

Supporting Information

Design, Synthesis, Structural and Spectroscopic Studies of Push-Pull Two-Photon Absorbing Chromophores with Acceptor Groups of Varying Strength

Alma R. Morales,[†] Andrew Frazer,[†] Adam W. Woodward,[†] Hyo-Yang Ahn-White,[†] Alexandr Fonari,[§] Paul Tongwa,[§] Tatiana Timofeeva,[§] Kevin D. Belfield,^{†‡*}

[†]*Department of Chemistry and [‡]CREOL, The College of Optics and Photonics, University of Central Florida, Orlando, FL 32816-2366, USA. Fax: 4078232252; Tel: 4078231028;*

[§]*Department of Biology and Chemistry, New Mexico Highlands University, Las Vegas, New Mexico, 87701, USA*

E-mail: belfield@ucf.edu

Table of Contents	Pages
Crystal Packing for 1 (a), 2 (b) and 6 (c)	S2
¹ H and ¹³ C NMR Spectra	S3-S27
Cartesian Coordinates /Å of the optimized ground state geometries of compounds 1-7 at B3LYP/6-311G** level of theory in the gas phase.	S28-S33

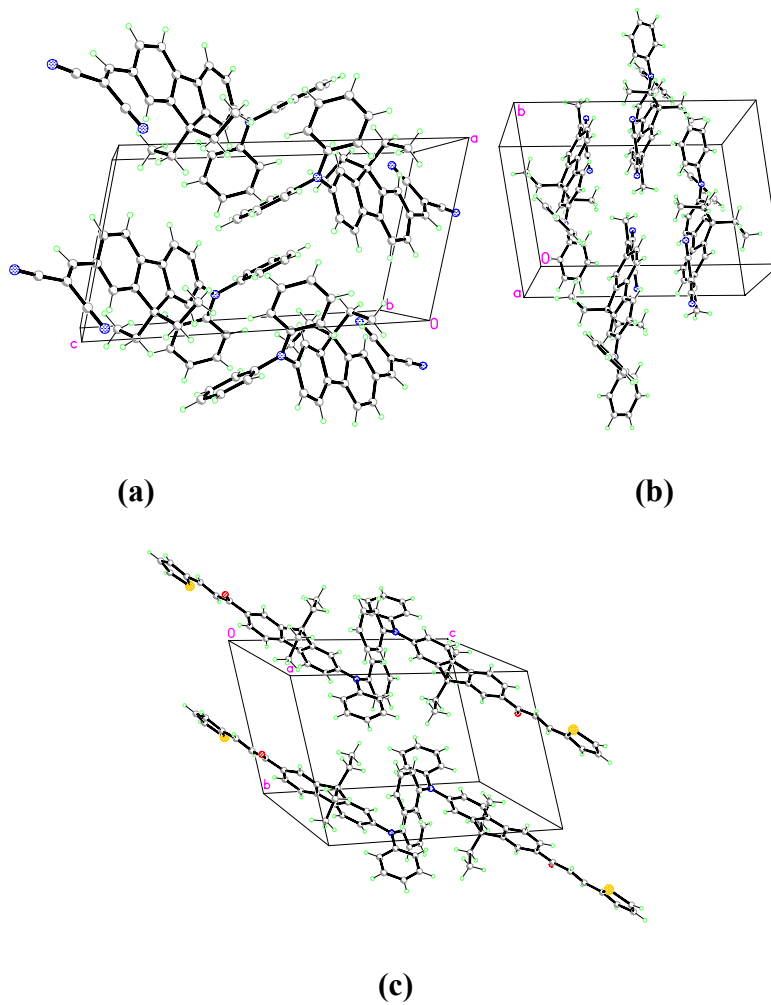


Figure S1. Crystal packing for **1** (a), **2** (b) and **6** (c).

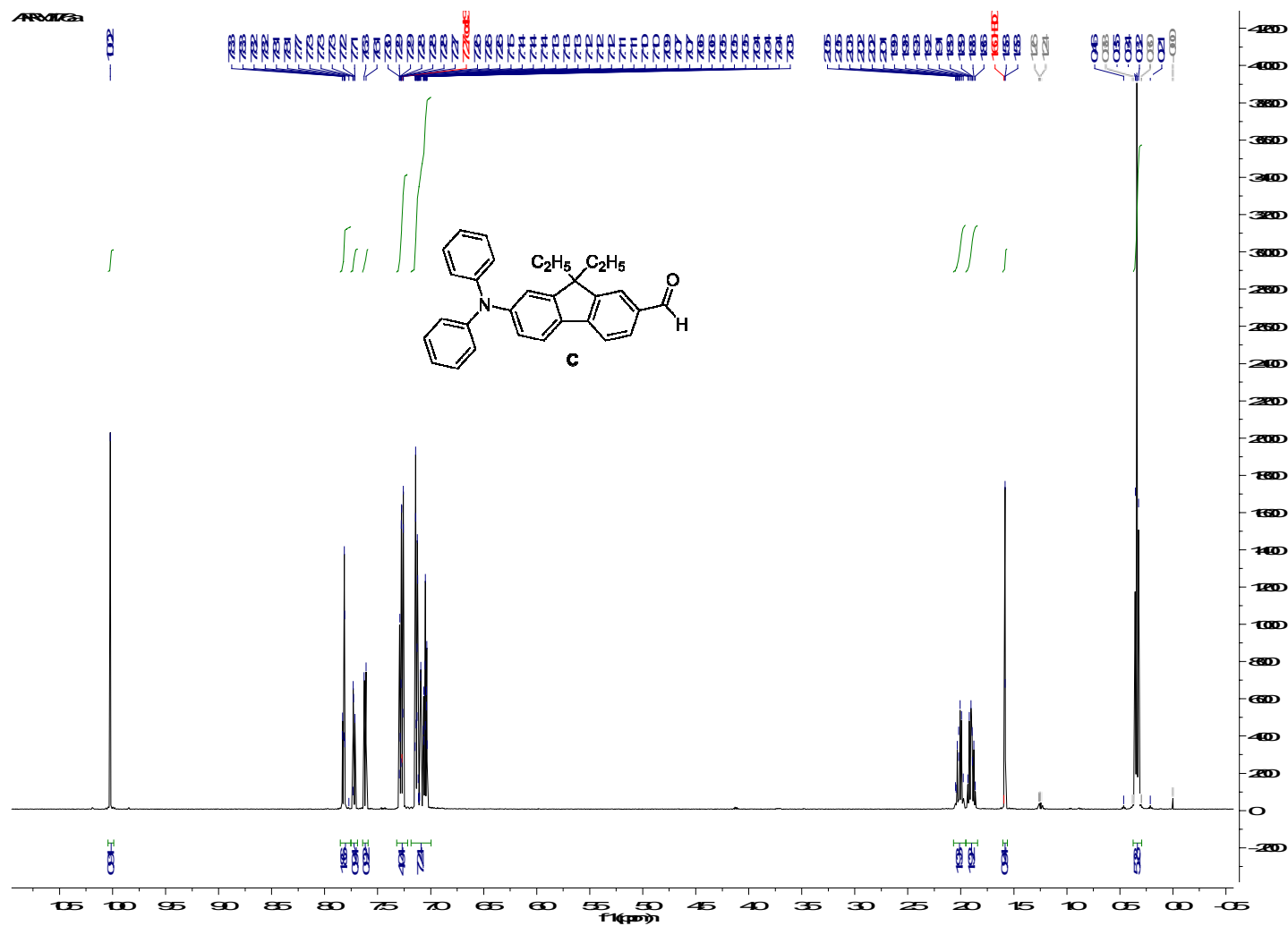


Figure S2. ¹H NMR spectrum of compound C.

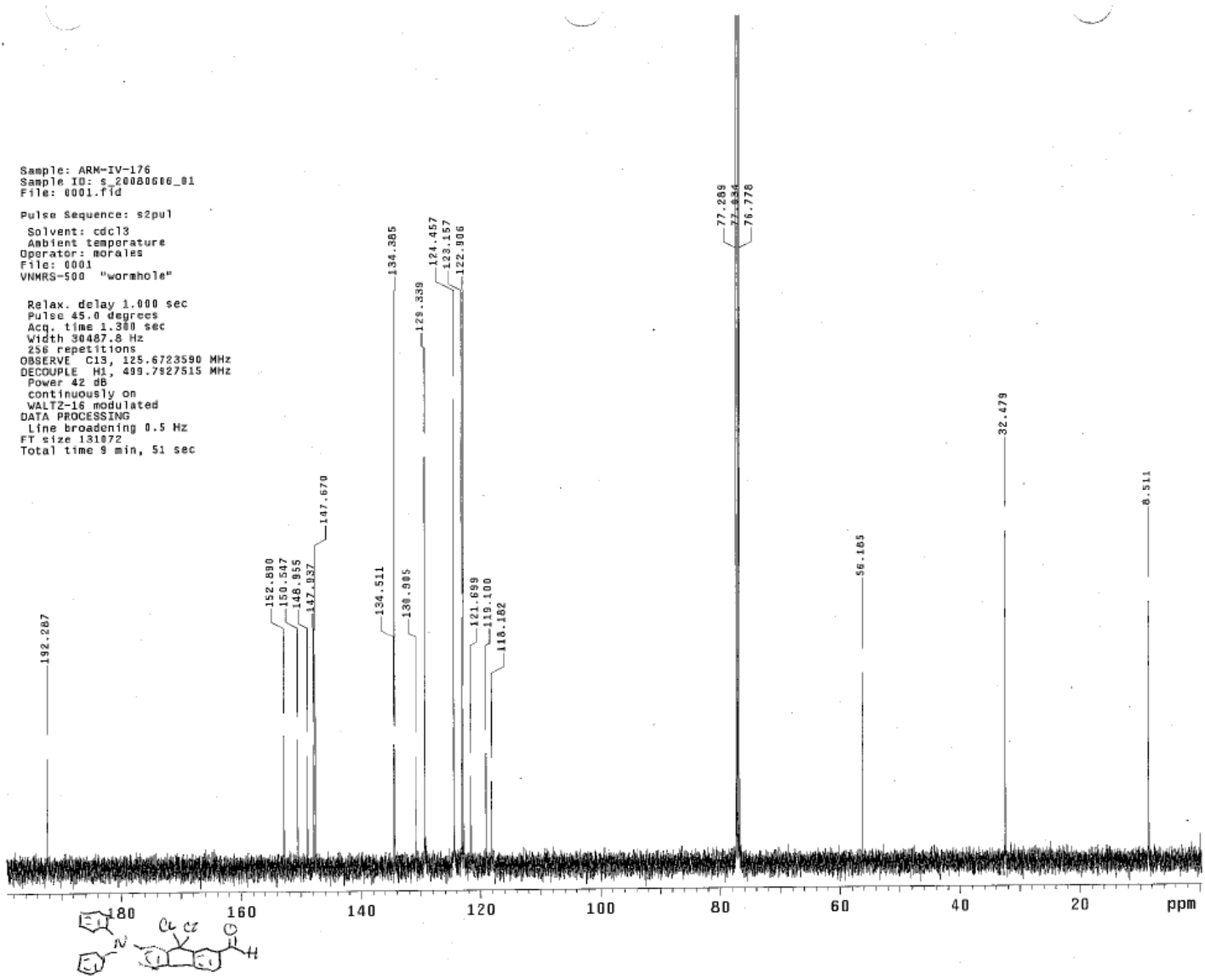


Figure S3. ¹³C NMR spectrum of compound C.

