

Supporting Information

Cross-dimerization of fluorenones for synthesis of dibenzo[g,p]chrysenes

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1. The analytical HPLC report for **27**, which was helped by Daicel Corporation CPI Company, Mr. Miyamoto.

YKM493 参考分析条件

Column: CHIRALPAK ID (0.46cmI.D. × 25cmL)

Eluent: n-Hex / THF = 70 / 30 < v / v >

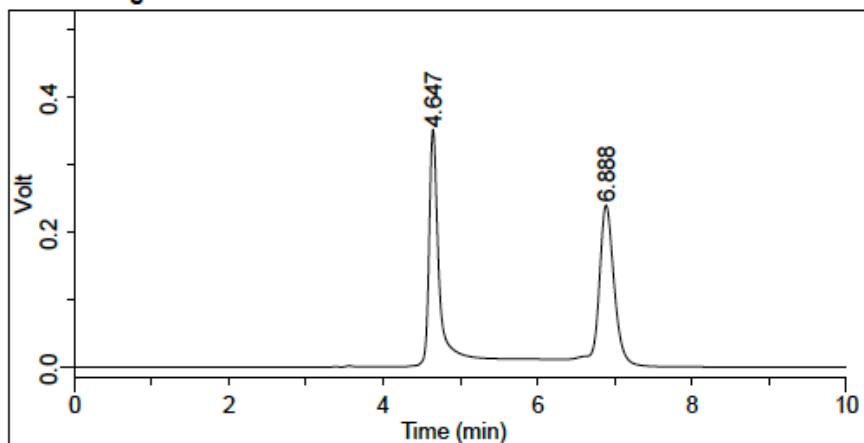
Flow Rate: 1.0mL/min.

Temp.: 25 °C

Det.: 306 nm (UV)

Injection: 10 μL (500mg/L in Eluent)

Chromatogram

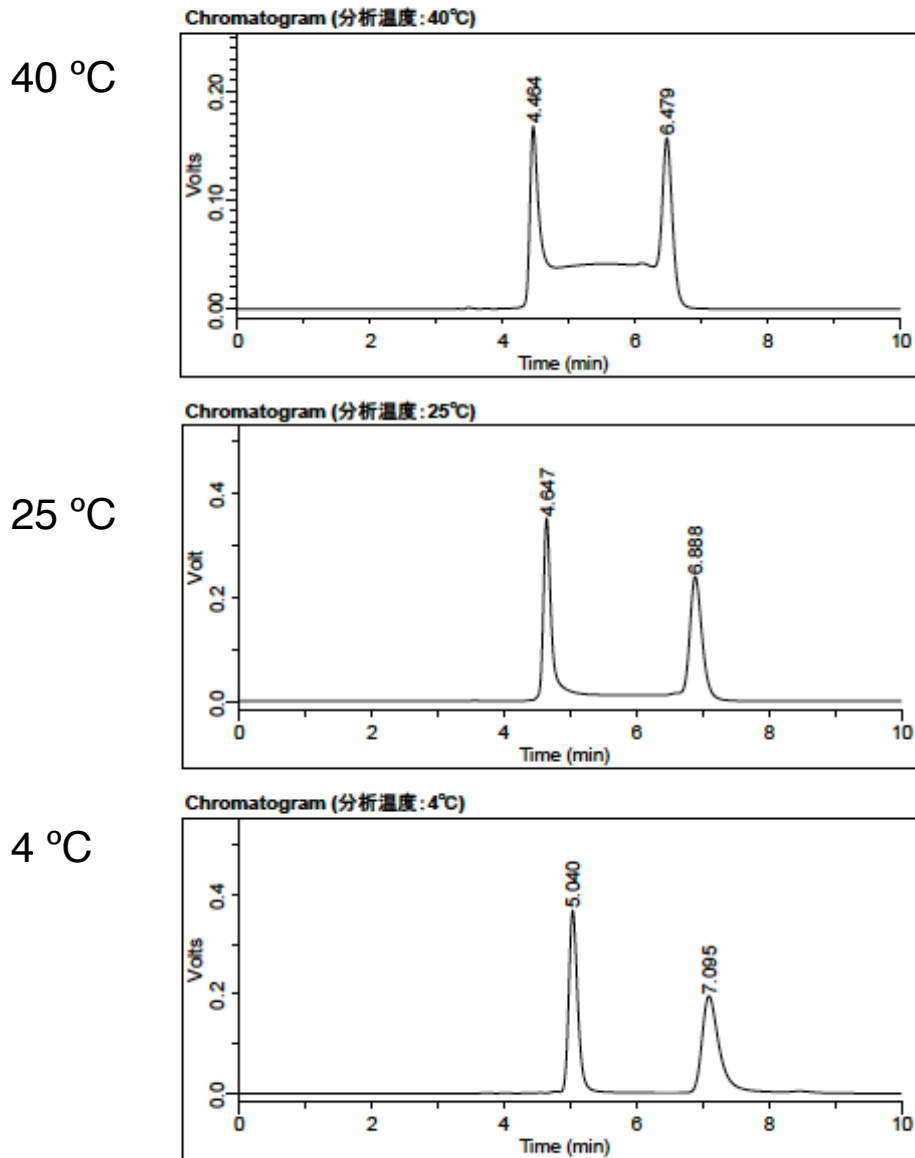


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n-Hex=n-Hexane

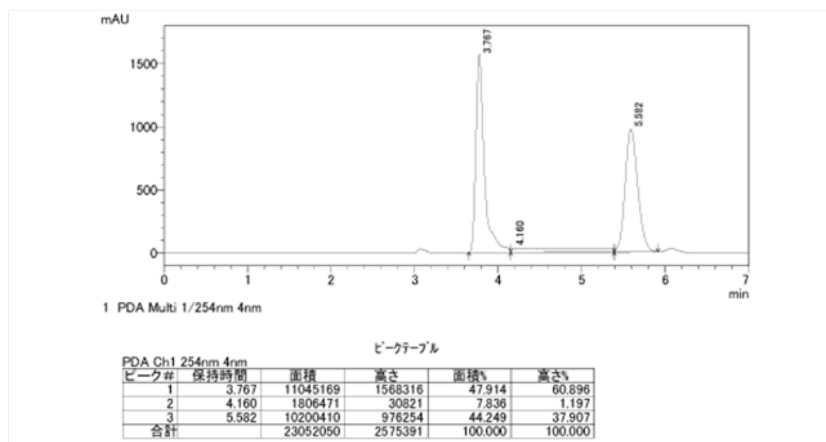
THF=Tetrahydrofuran

YKM493 分析温度の違いによるクロマトグラムの比較

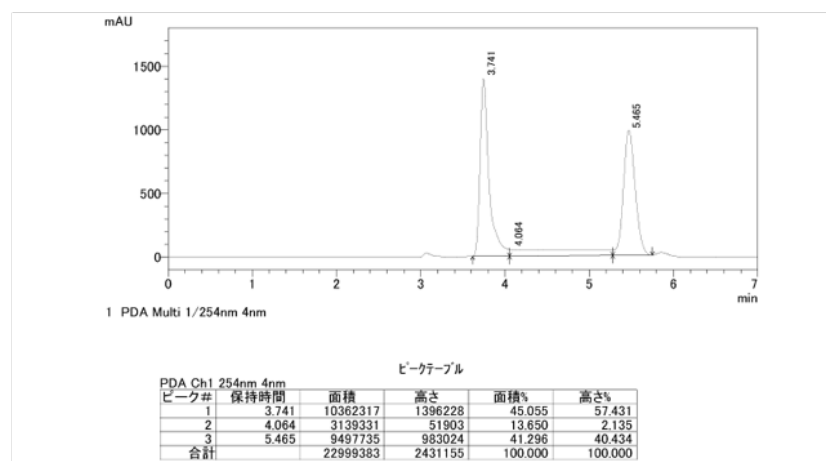


2. The temperature- and time-dependent chiral HPLC analysis of compound **27**

27 °C
1.0 mL/min



31 °C
1.0 mL/min



41 °C
1.0 mL/min

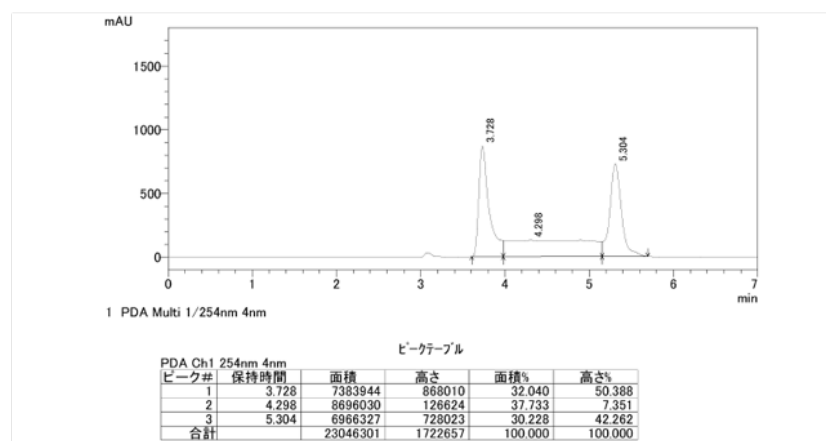
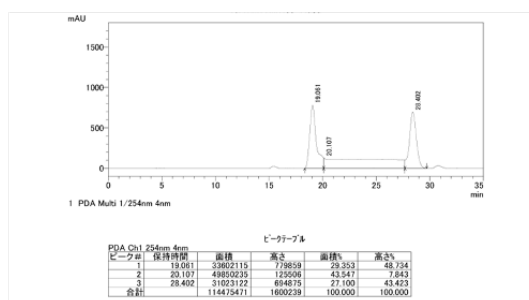
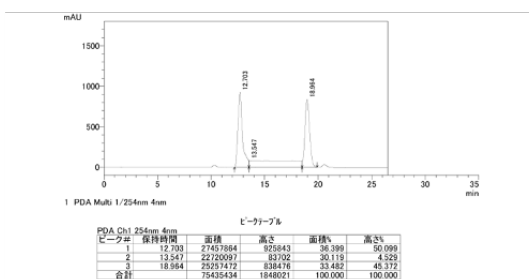


Figure S1. Temperature-dependent chiral HPLC analysis of **27** using CHIRALPAK ID-3 (4.6 mm I.D. × 25 cm L) as a stationary phase. Flow rate: 1.0 mL/min, eluent: hexane/EtOAc 1:1, detection: 254 nm, temperature: 27 - 41 °C.

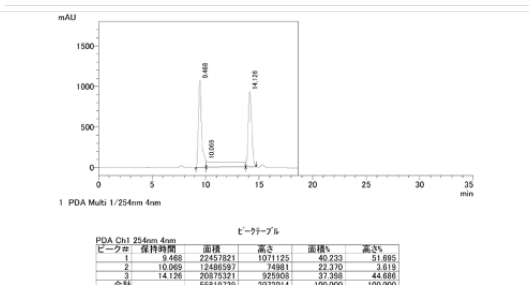
27 °C 0.2 mL/min



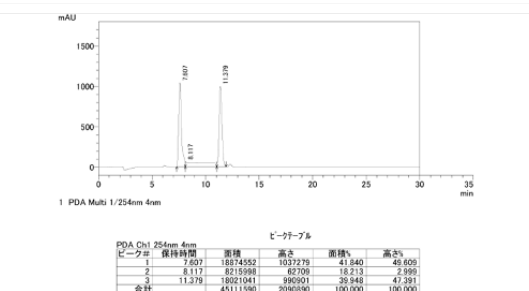
0.3 mL/min



0.4 mL/min



0.5 mL/min



1.0 mL/min

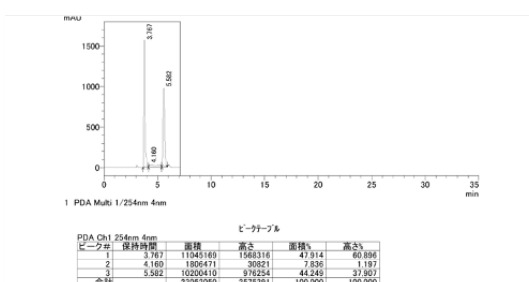
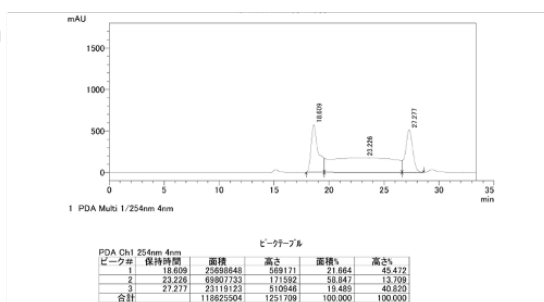
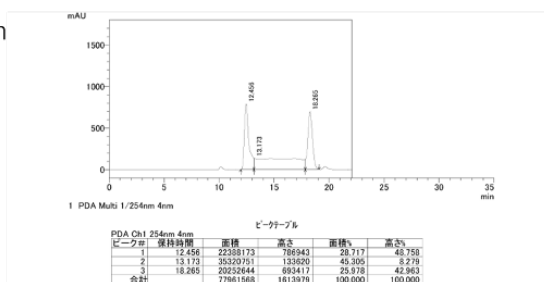


Figure S2. Time-dependent chiral HPLC analysis of **27** using CHIRALPAK ID3 (4.6 mmI.D.× 25 cmL) as a stationary phase. Flow rate: 0.2-1.0 mL/min, eluent: hexane/EtOAc 1:1, detection: 254 nm, temperature: 27 °C.

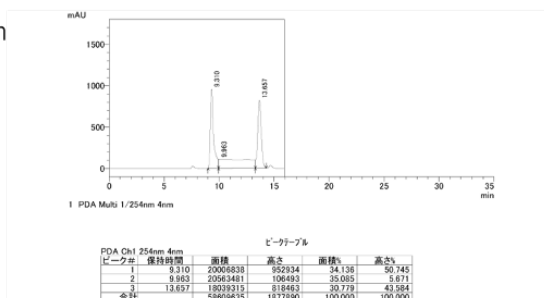
31 °C 0.2 mL/min



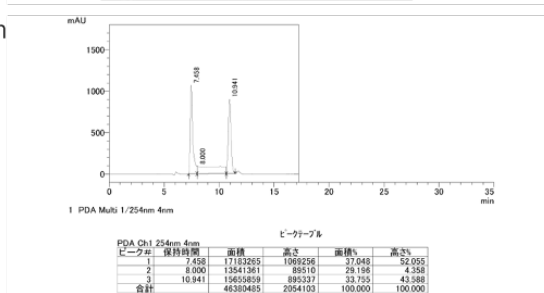
0.3 mL/min



0.4 mL/min



0.5 mL/min



1.0 mL/min

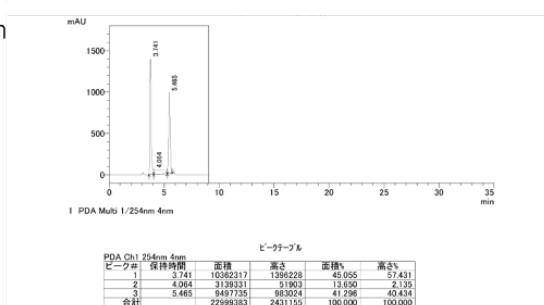


Figure S3. Time-dependent chiral HPLC analysis of **27** using CHIRALPAK ID3 (4.6 mm I.D. x 25 cm L) as a stationary phase. Flow rate: 0.2-1.0 mL/min, eluent: hexane/EtOAc 1:1, detection: 254 nm, temperature: 31 °C.

3. ORTEP drawings of DBC-**27** core with description of the selected bond-lengths and -angles, and its molecular packing structures (Figure S4).

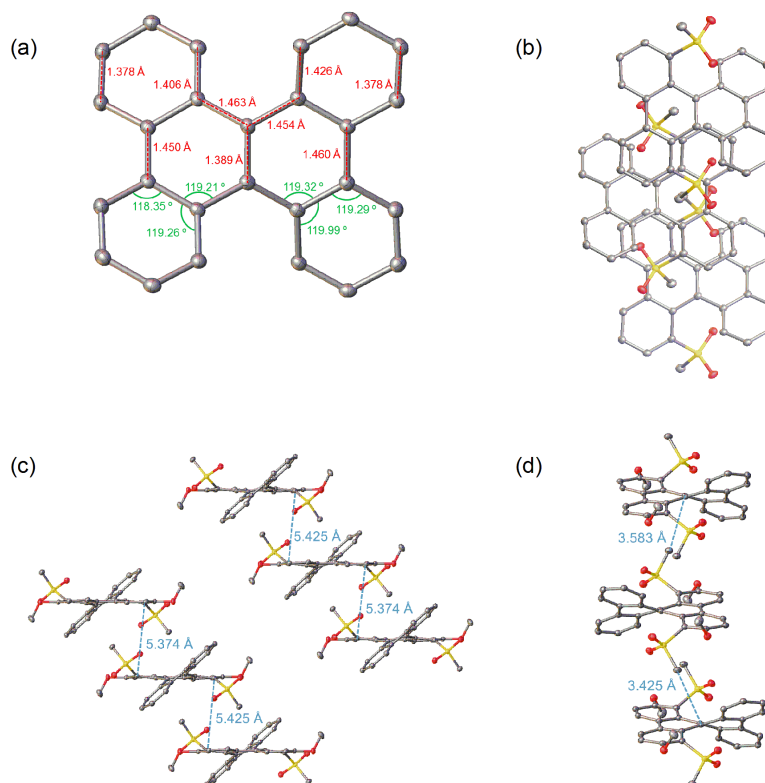
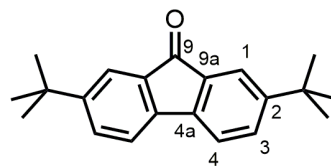
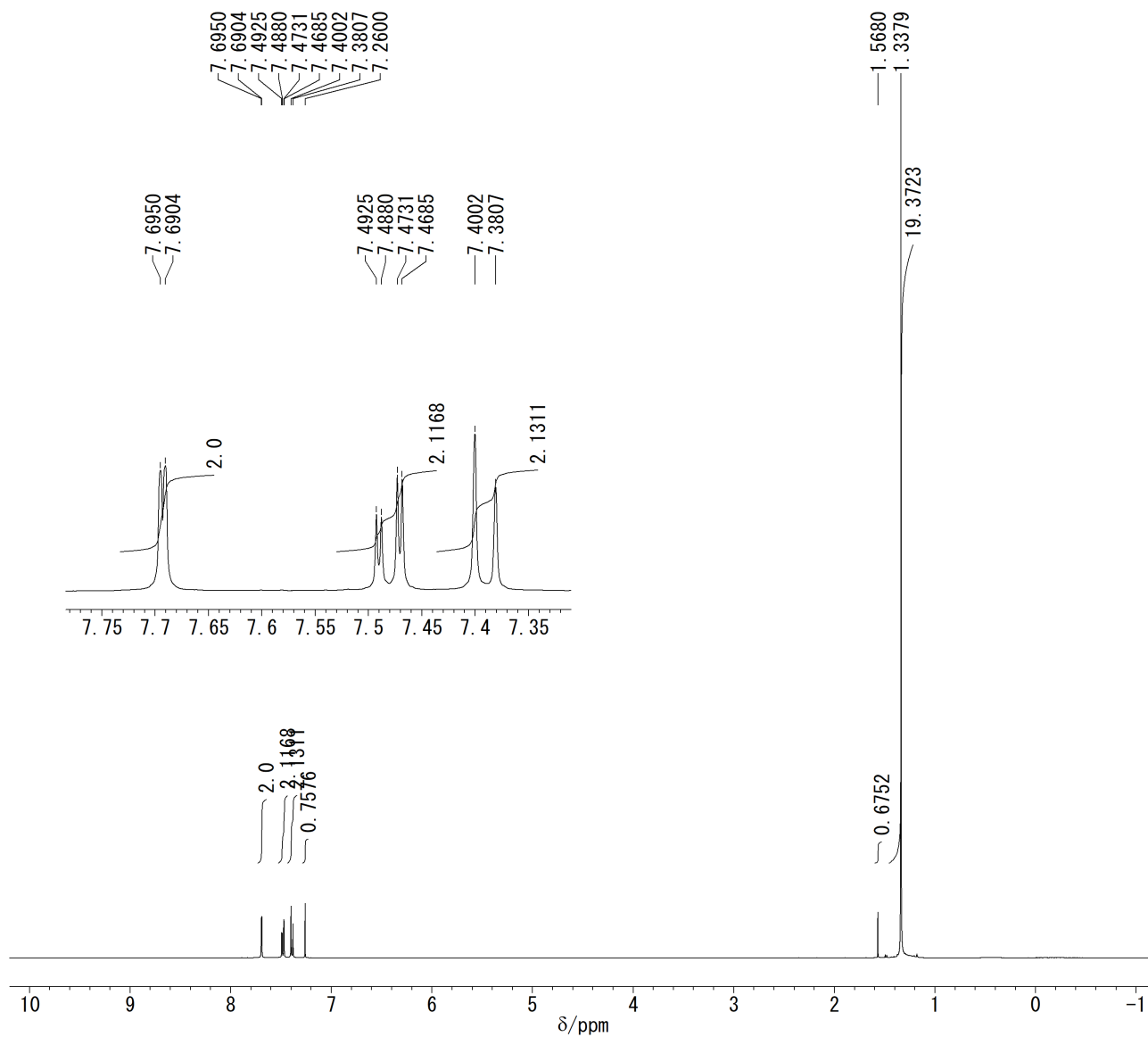


Figure S4. Molecular structures with ORTEP drawing of **27** with thermal ellipsoids at the 50% probability level (the hydrogen atoms are omitted for clarity); (a) the selected bond-lengths and angles (peripheral substituents are removed for ease of viewing); (b) packing structure, top view; (c) packing structure, side view from a *bay* region with description of the shortest intramolecular layer distance of 5.374 Å between two *ipso*-positioned carbons of methanesulfonyl groups (*tert*-butyl groups are omitted for ease of viewing); (d) packing structure, side view from a *cove* region with description of the shortest intramolecular distance of 3.425 Å between the methyl carbon of methanesulfonyl group and the one carbon of intersectional carbon-carbon double bond .

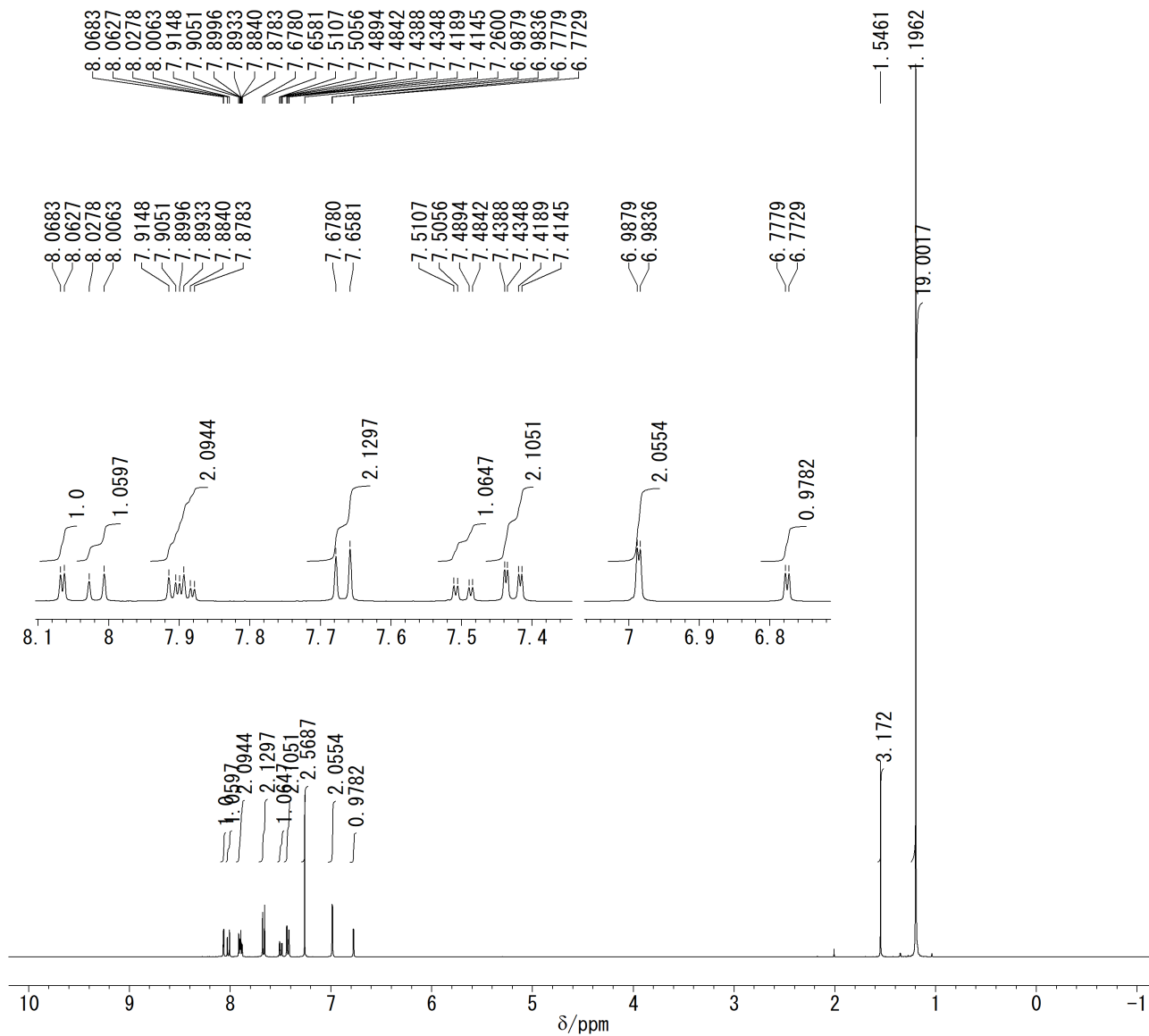
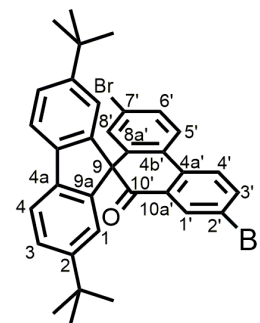
4. ^1H NMR and ^{13}C NMR spectra for all new compounds.



