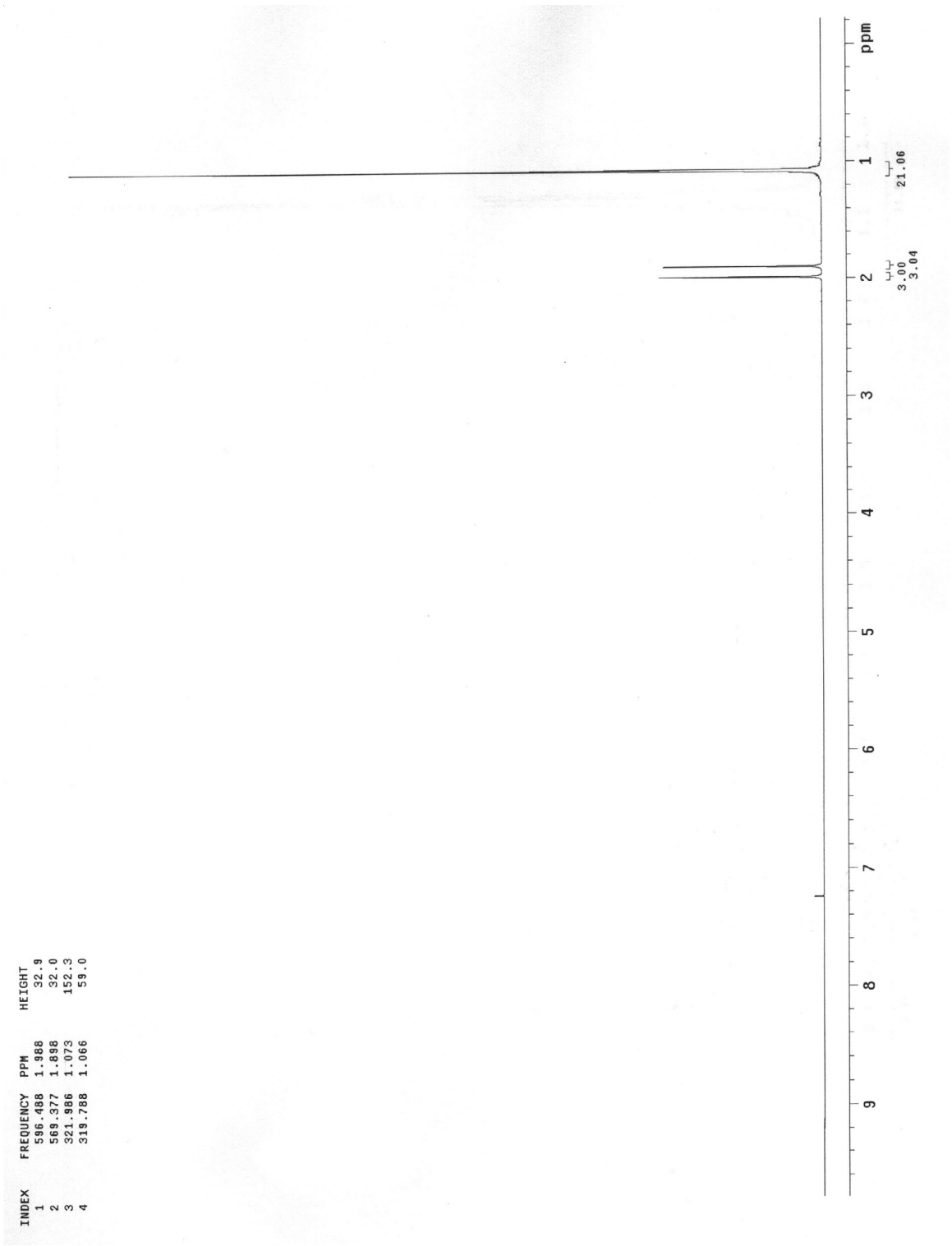


Fig. S1. ^{1}H NMR Spectrum of Compound **9**.

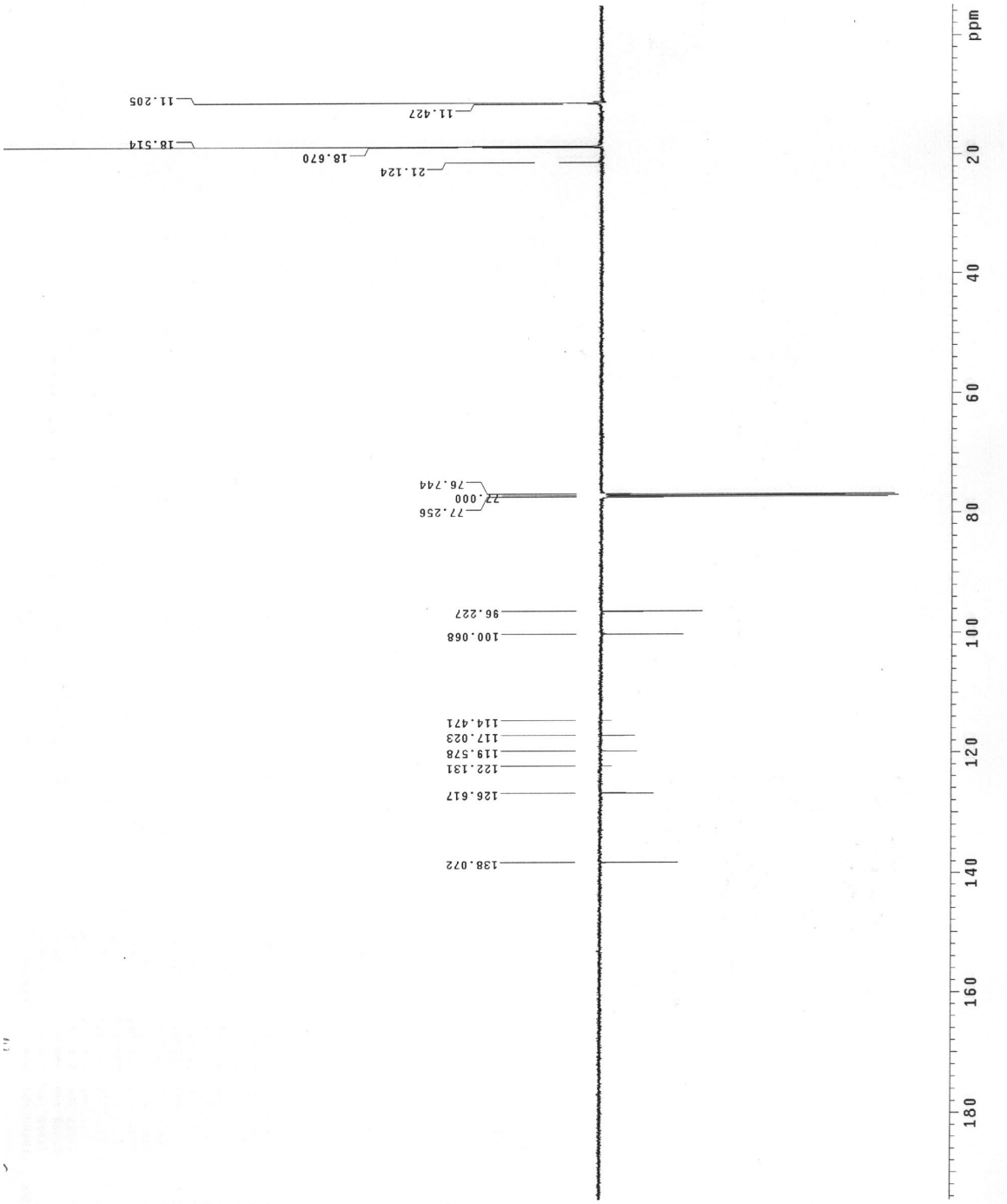


Fig. S2. ^{13}C NMR Spectrum of Compound **9**.