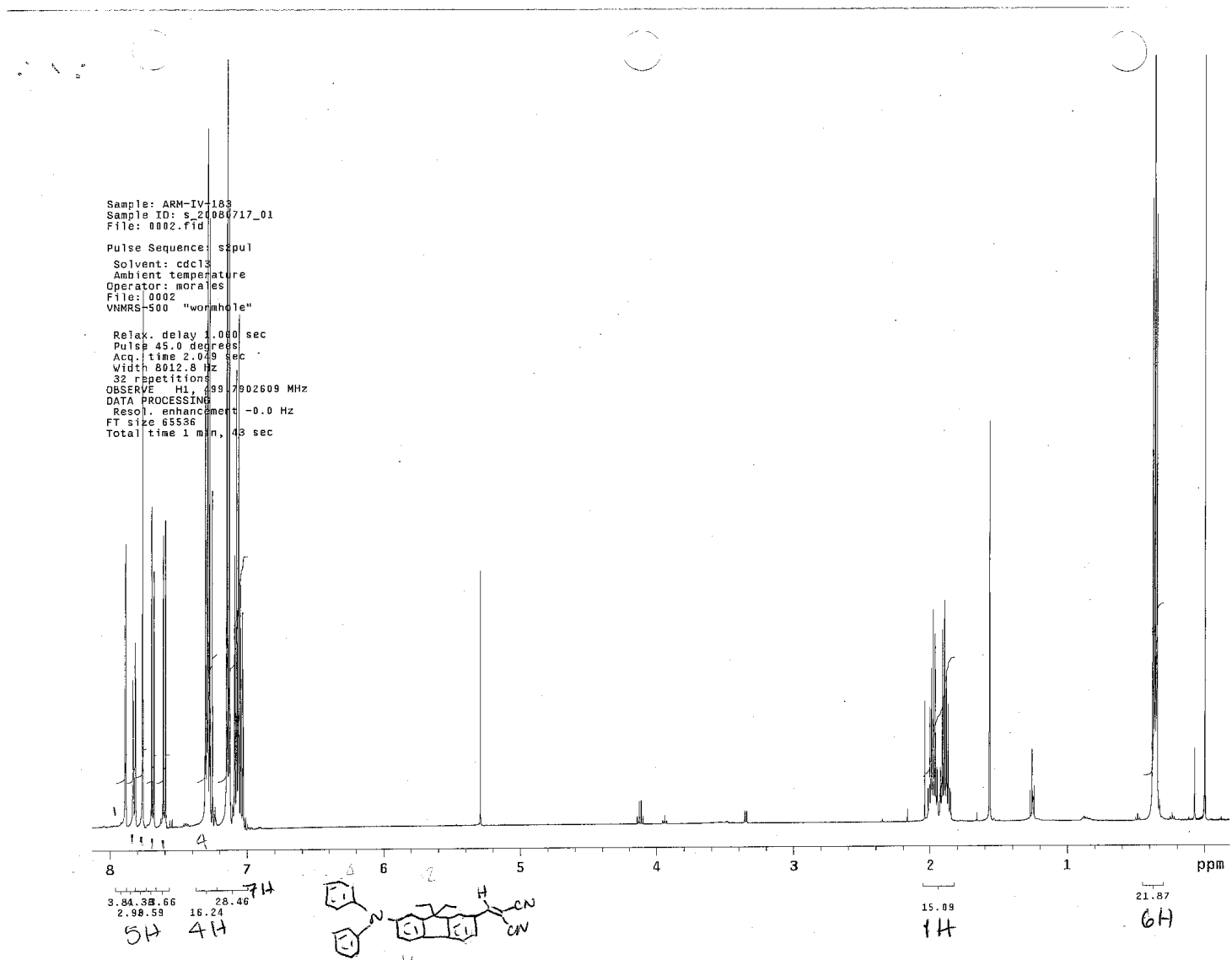


Figure S4. ^1H NMR spectrum of compound 1.

ARM-IV-184 precipitate in ether

Sample: ARM-IV-183
Sample ID: s_20080717_01
File: 0002.fid

Pulse Sequence: s2pu1

Solvent: cdc13
Ambient temperature
Operator: morales
File: 0002
VNMR5-500 "wormhole"

Relax. delay 1.000 sec
Pulse 45.0 degrees
Acq. time 1.300 sec
Width 30487.8 Hz
256 repetitions
OBSERVE C13, 125.6723590 MHz
DECOUPLE H1, 499.7927515 MHz
Power 42 dB
continuously on
WALTZ-16 modulated
DATA PROCESSING
Line broadening 0.5 Hz
FT size 131072
Total time 9 min 51 sec

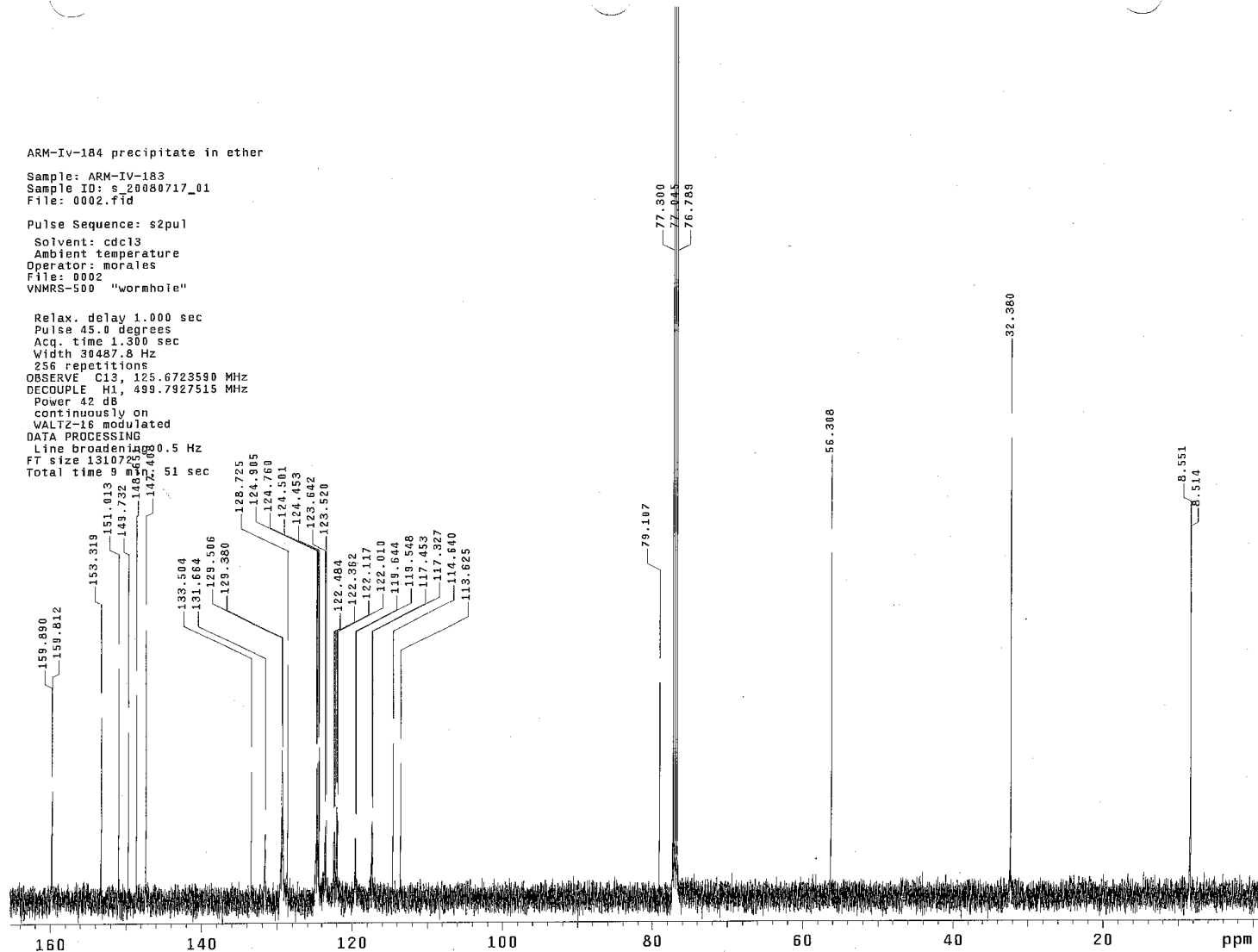


Figure S5. ^{13}C NMR spectrum of compound 1.

ARMV196
after column

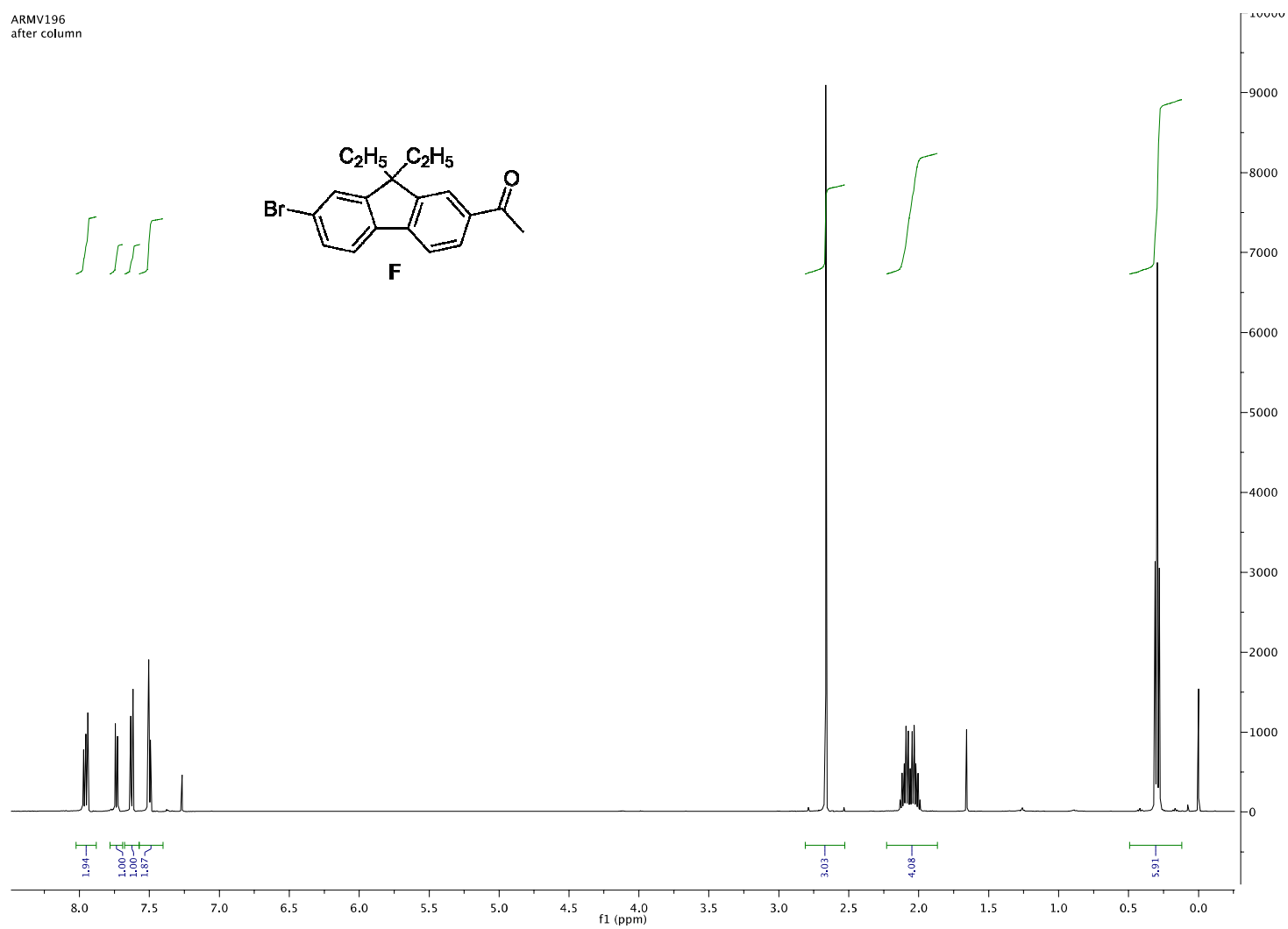


Figure S6. ¹H NMR spectrum of compound F.