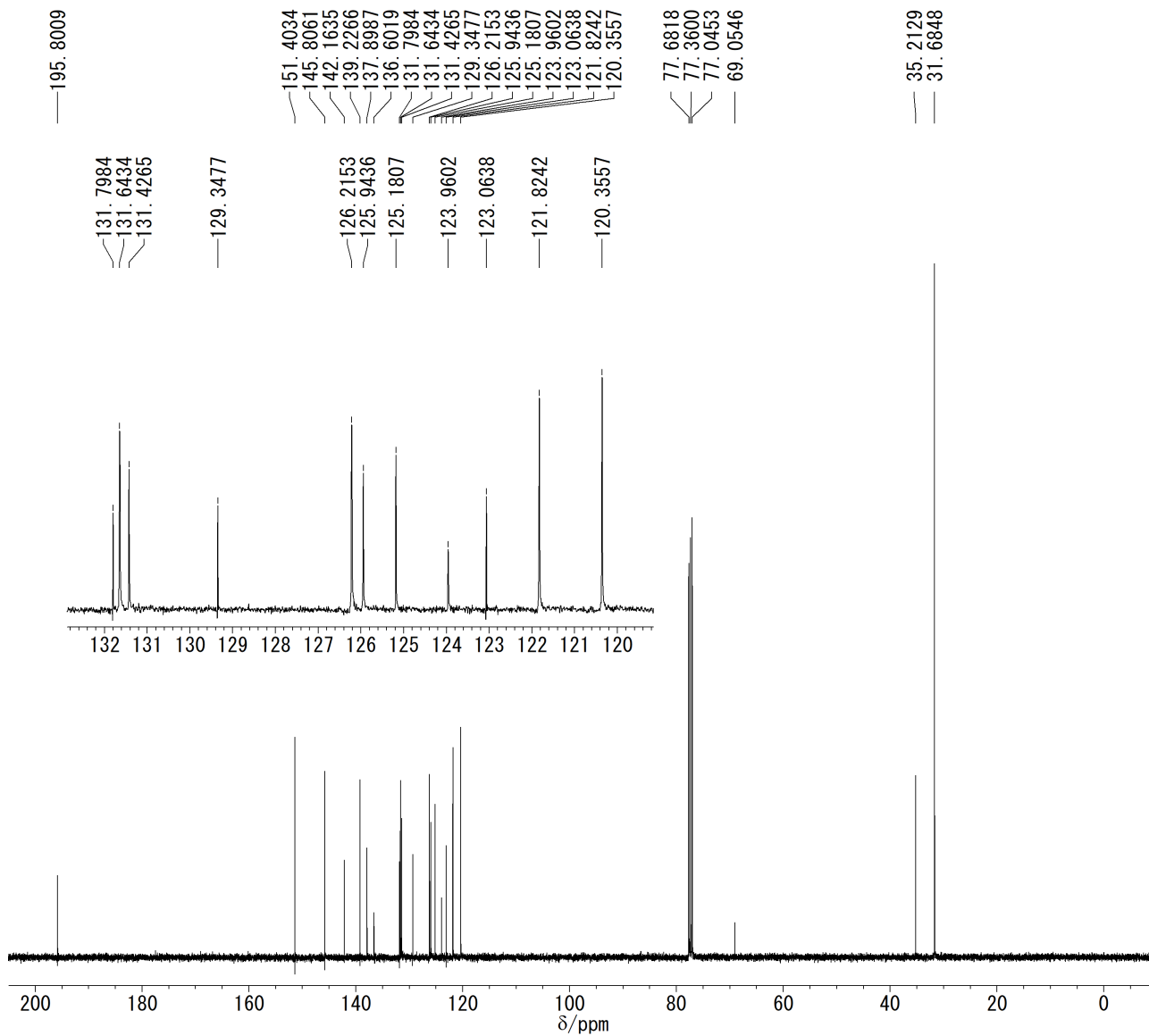
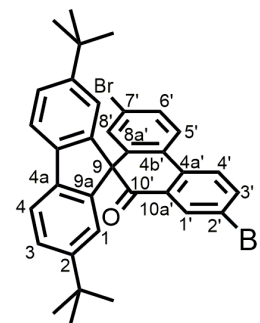
Compound **1** (^1H NMR spectrum, 400 MHz in CDCl_3).



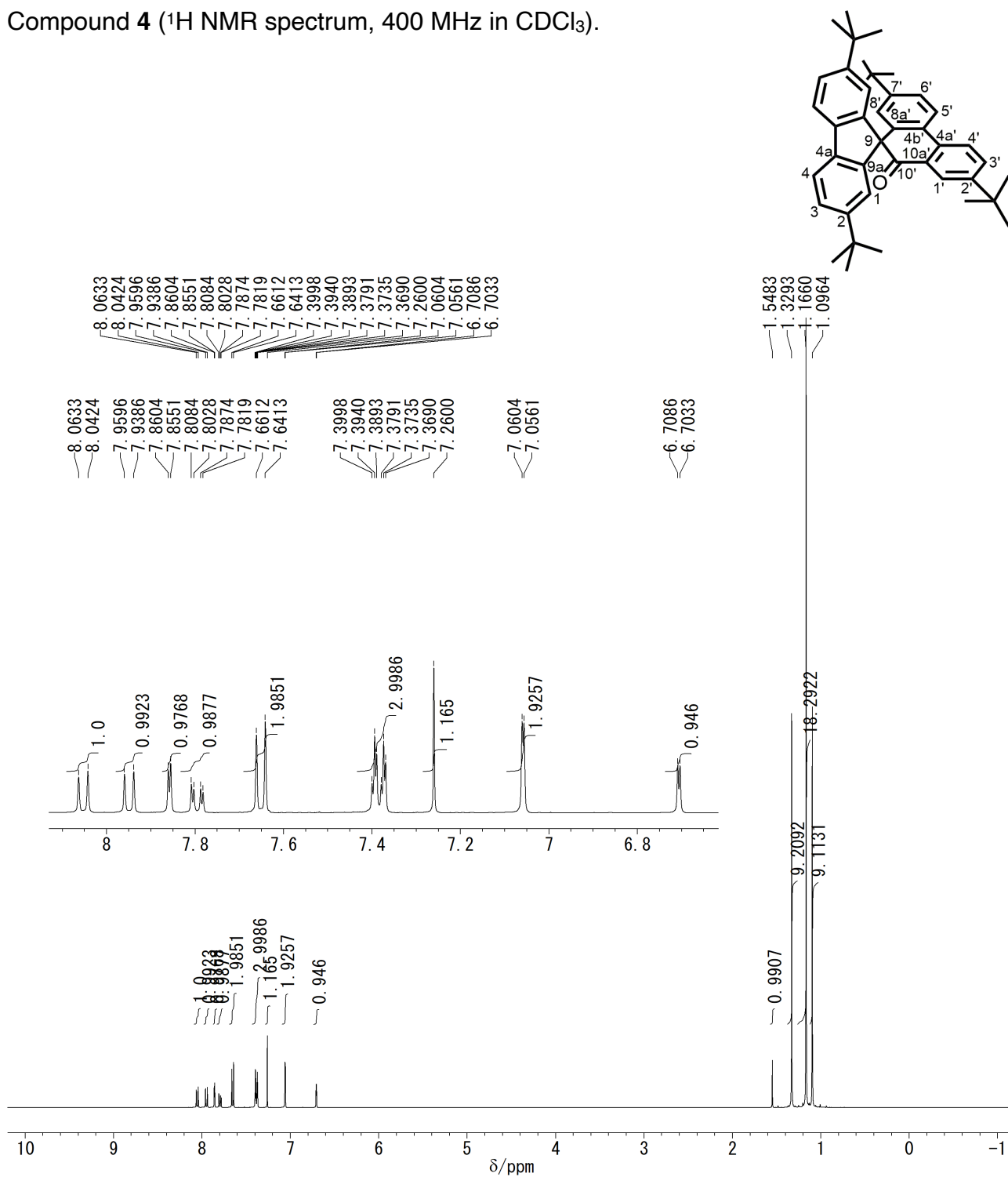
Compound 3 (¹H NMR spectrum, 400 MHz in CDCl₃).



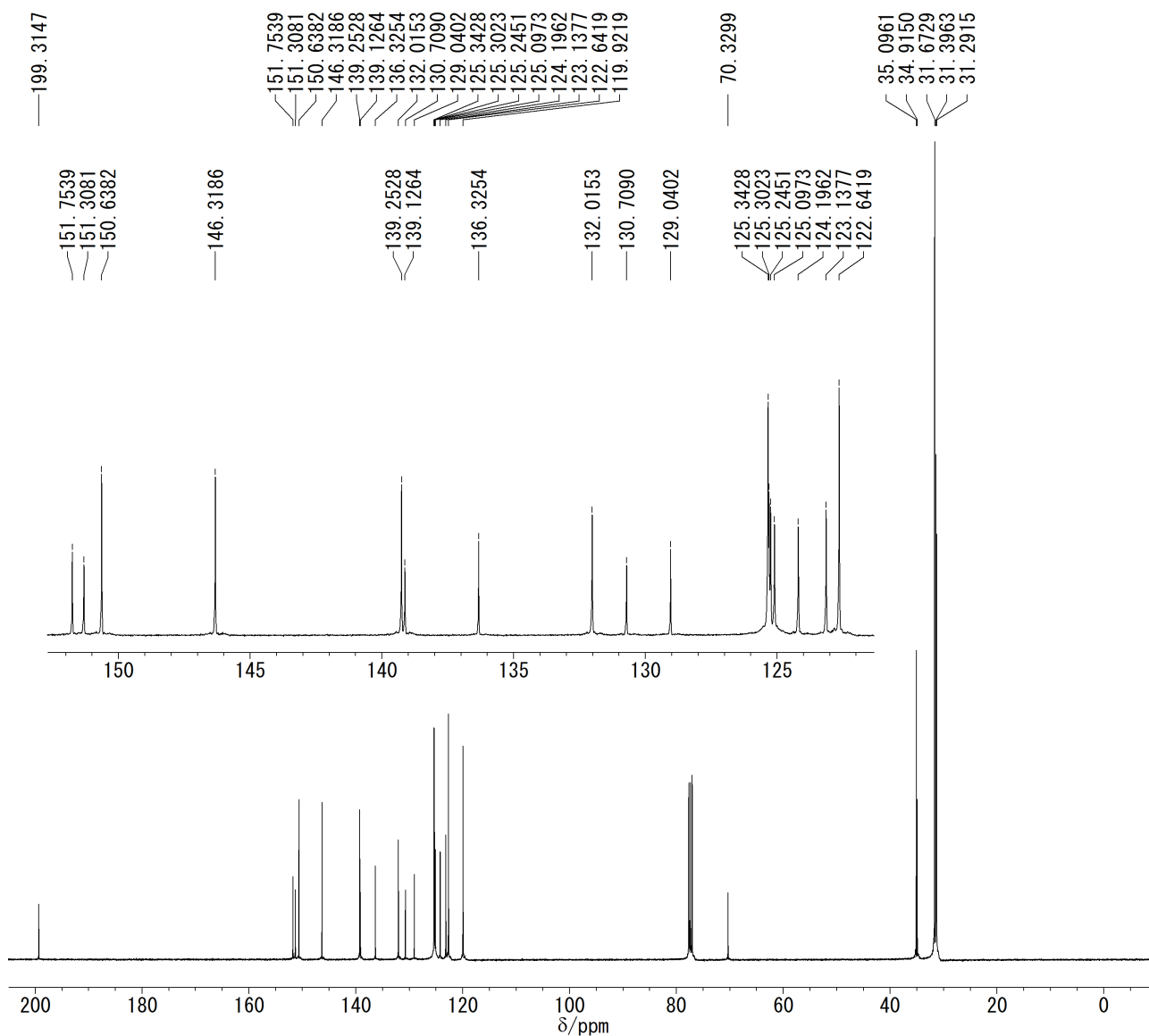
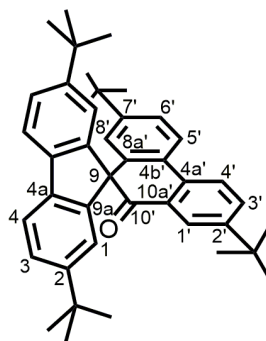
Compound 3 (^{13}C NMR spectrum, 100 MHz in CDCl_3).



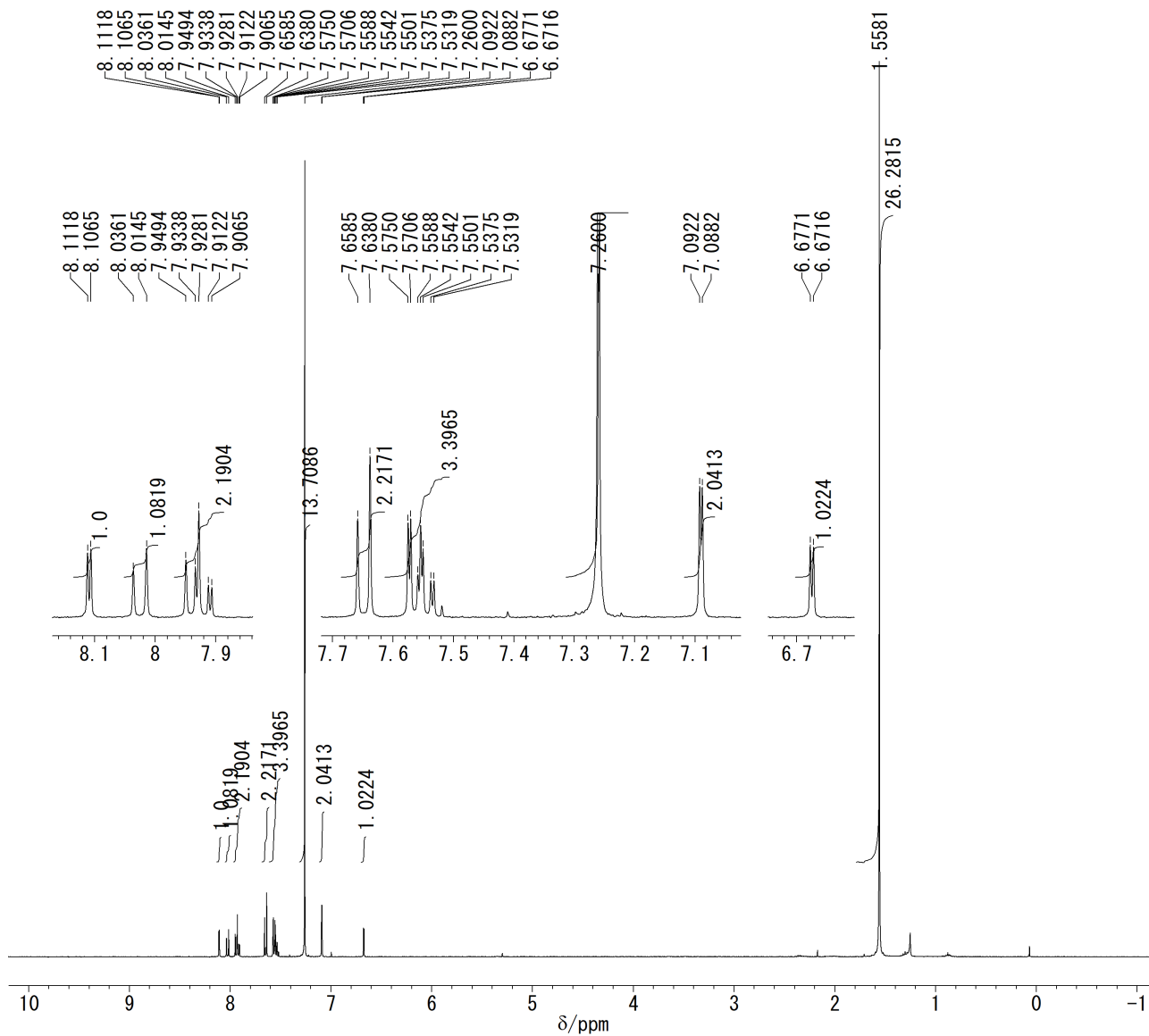
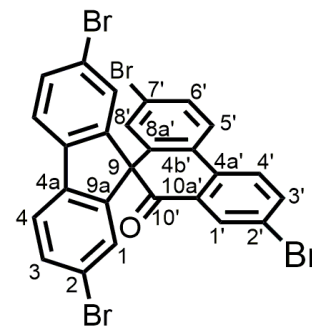
Compound 4 (¹H NMR spectrum, 400 MHz in CDCl₃).



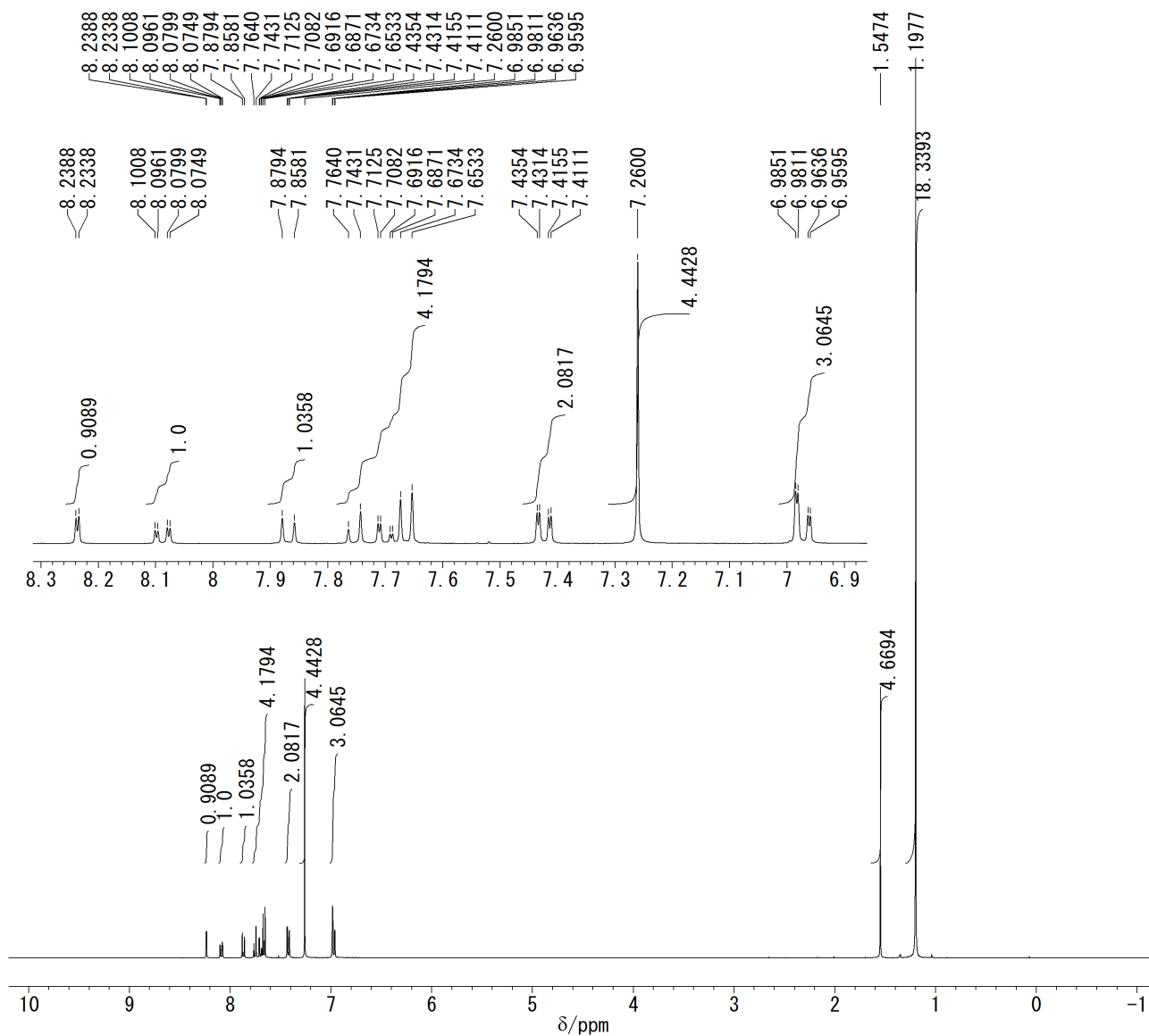
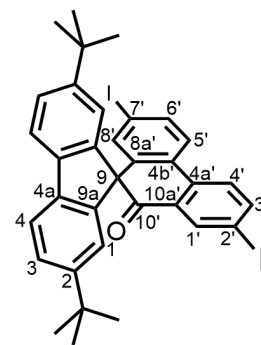
Compound 4 (¹³C NMR spectrum, 100 MHz in CDCl₃).



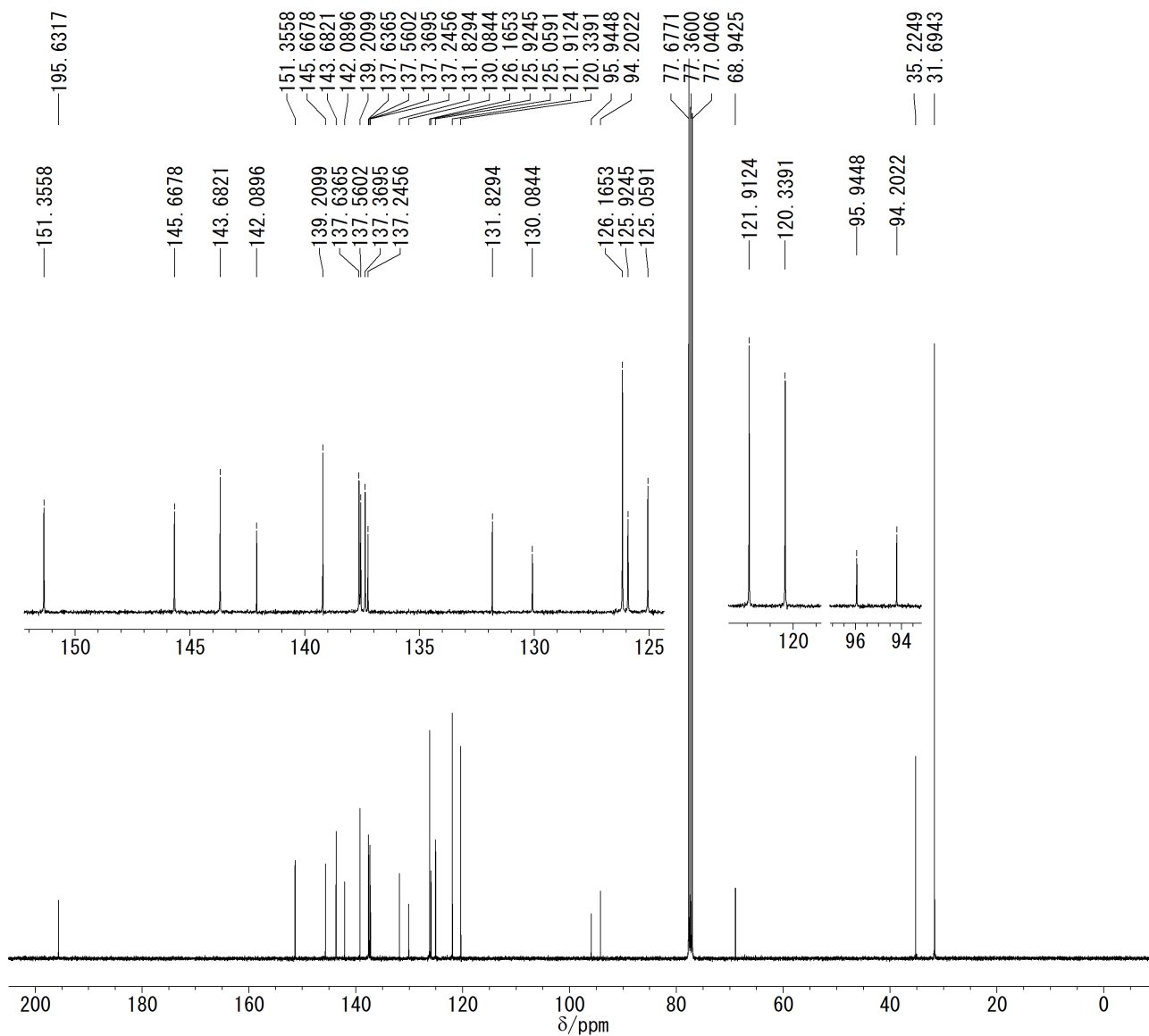
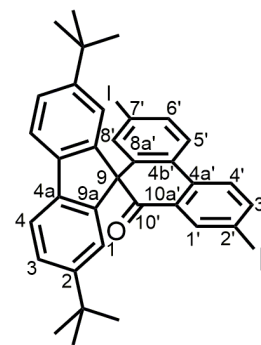
Compound 5 (¹H NMR spectrum, 400 MHz in CDCl₃).