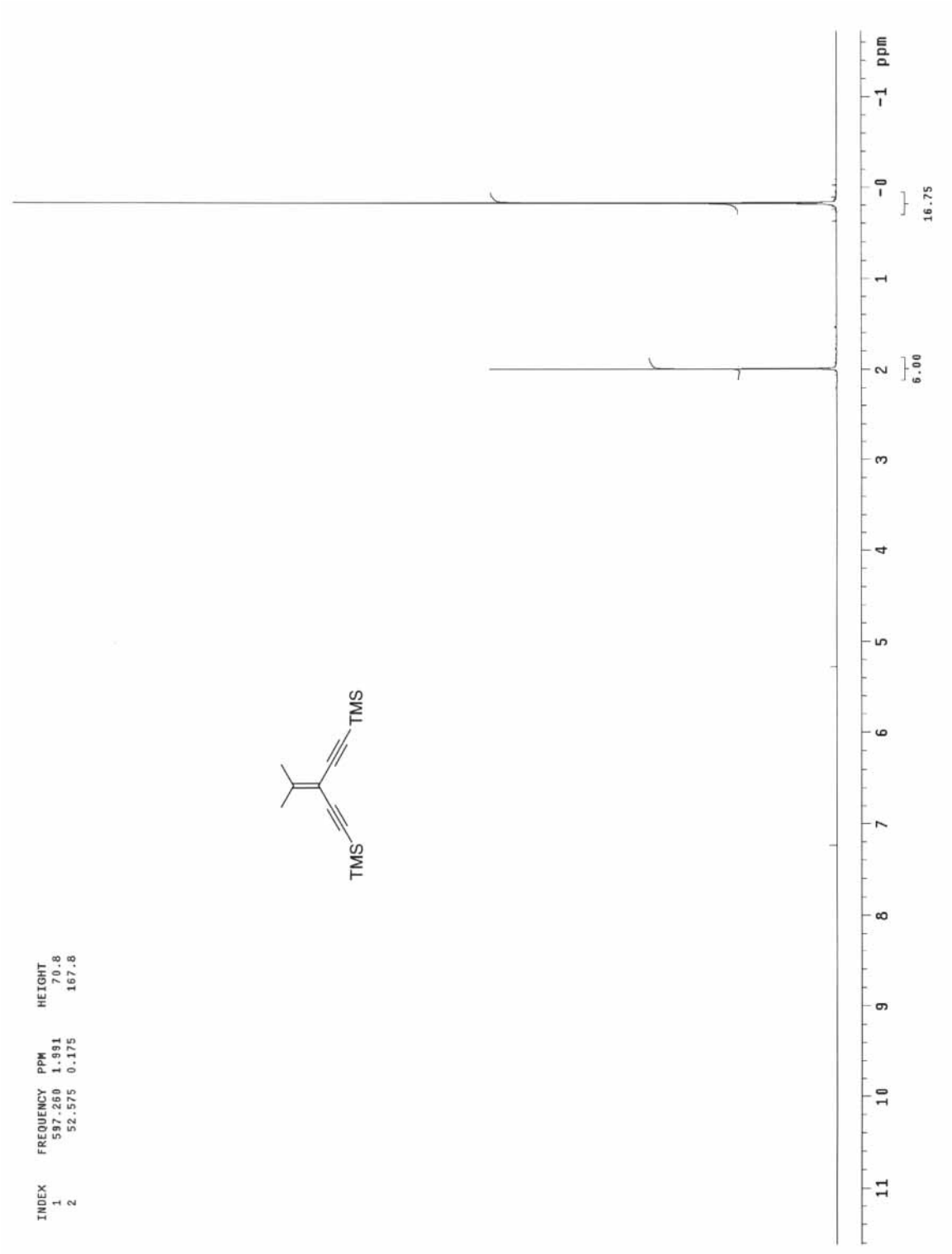


Fig. S3. ^{1}H NMR Spectrum of Compound **10**.

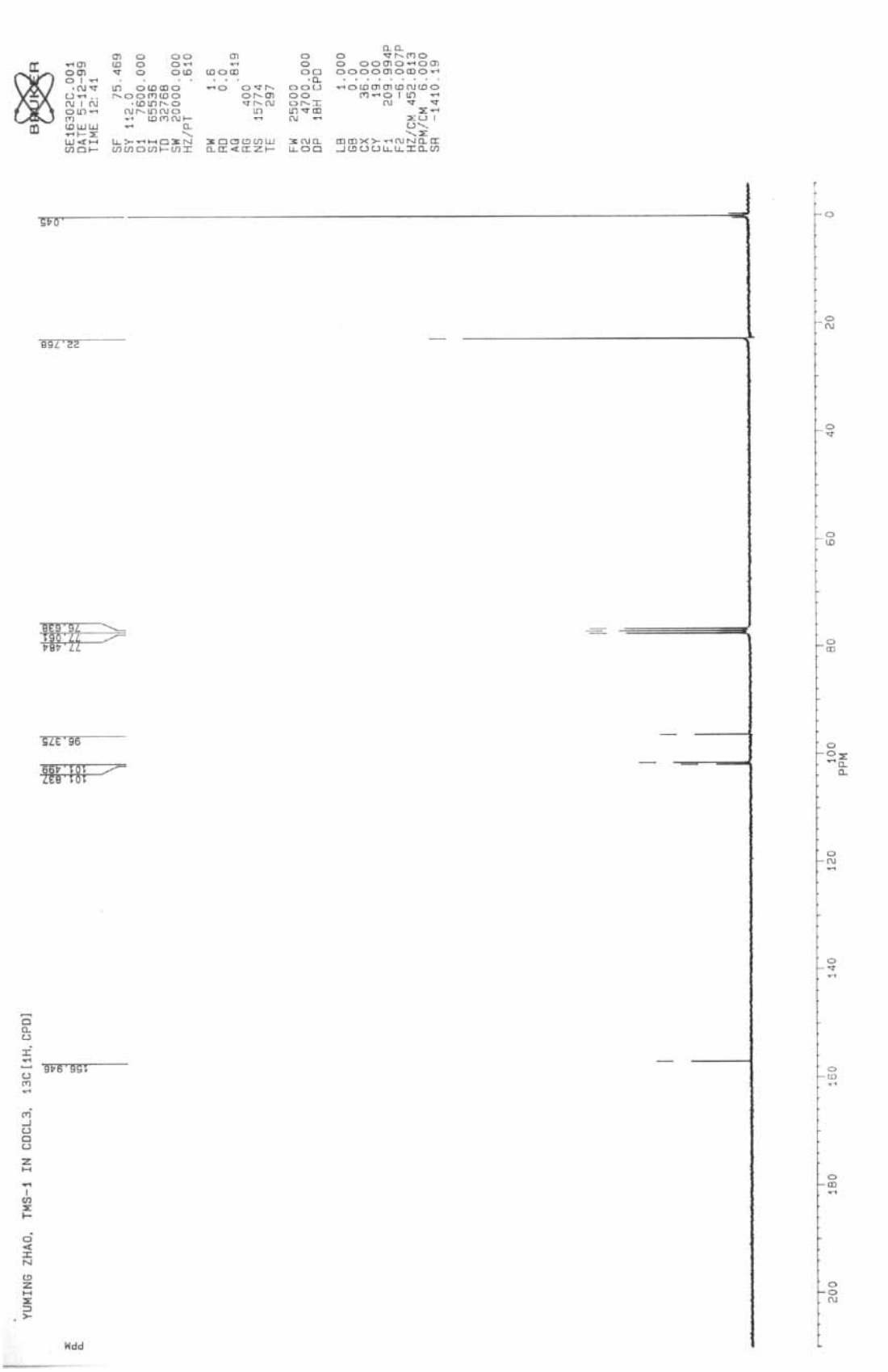


Fig. S4. ^{13}C NMR Spectrum of Compound **10**.

