

Supplementary Materials

Broadband Visible Light-Absorbing [70]Fullerene-BODIPY-Triphenylamine Triad: Synthesis and Application as Heavy Atom-Free Organic Triplet Photosensitizer for Photooxidation

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1. The spectral response of DHN with MB as the sensitizer.

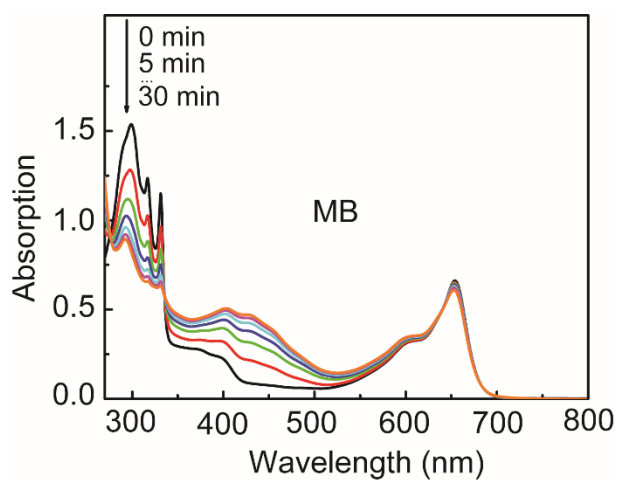


Figure S1. Absorption spectral change for the photooxidation of DHN using **MB** as the sensitizer. $c[\text{MB}] = 1.0 \times 10^{-5} \text{ mol L}^{-1}$, $c[\text{DHN}] = 1.0 \times 10^{-4} \text{ mol L}^{-1}$. In CH_2Cl_2 -MeOH (9/1, v/v).

2. The photostability of C_{70} -B-T.

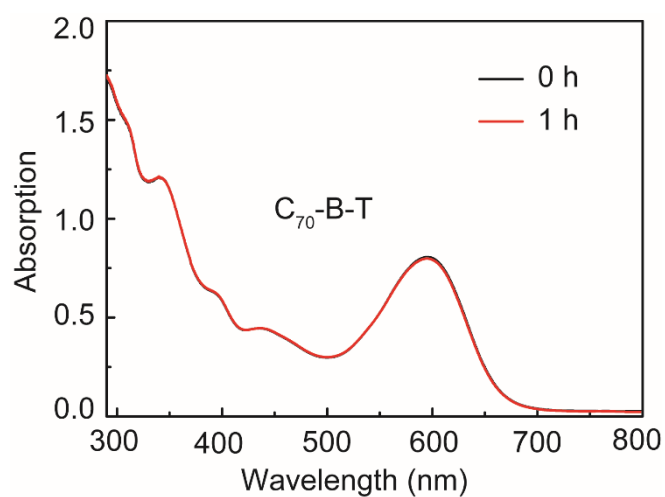
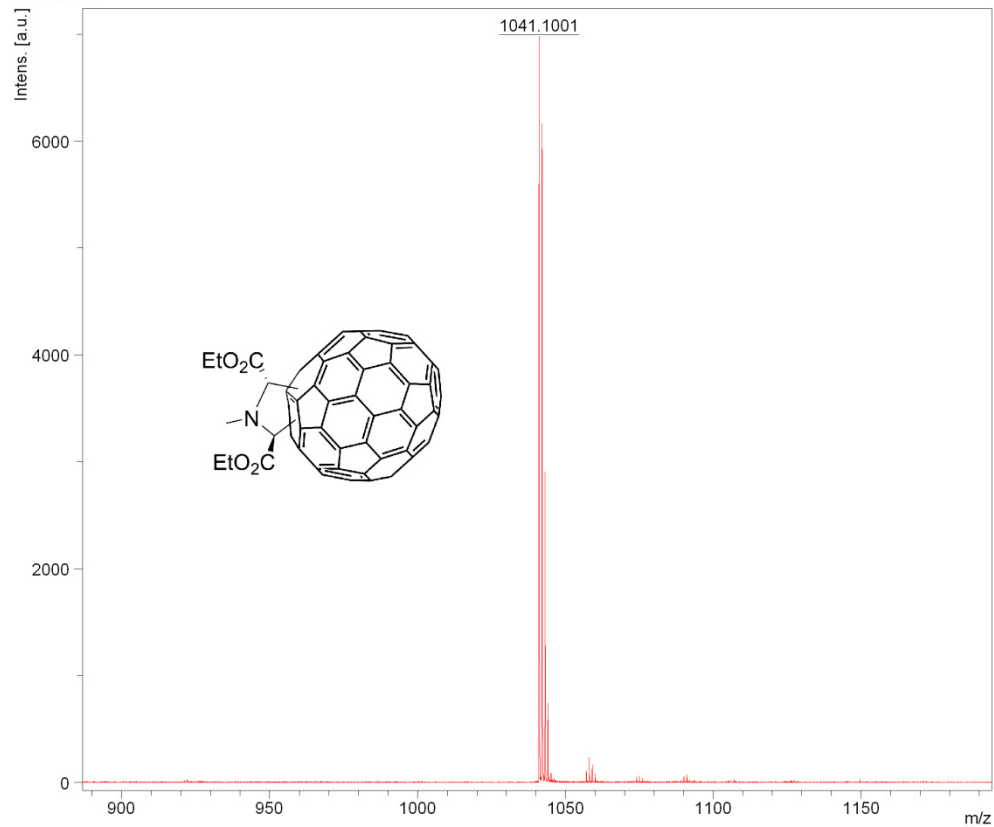


Figure S2. The stability of C_{70} -B-T. $c = 1.0 \times 10^{-5} \text{ mol L}^{-1}$ in CH_2Cl_2 -MeOH (9/1, v/v). After being exposed to light for 1 h, no bleaching is observed.

3. High resolution mass spectra

Comment 1

Comment 2



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Name of spectrum used for calibration
Calibration reference list used sample