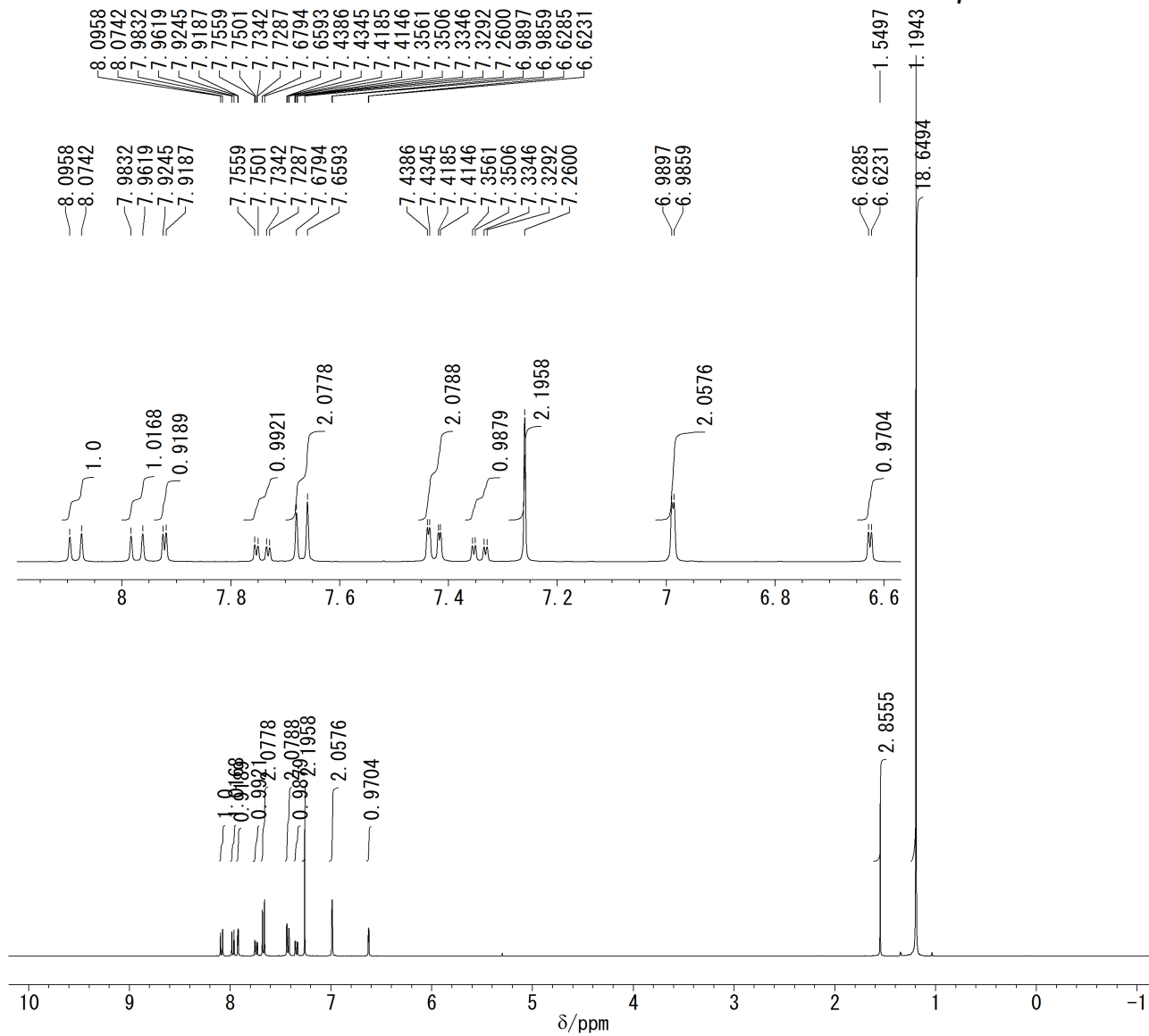
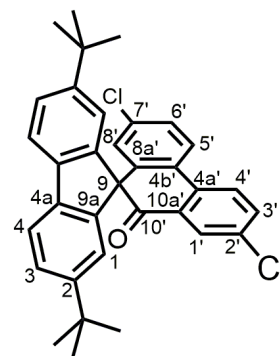
Compound 6 (¹H NMR spectrum, 400 MHz in CDCl₃).



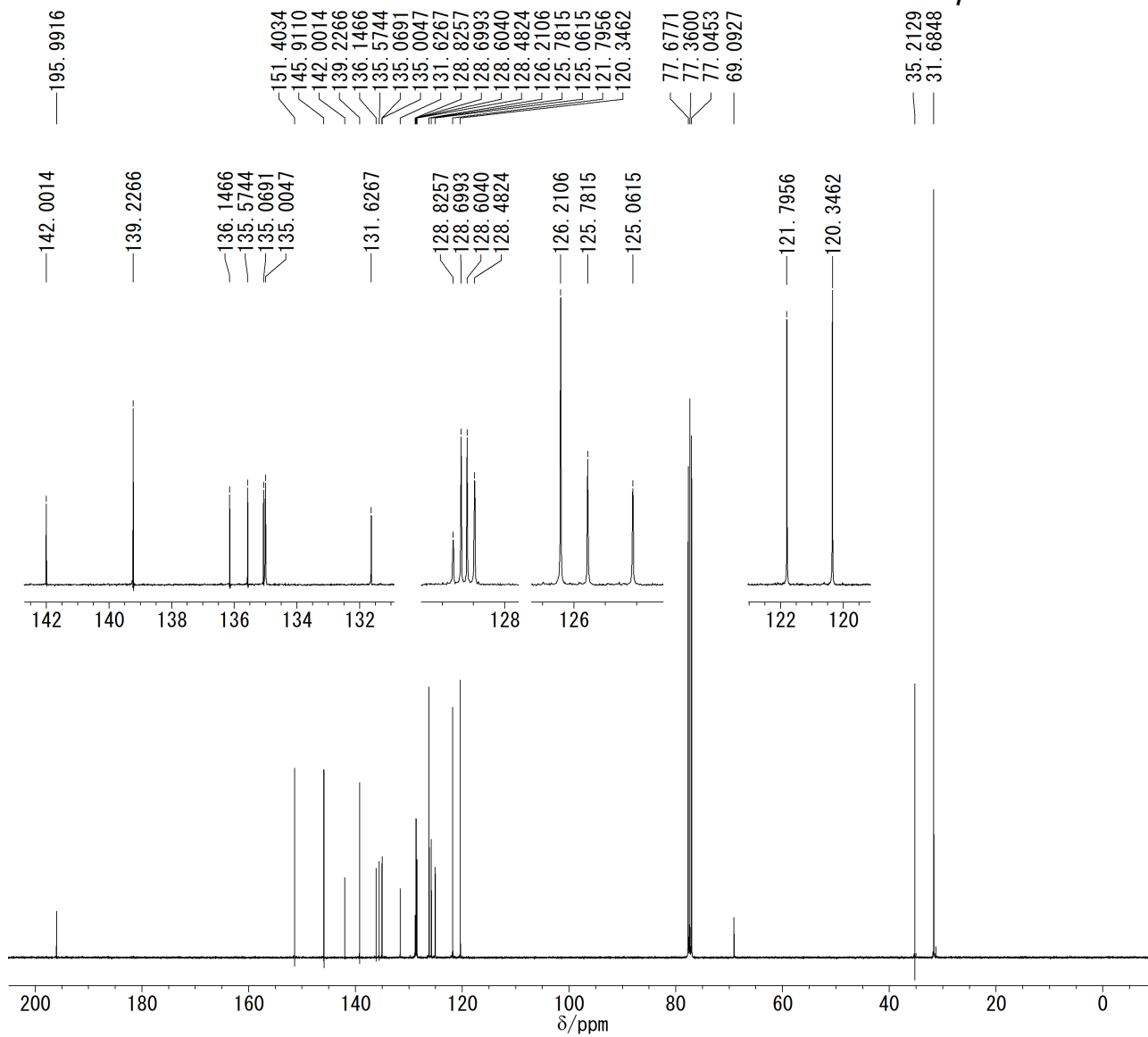
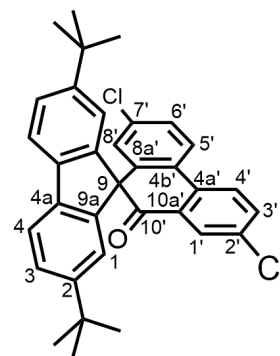
Compound **6** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



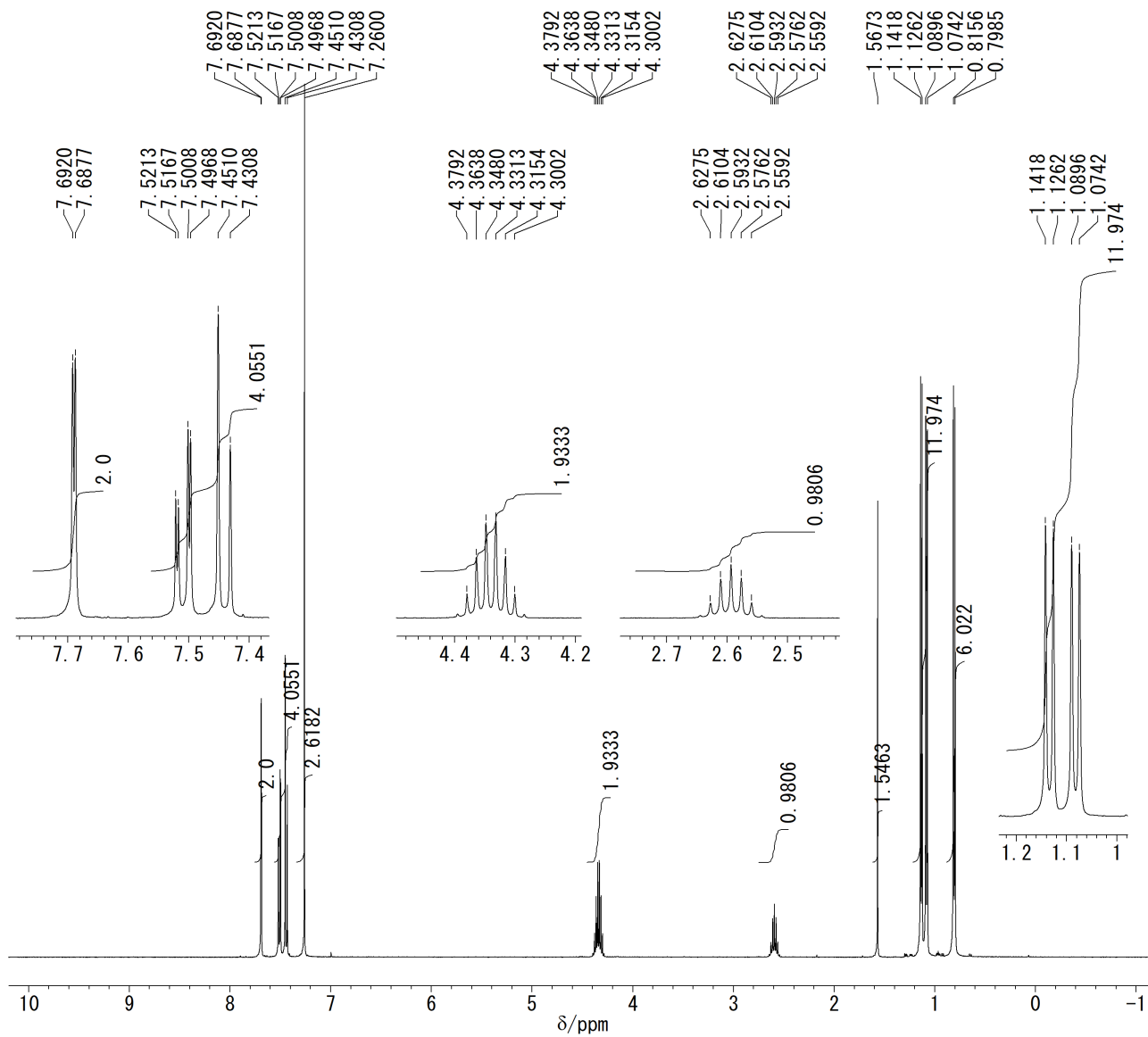
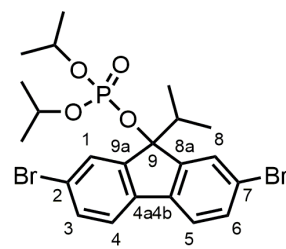
Compound 7 (¹H NMR spectrum, 400 MHz in CDCl₃).



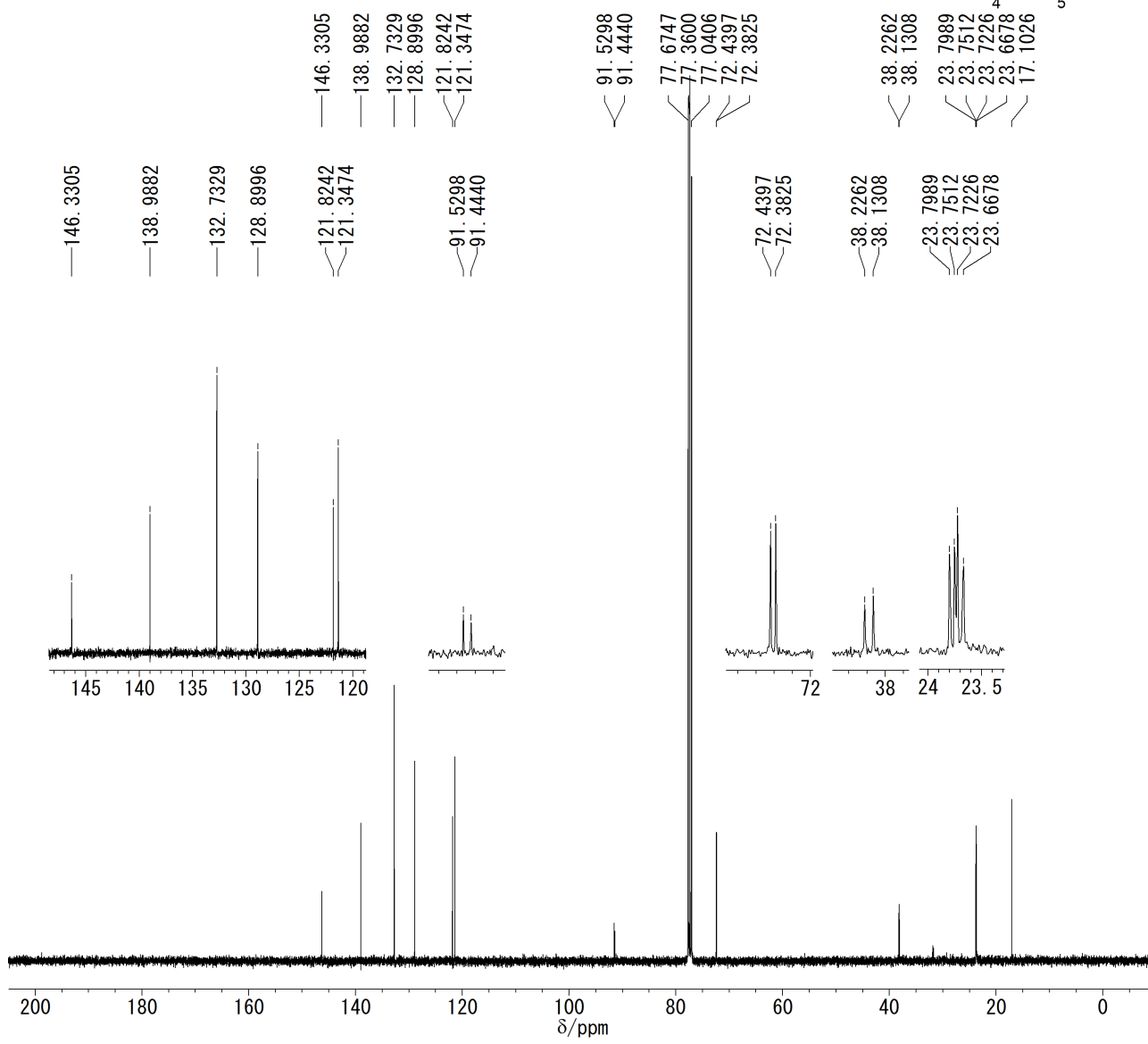
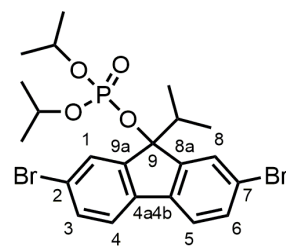
Compound 7 (^{13}C NMR spectrum, 100 MHz in CDCl_3).



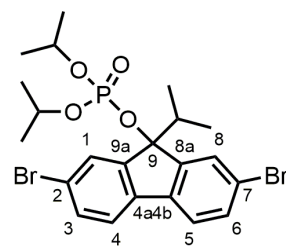
Compound **8** (^1H NMR spectrum, 400 MHz in CDCl_3).



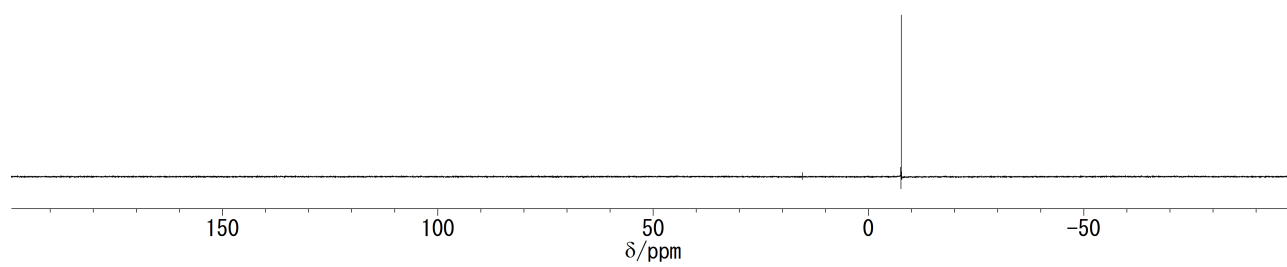
Compound **8** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



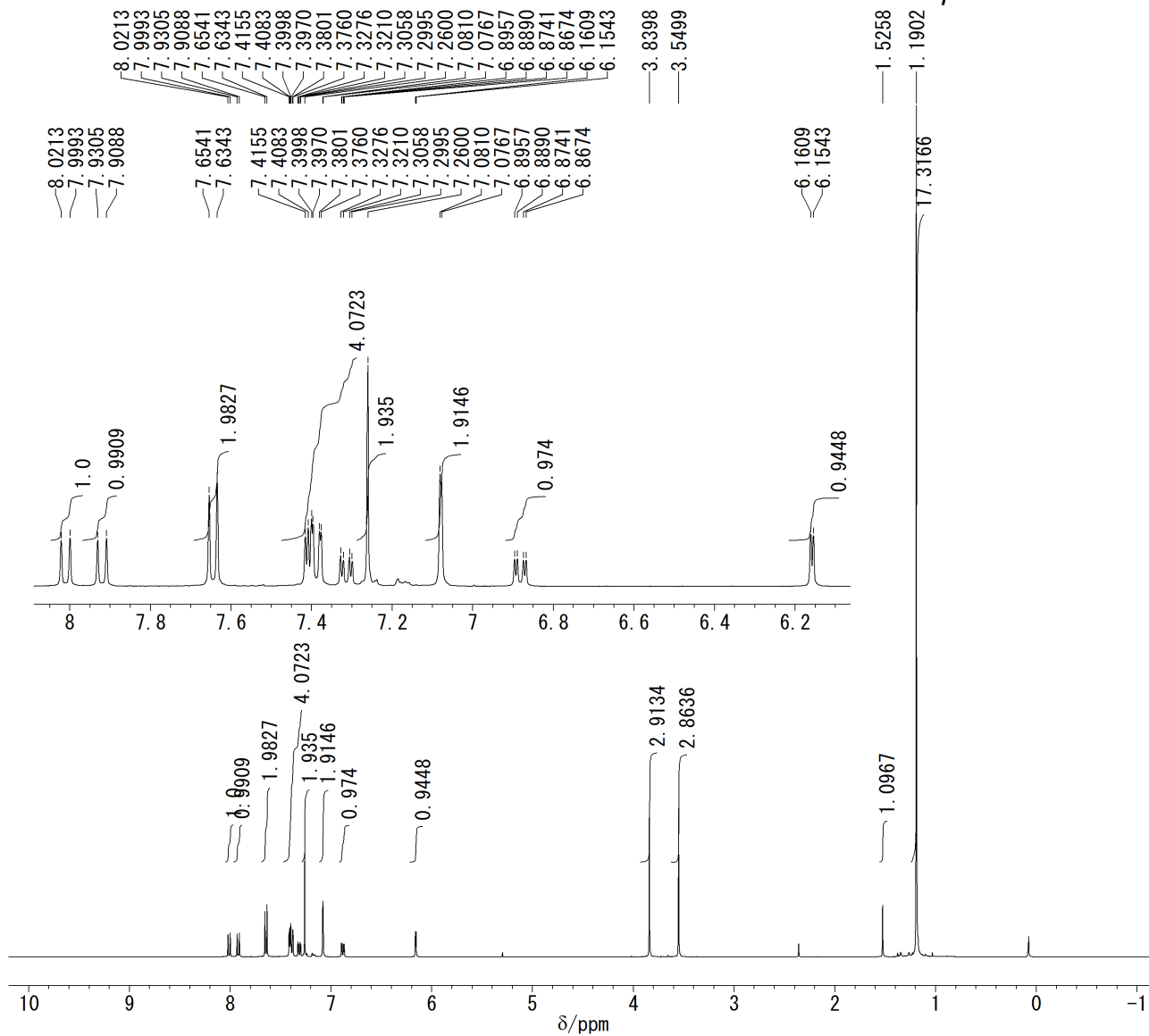
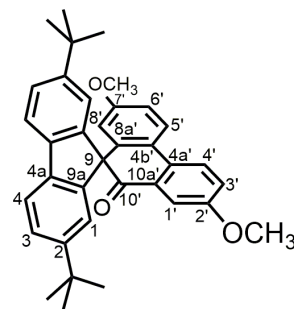
Compound **8** (^{31}P NMR spectrum, 162 MHz in CDCl_3)



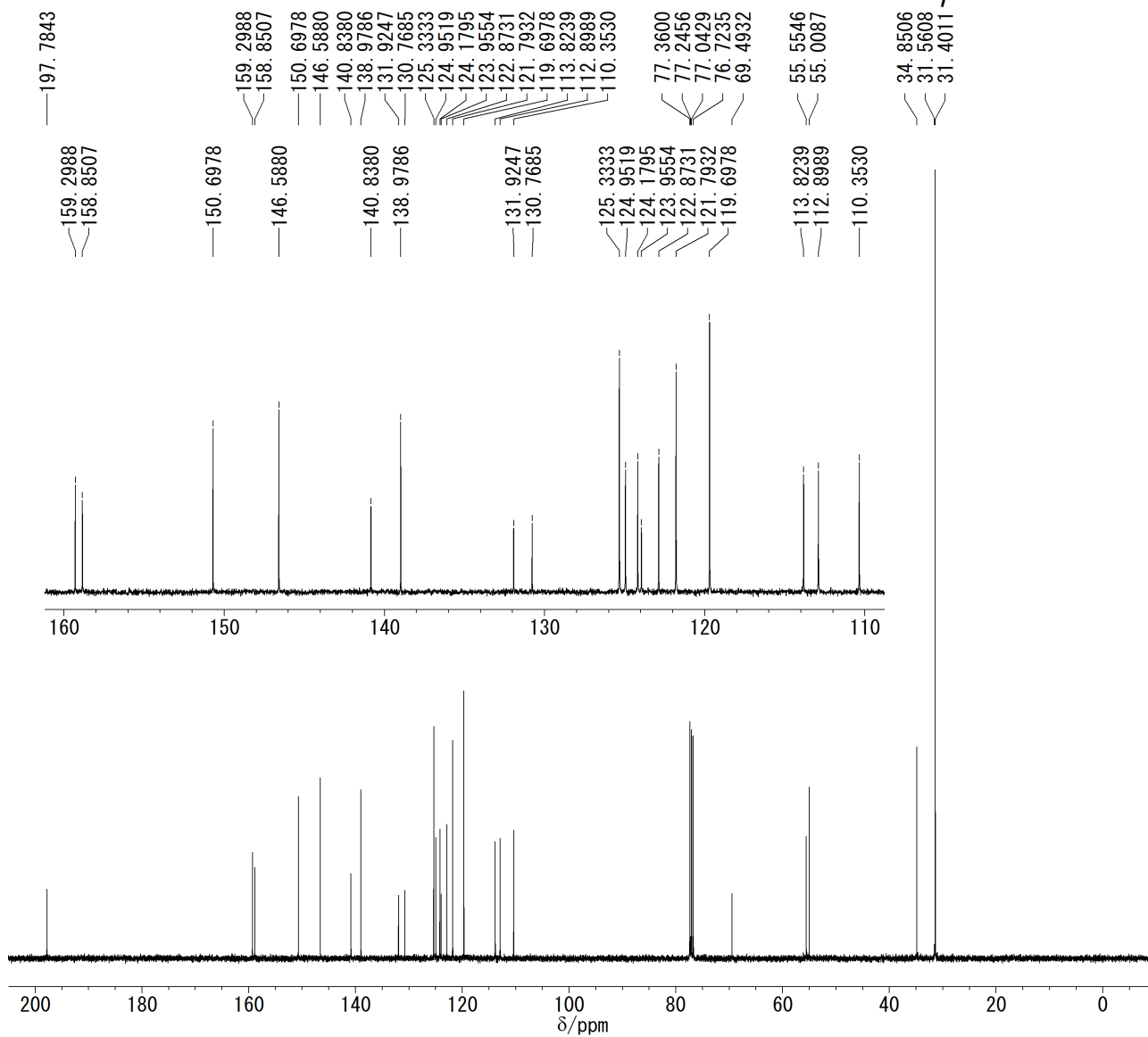
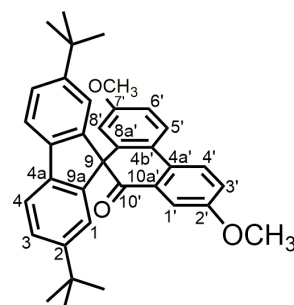
7.5894