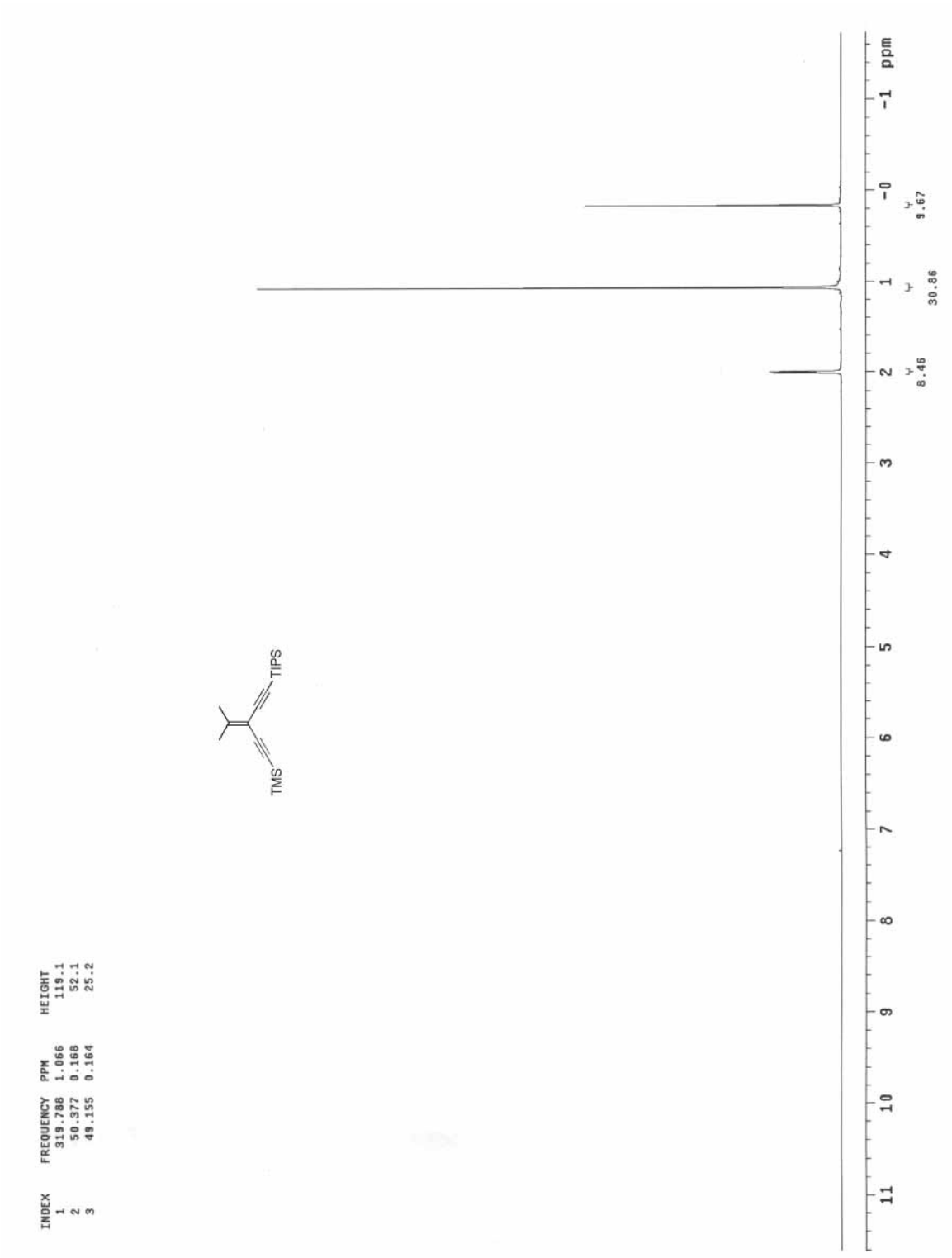


Fig. S5. ^{1}H NMR Spectrum of Compound **11**.

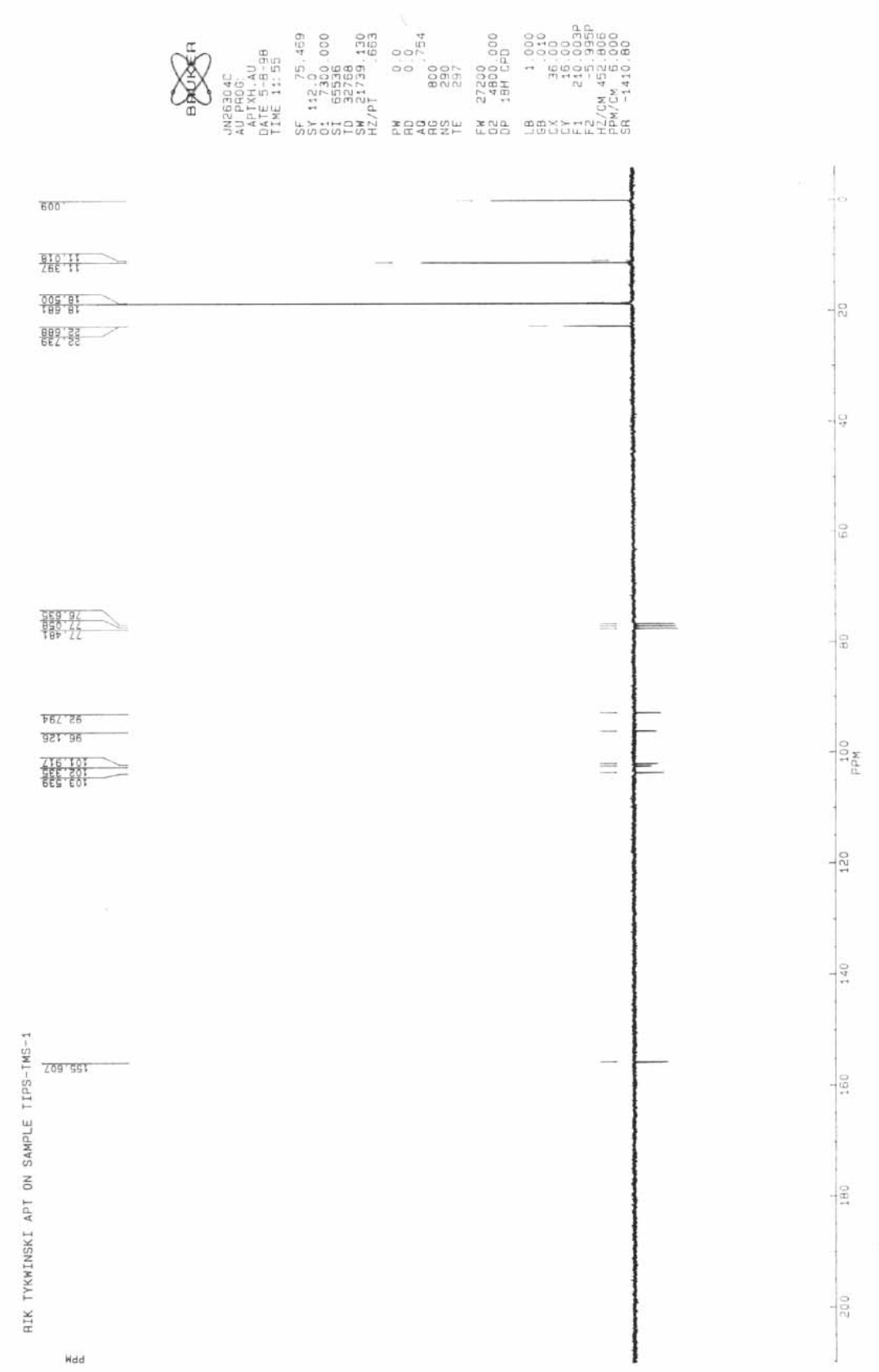


Fig. S6. ^{13}C NMR Spectrum of Compound **11**.

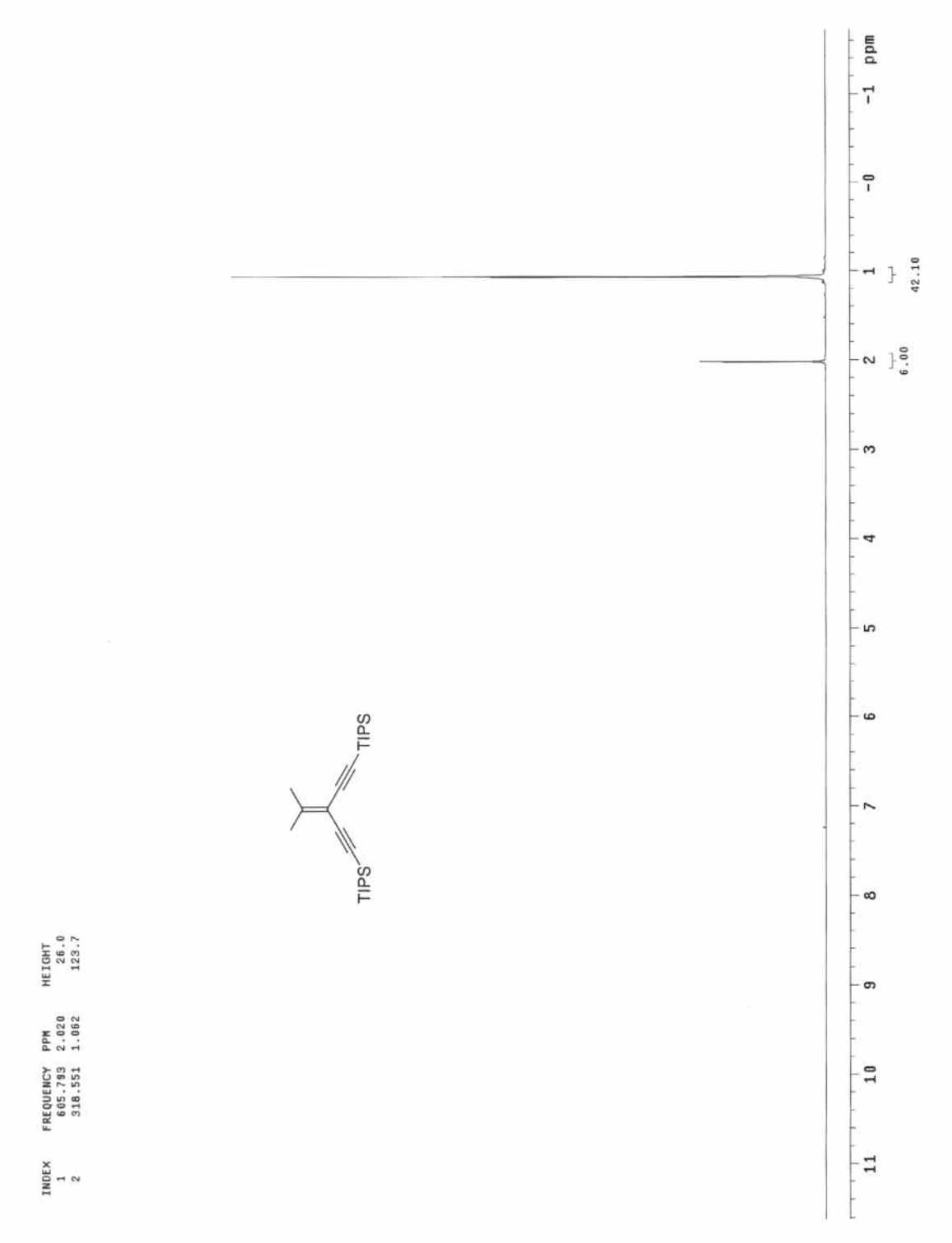


Fig. S7. ^{1}H NMR Spectrum of Compound **12**.