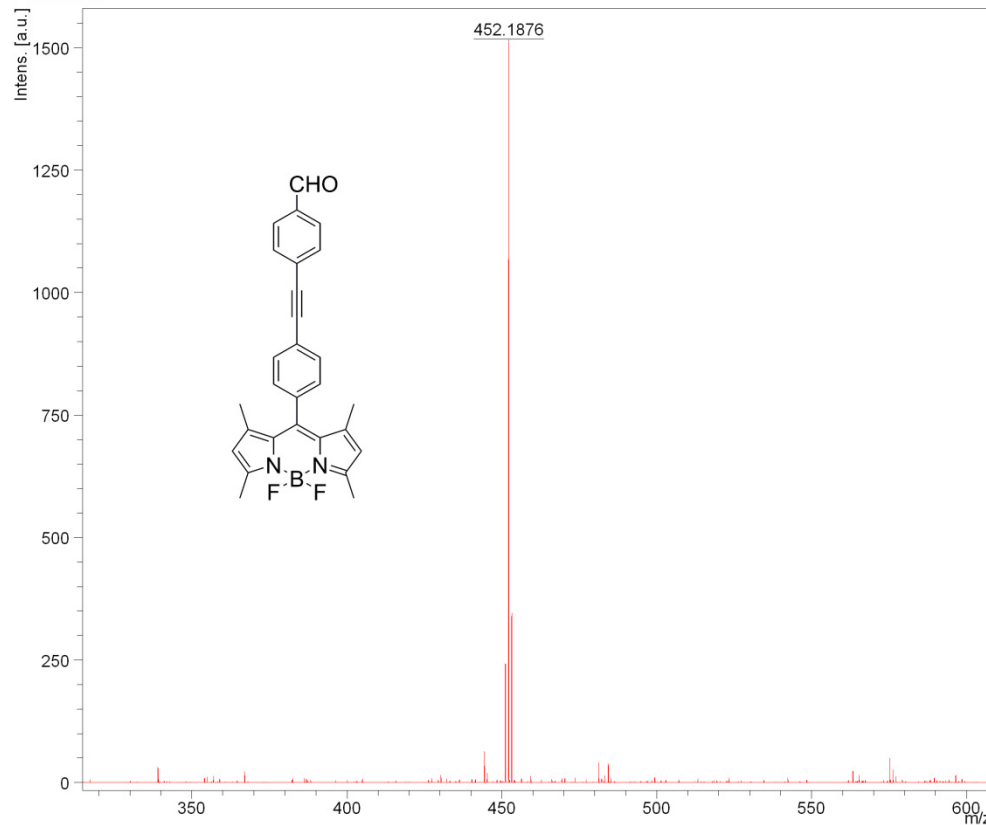
Instrument Info

User BDAL@CN
Instrument FLEX-PC
Instrument type ultraflexTOF/TOF

Figure S3. The high resolution mass spectrum (HRMS) of C₇₀-1.

Comment 1

Comment 2



Acquisition Parameter

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Calibration reference list used sample

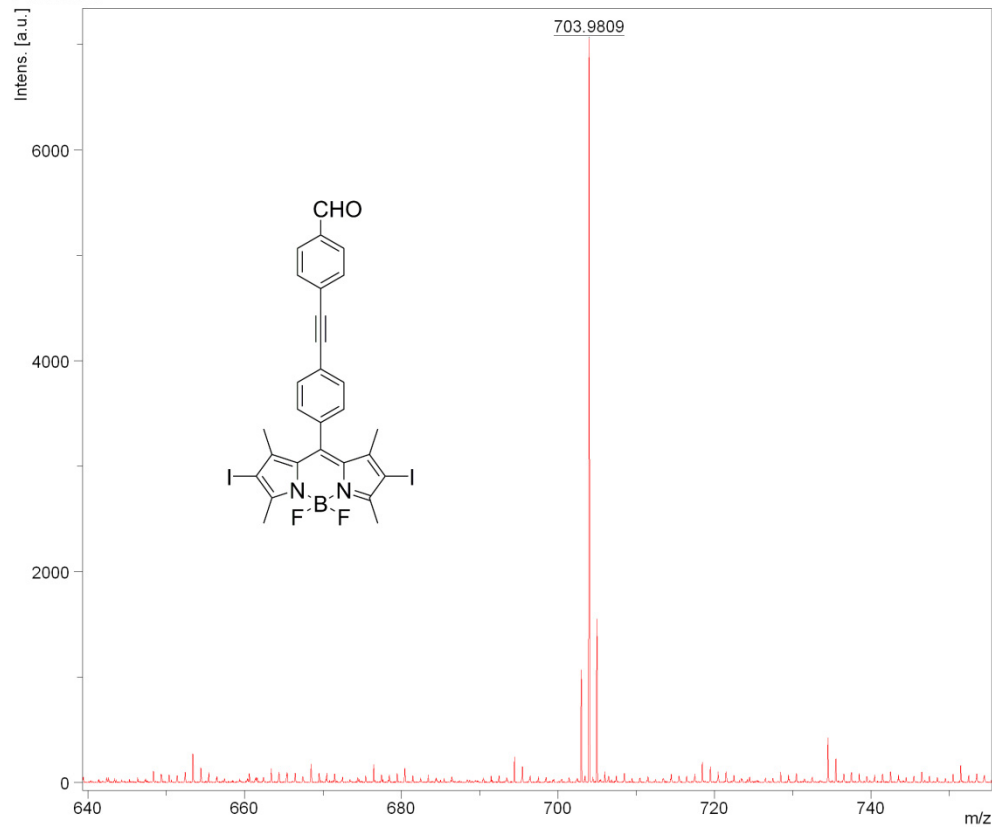
Instrument Info

User BDAL@CN
Instrument FLEX-PC
Instrument type ultraflexTOF/TOF

Figure S4. The high resolution mass spectrum (HRMS) of **5**.

Comment 1

Comment 2



Acquisition Parameter

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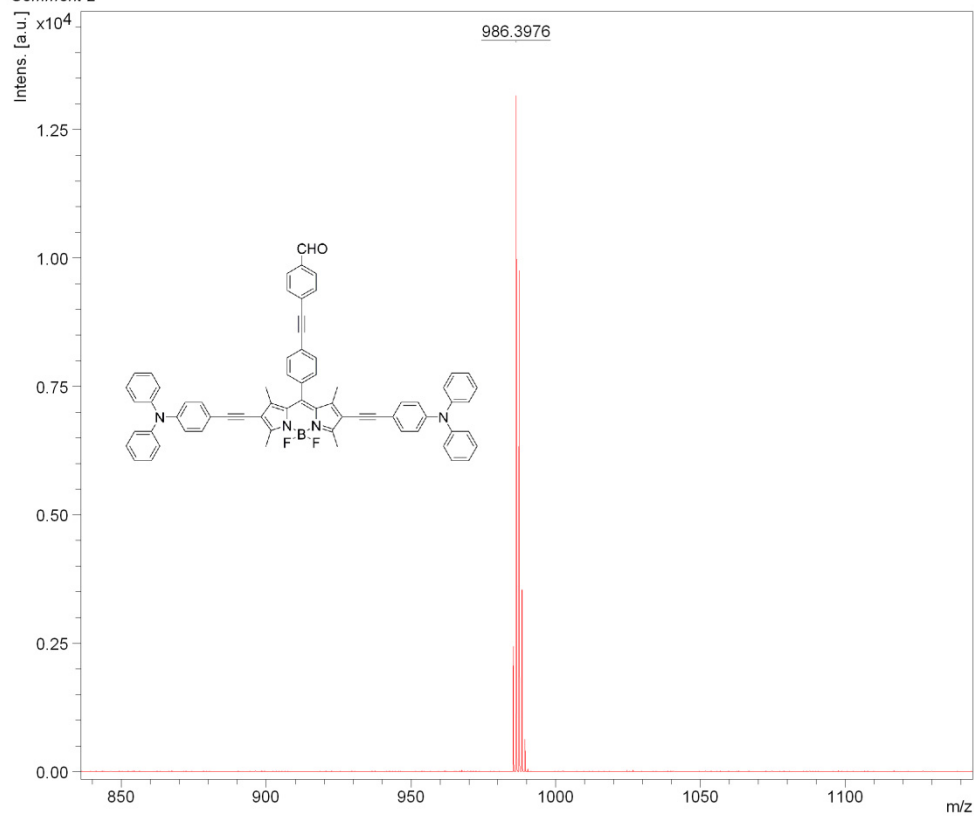
Instrument Info

User BDAL@CN
Instrument FLEX-PC
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Figure S5. The high resolution mass spectrum (HRMS) of 6.