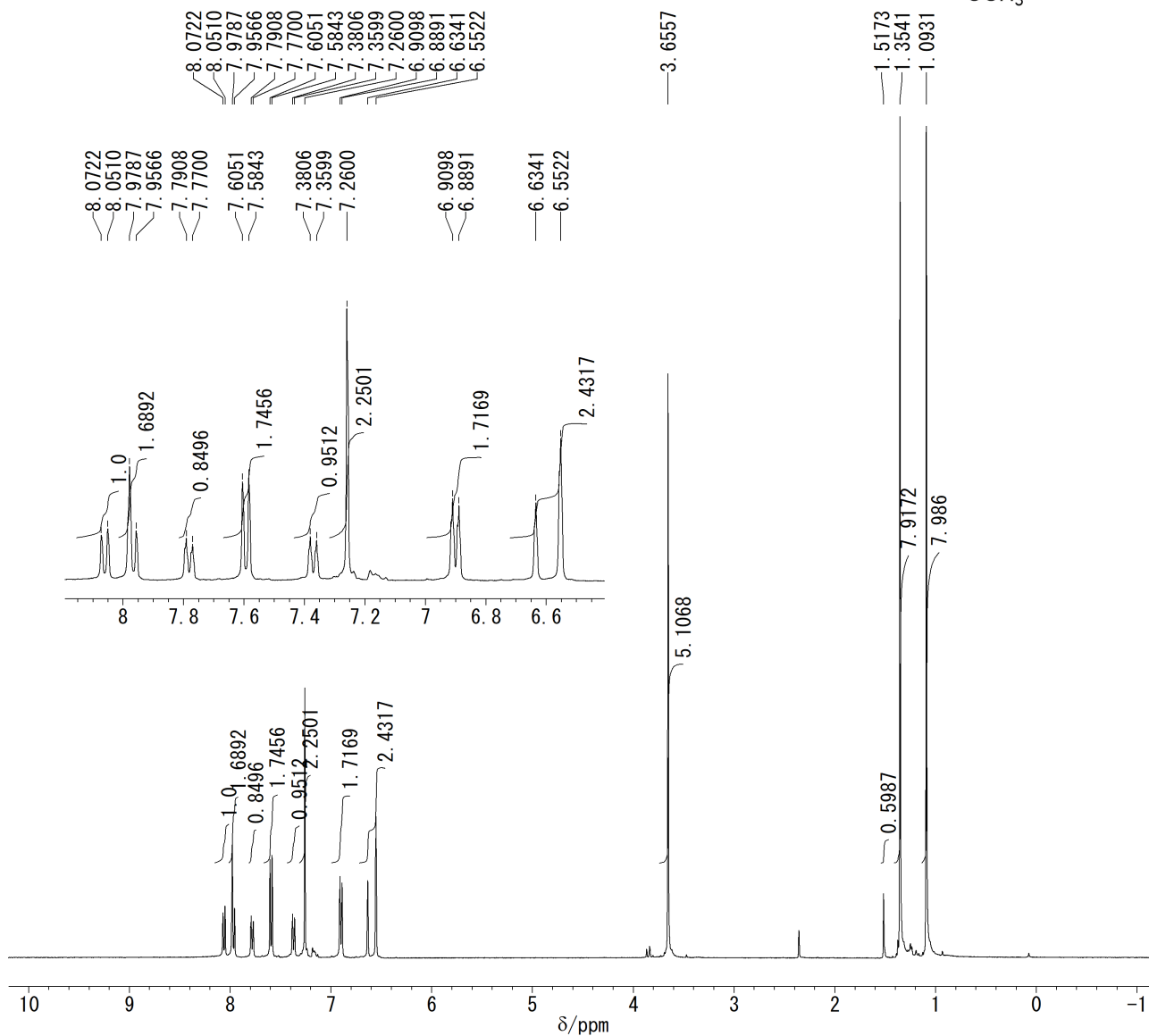
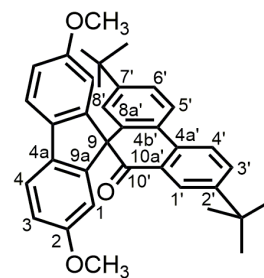
Compound **9** (^1H NMR spectrum, 400 MHz in CDCl_3).



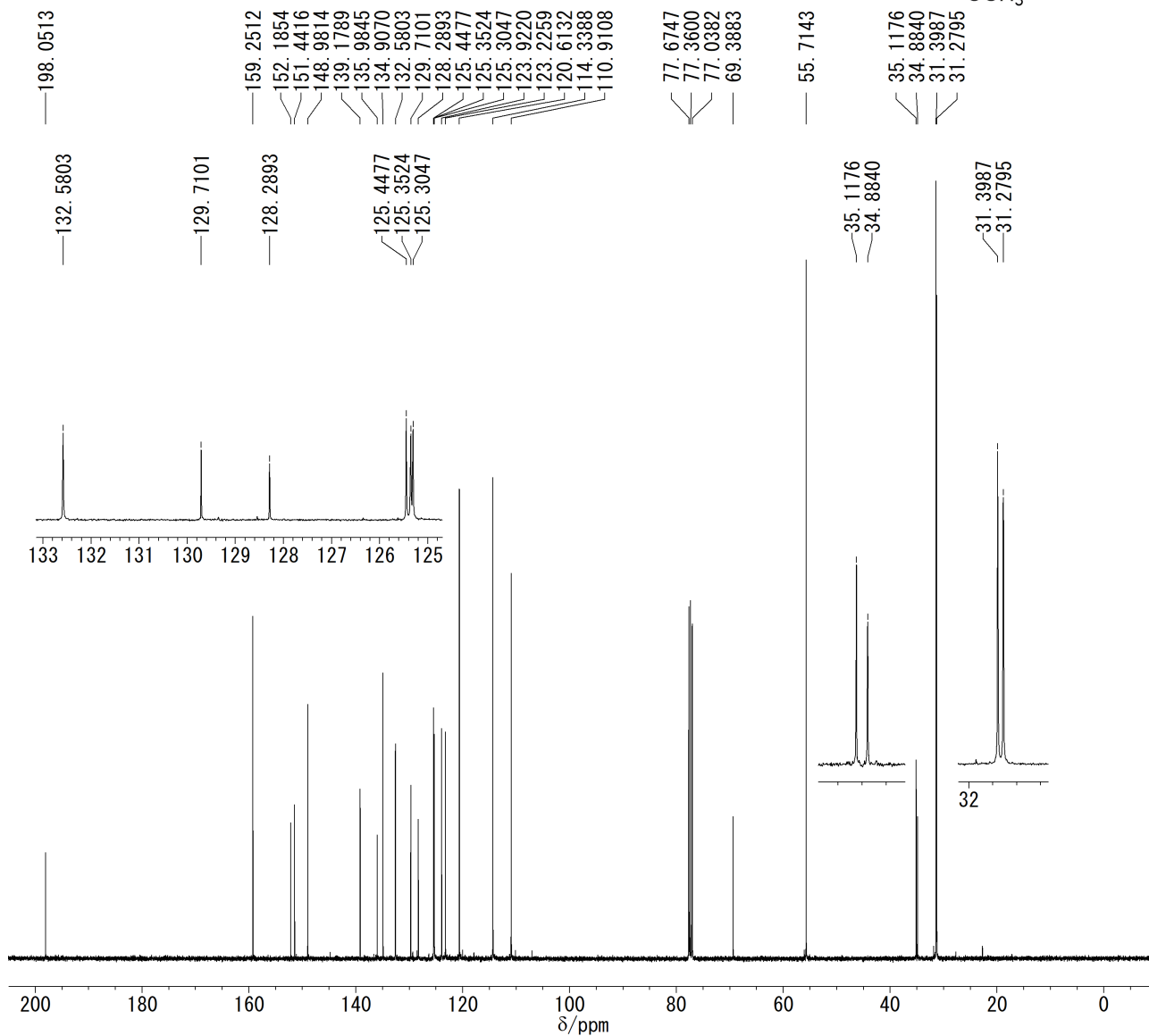
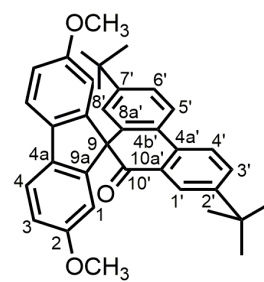
Compound **9** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



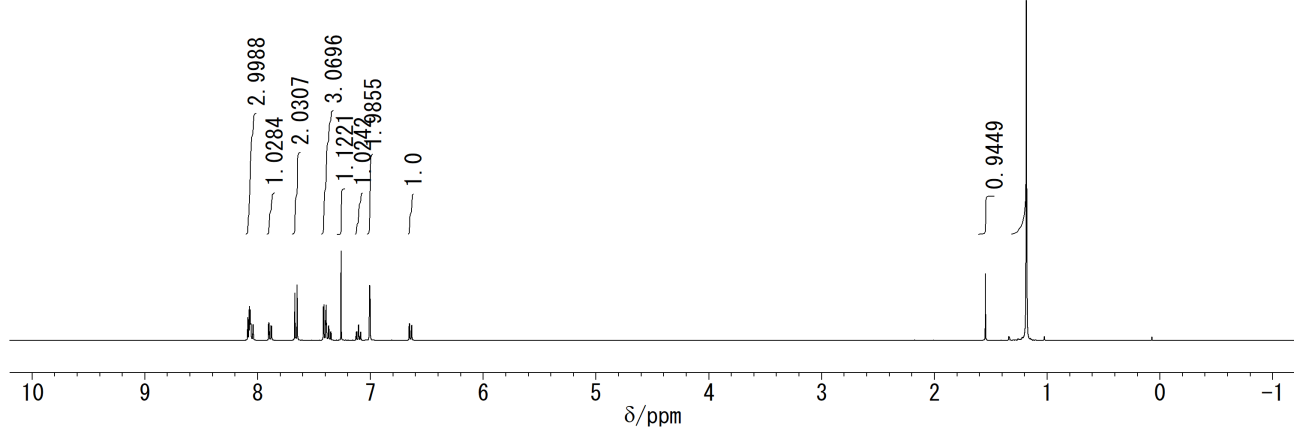
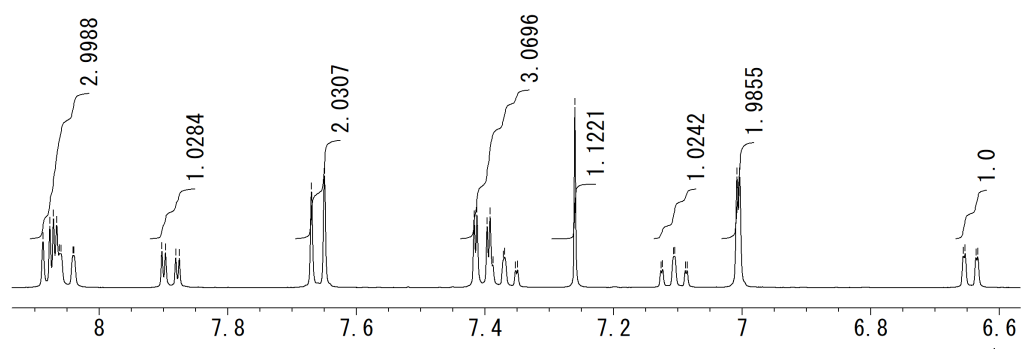
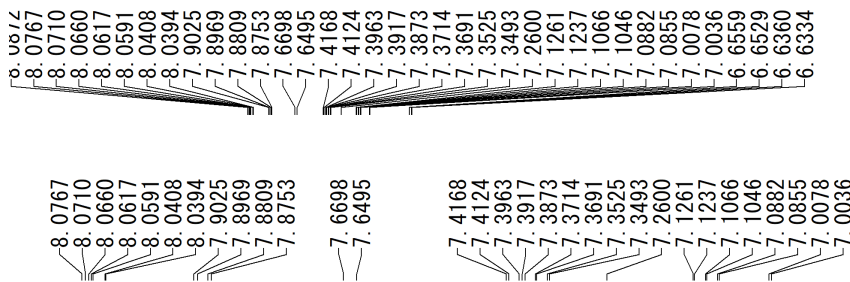
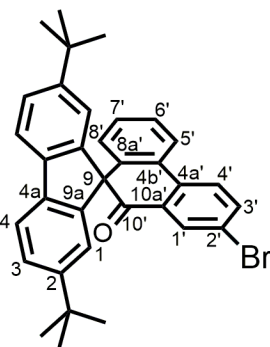
Compound *iso-9* (¹H NMR spectrum, 400 MHz in CDCl₃).



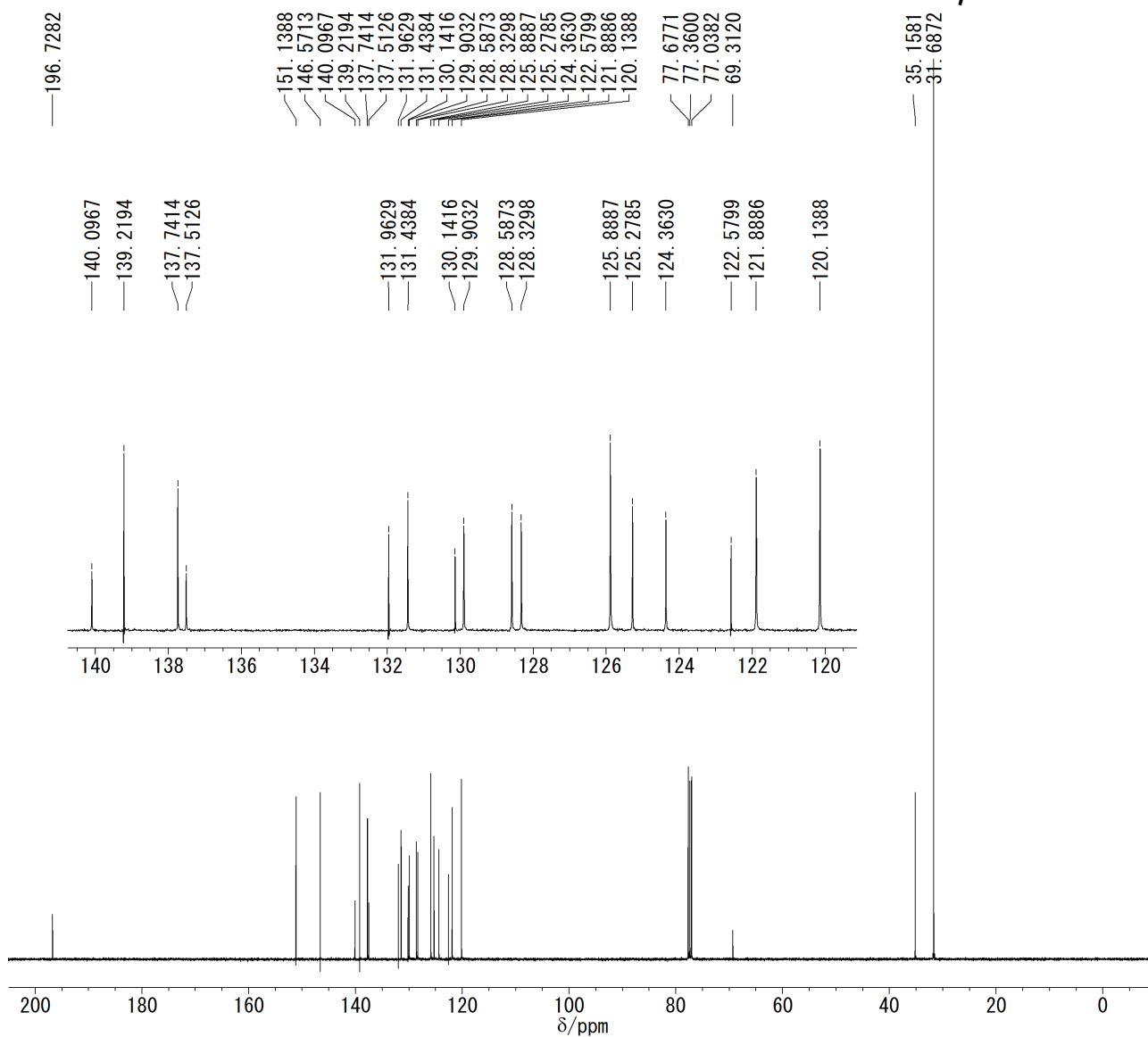
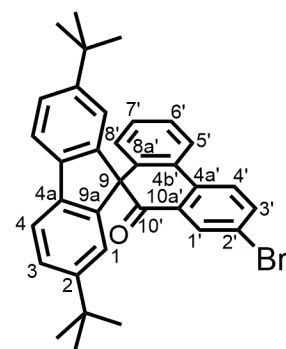
Compound *iso-9* (^{13}C NMR spectrum, 100 MHz in CDCl_3).



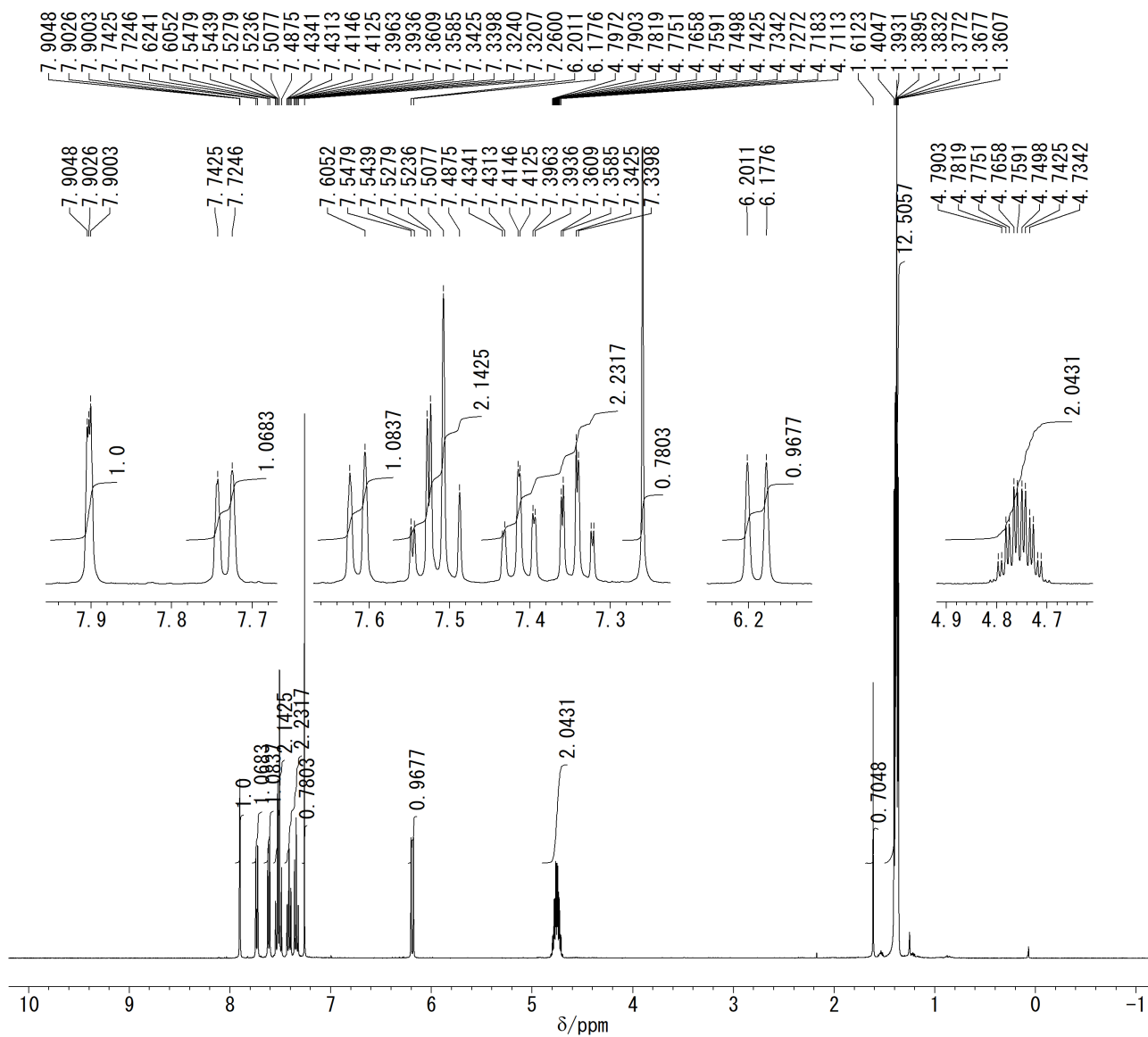
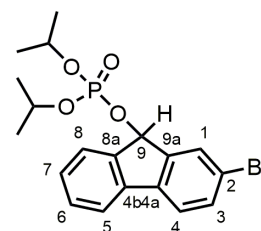
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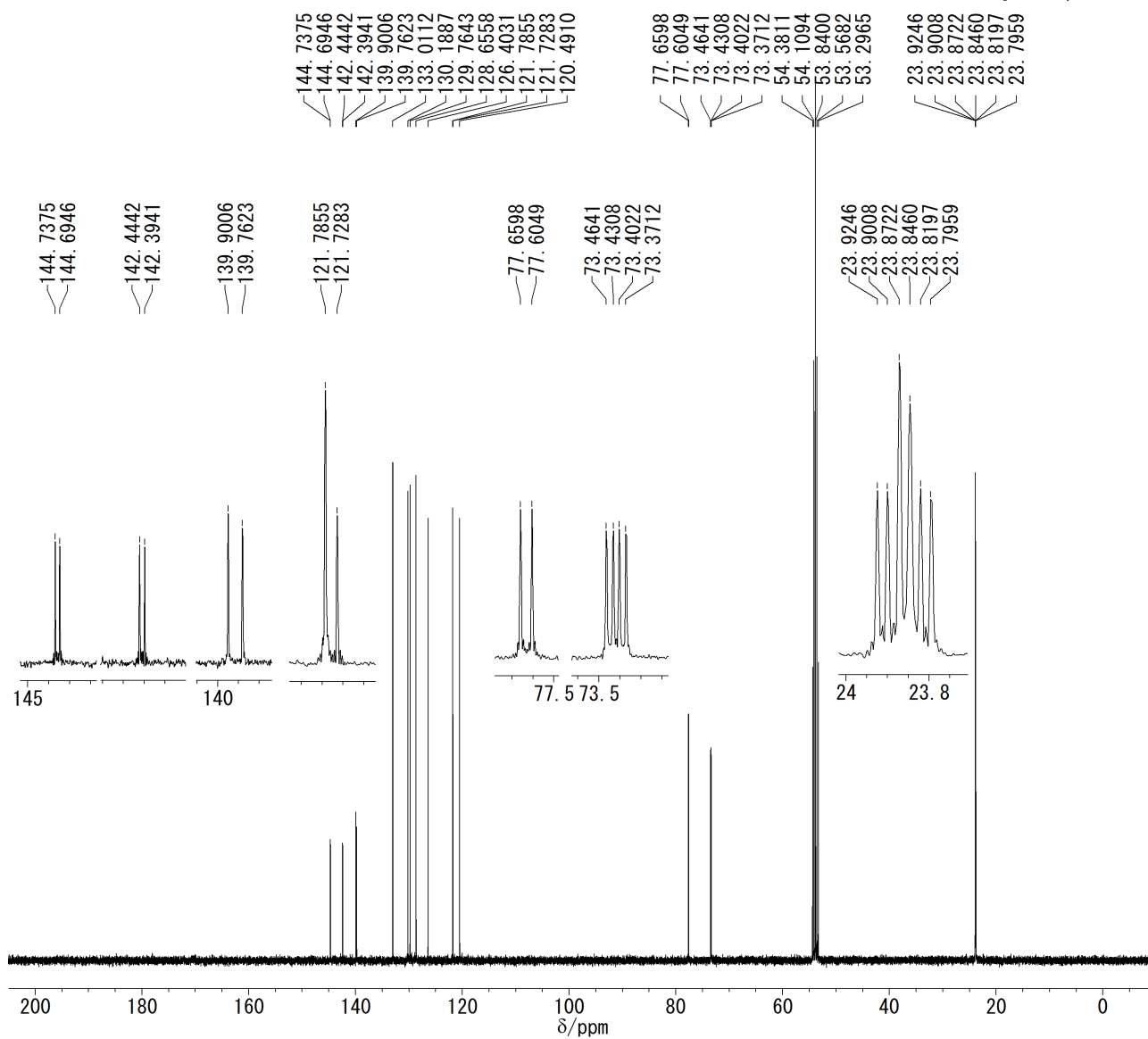
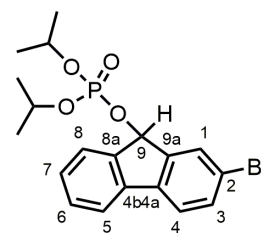
Compound **10** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