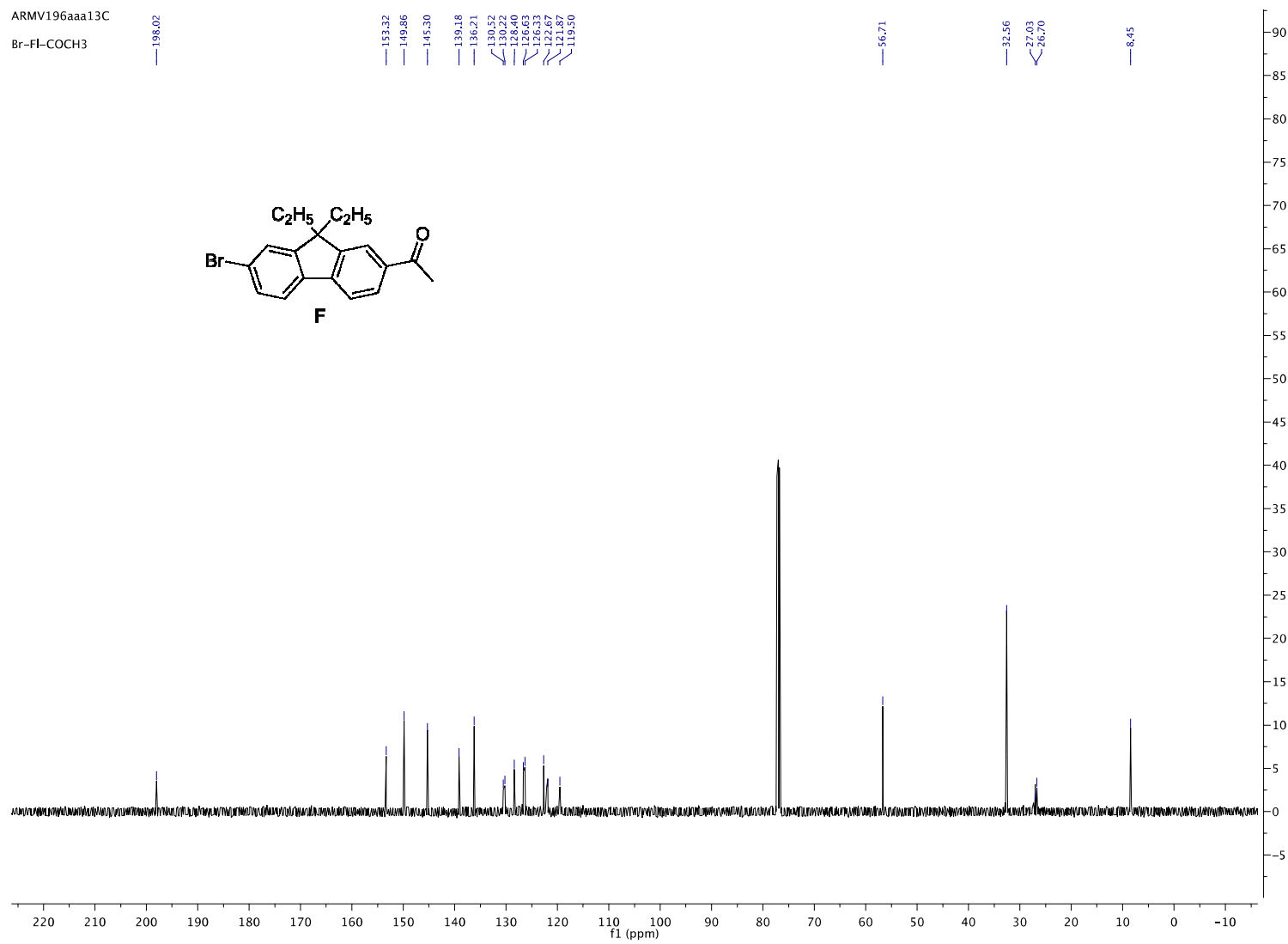


Figure S7. ¹³C NMR spectrum of compound F.

ARMV198aaa
Ph2FCOCH3

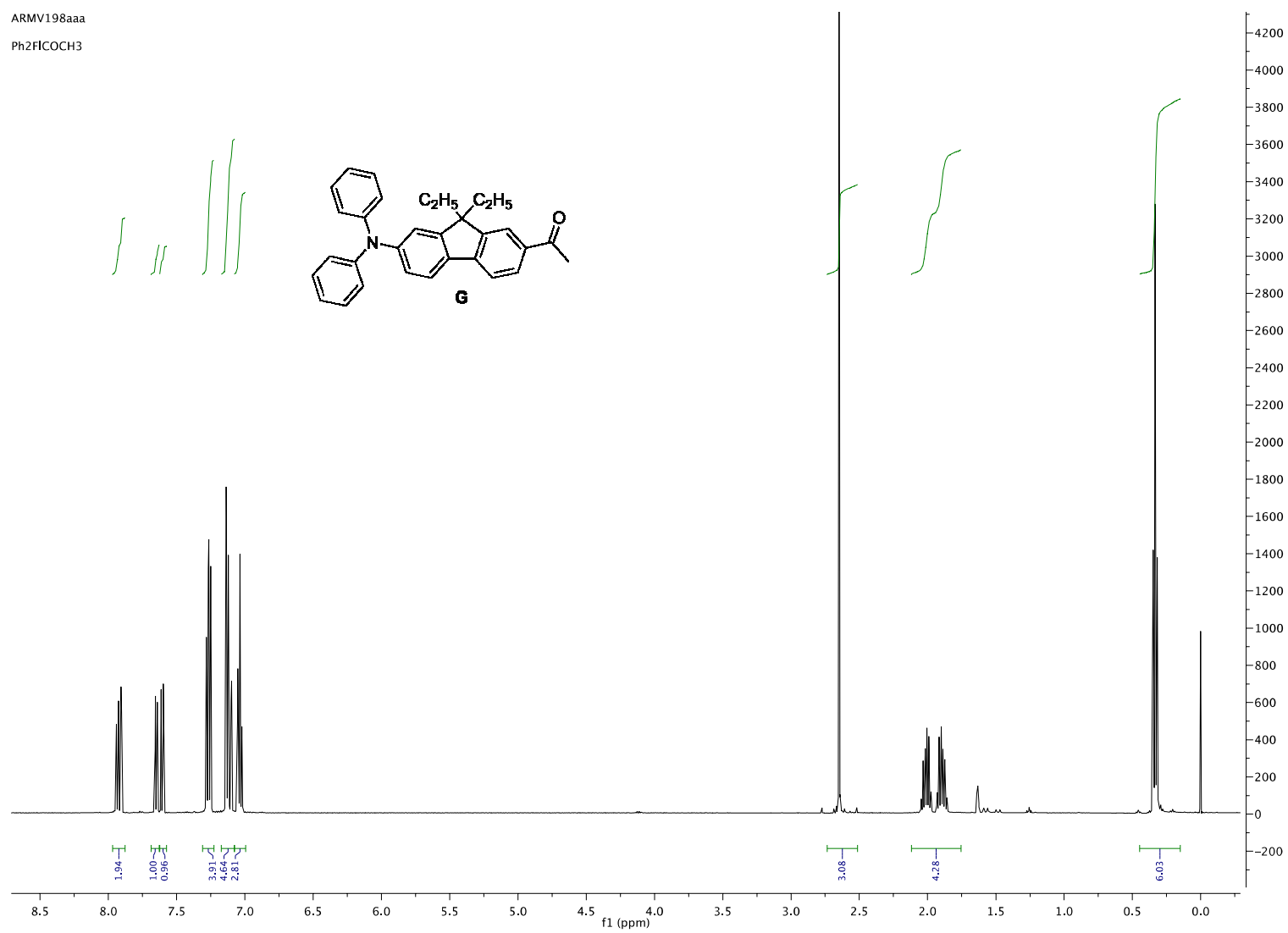


Figure S8. ¹H NMR spectrum of compound G.

ARMV198aaa13C

Ph2FCOCH3

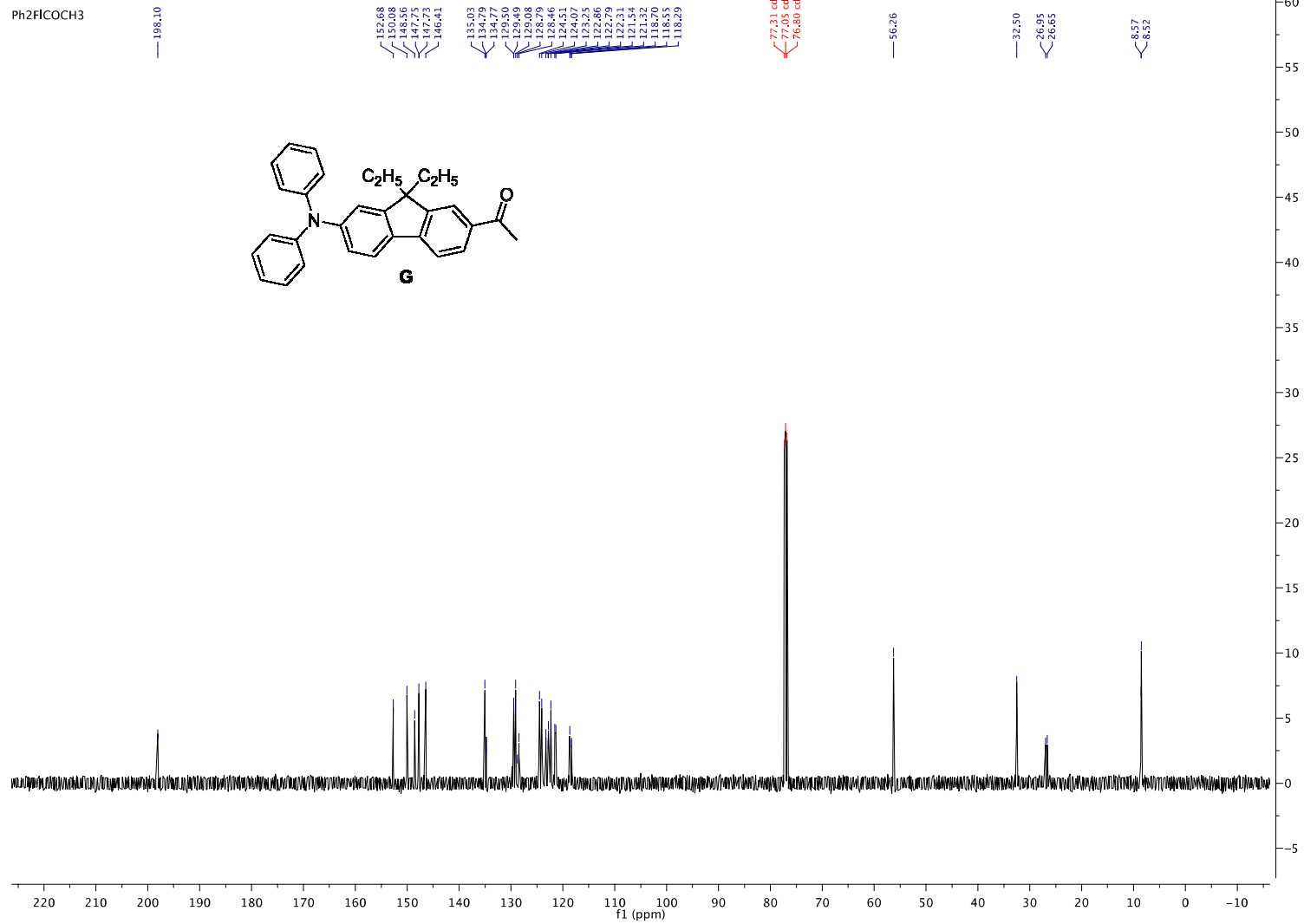


Figure S9. ^{13}C NMR spectrum of compound G.