Comment 1

Comment 2



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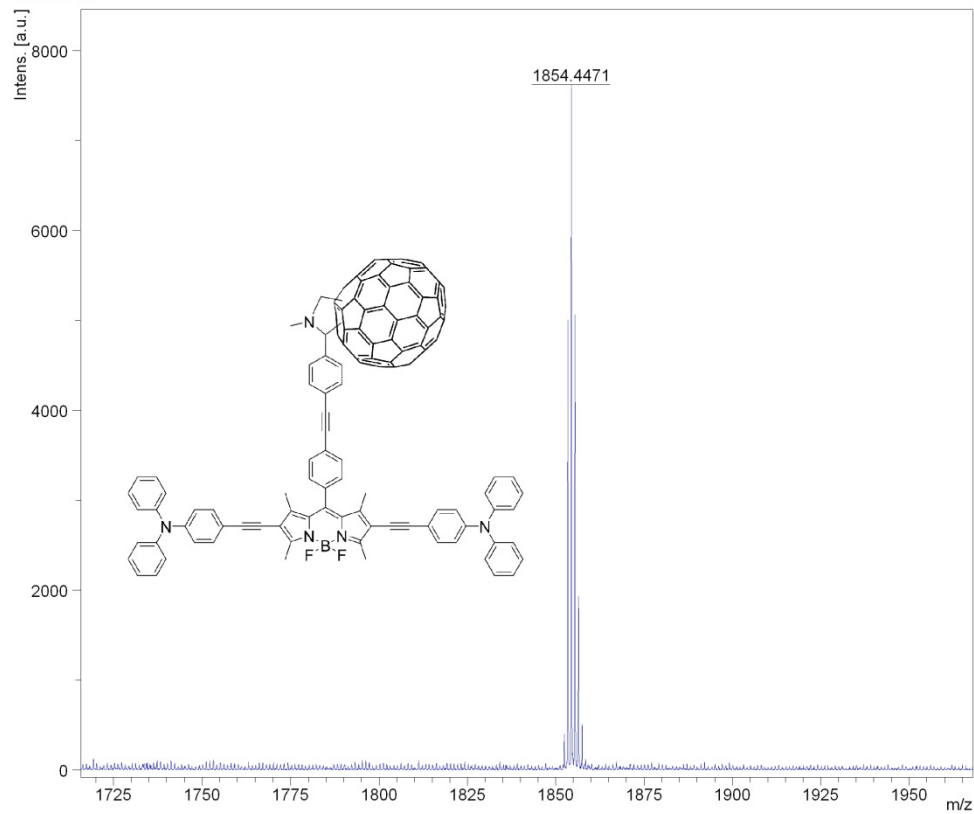
Instrument Info

User BDAL@CN
Instrument FLEX-PC
Instrument type ultraflexTOF/TOF

Figure S6. The high resolution mass spectrum (HRMS) of B-T.

Comment 1

Comment 2



Acquisition Parameter

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Calibration reference list used sample

Instrument Info

User BDAL@CN
Instrument FLEX-PC
Instrument type ultraflexTOF/TOF

Figure S7. The high resolution mass spectrum (HRMS) of C₇₀-B-T.

4. ¹H NMR and ¹³C NMR spectra

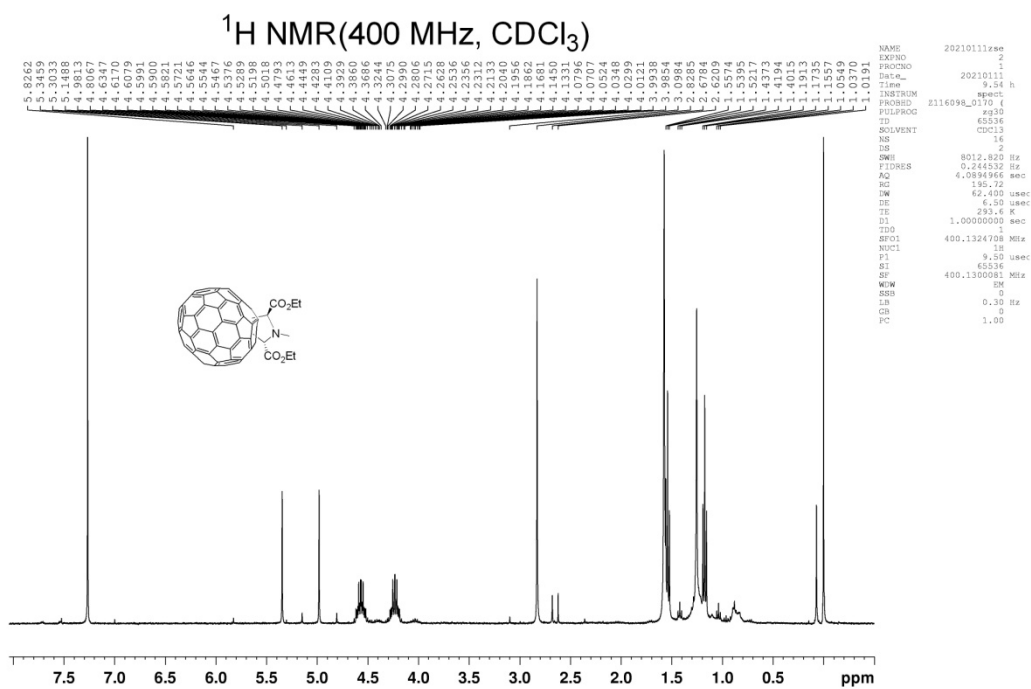


Figure S8. ¹H NMR of C₇₀-1 in CDCl₃ (400 MHz).

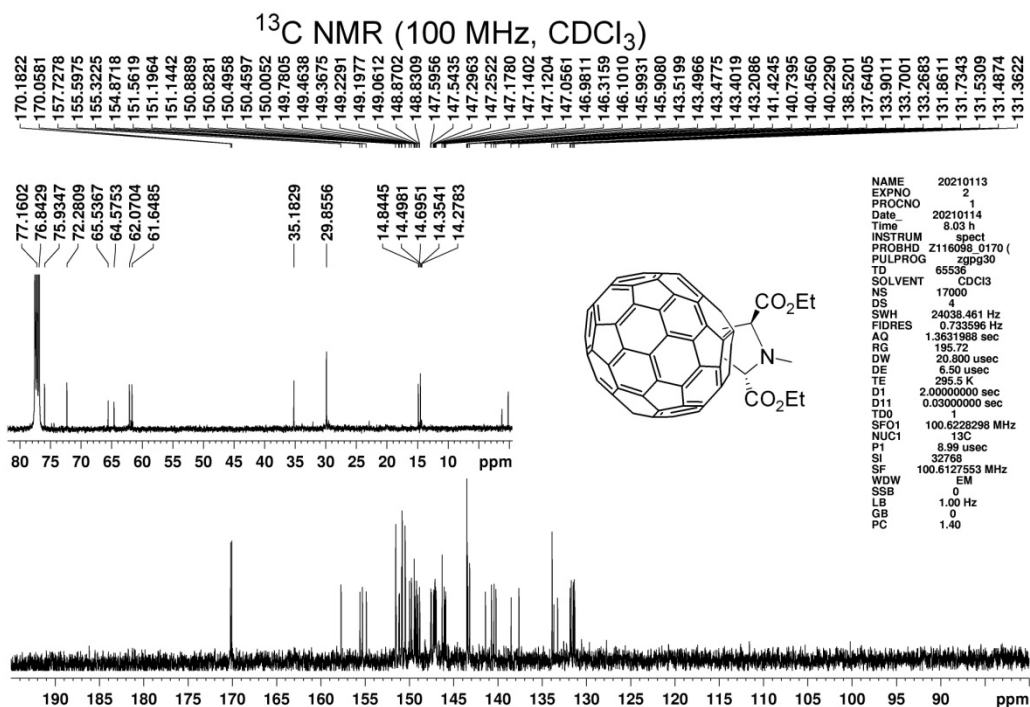


Figure S9. ¹³C NMR of C₇₀-1 in CDCl₃ (100 MHz).