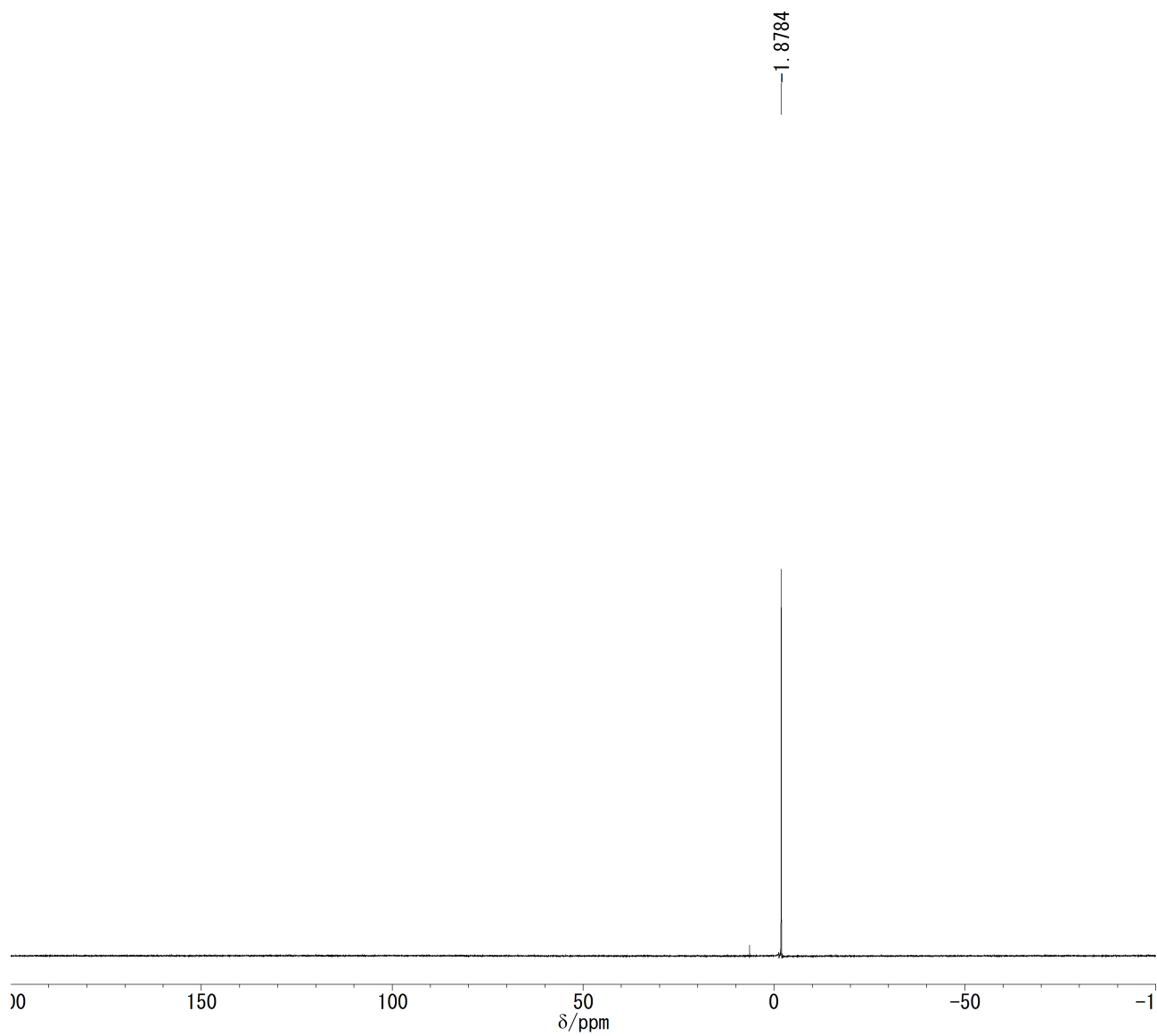
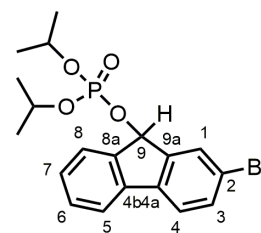
Compound **11** (¹H NMR spectrum, 400 MHz in CDCl₃).



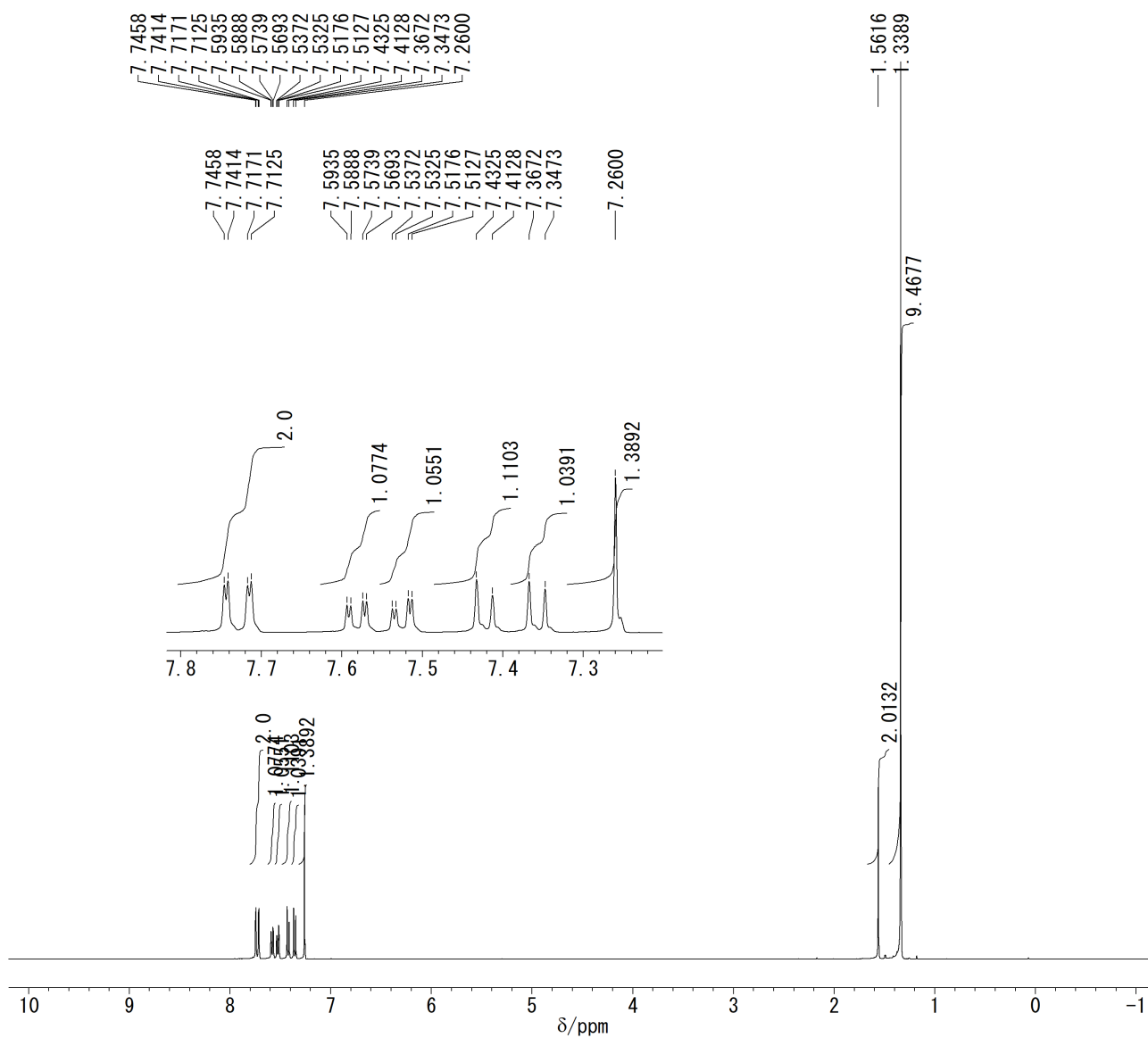
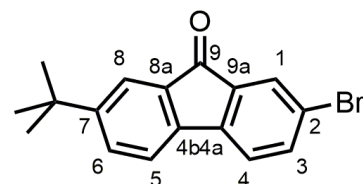
Compound **11** (^{13}C NMR spectrum, 100 MHz in CD_2Cl_2).



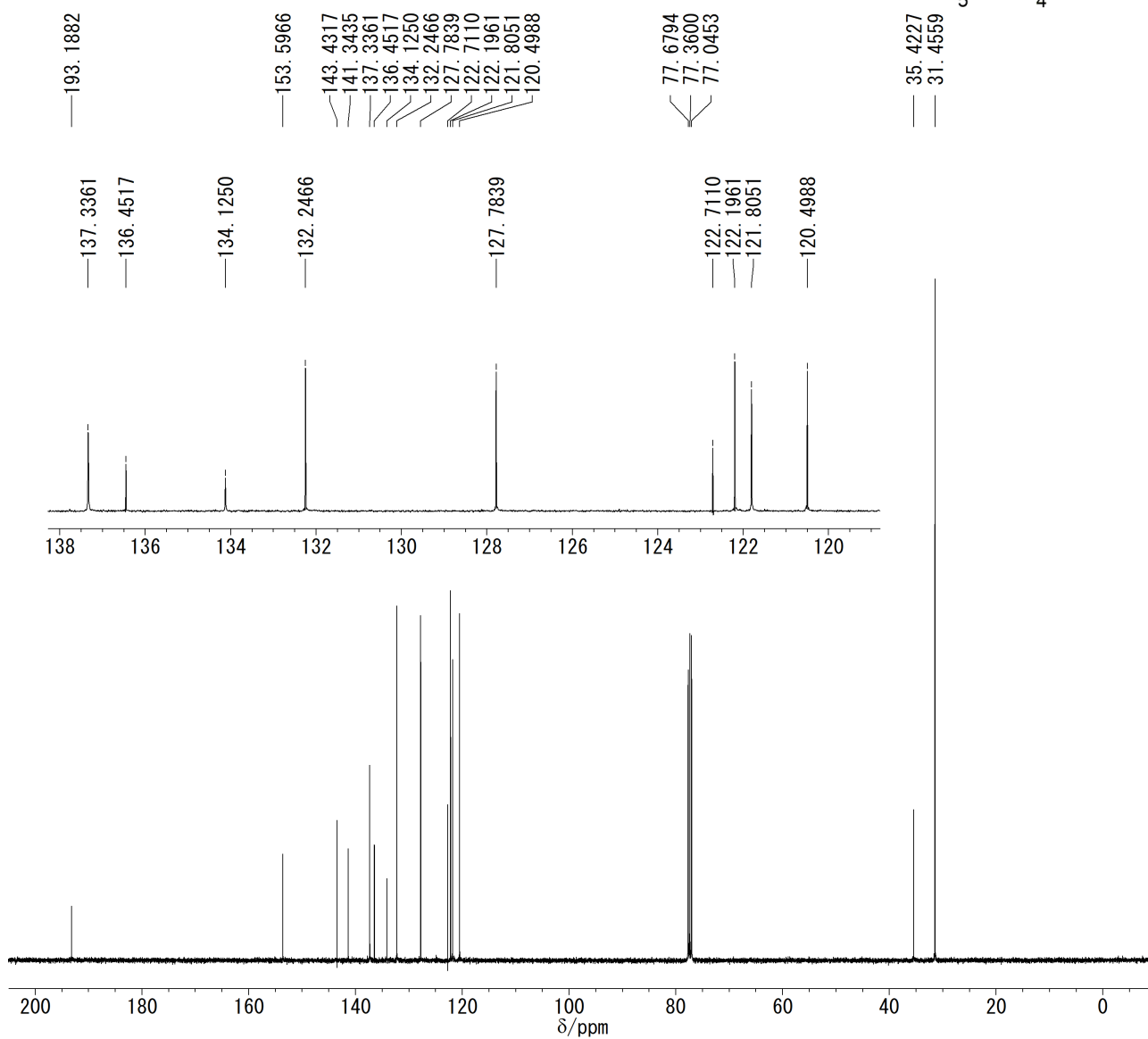
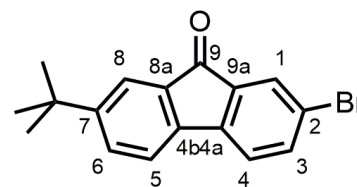
Compound **11** (^{31}P NMR spectrum, 162 MHz in CDCl_3).



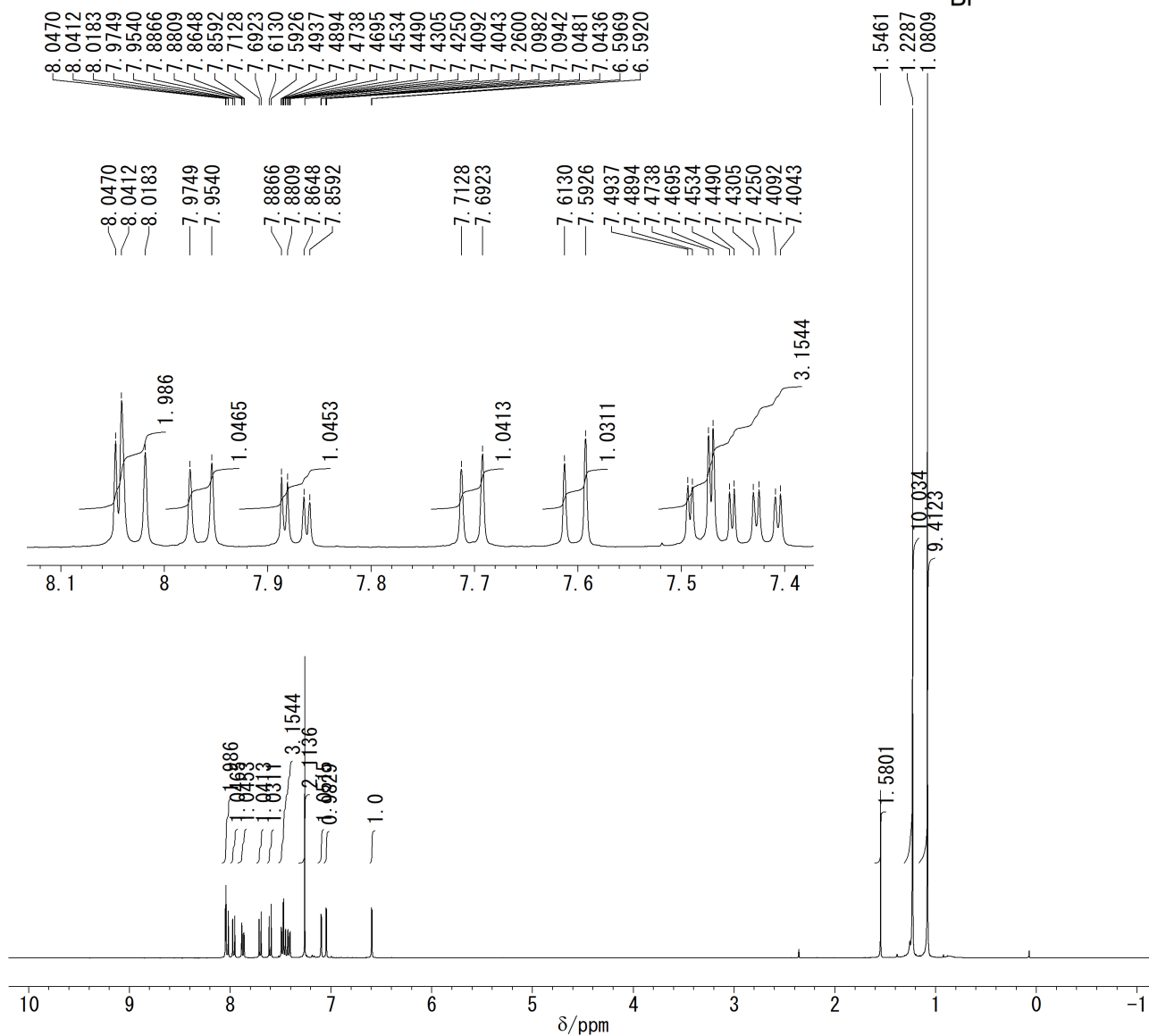
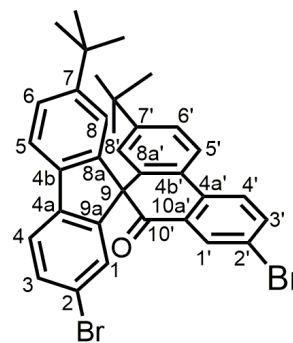
Compound **12** (¹H NMR spectrum, 400 MHz in CDCl₃).



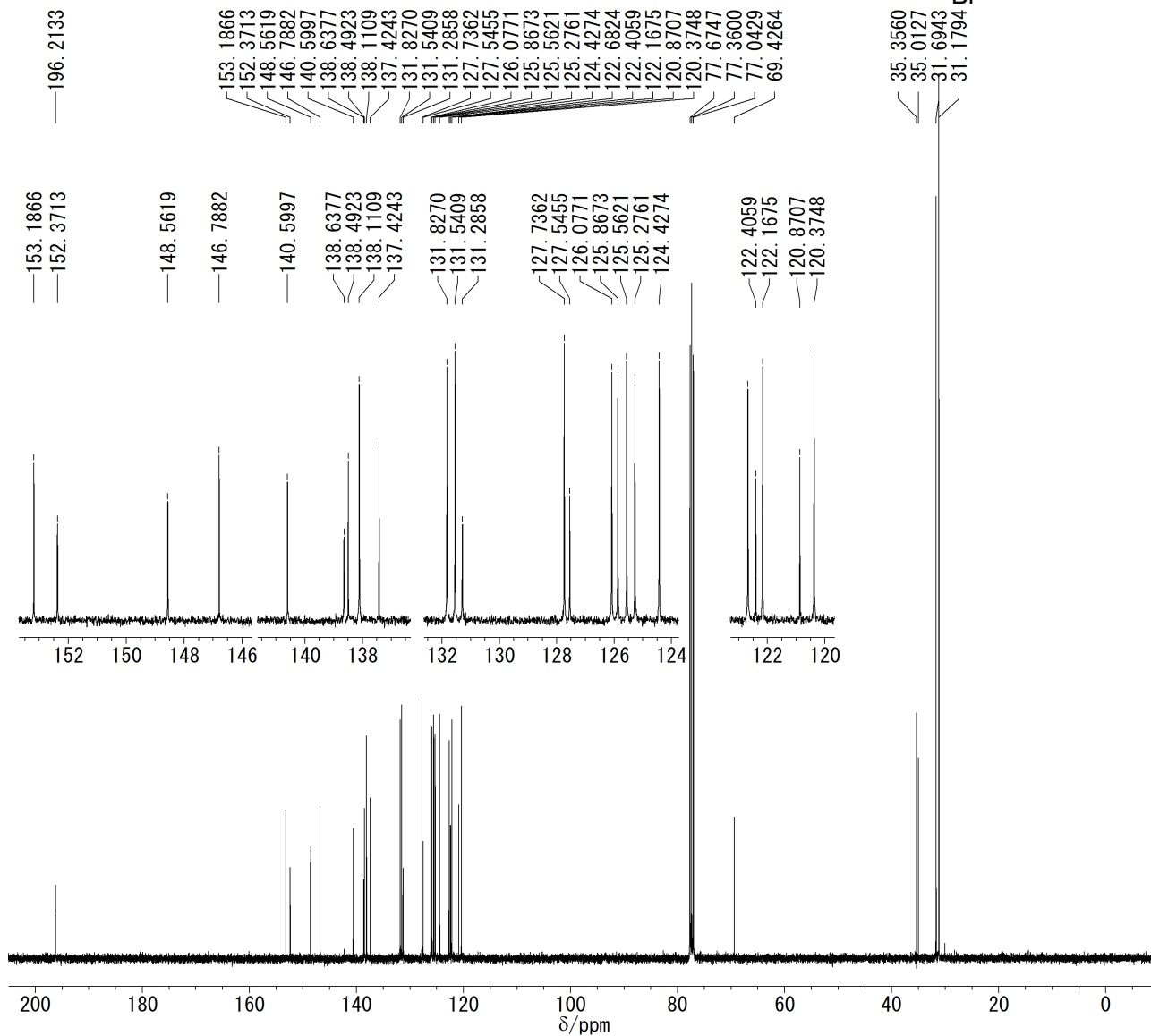
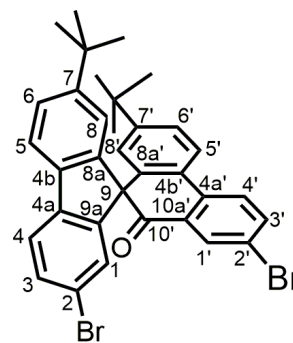
Compound **12** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



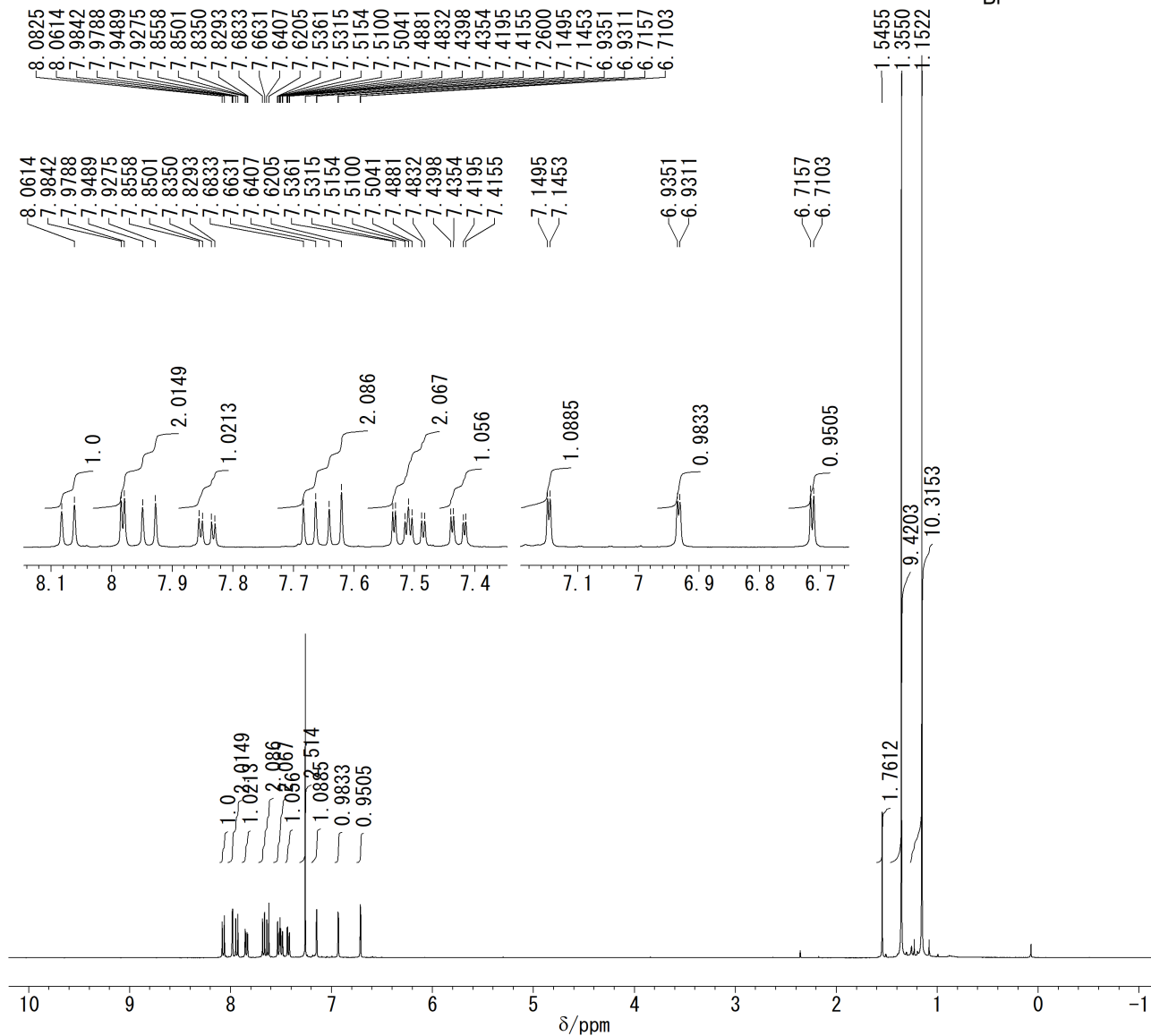
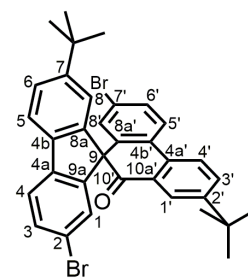
Compound **13** (¹H NMR spectrum, 400 MHz in CDCl₃).