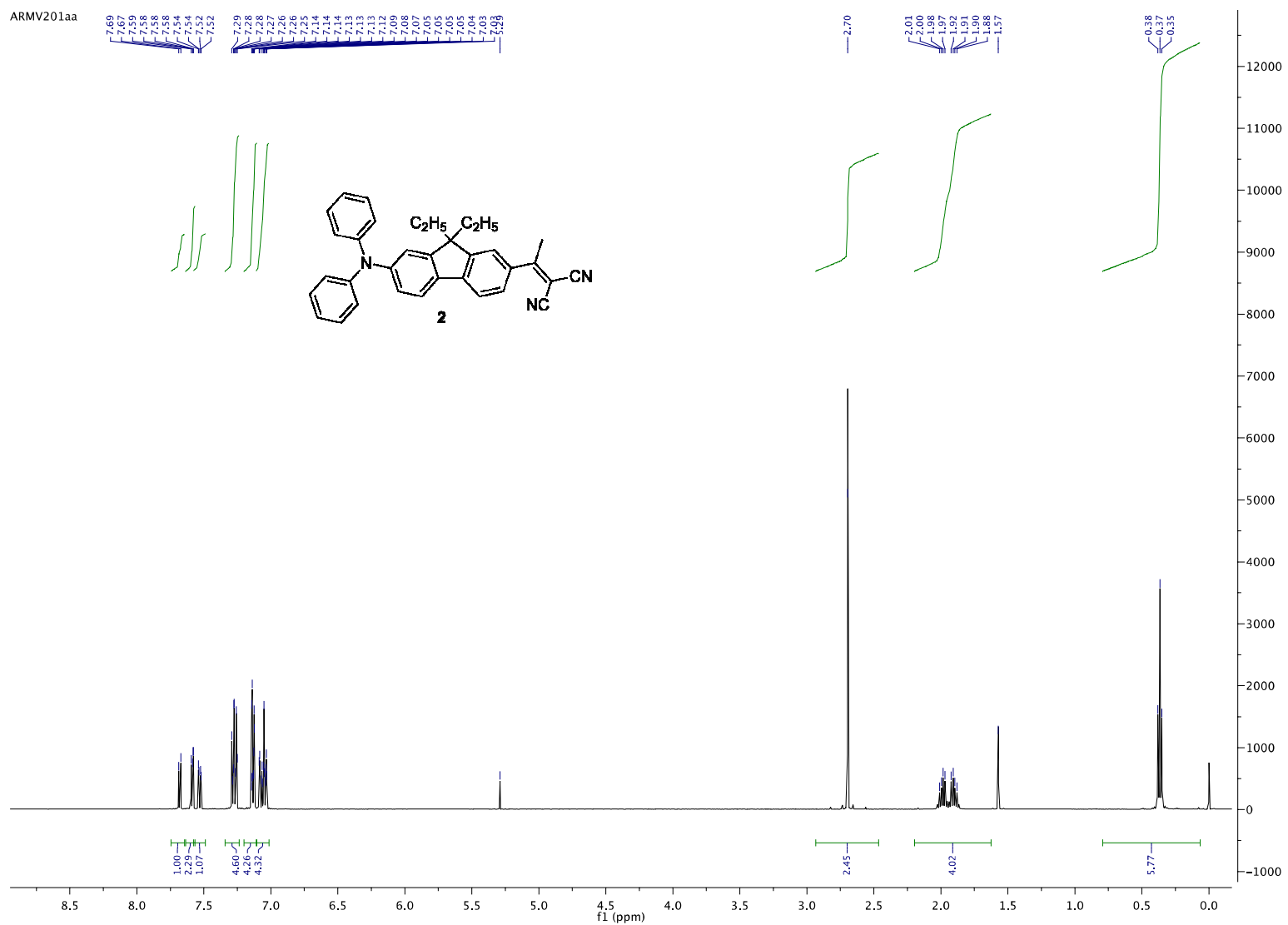


Figure S10. 1H NMR spectrum of compound **2**.

ARMv201aa13C

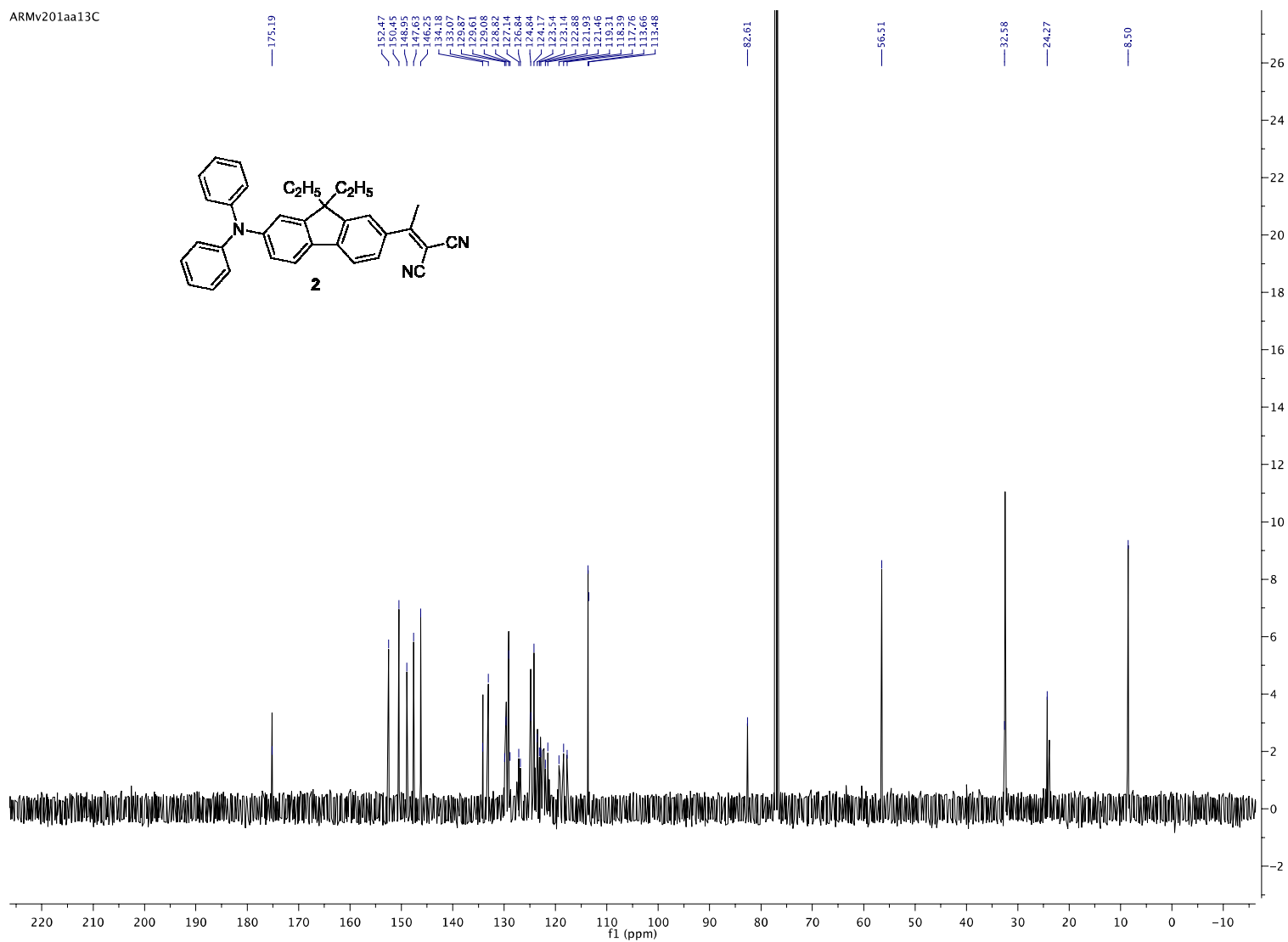


Figure S11. ¹³C NMR spectrum of compound 2.

ARMV191

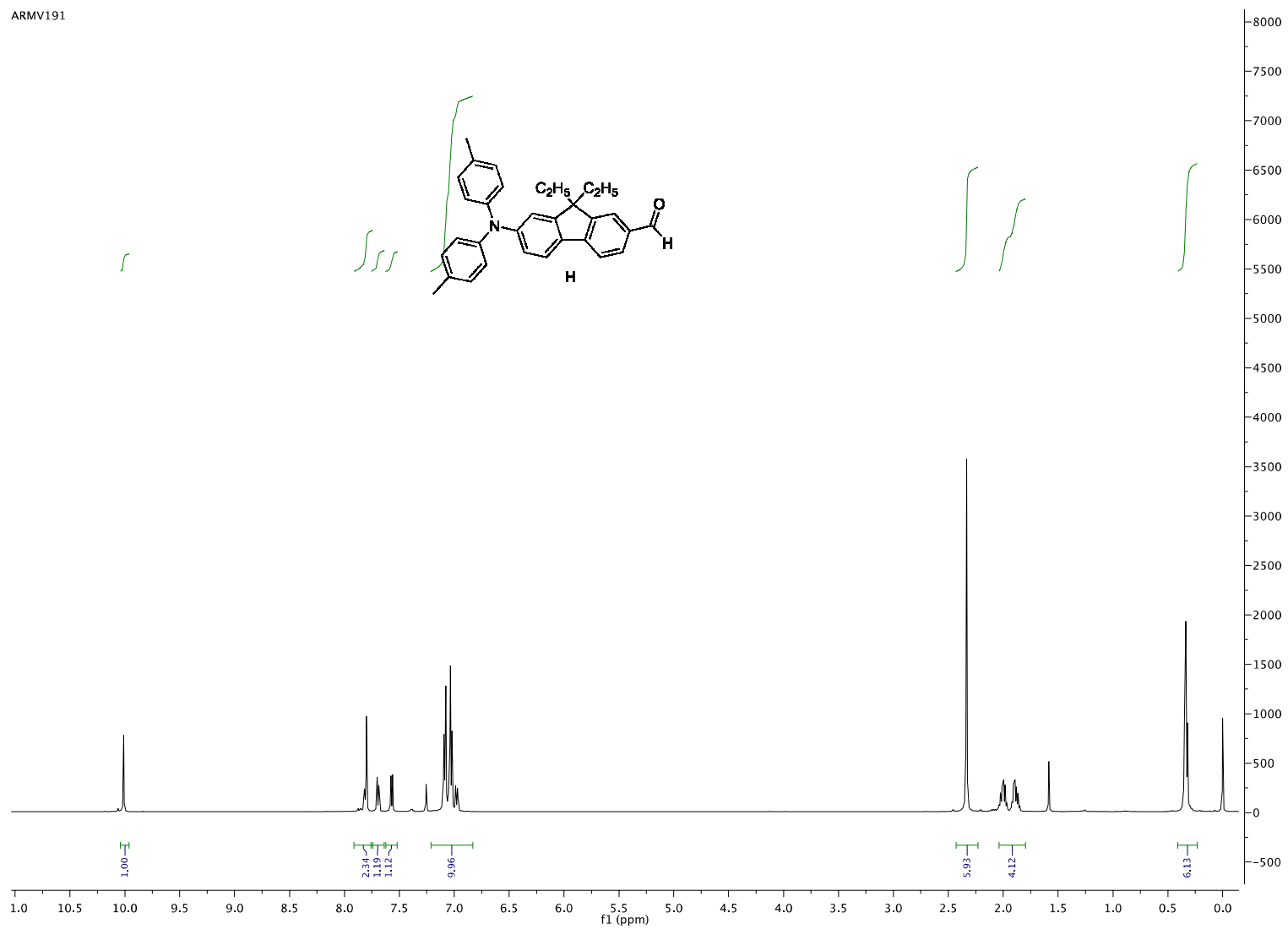


Figure S12. ¹H NMR spectrum of compound H.