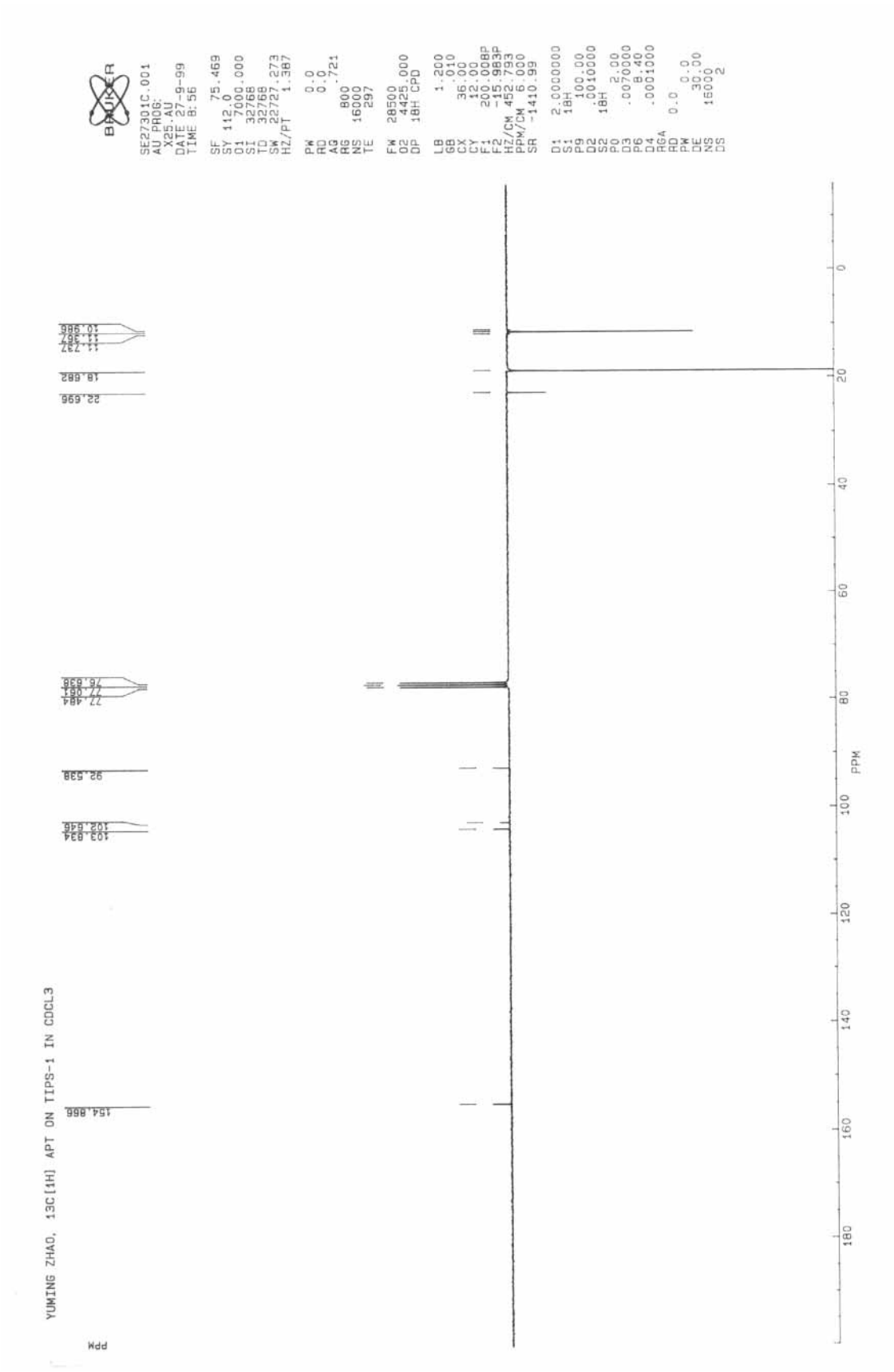


Fig. S8. ^{13}C NMR Spectrum of Compound **12**.

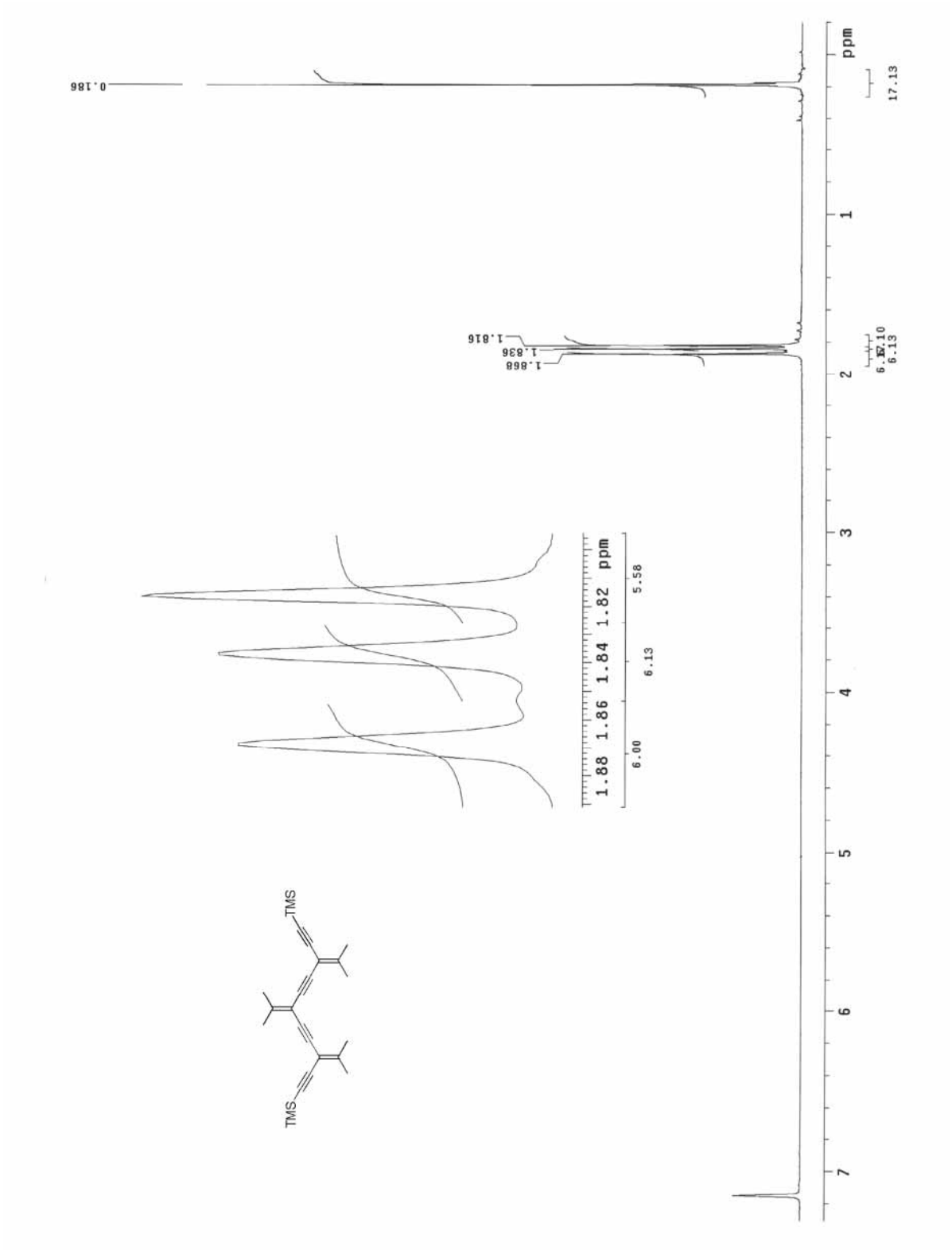


Fig. S9. ^{1}H NMR Spectrum of Compound **13**.