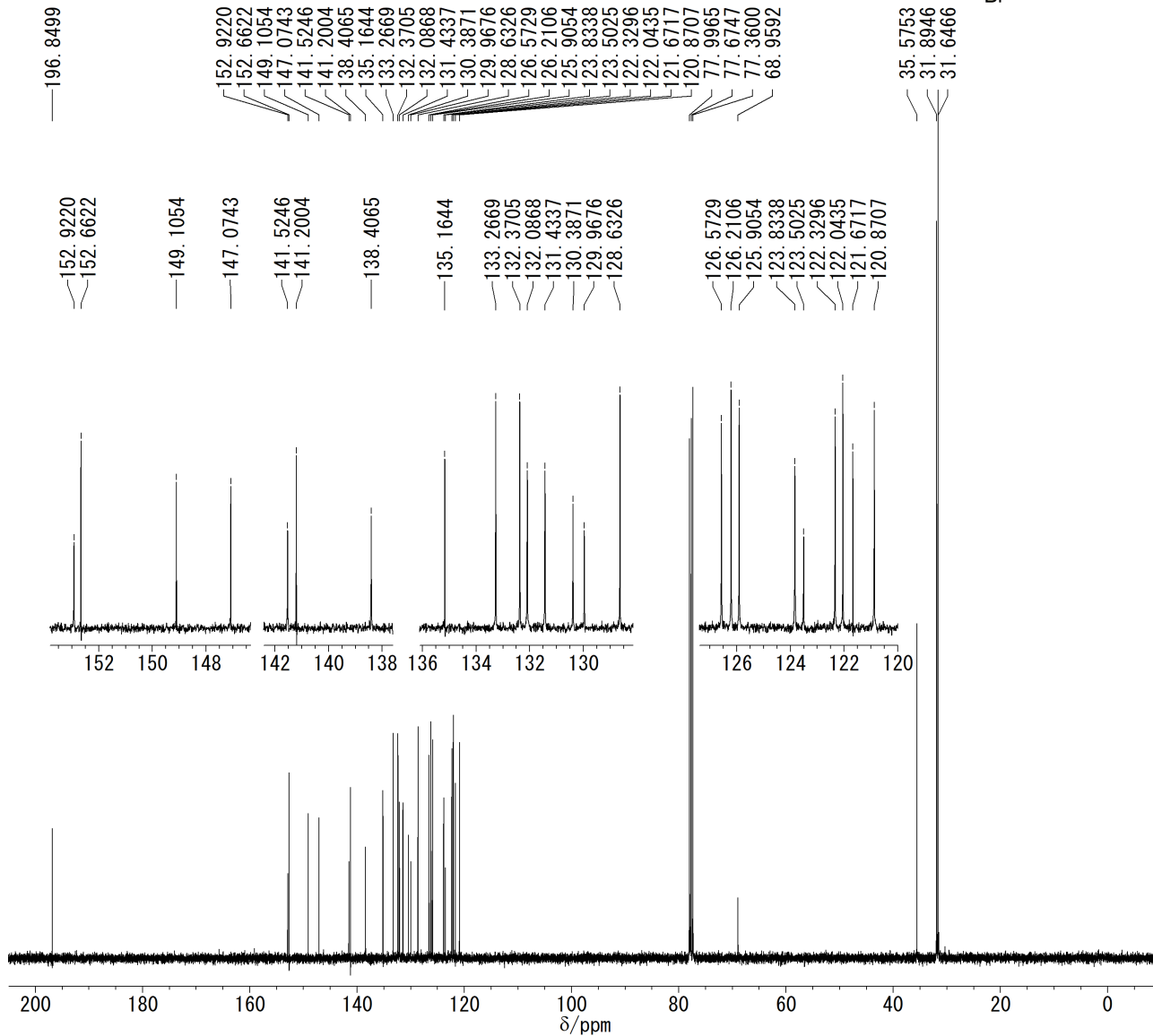
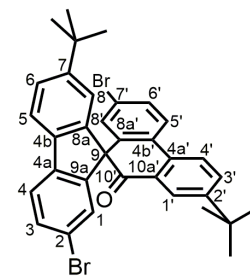
Compound **13** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



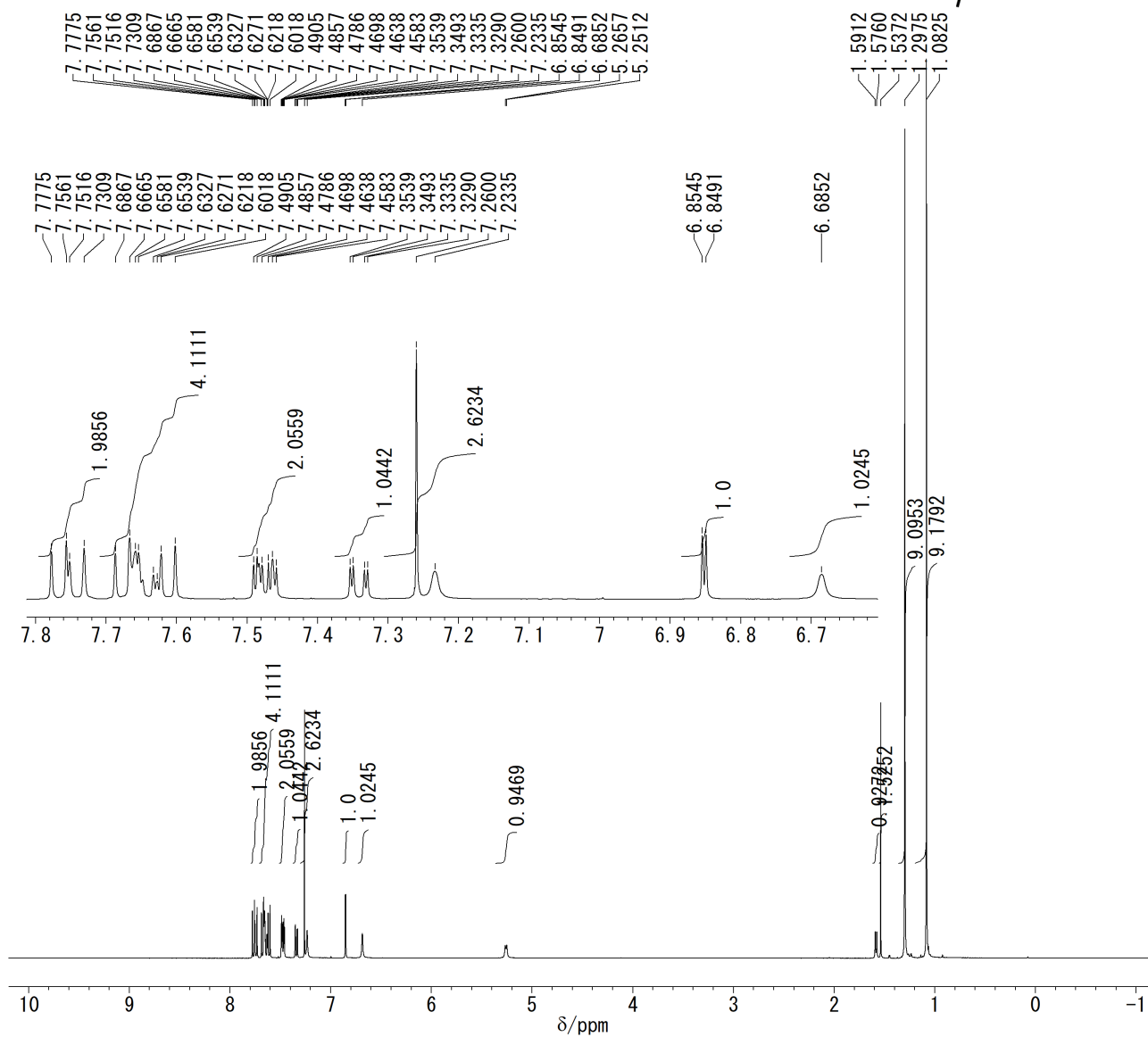
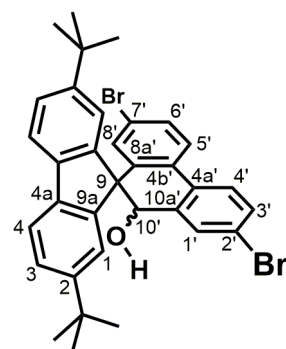
Compound *iso-13* (¹H NMR spectrum, 400 MHz in CDCl₃).



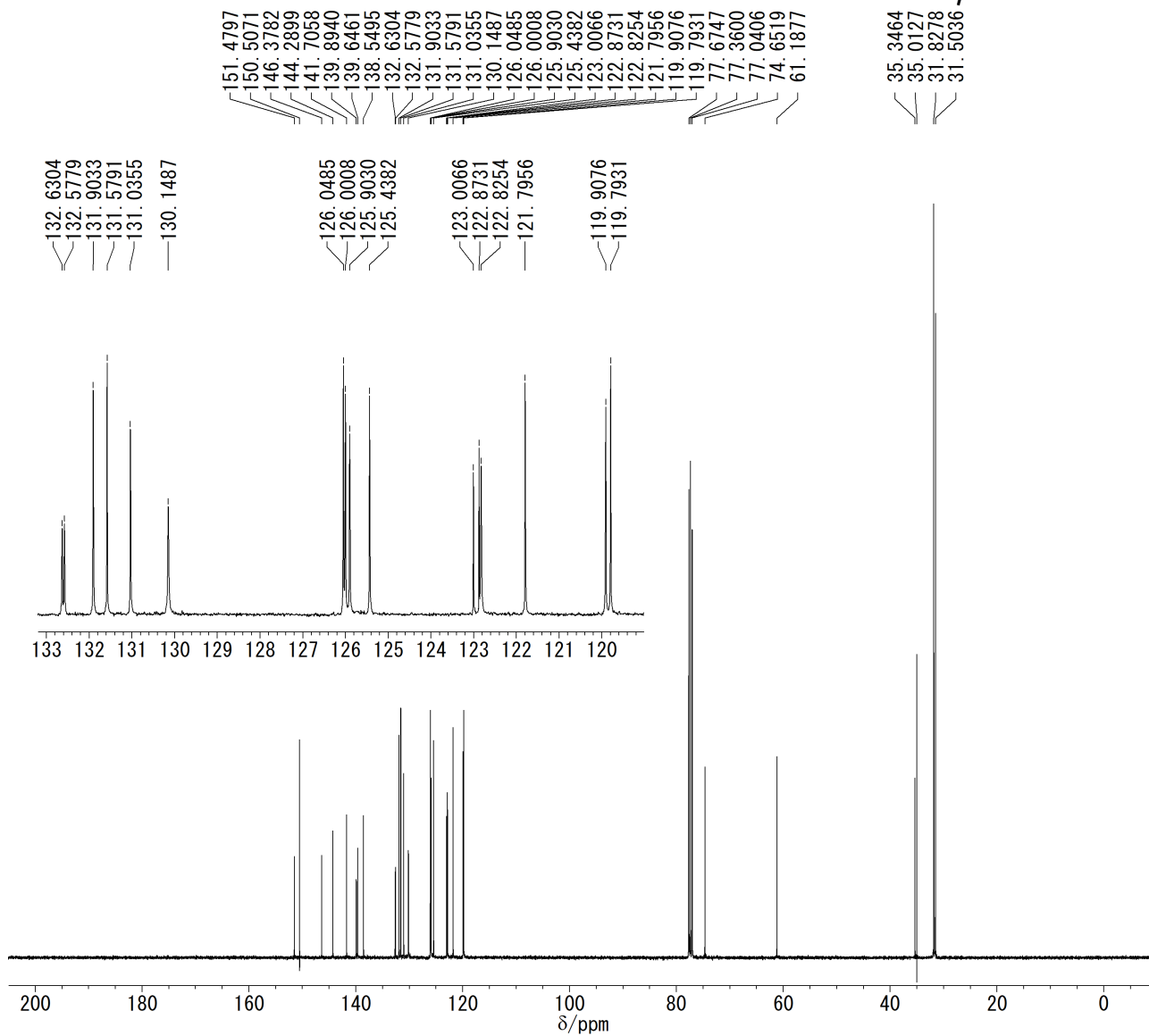
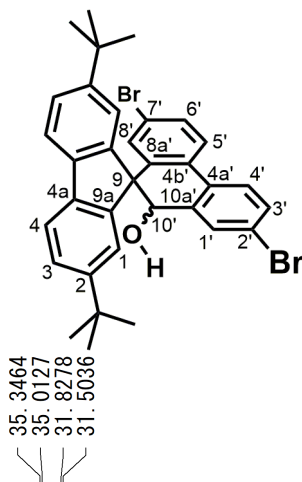
Compound *iso-13* (^{13}C NMR spectrum, 100 MHz in CDCl_3).



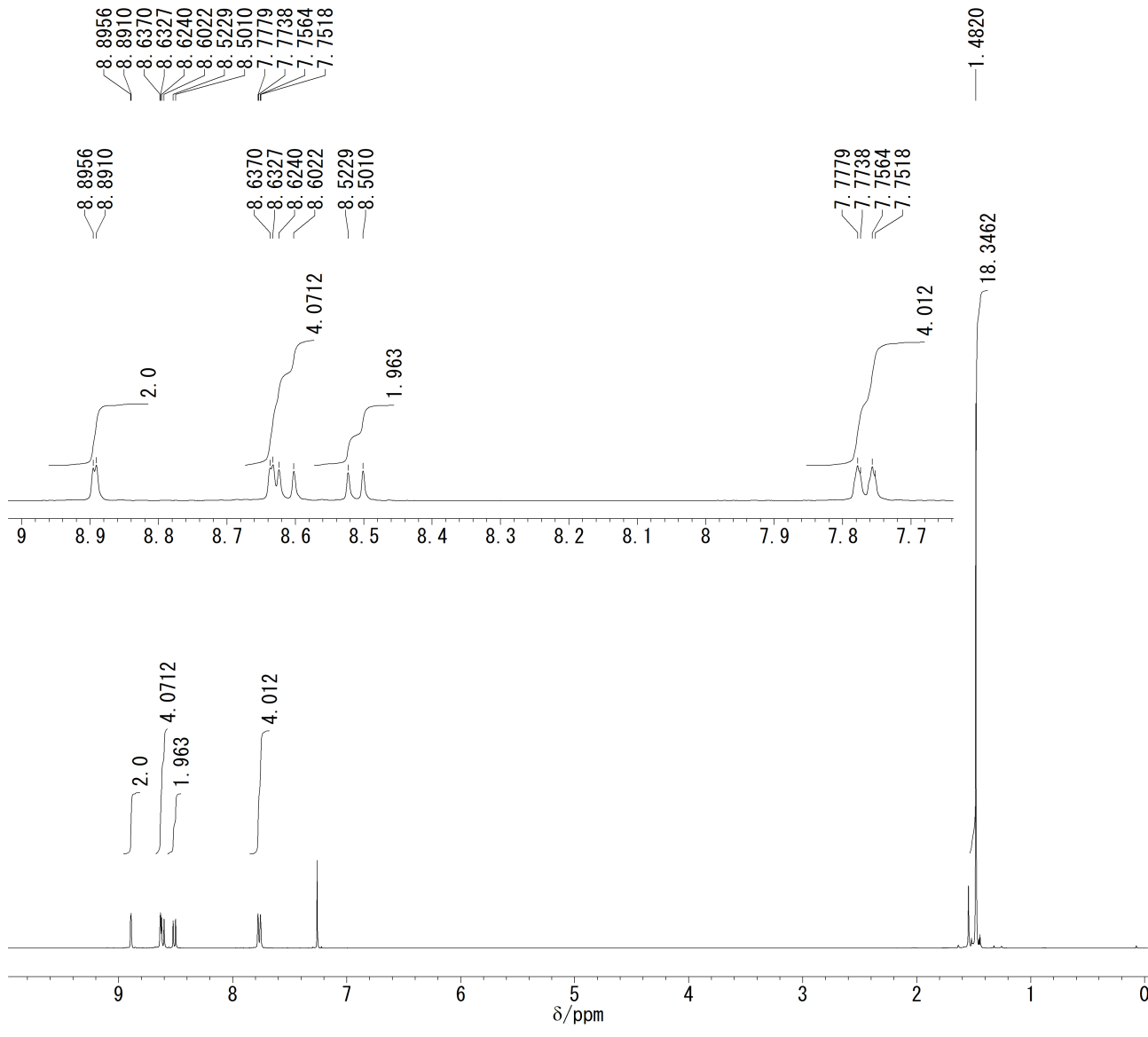
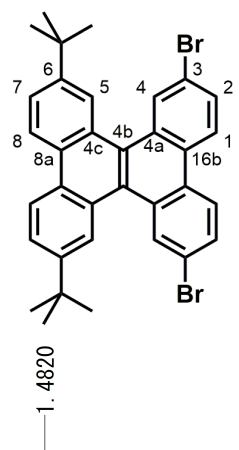
Compound **14** (^1H NMR spectrum, 400 MHz in CDCl_3).



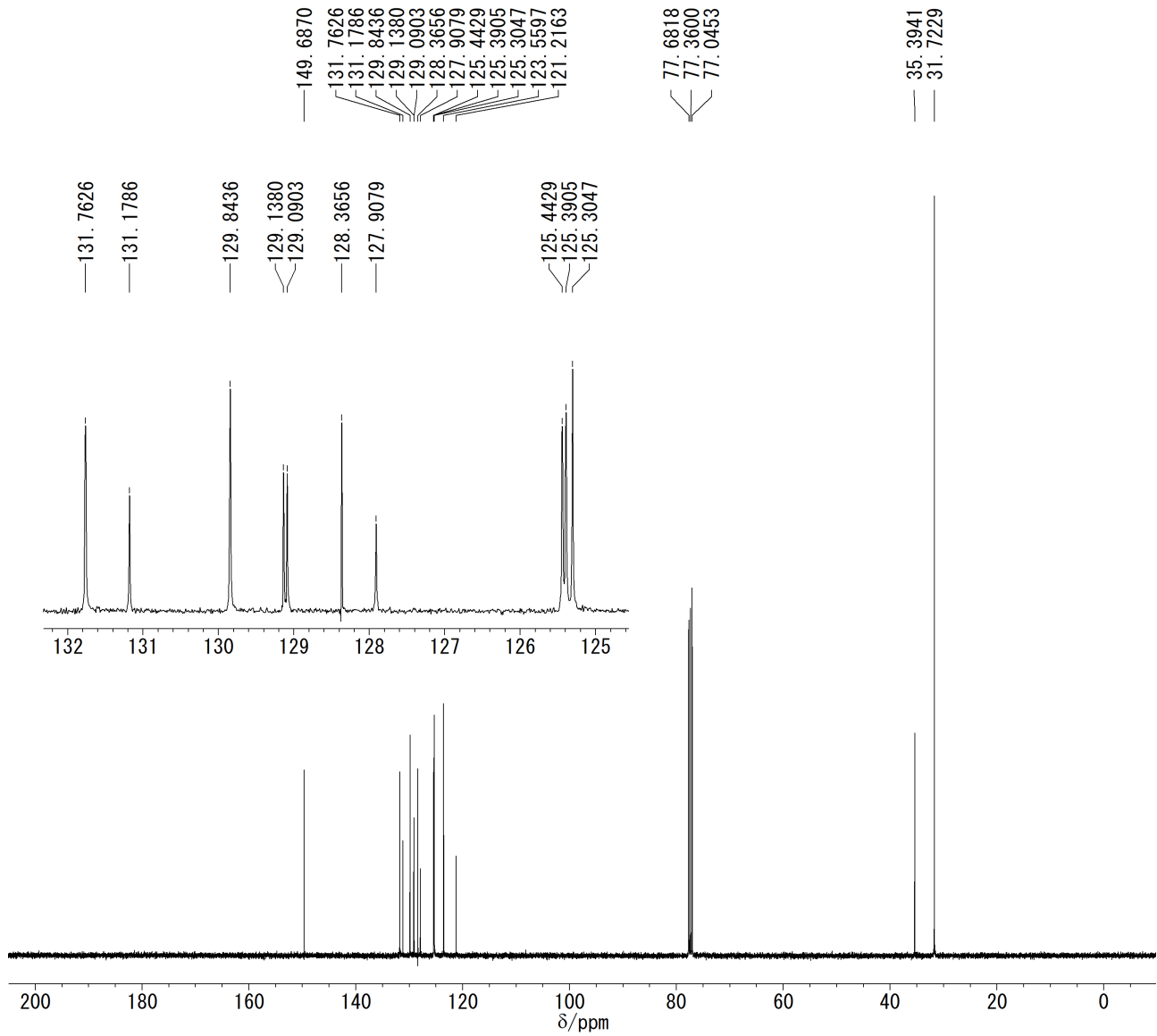
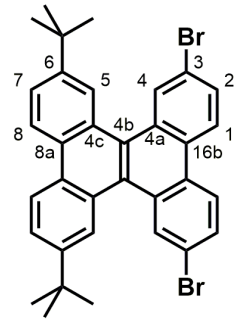
Compound **14** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



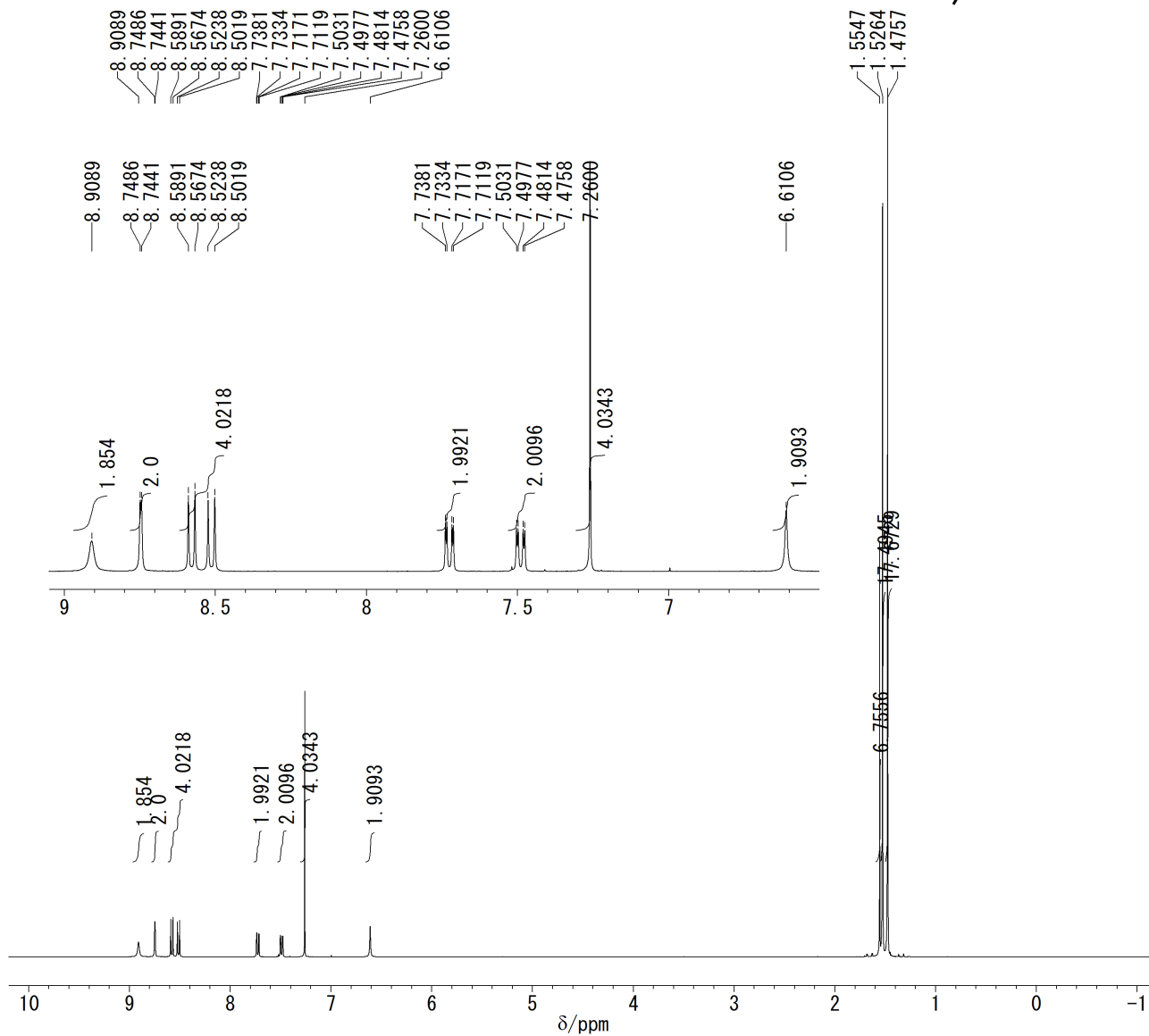
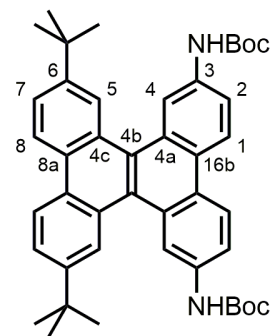
Compound **15** (¹H NMR spectrum, 400 MHz in CDCl₃).