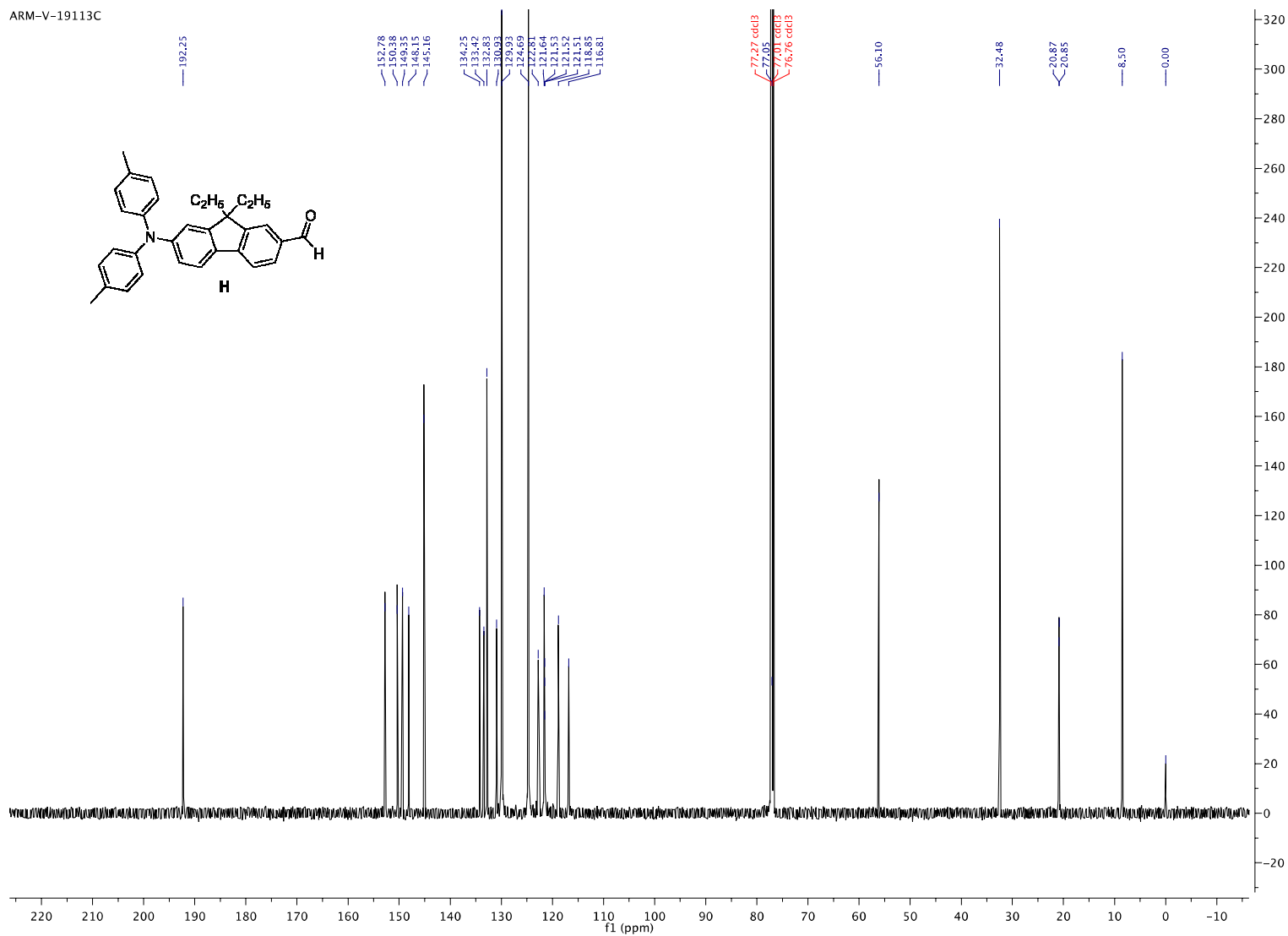


Figure S13. ^{13}C NMR spectrum of compound **H**.

ARMV192

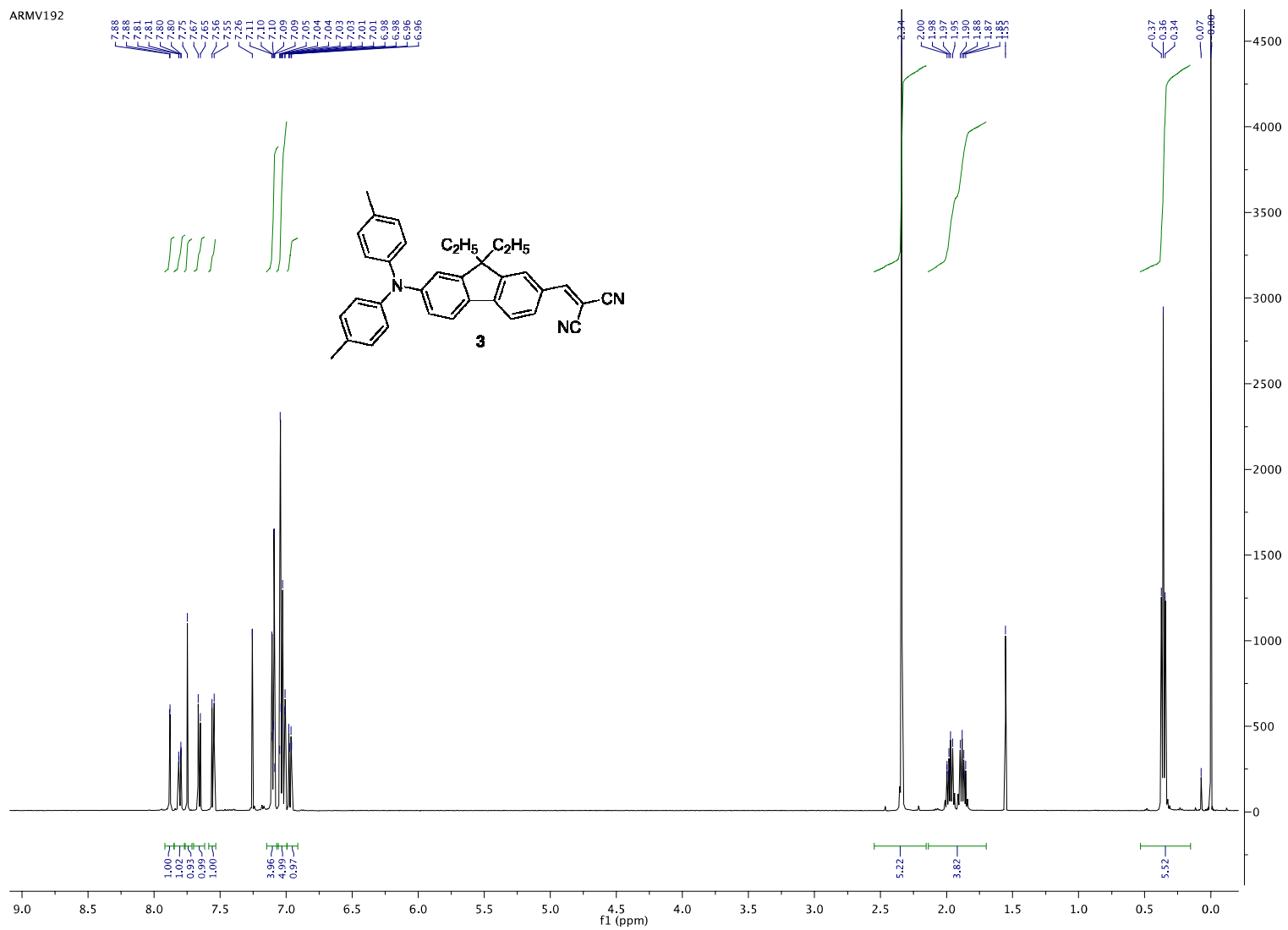


Figure S14. 1H NMR spectrum of compound 3.

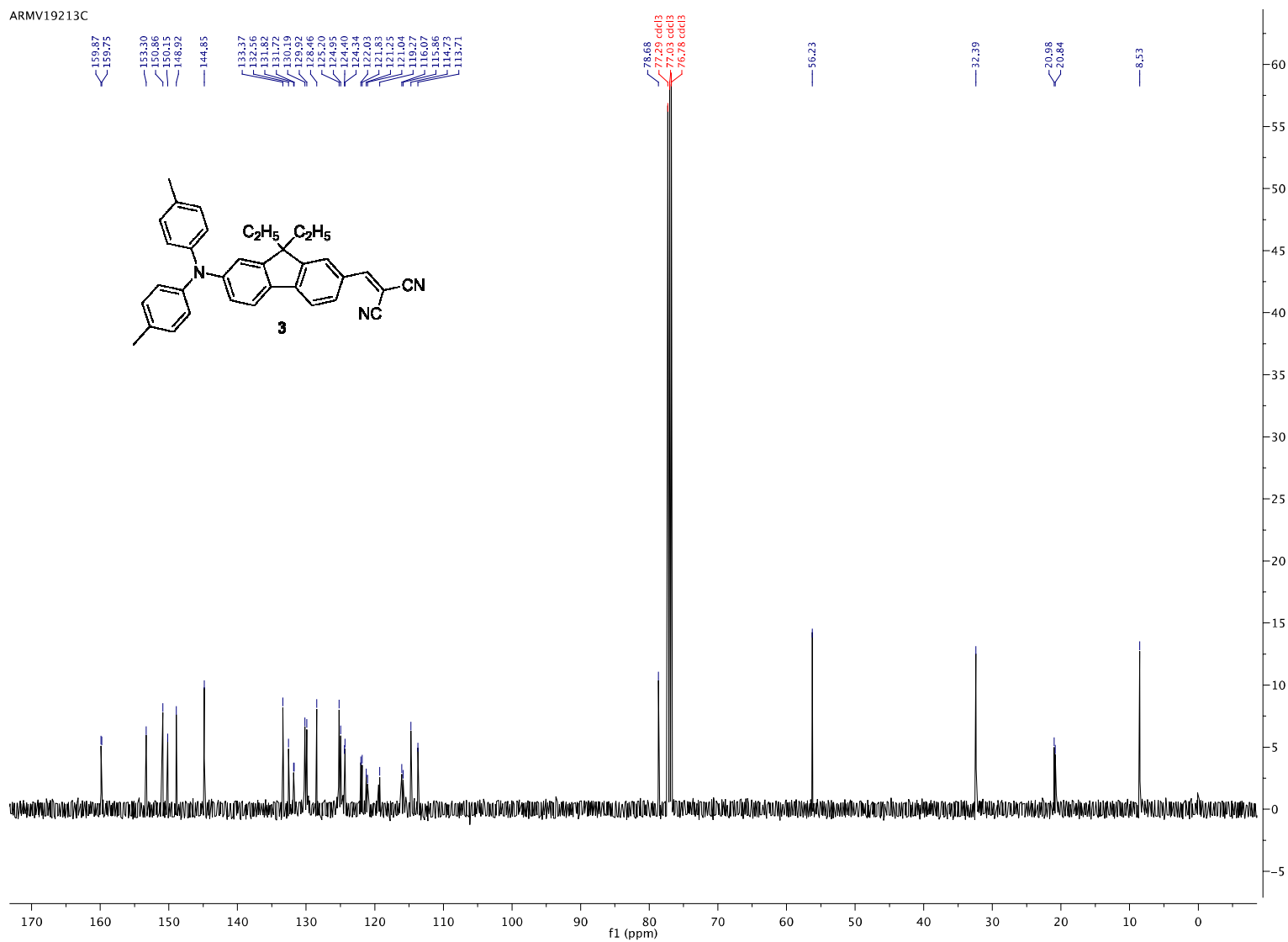


Figure S15. ^{13}C NMR spectrum of compound **3**.

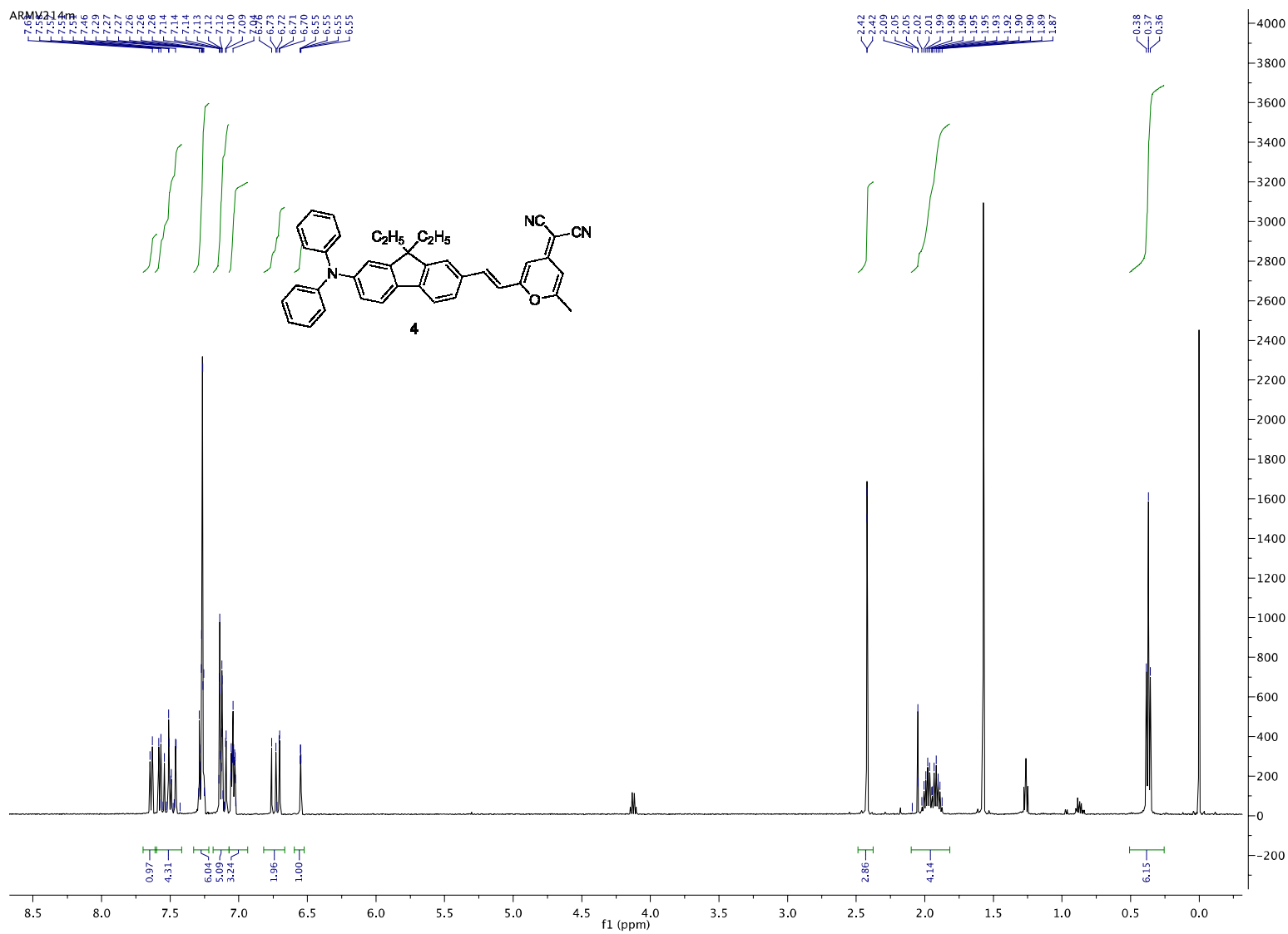


Figure S16. ¹H NMR spectrum of compound 4.