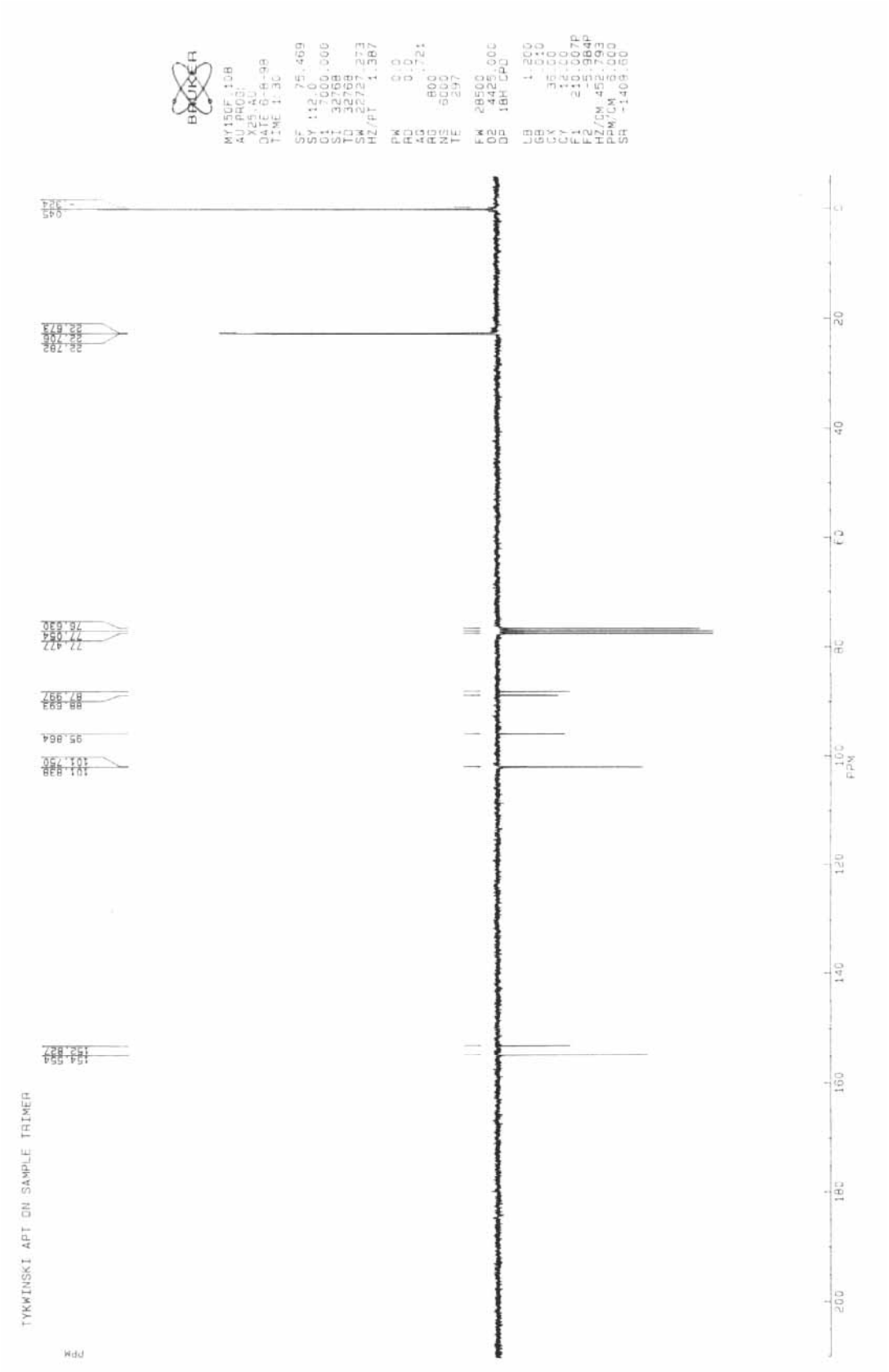


Fig. S10. ^{13}C NMR Spectrum of Compound **13**.

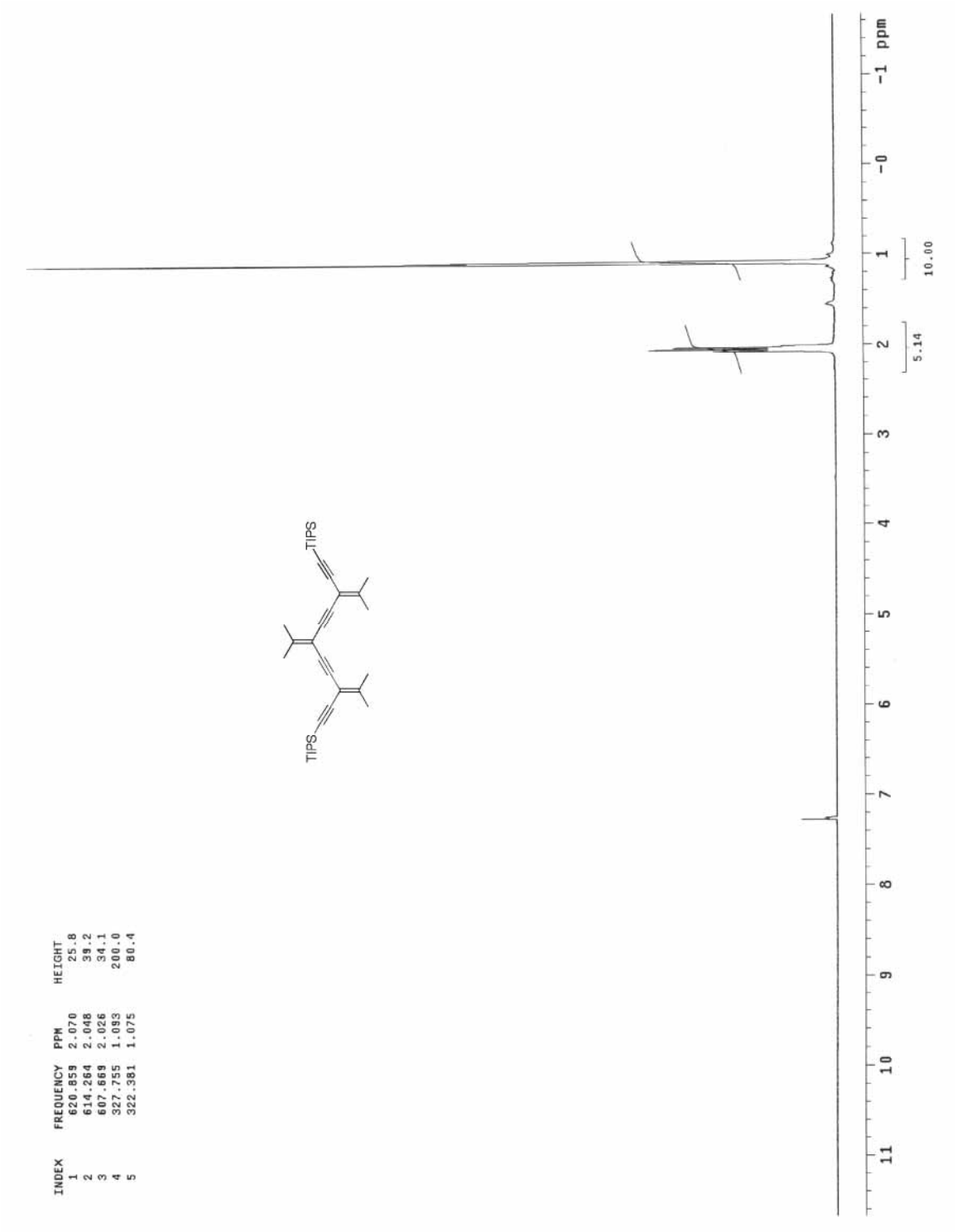


Fig. S11. ^{1}H NMR Spectrum of Compound **14**.