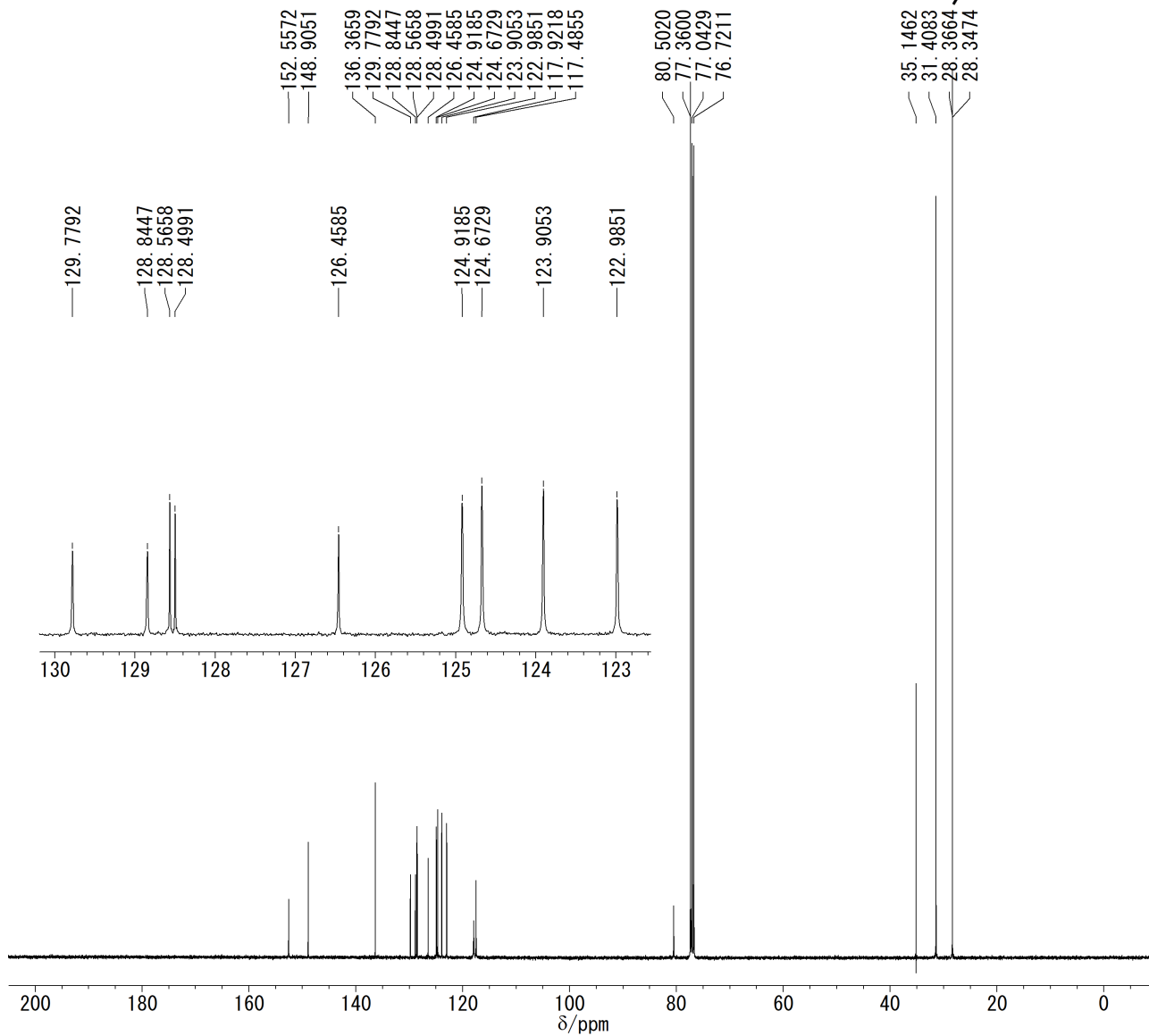
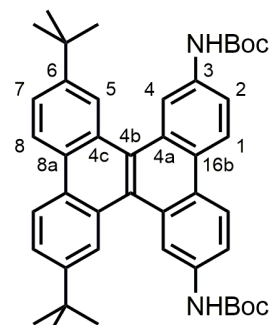
Compound **15** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



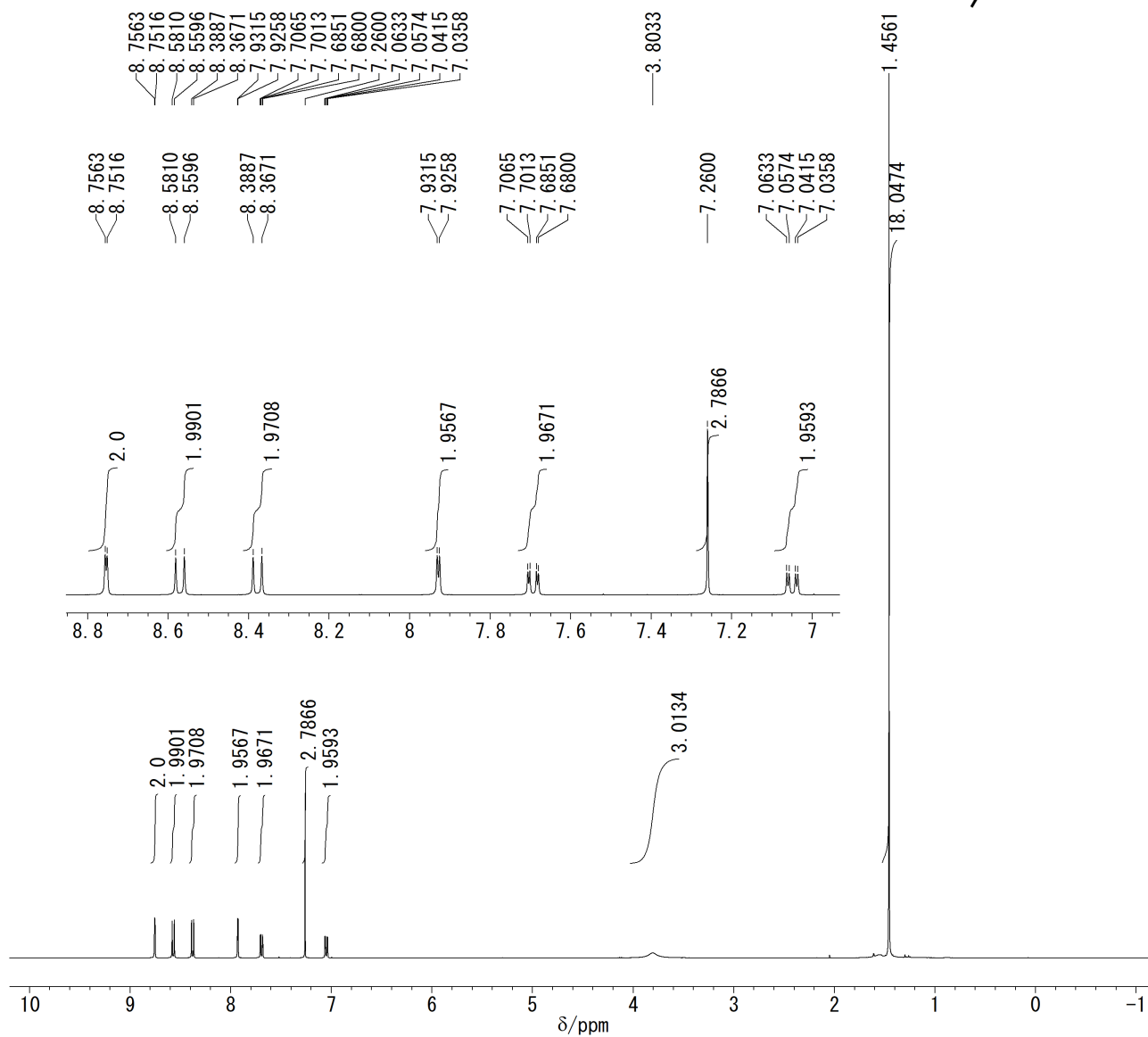
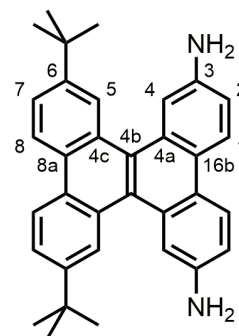
Compound **16** (¹H NMR spectrum, 400 MHz in CDCl₃).



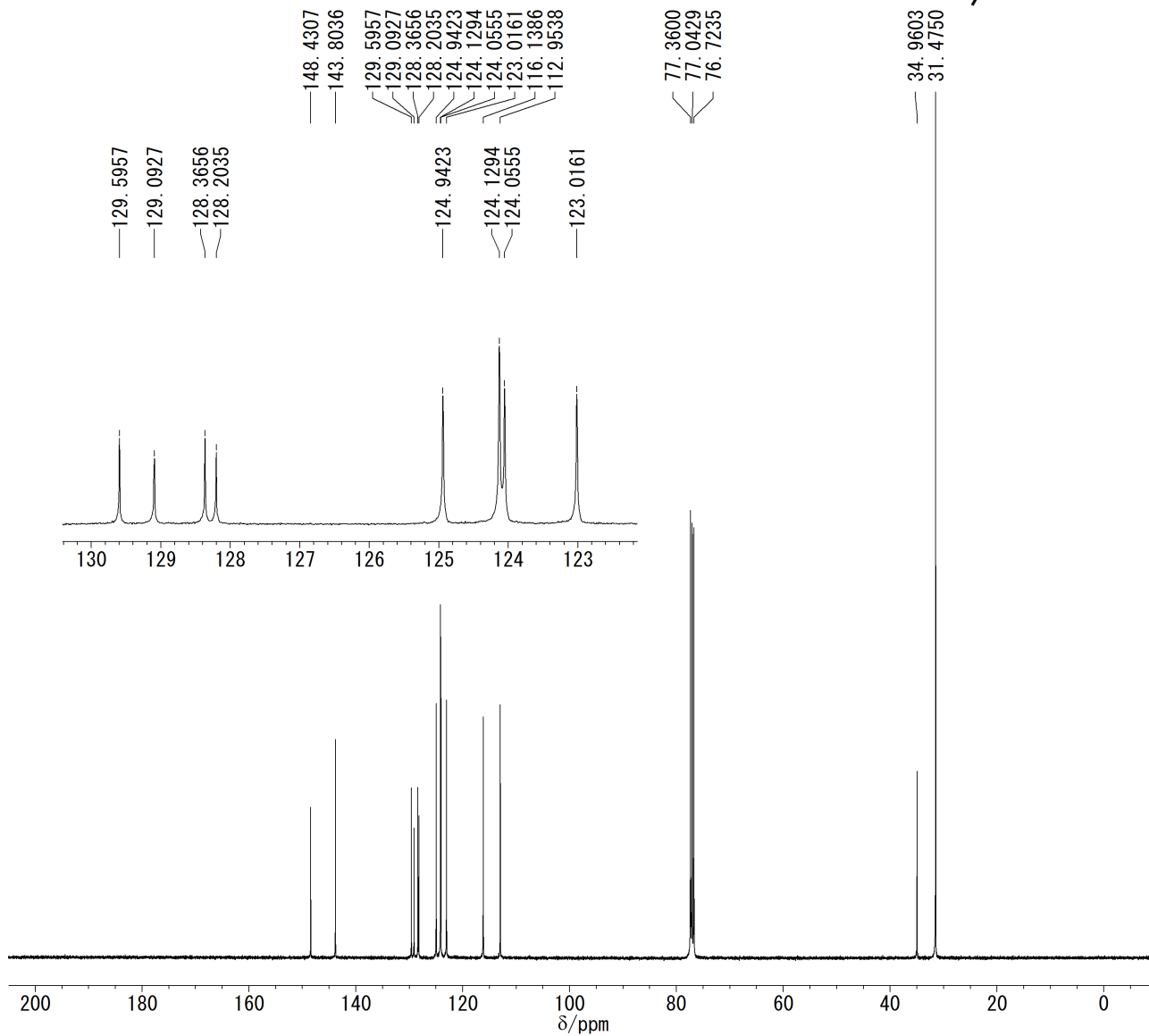
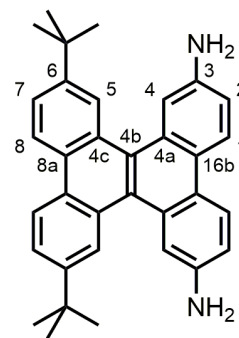
Compound **16** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



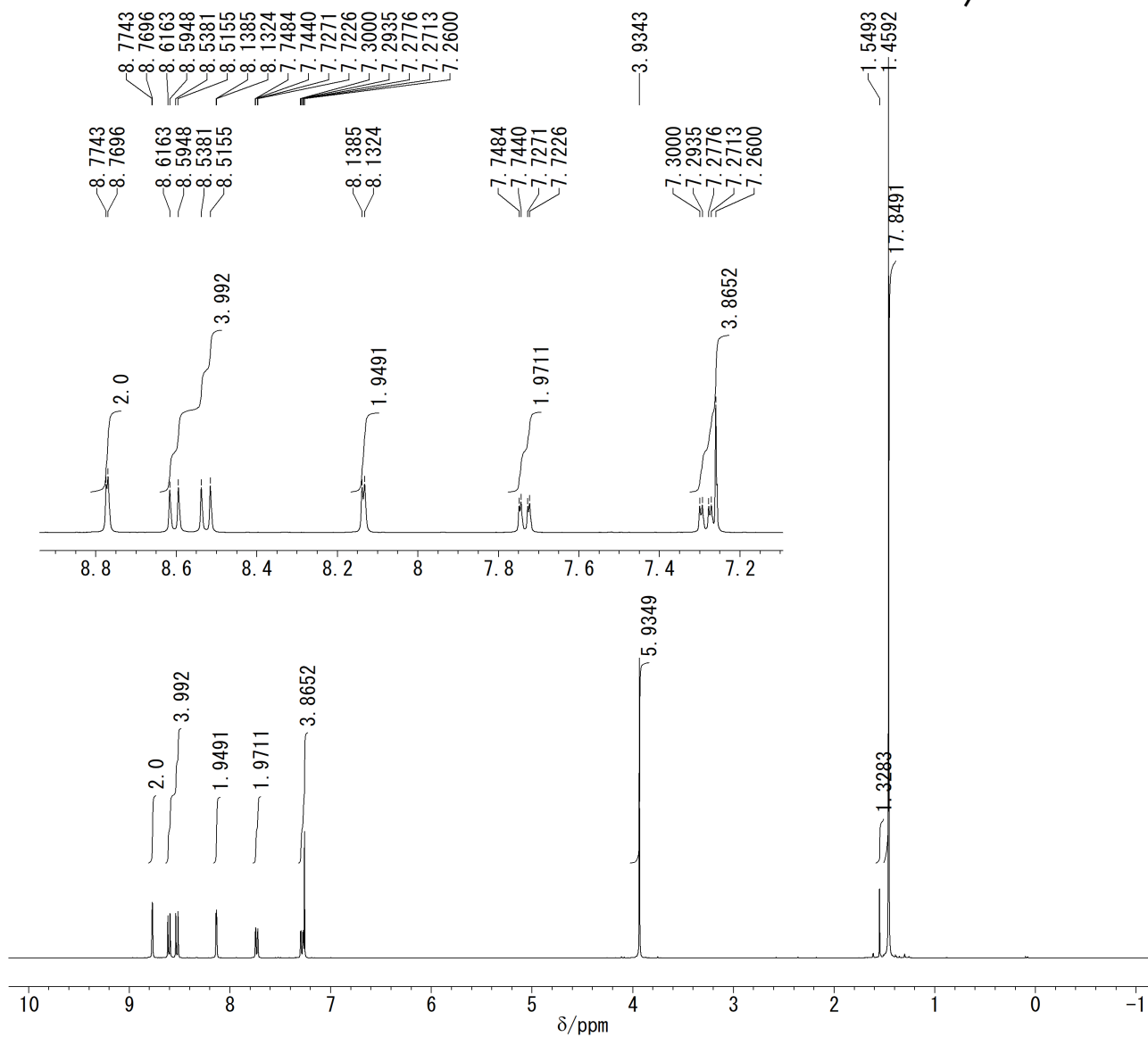
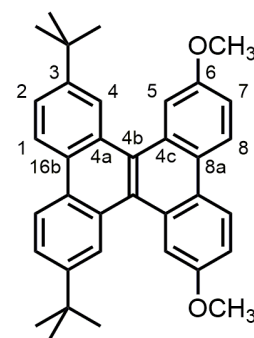
Compound 17 (¹H NMR spectrum, 400 MHz in CDCl₃).



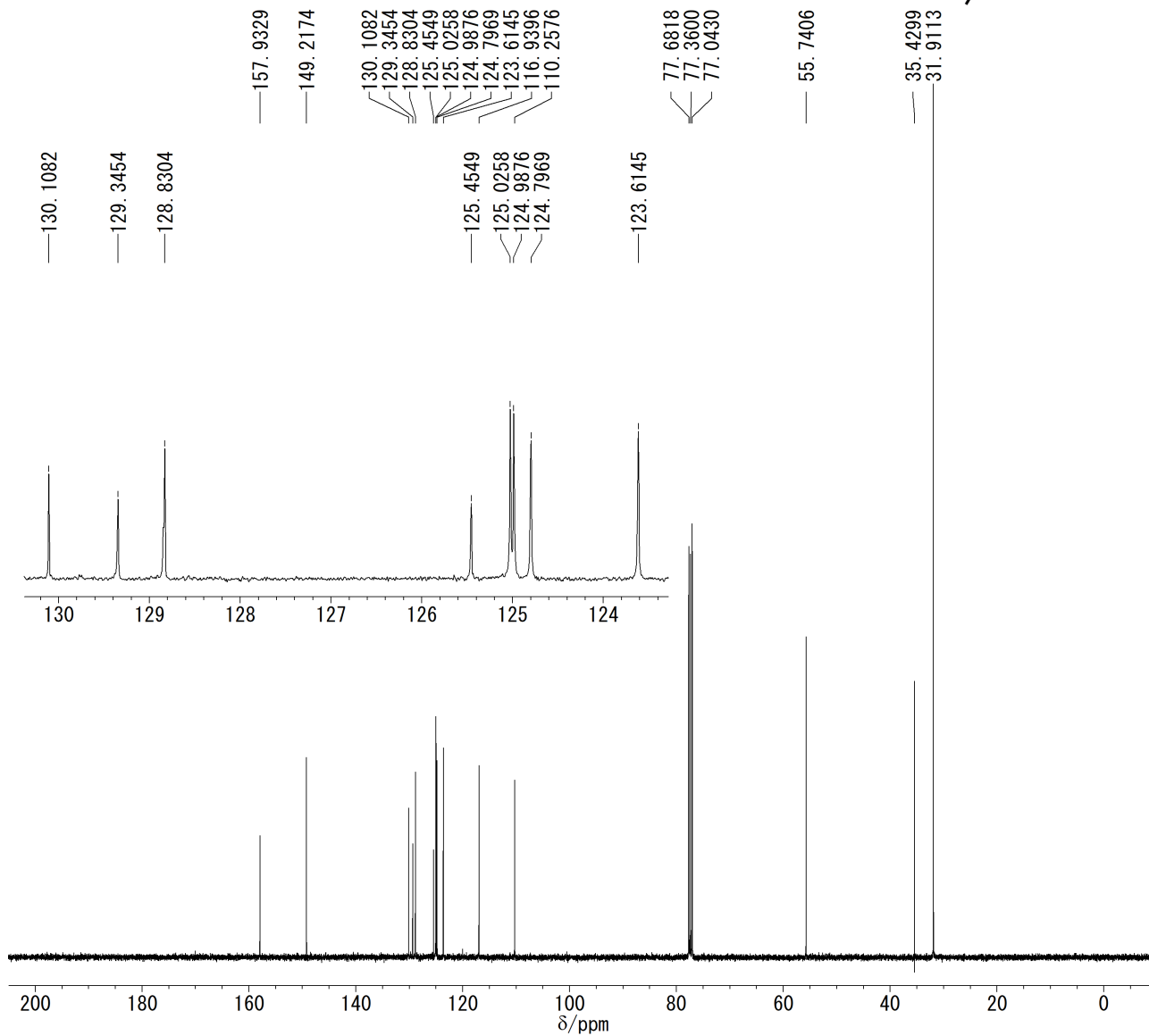
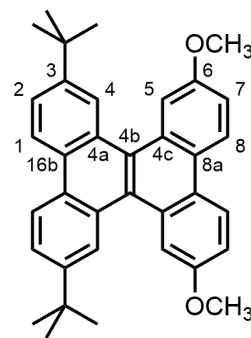
Compound **17** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



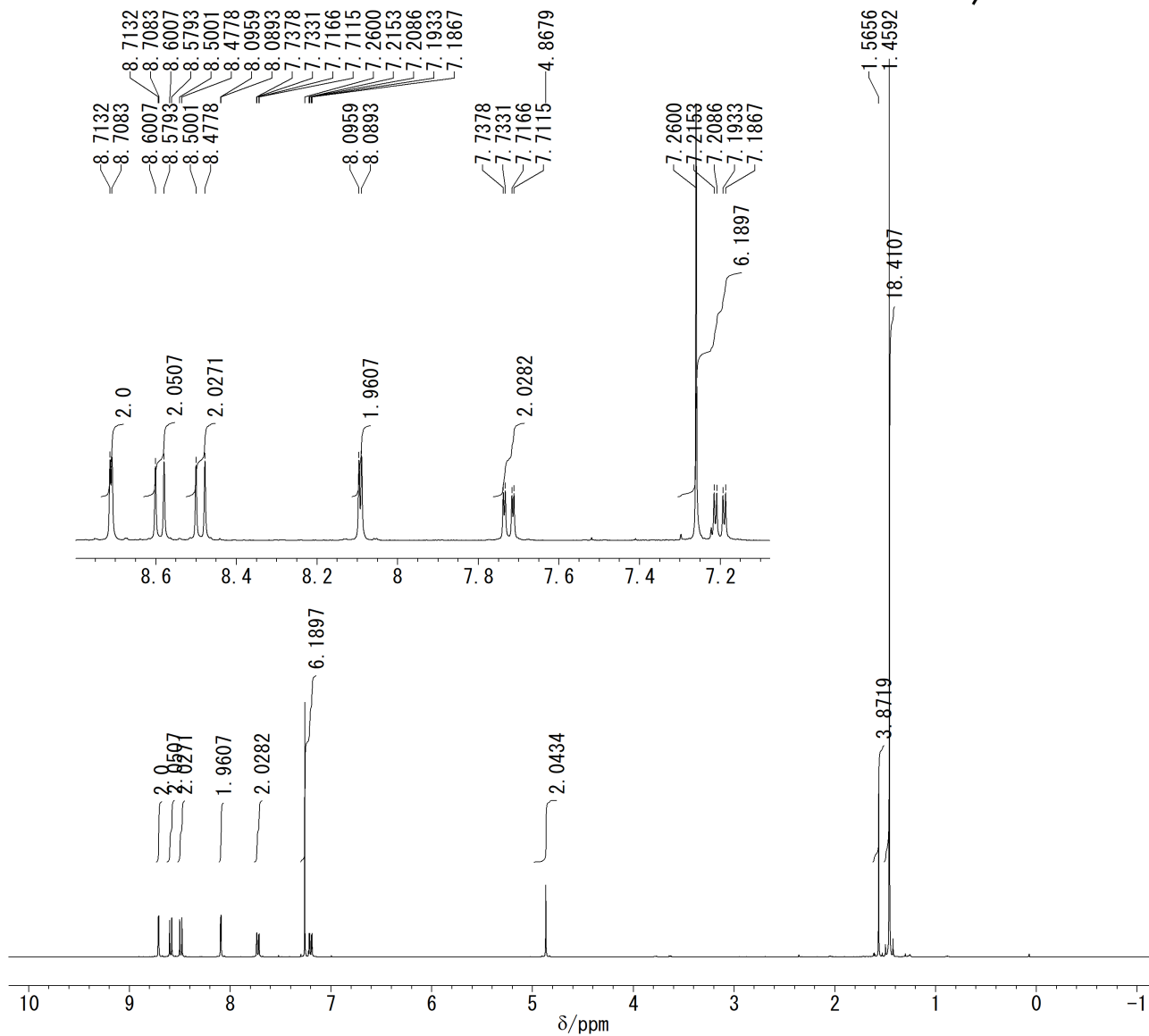
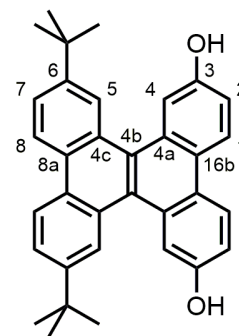
Compound **18** (¹H NMR spectrum, 400 MHz in CDCl₃).