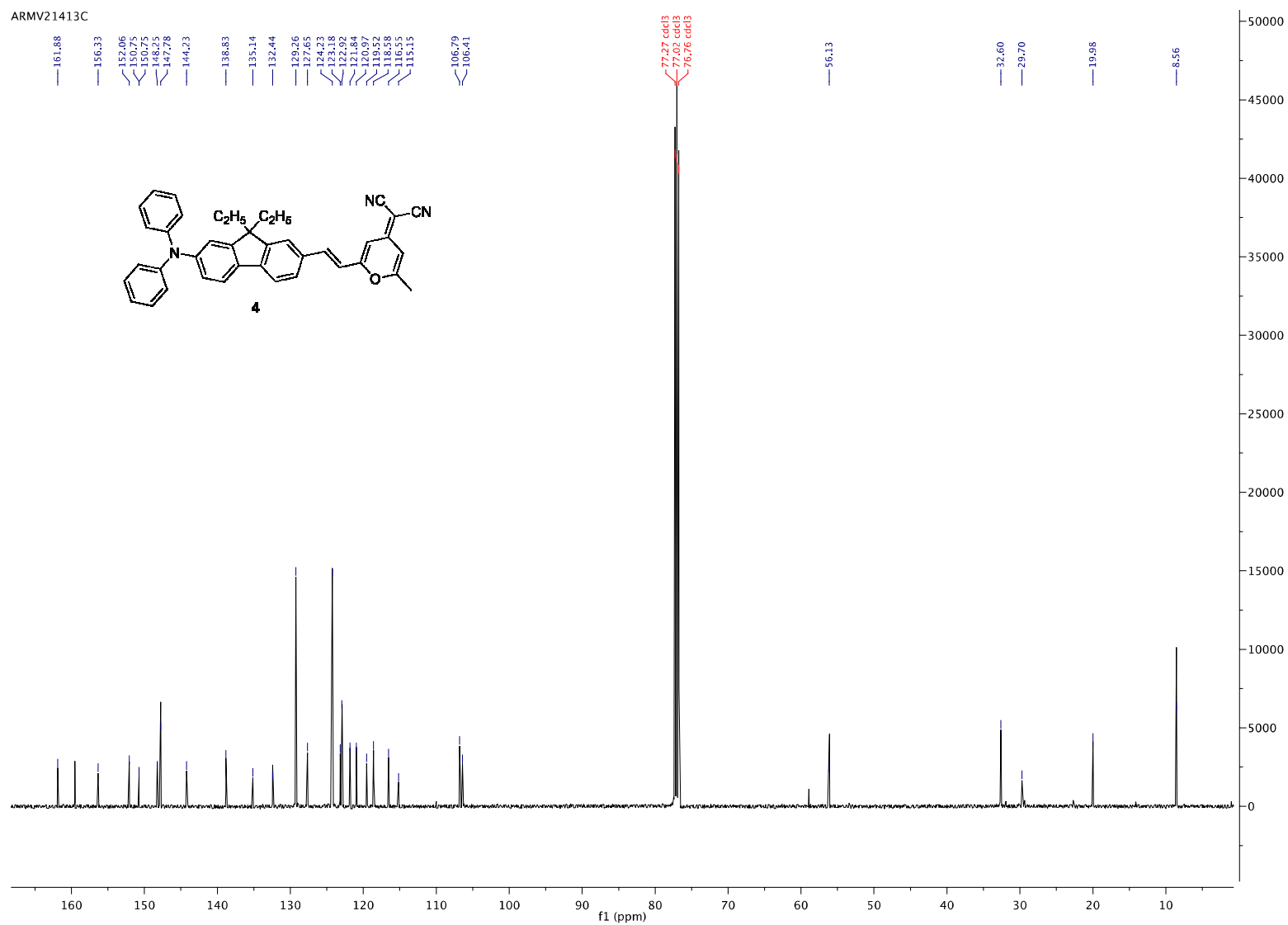


Figure S17. ^{13}C NMR spectrum of compound 4.

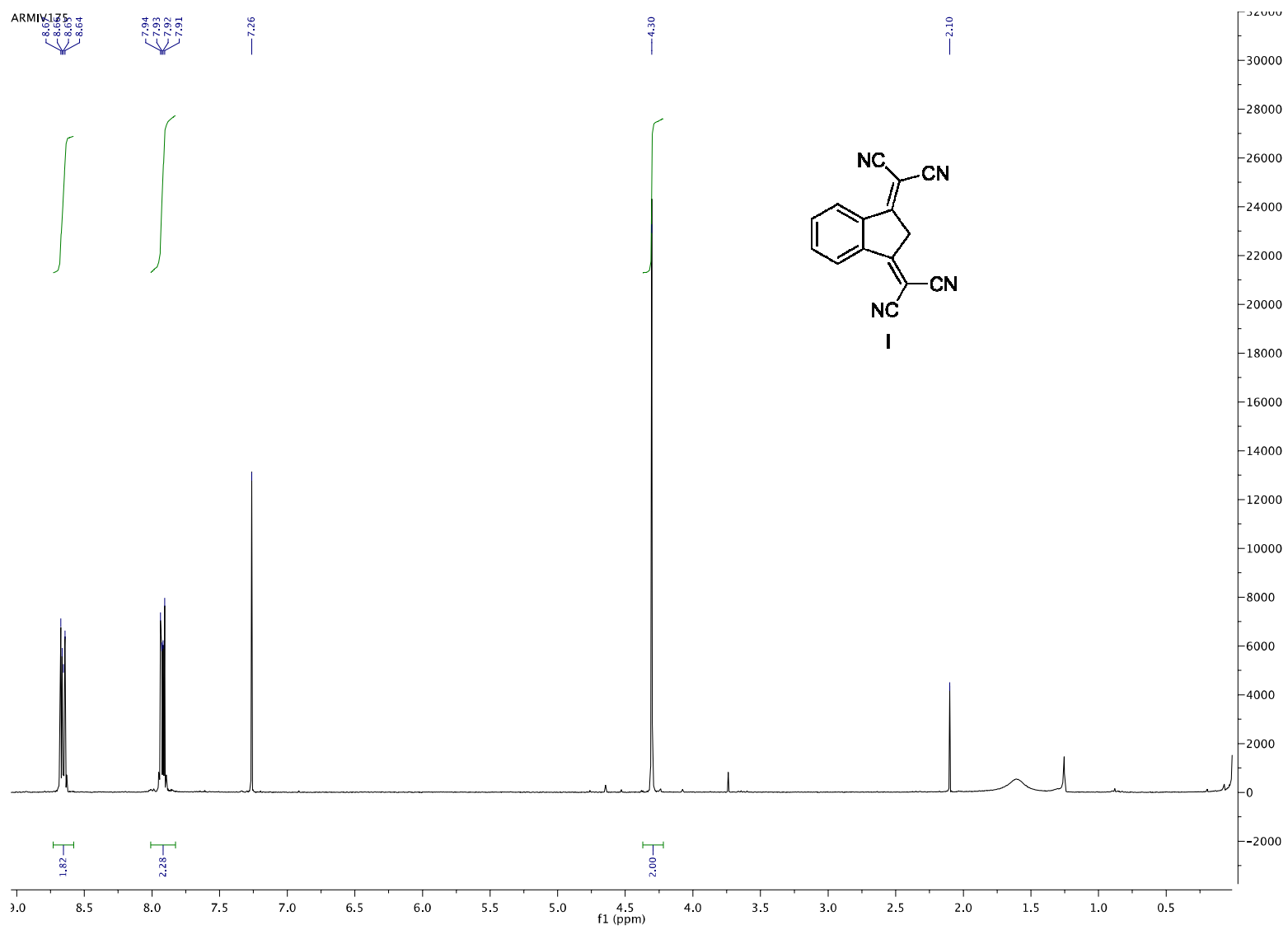


Figure S18. ^1H NMR spectrum of compound I.

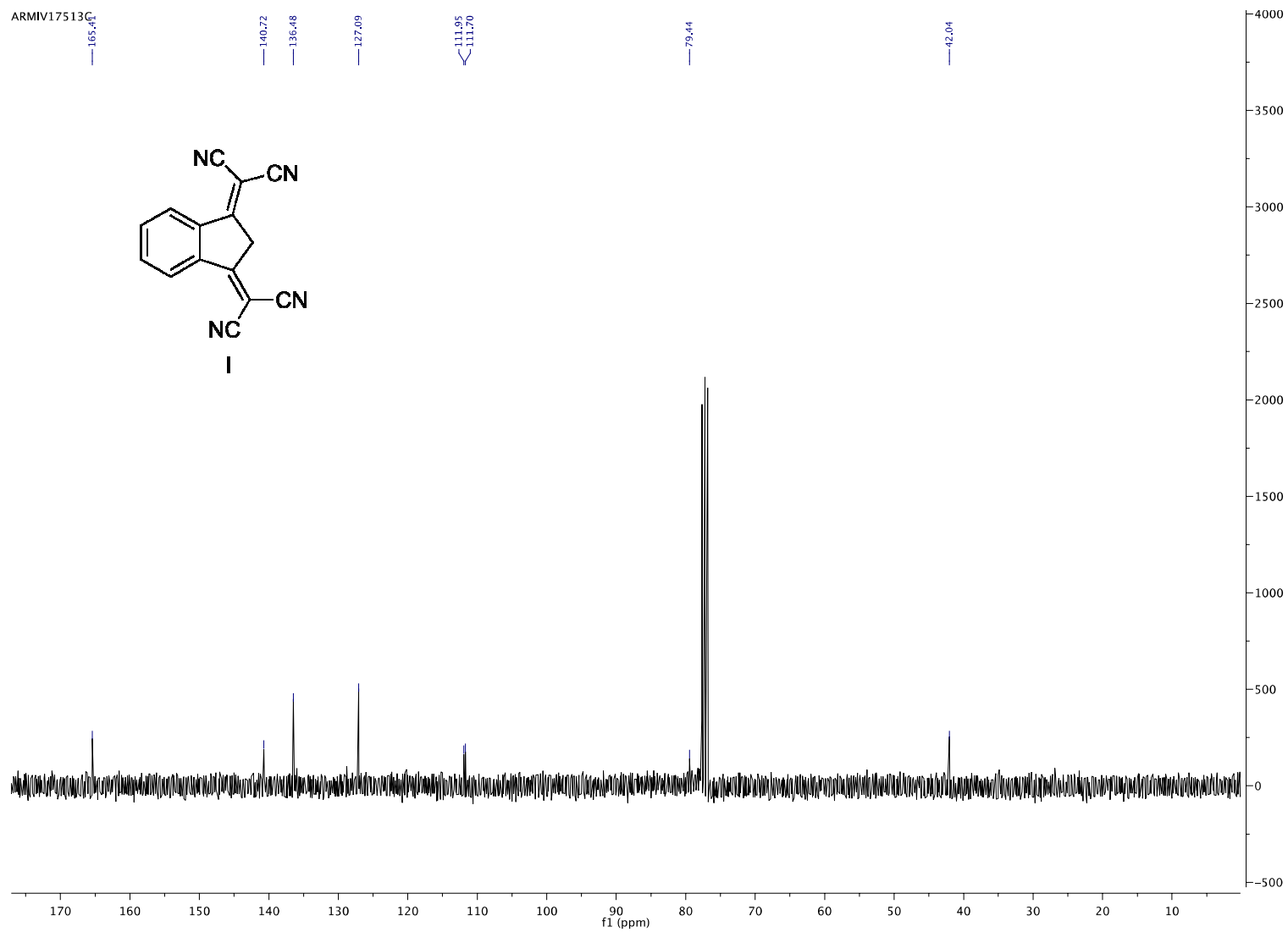


Figure S19. ^{13}C NMR spectrum of compound I.