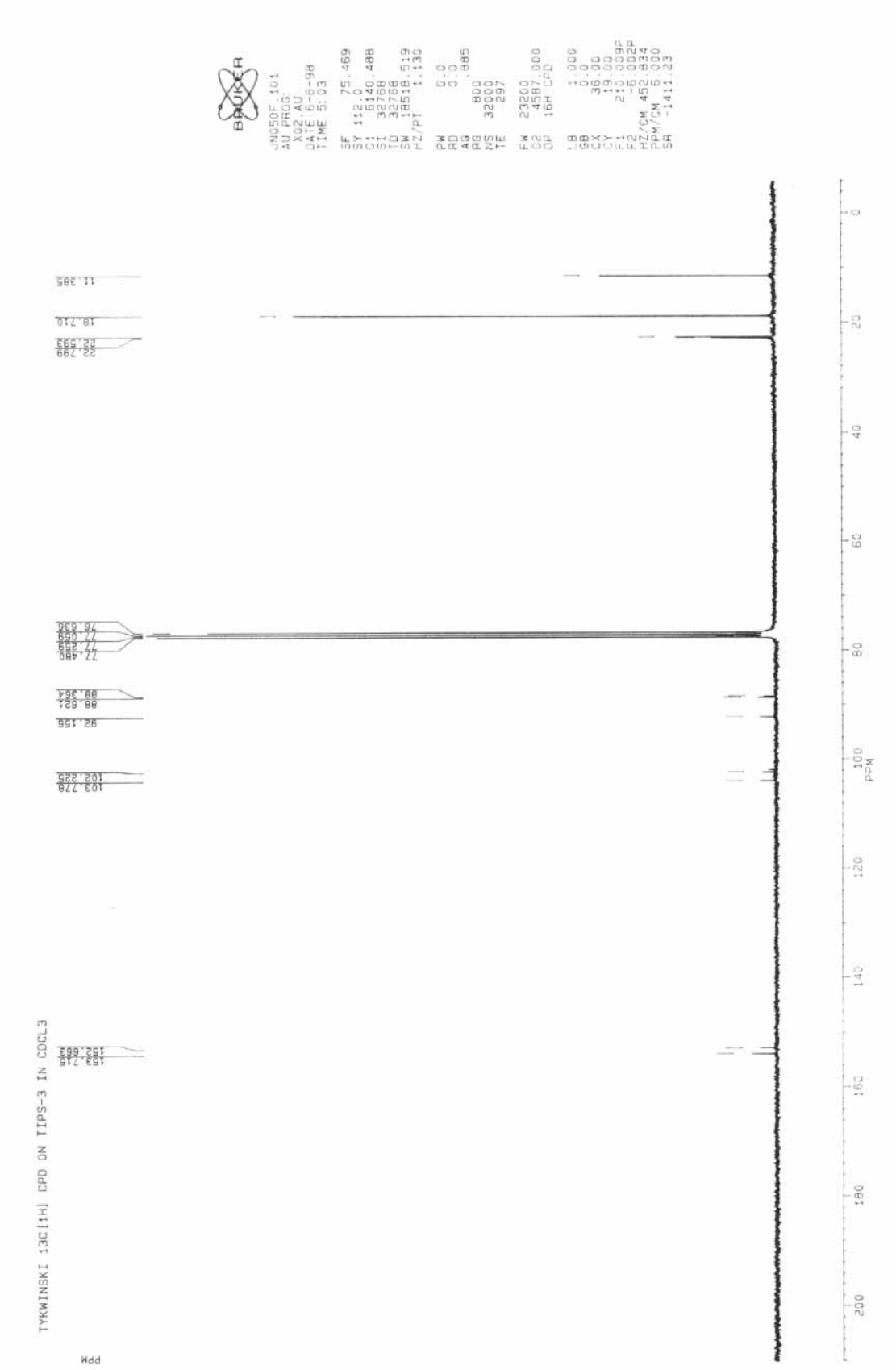


Fig. S12. ^{13}C NMR Spectrum of Compound **14**.

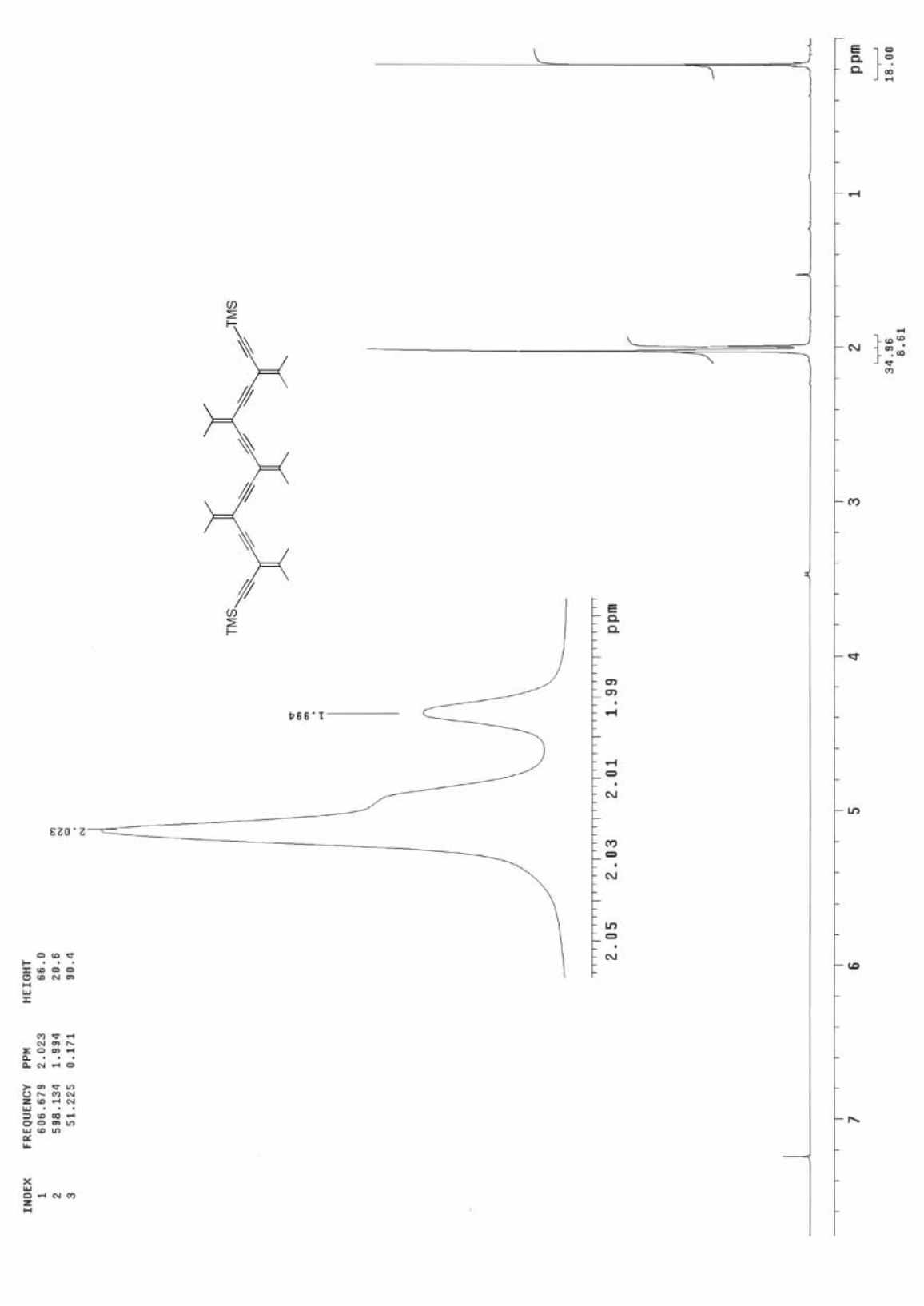


Fig. S13. ^{1}H NMR Spectrum of Compound **15**.