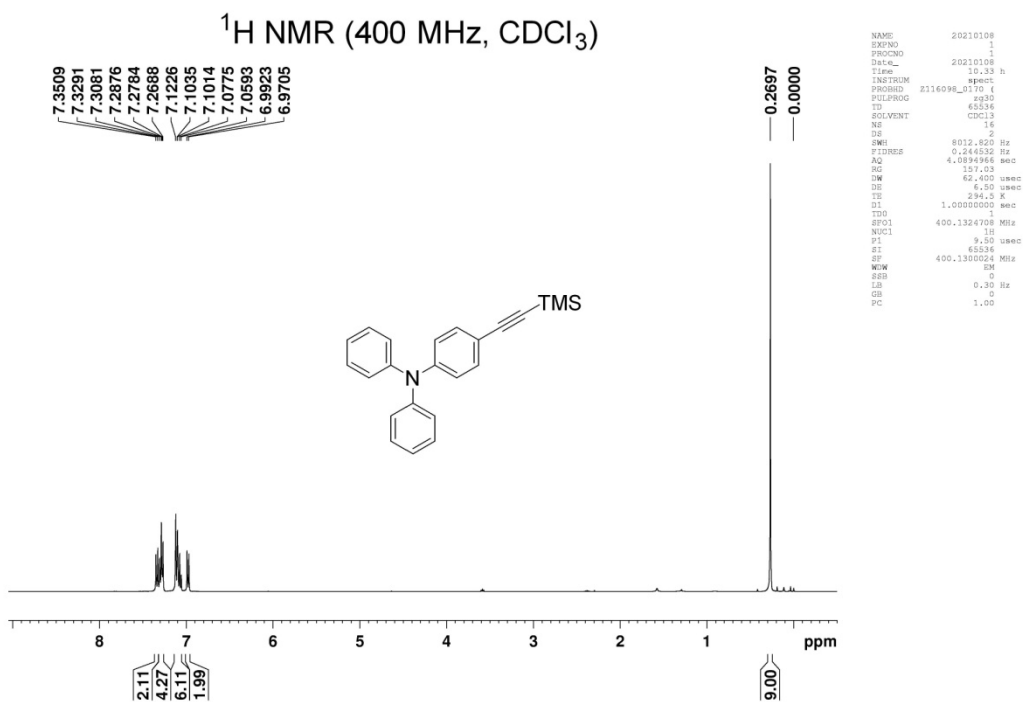


Figure S10. ¹H NMR of **2** in CDCl₃ (400 MHz).

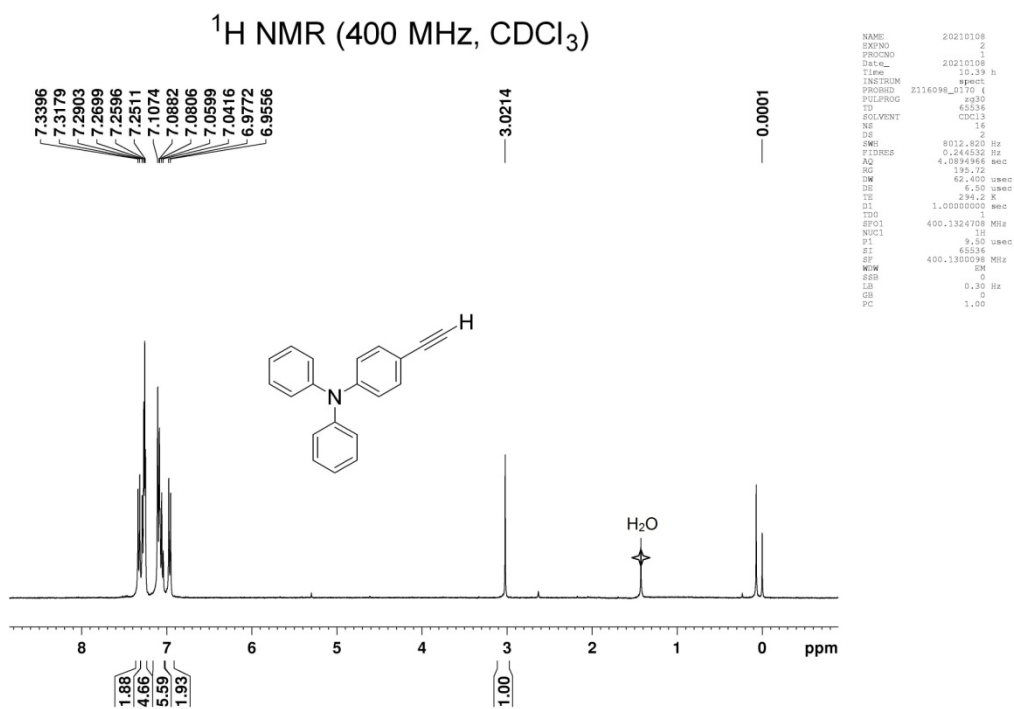


Figure S11. ¹H NMR of **3** in CDCl₃ (400 MHz).

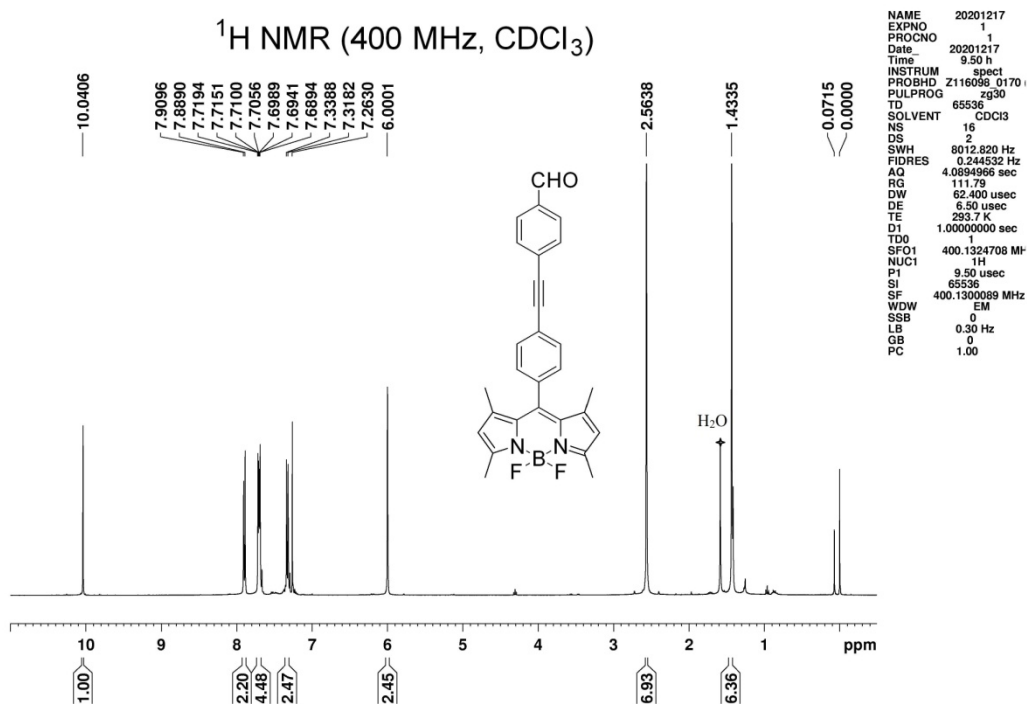


Figure S12. ¹H NMR of **5** in CDCl₃ (400 MHz).