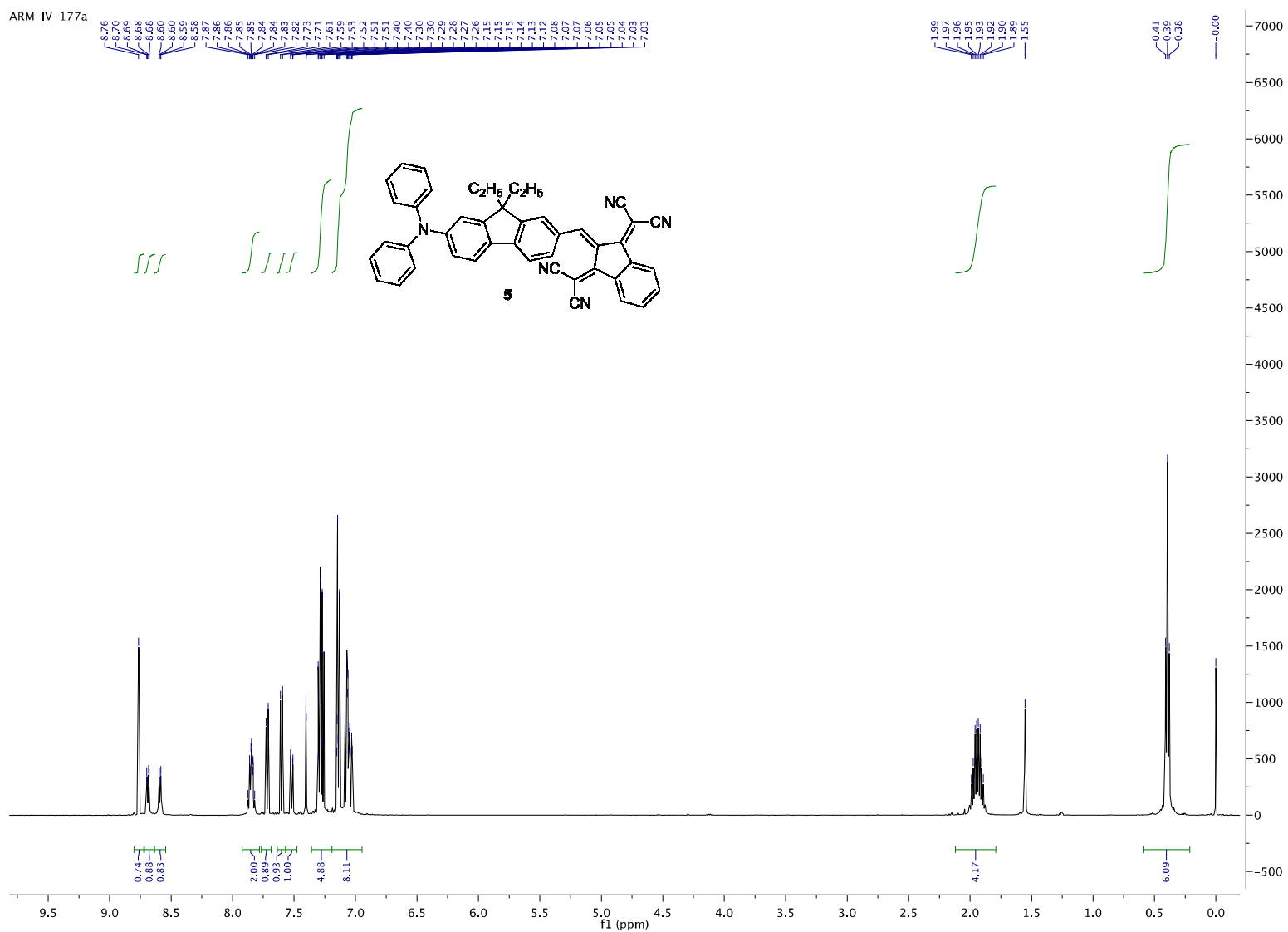


Figure S20. 1H NMR spectrum of compound **5**.

ARMIV17713C

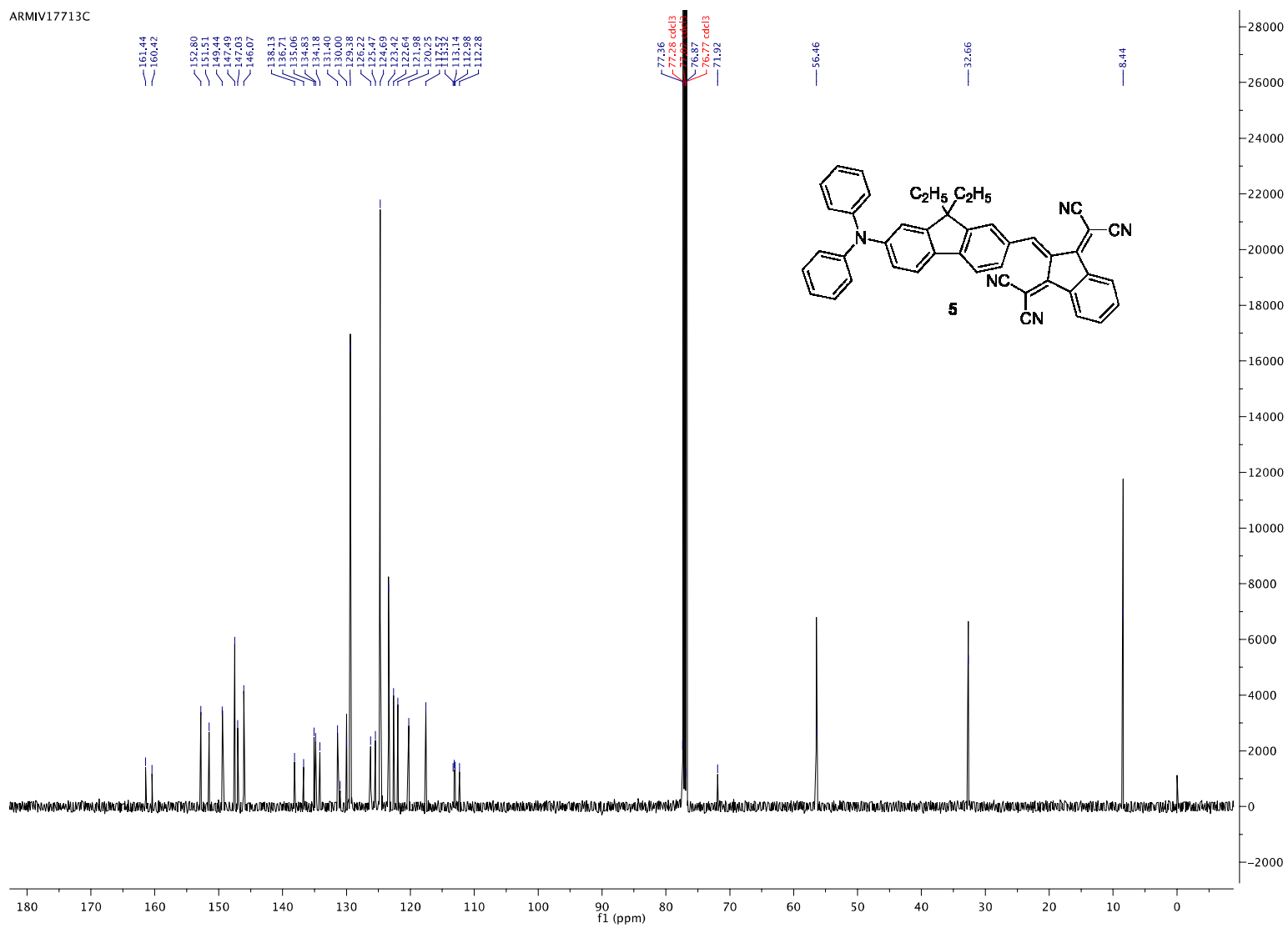


Figure S21. ^{13}C NMR spectrum of compound 5.

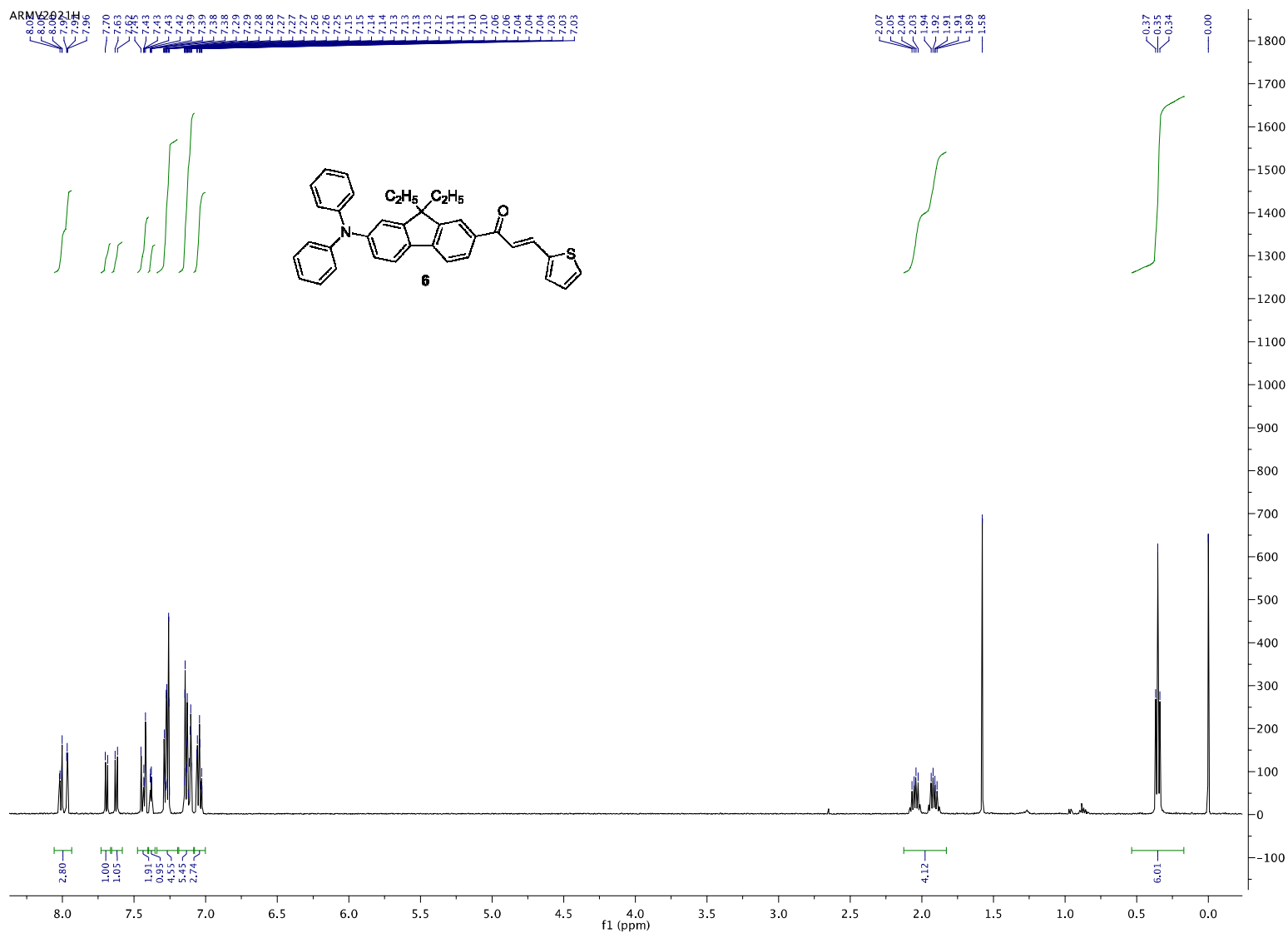


Figure S22. ¹H NMR spectrum of compound 6.