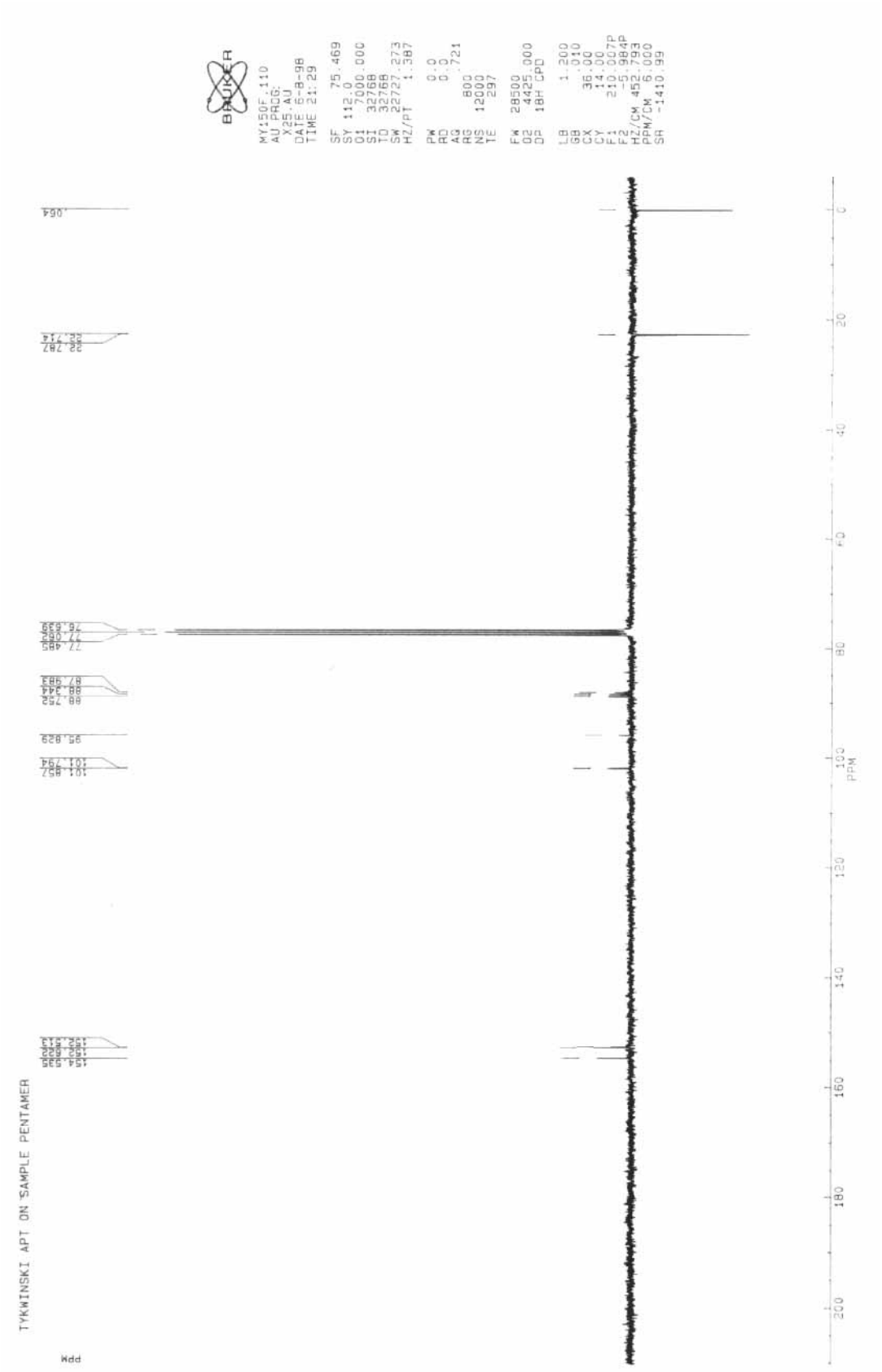
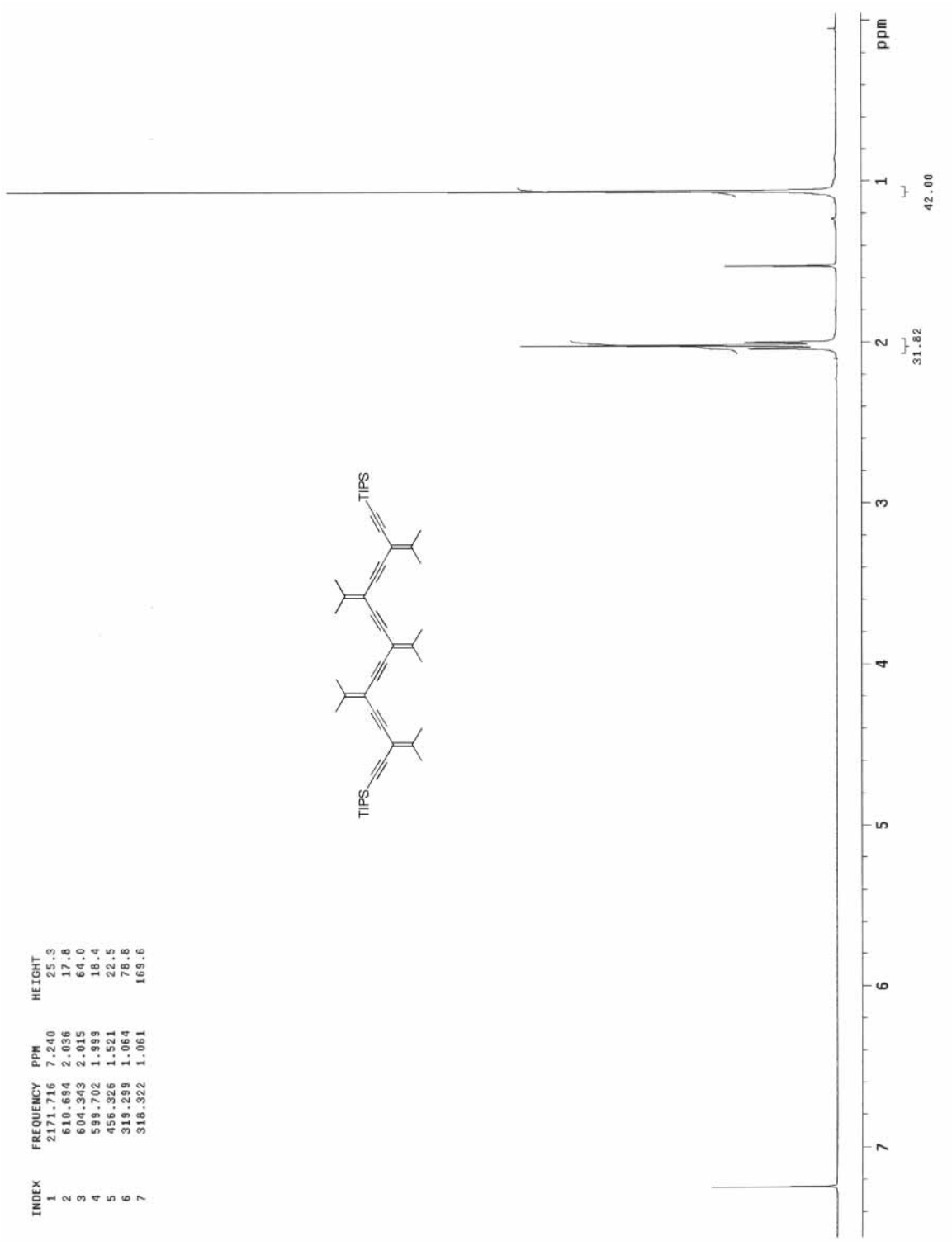


Fig. S14. ^{13}C NMR Spectrum of Compound **15**.



INDEX	FREQUENCY	PPM	HEIGHT
1	2171.716	7.240	25.3
2	610.694	2.036	17.8
3	604.343	2.015	64.0
4	599.702	1.999	18.4
5	456.326	1.521	22.5
6	319.239	1.064	78.8
7	318.322	1.061	169.6

Fig. S15. ^{1}H NMR Spectrum of Compound **16**.

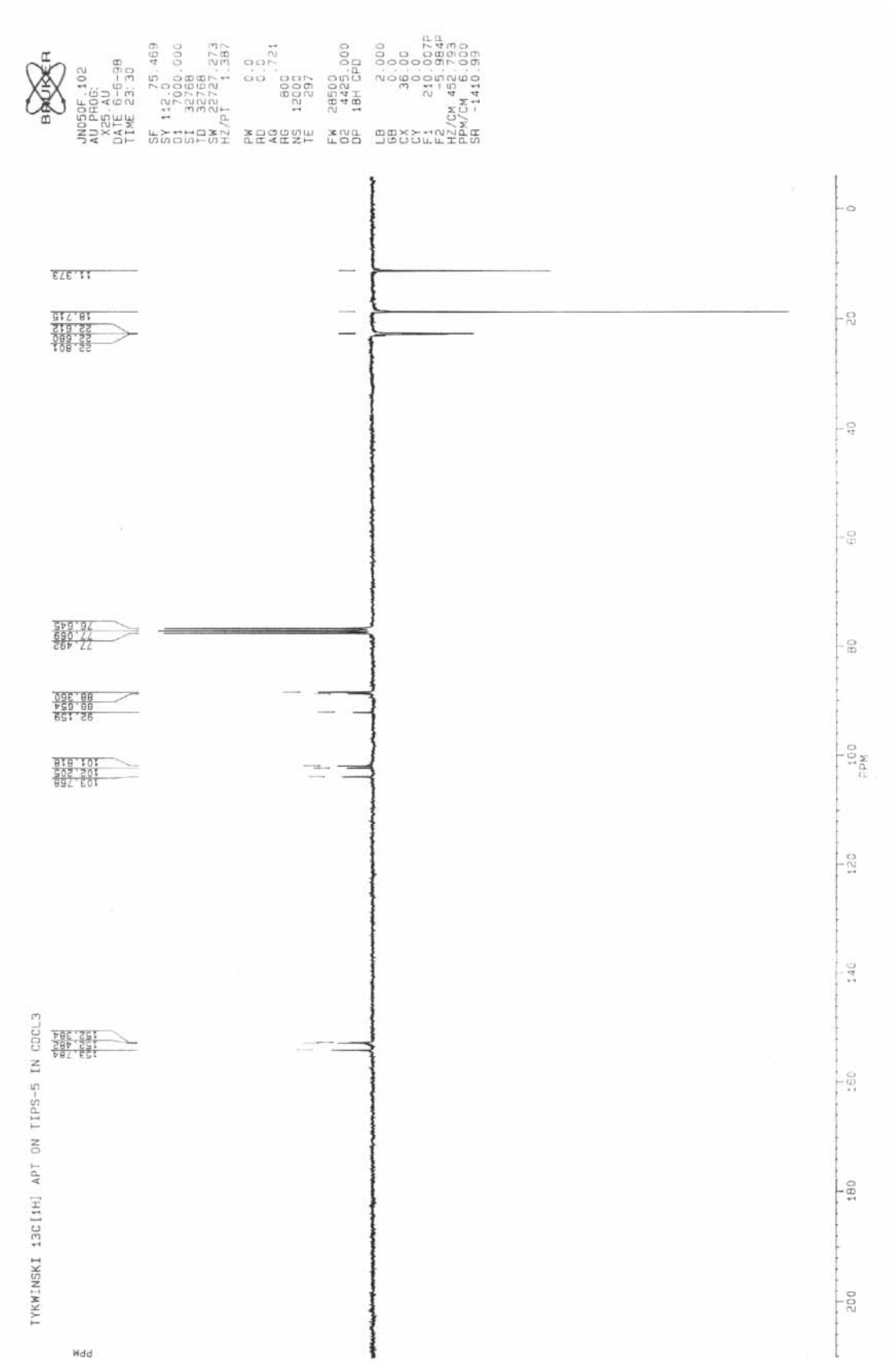


Fig. S16. ^{13}C NMR Spectrum of Compound **16**.