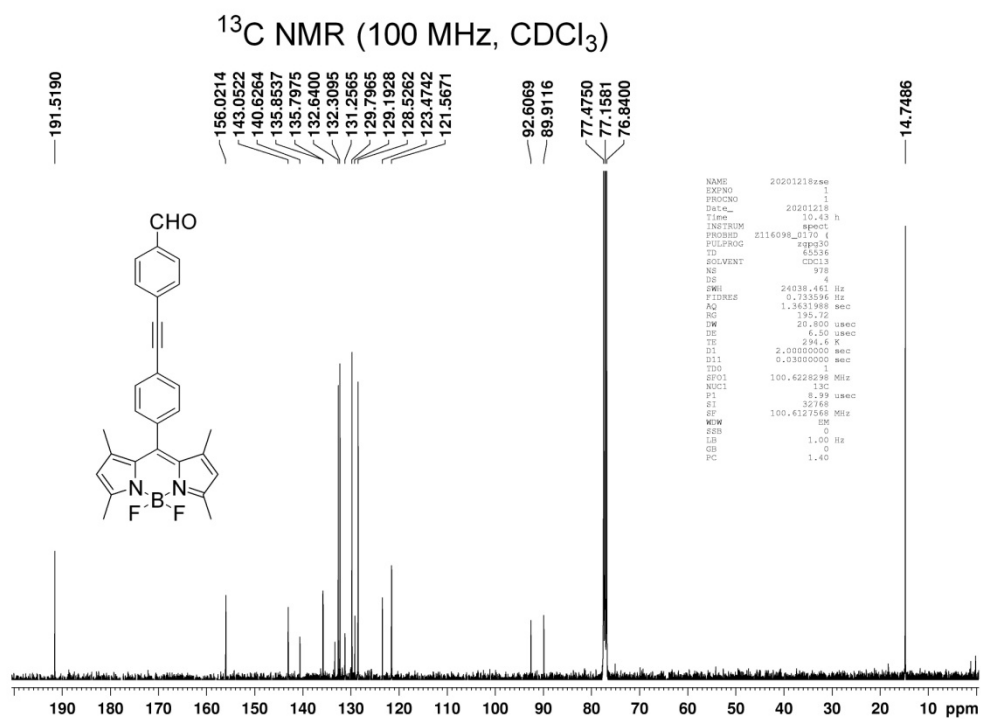


Figure S13. ¹³C NMR of **5** in CDCl₃ (100 MHz).

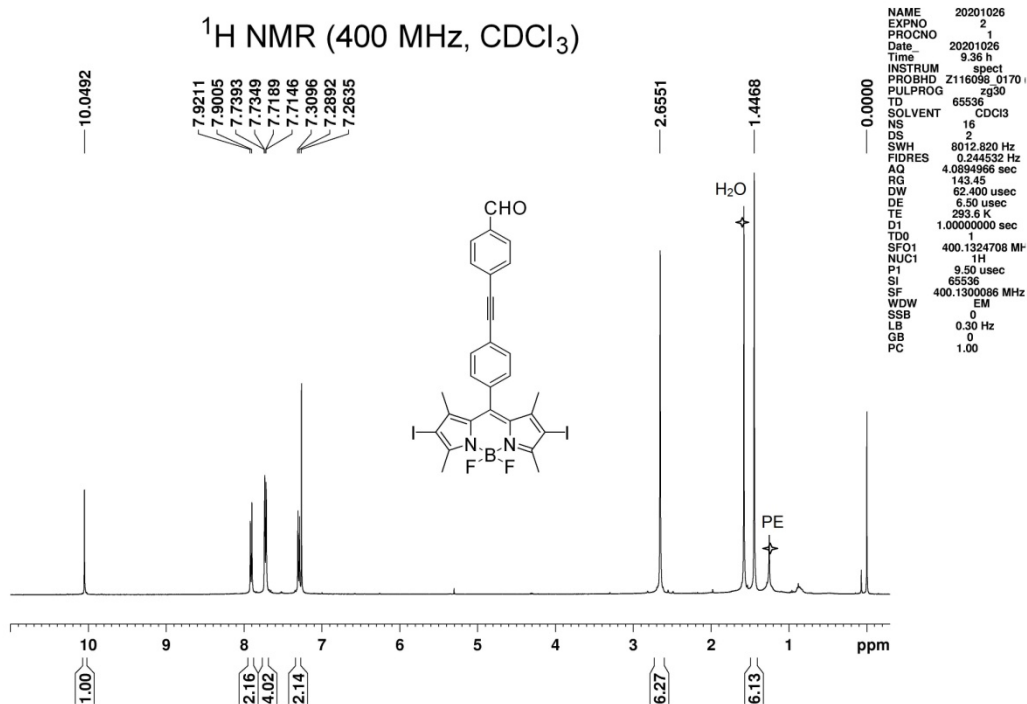


Figure S14. ¹H NMR of **6** in CDCl₃ (400 MHz).