ARM-V-20213C

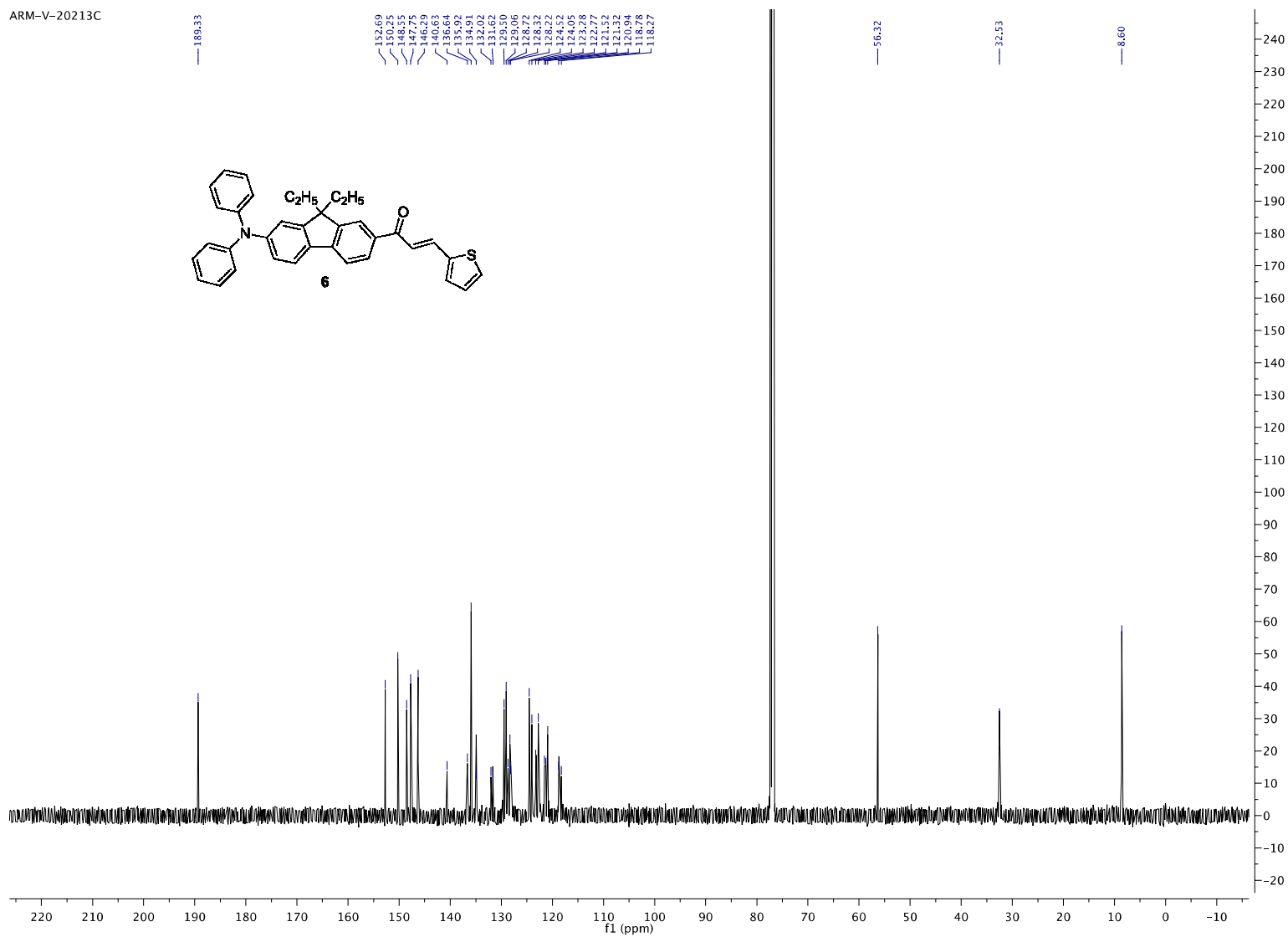


Figure S23. ^{13}C NMR spectrum of compound 6.

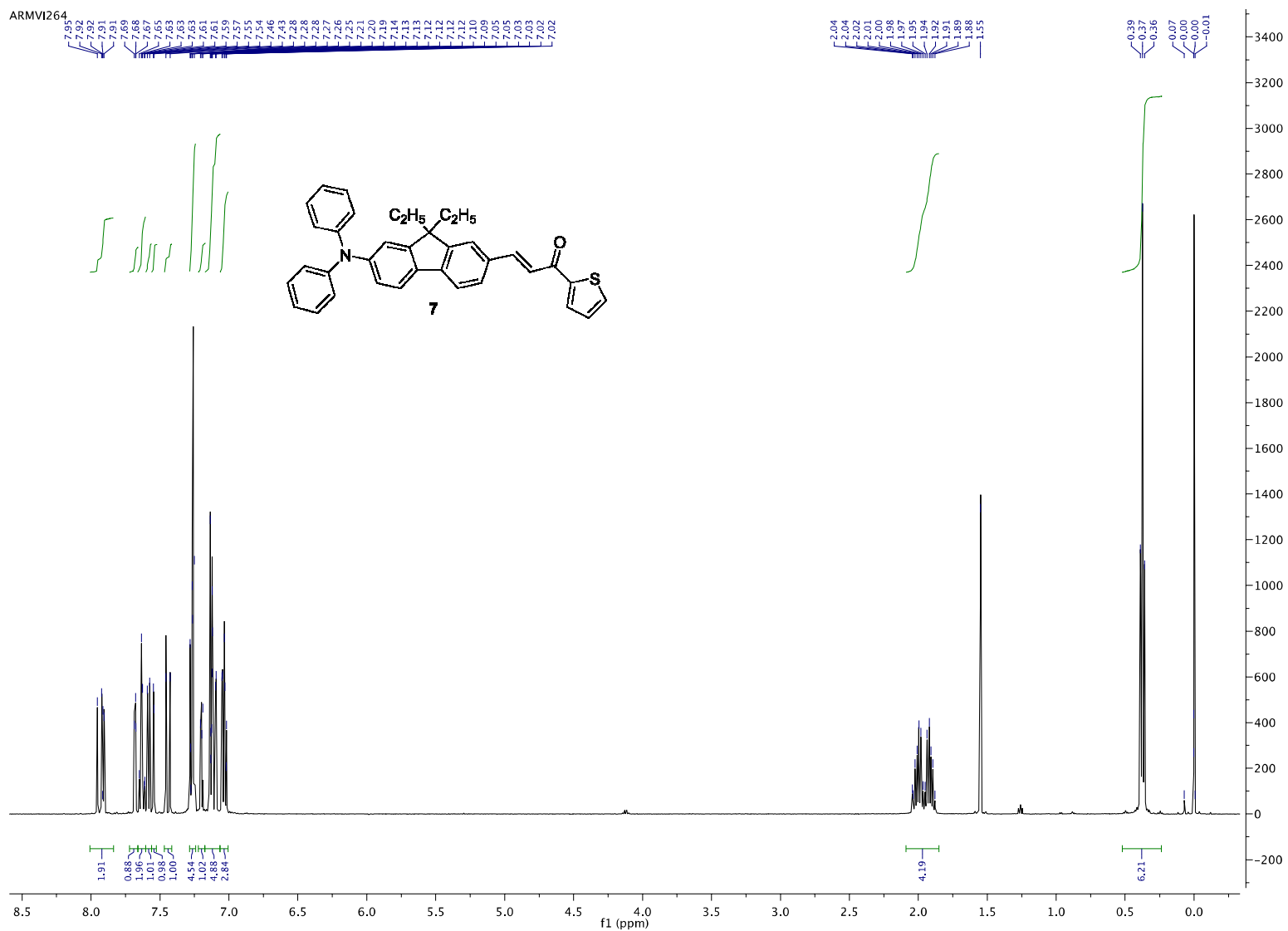


Figure S24. ¹H NMR spectrum of compound 7.

ARMVI264b13C

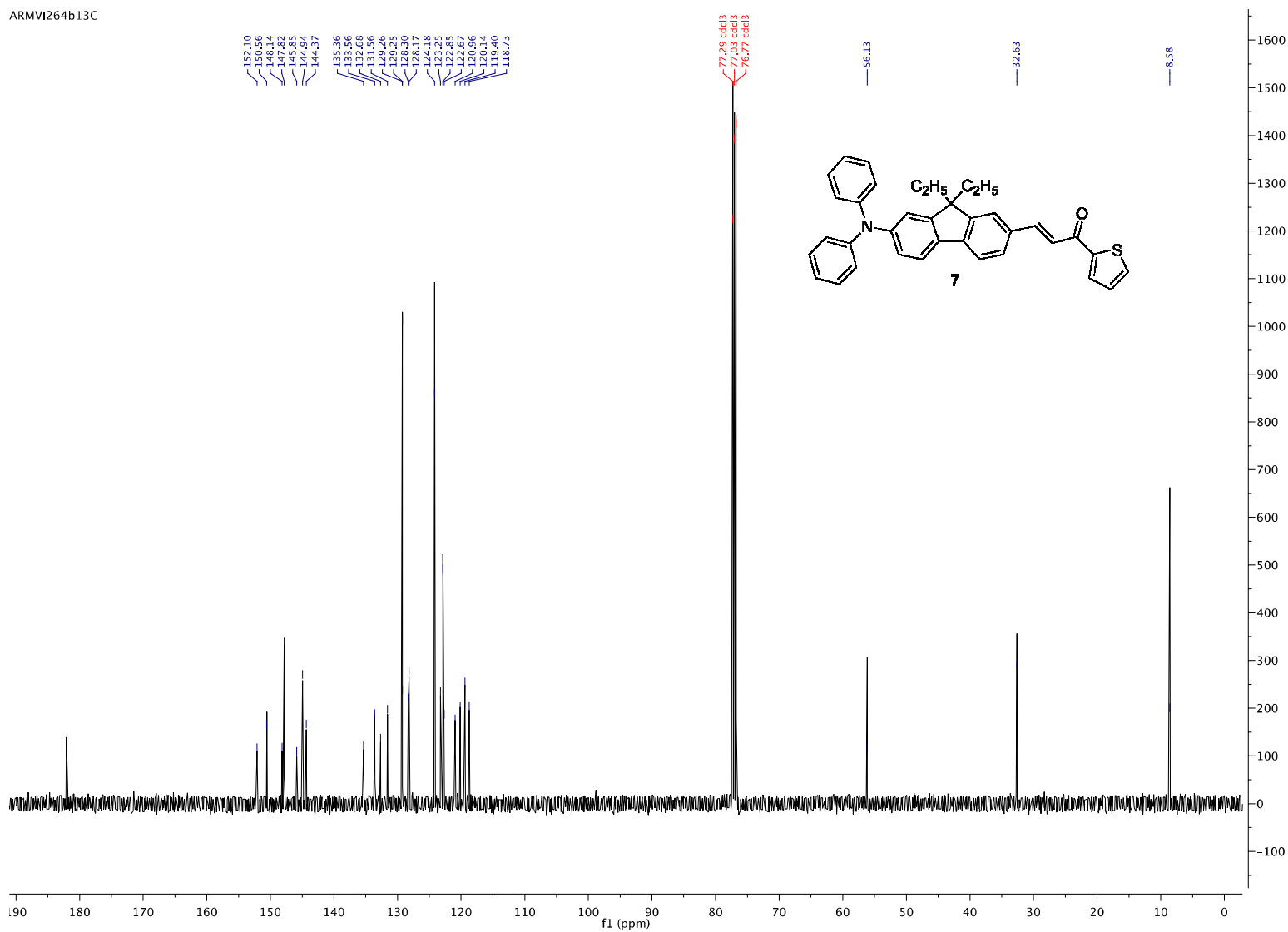


Figure S25. ¹³C NMR spectrum of compound 7.