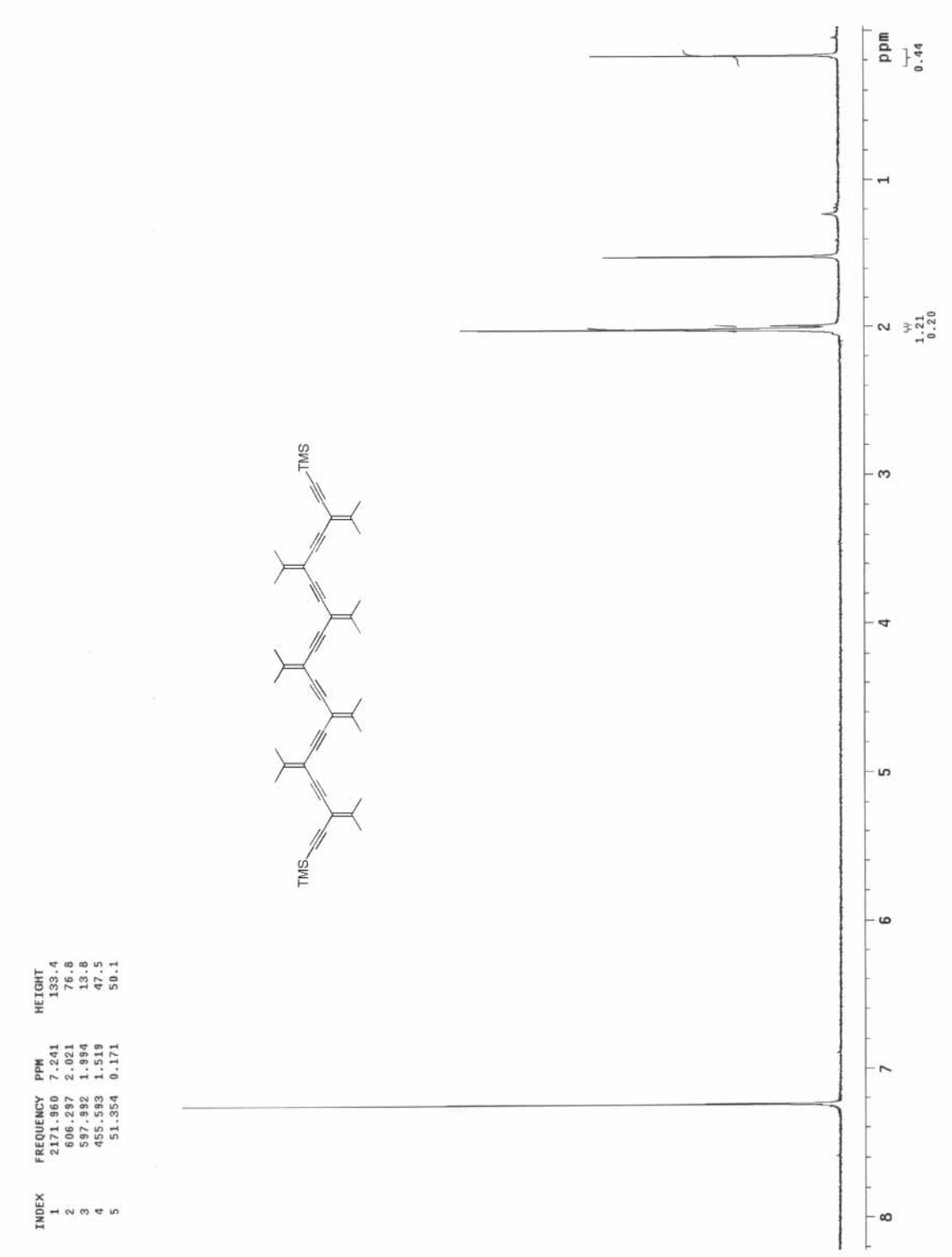


Fig. S17. ^{1}H NMR Spectrum of Compound **17**.

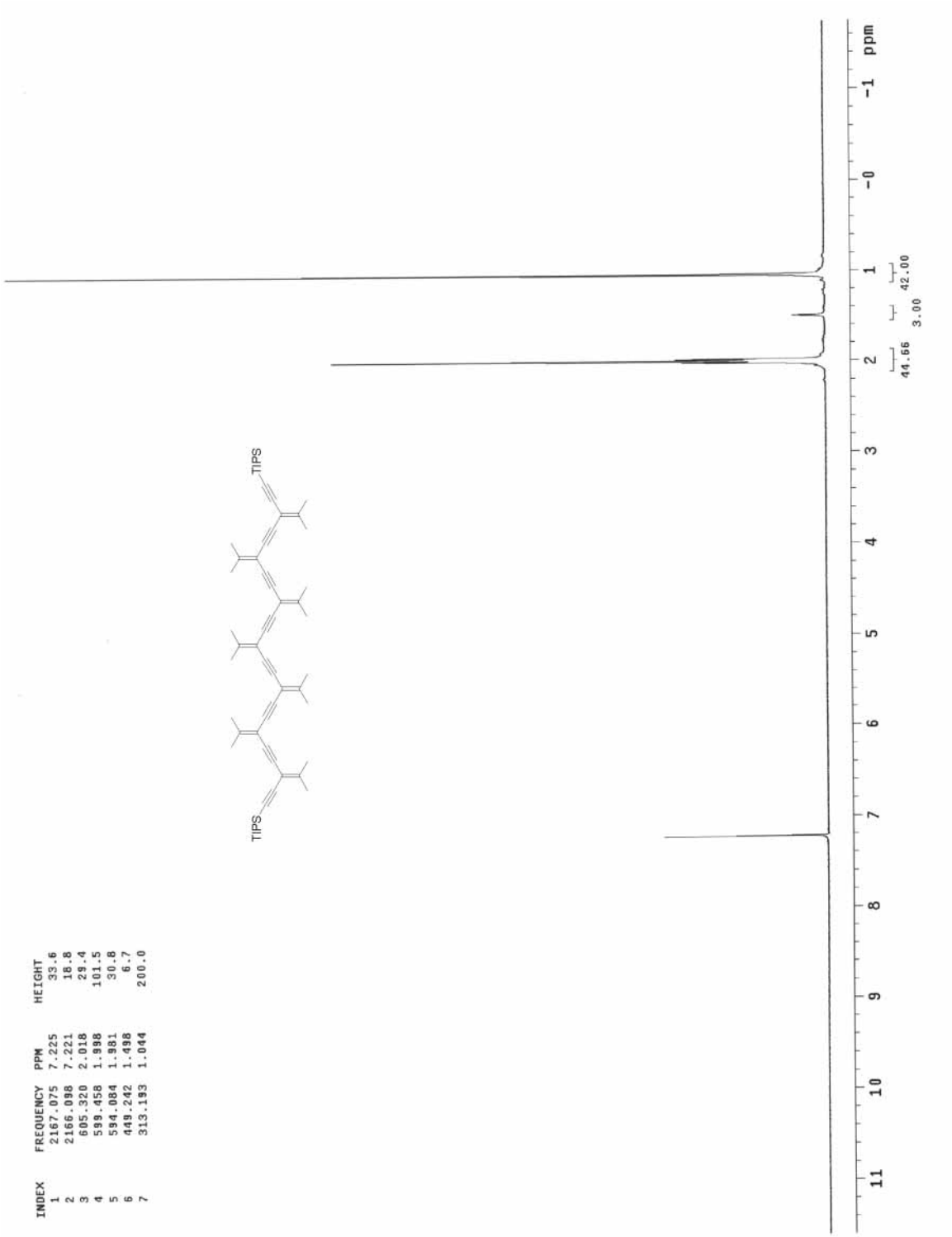


Fig. S18. ^{1}H NMR Spectrum of Compound **18**.