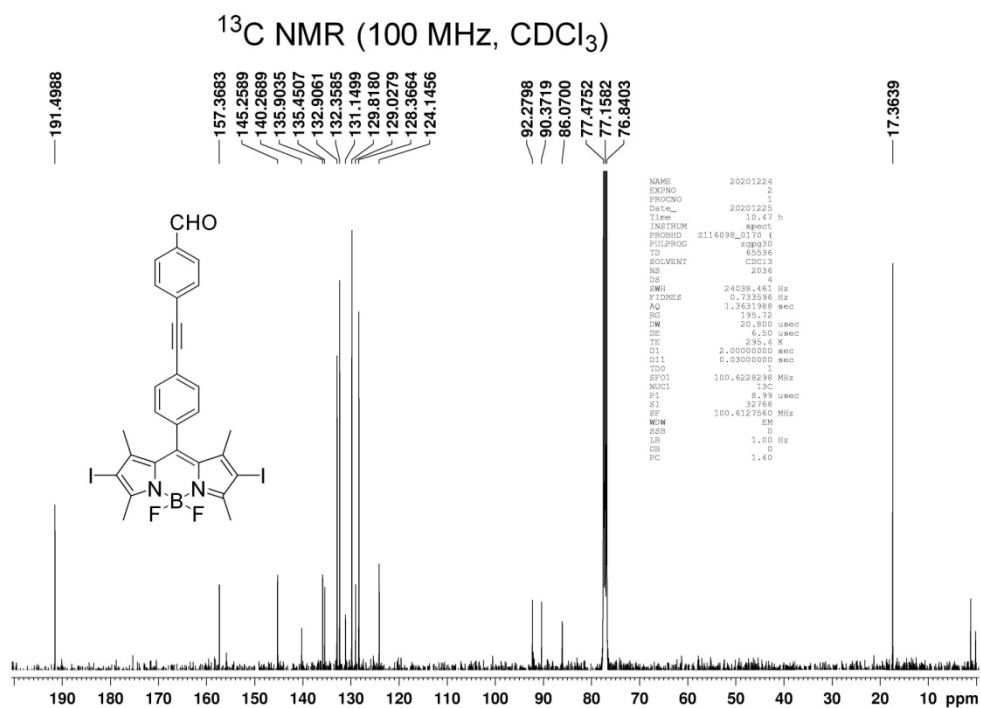
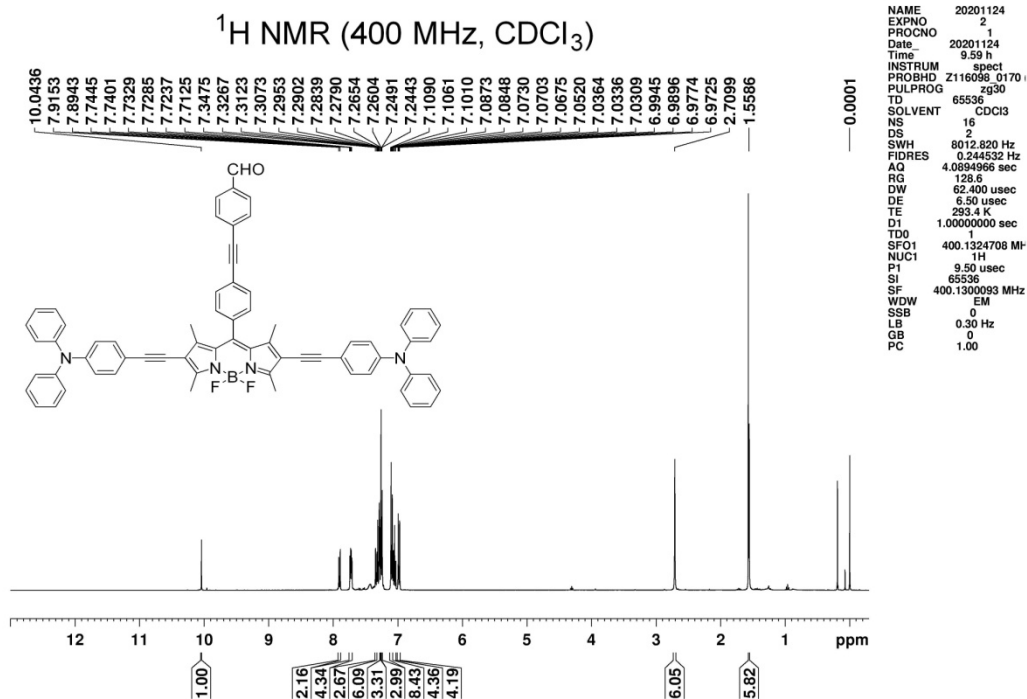


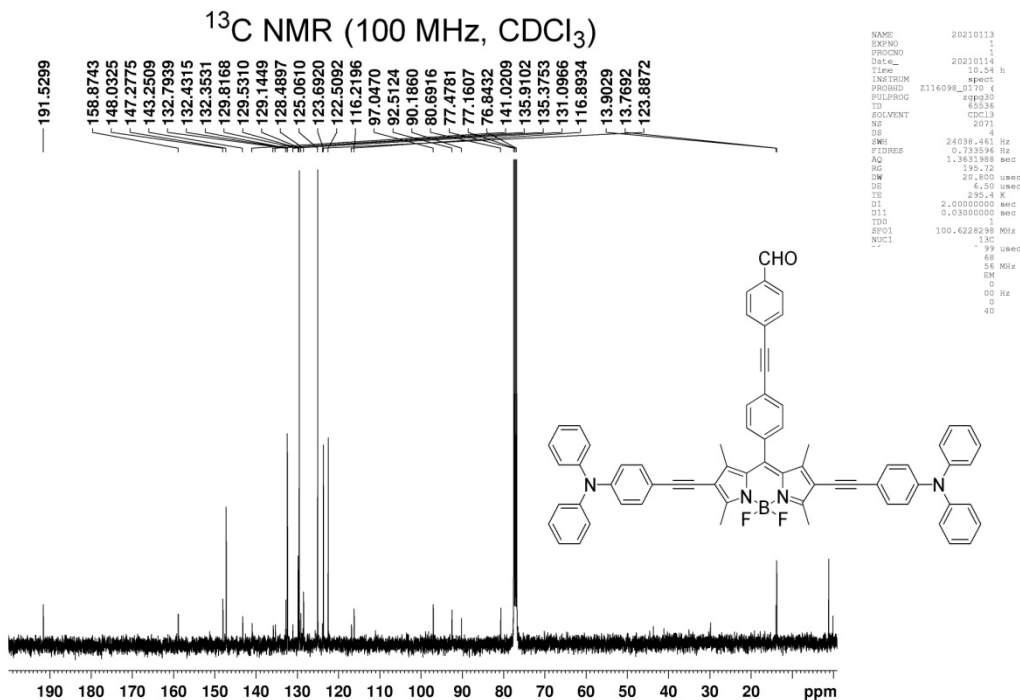
Figure S15. ¹³C NMR of **6** in CDCl₃ (100 MHz).



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PROCNO   1
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PULPROG  zg30
TD        65536
SOLVENT  CDCl3
NS        16
DS        2
SWH       8012.820 Hz
FIDRES   0.244532 Hz
AQ        4.0684966 sec
RG        128.8
DW        62.400 usec
DE        6.50 usec
TE        293.4 K
D1        1.00000000 sec
TD0       400.1324708 MHz
SFO1      400.1324708 MHz
NUC1      1H
P1        9.50 usec
SI        65536
SF        400.1300093 MHz
WDW       EM
SSB       0
LB        0.30 Hz
GB        0
PC        1.00
  
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Figure S16. ¹H NMR of B-T in CDCl₃ (400 MHz).



```

NAME      20210113
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PROCNO   1
Date_    20210114
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PULPROG  zgpg30
TD        65536
SOLVENT  CDCl3
NS        2071
DS        4
SWH       24038.461 Hz
FIDRES   0.733596 Hz
AQ        1.3631968 sec
RG        195.72
DW        20.800 usec
DE        6.50 usec
TE        295.4 K
D1        2.00000000 sec
D11       0.03000000 sec
TD0       1
SFO1      100.6228298 MHz
NUC1      13C
P1        99 usec
SI        65
SF        56 MHz
WDW       EM
SSB       0
LB        0.00 Hz
GB        0
PC        40
  
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Figure S17. ¹³C NMR of B-T in CDCl₃ (100 MHz).

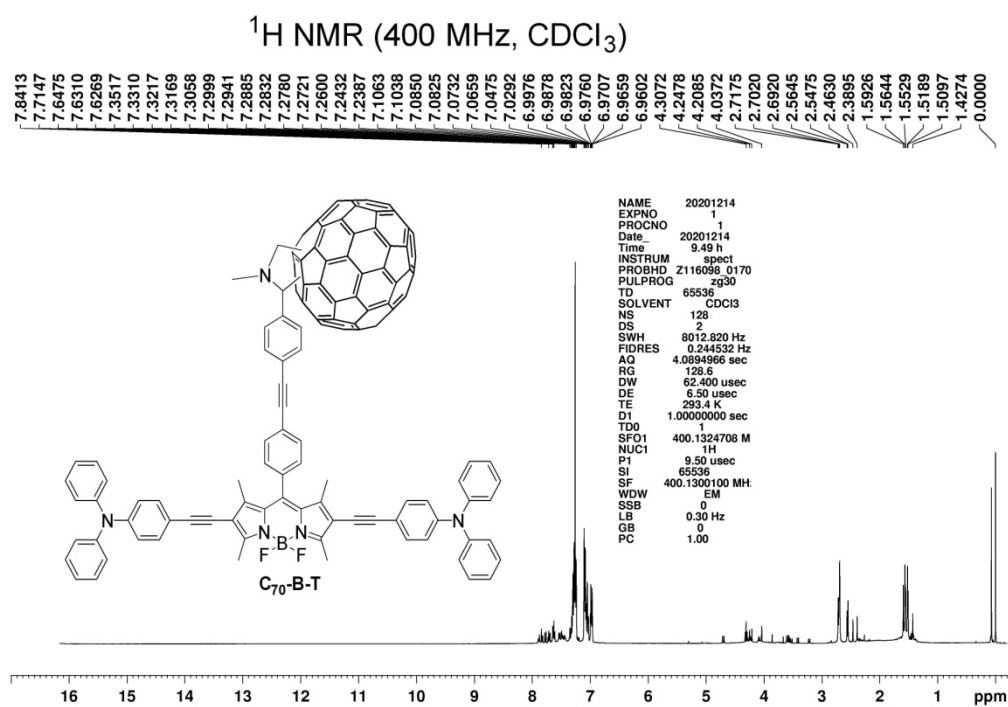


Figure S18. ¹H NMR of C₇₀-B-T in CDCl₃ (400 MHz).

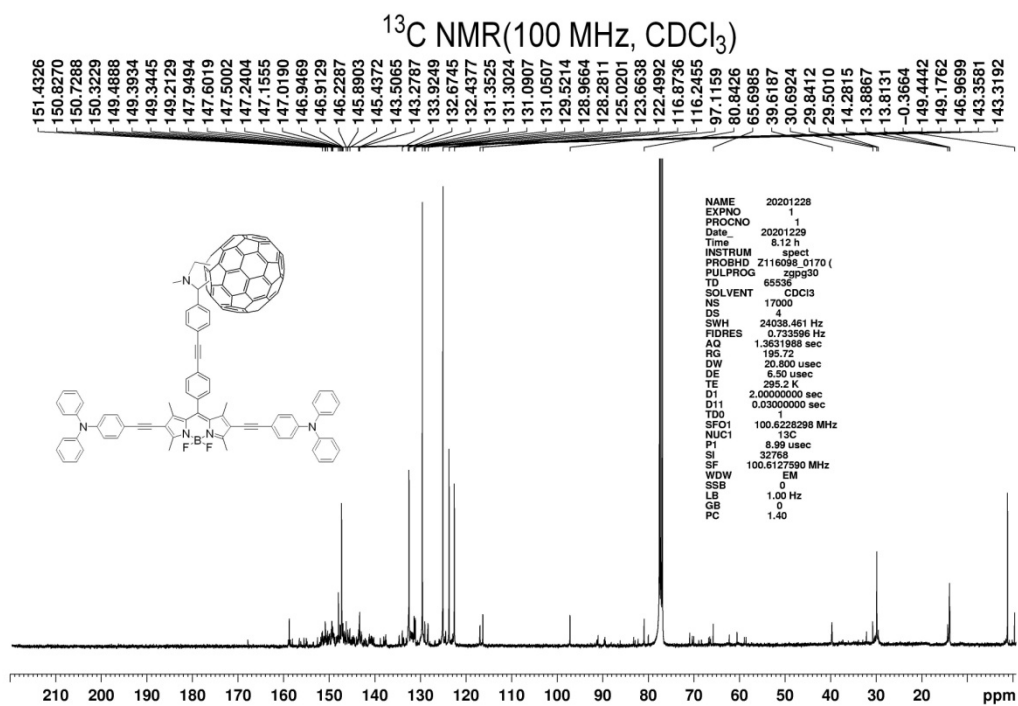


Figure S19. ¹³C NMR of C₇₀-B-T in CDCl₃ (100 MHz).

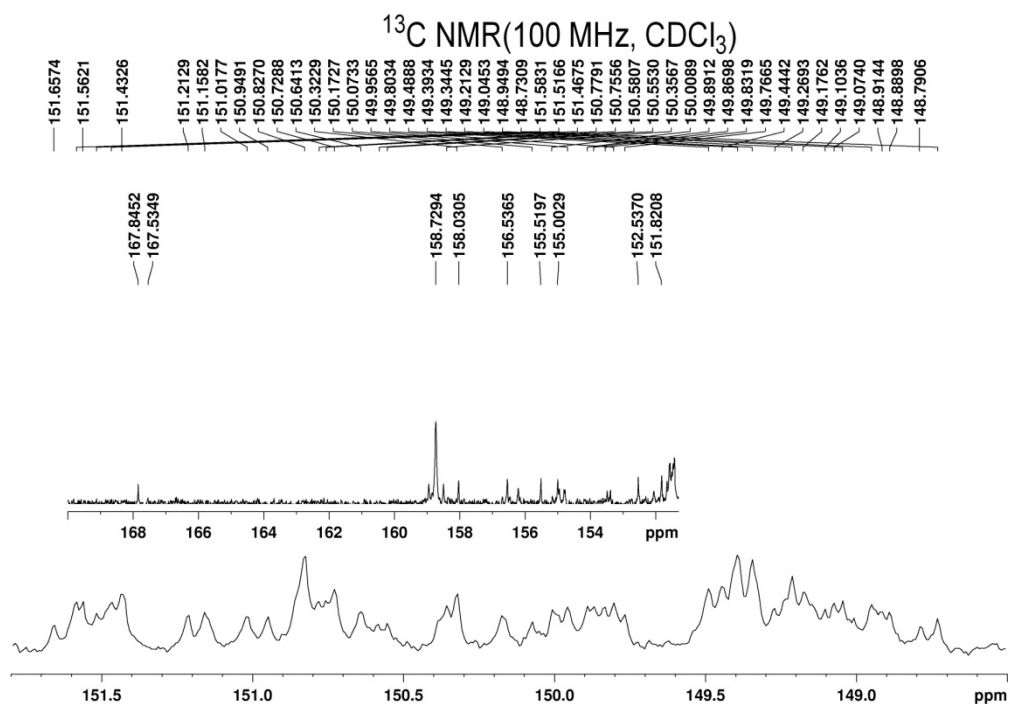


Figure S20. Expansion of the ^{13}C NMR of $\text{C}_{70}\text{-B-T}$.

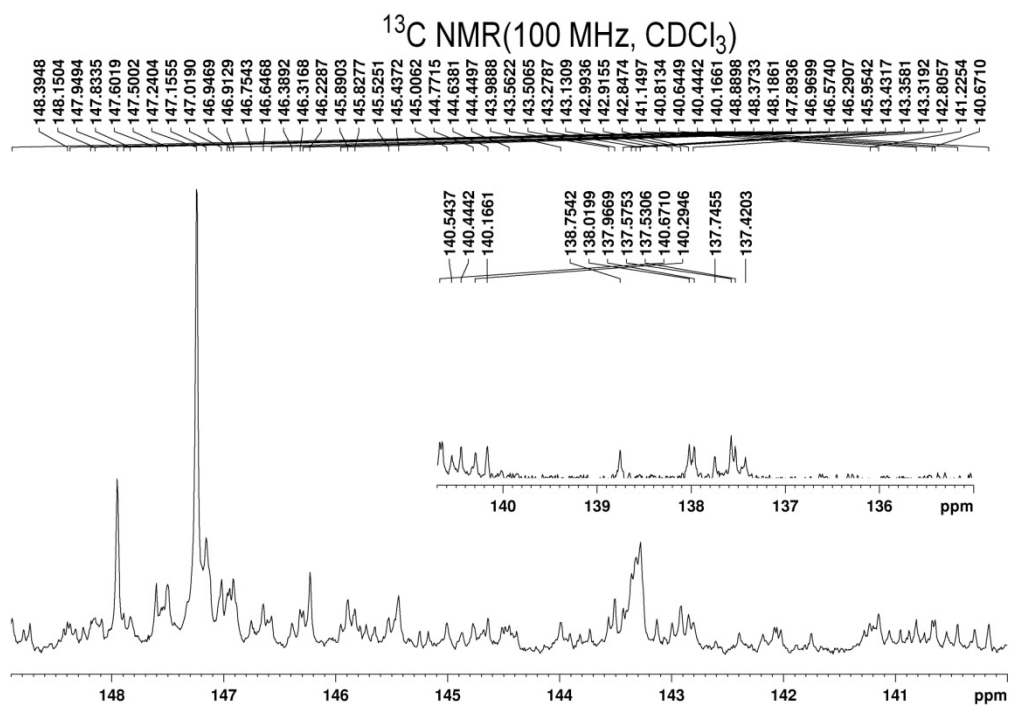


Figure S21. Expansion of the ^{13}C NMR of $\text{C}_{70}\text{-B-T}$.

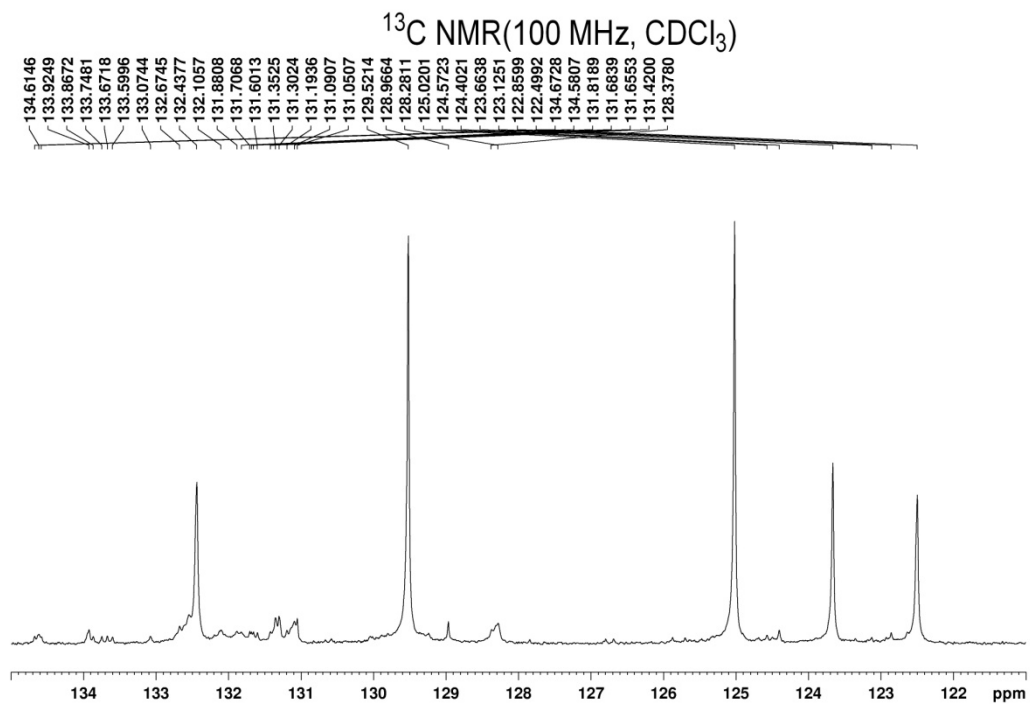


Figure S22. Expansion of the ¹³C NMR of C₇₀-B-T.

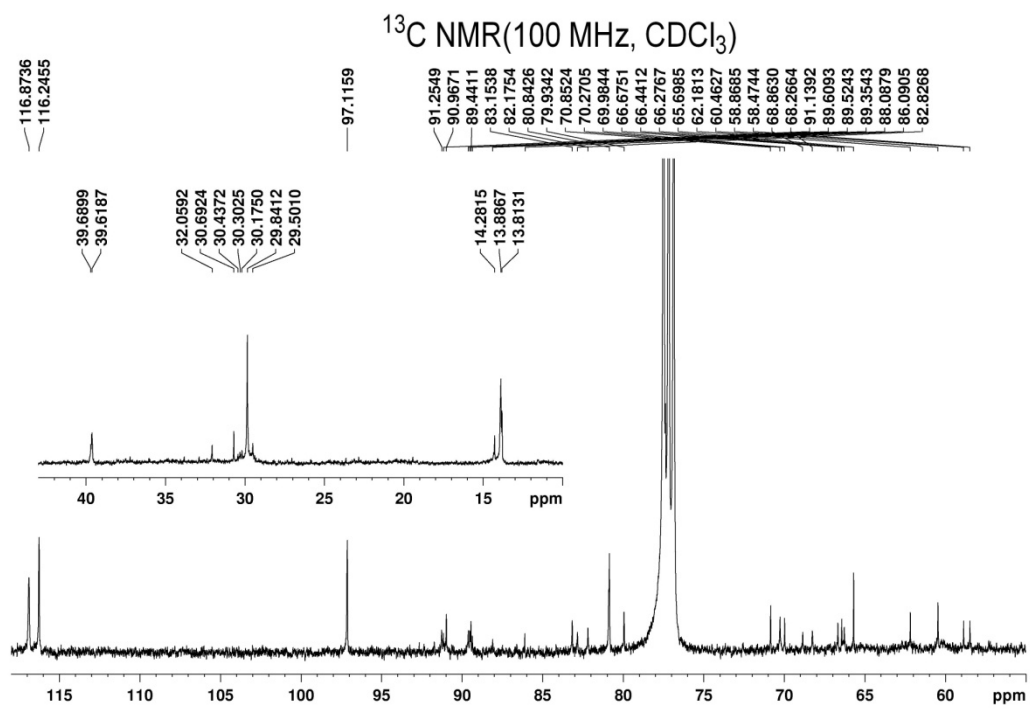


Figure S23. Expansion of the ¹³C NMR of C₇₀-B-T.