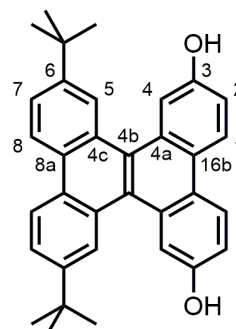
Compound **18** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



Compound **19** (¹H NMR spectrum, 400 MHz in CDCl₃).



Compound **19** (^{13}C NMR spectrum, 100 MHz in $\text{DMSO-}d_6$).



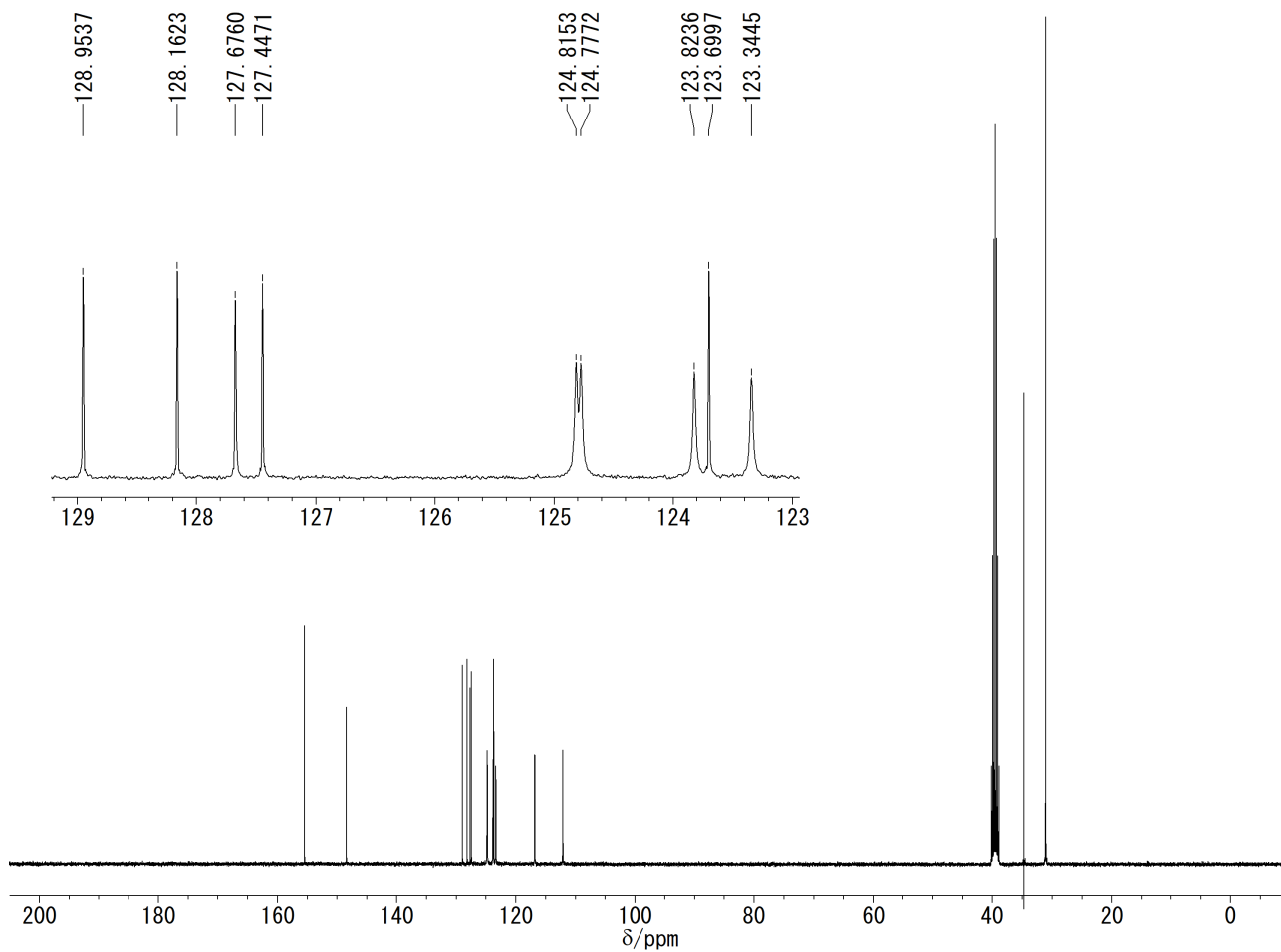
155.4625
148.4539
128.9537
128.1623
127.6760
127.4471
124.8153
124.7772
123.8236
123.6997
123.3445
116.8150
112.1140

40.1470
39.9396
39.7298
39.5200
39.3102
39.1004
38.8930
34.7046
31.0787

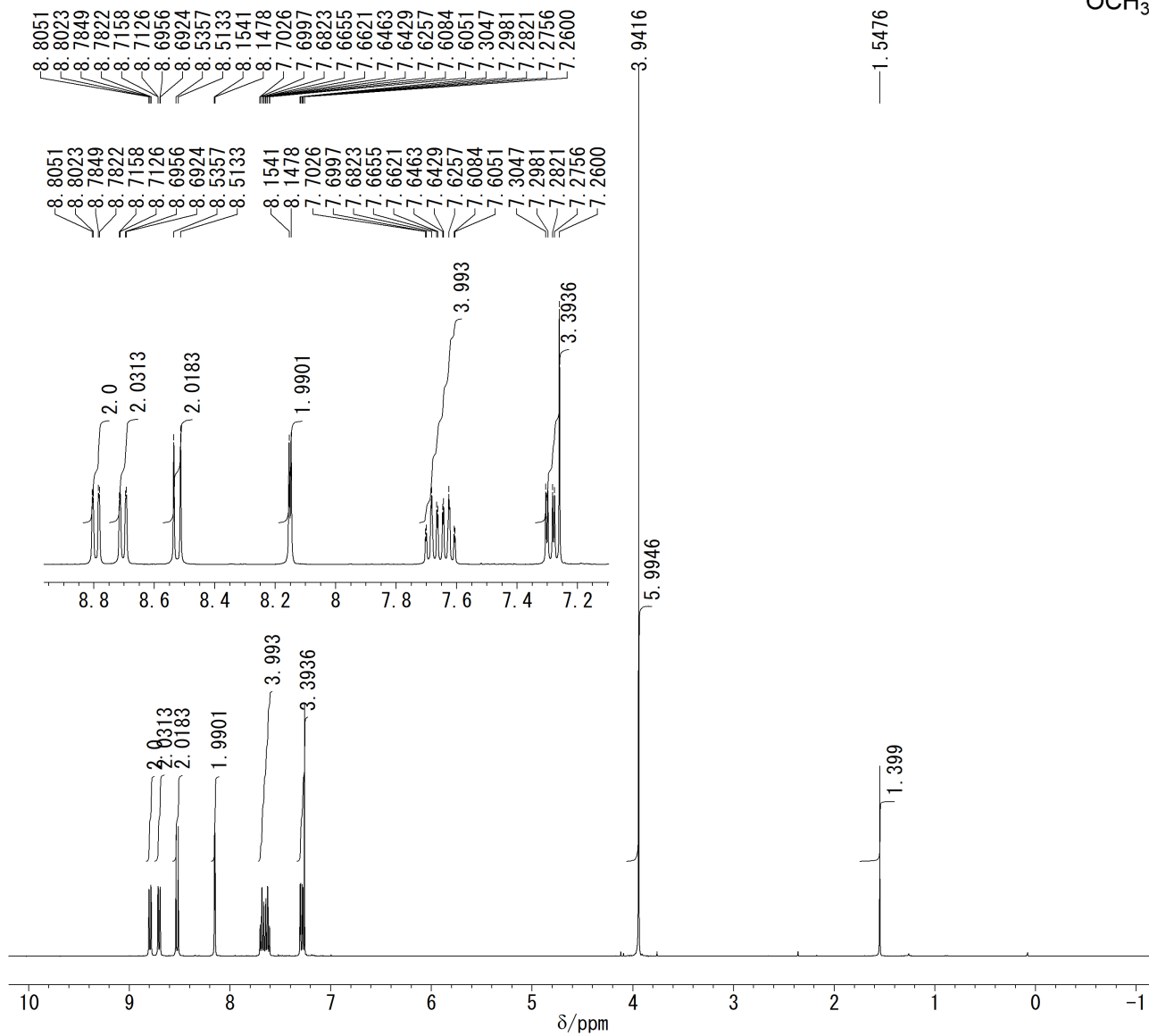
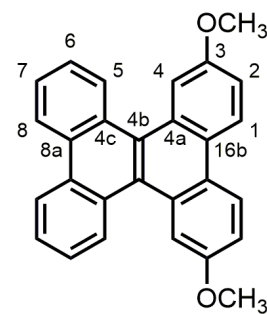
128.9537
128.1623
127.6760
127.4471

124.8153
124.7772

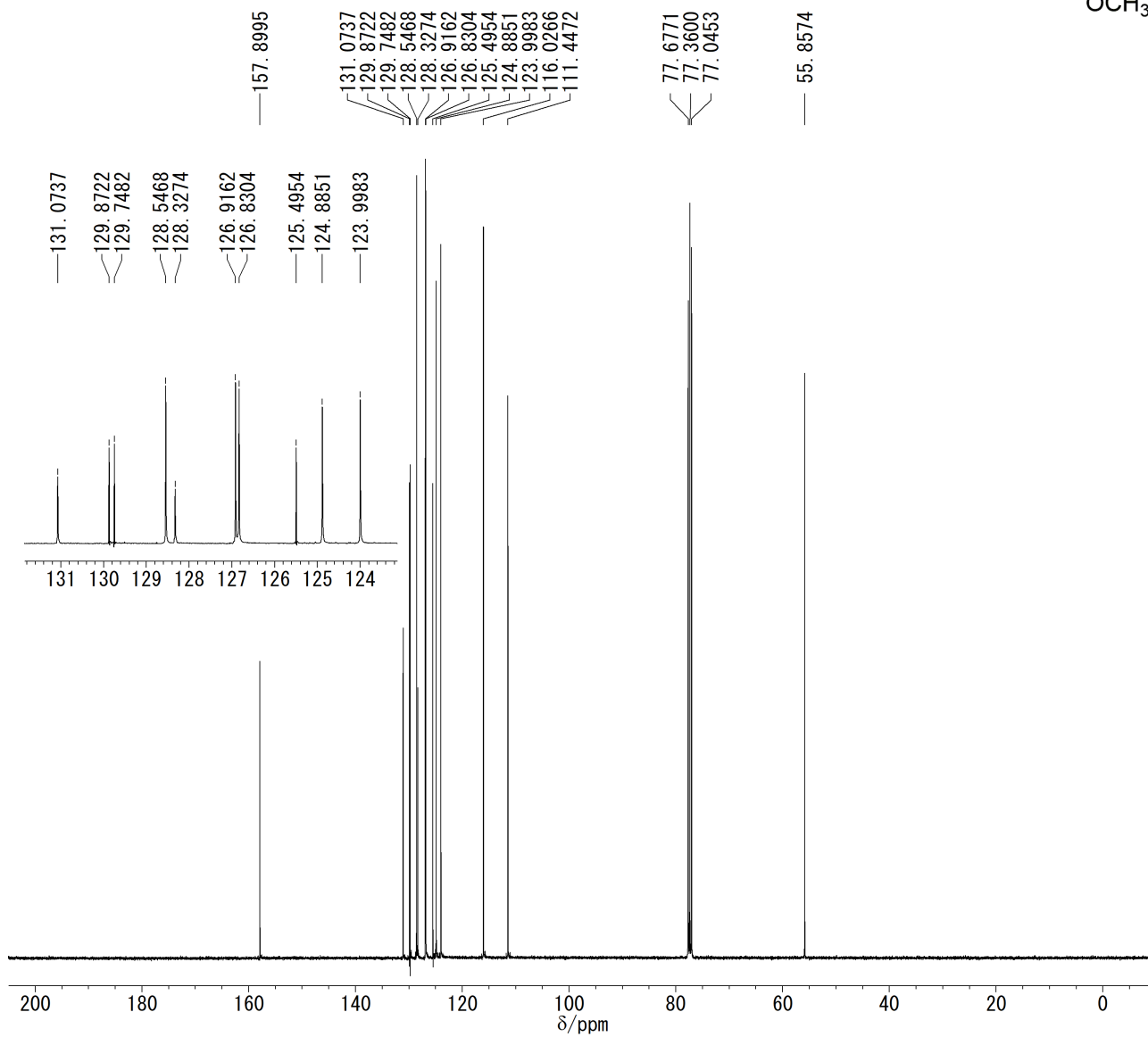
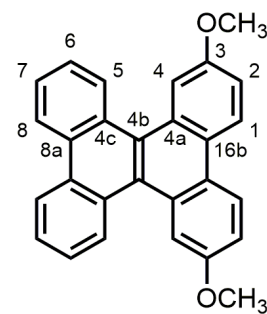
123.8236
123.6997
123.3445



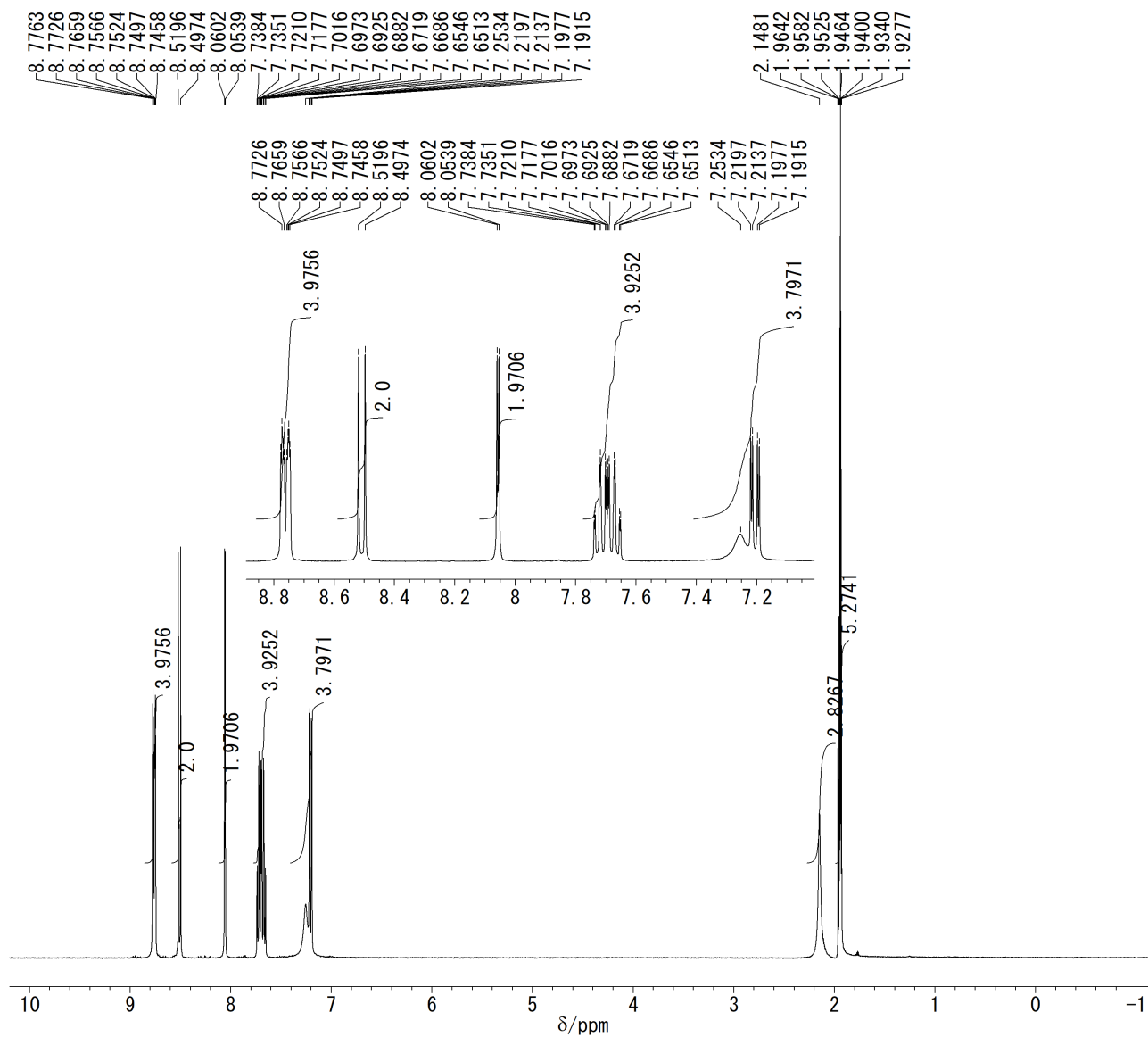
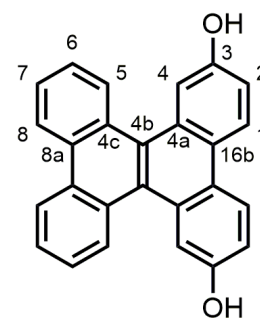
Compound **20** (^1H NMR spectrum, 400 MHz in CDCl_3).



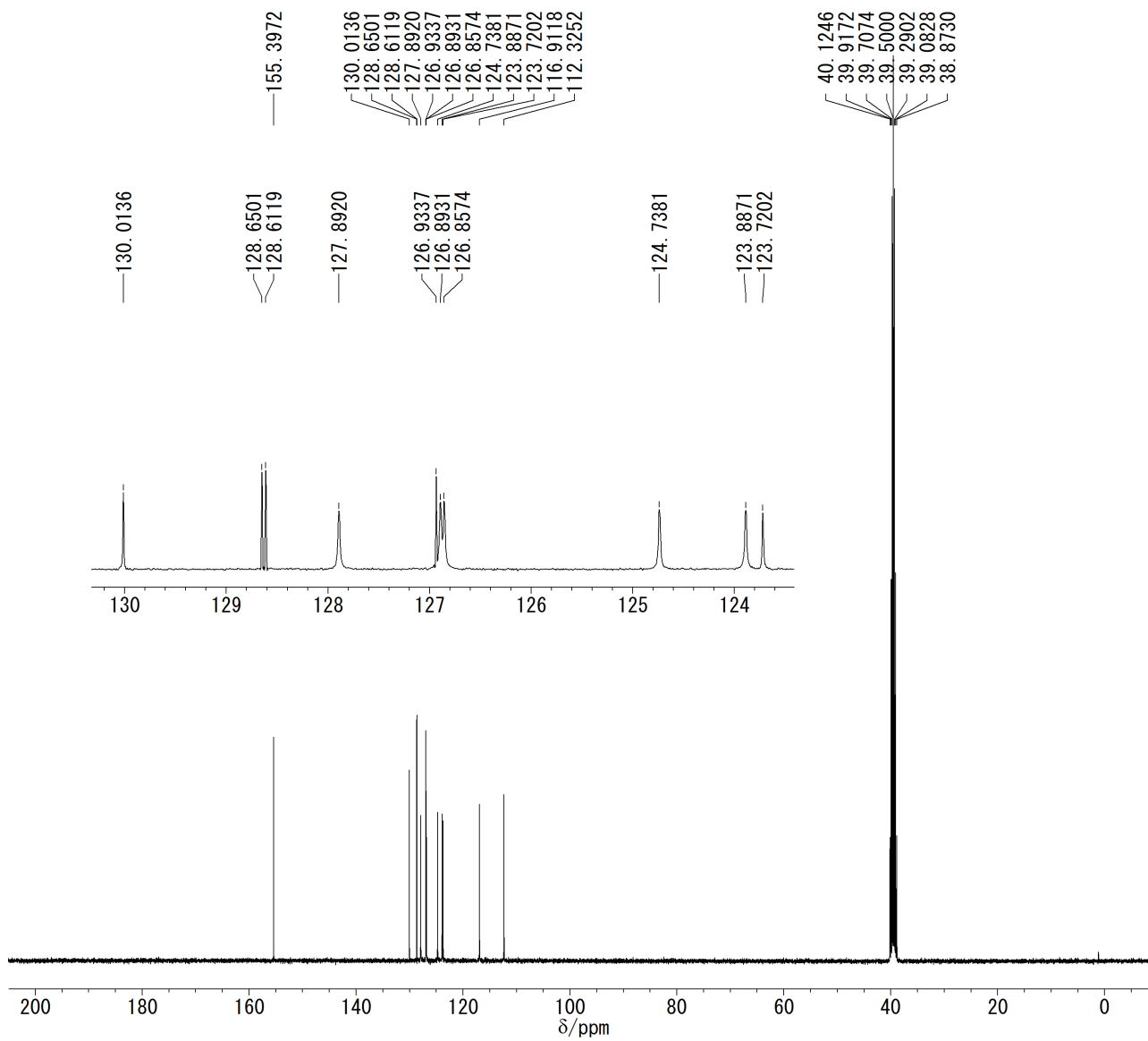
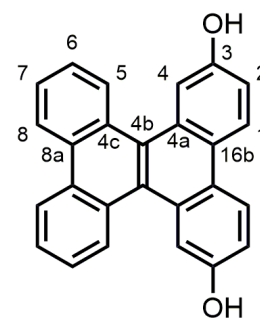
Compound **20** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



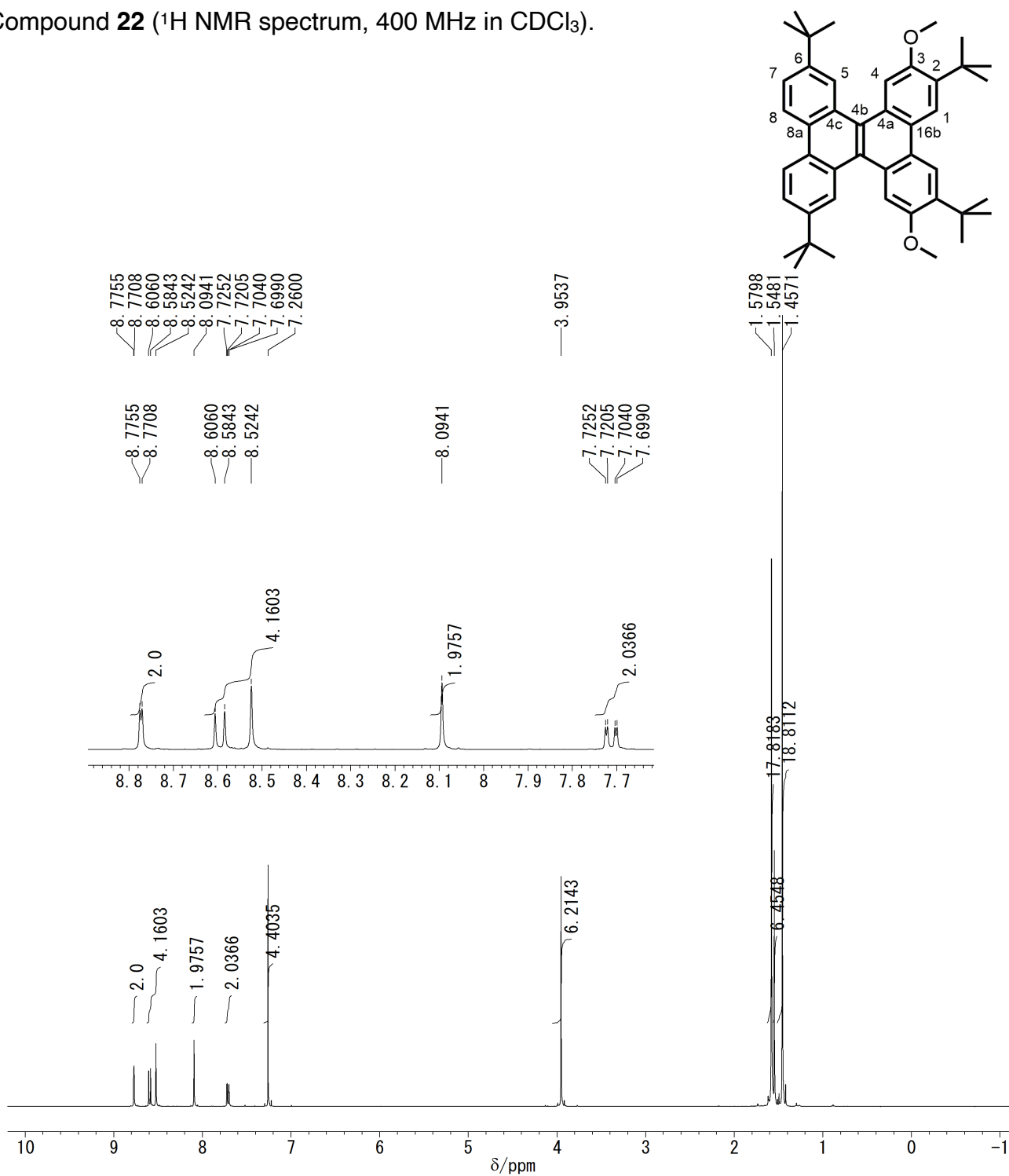
Compound **21** (¹H NMR spectrum, 400 MHz in CD₃CN).



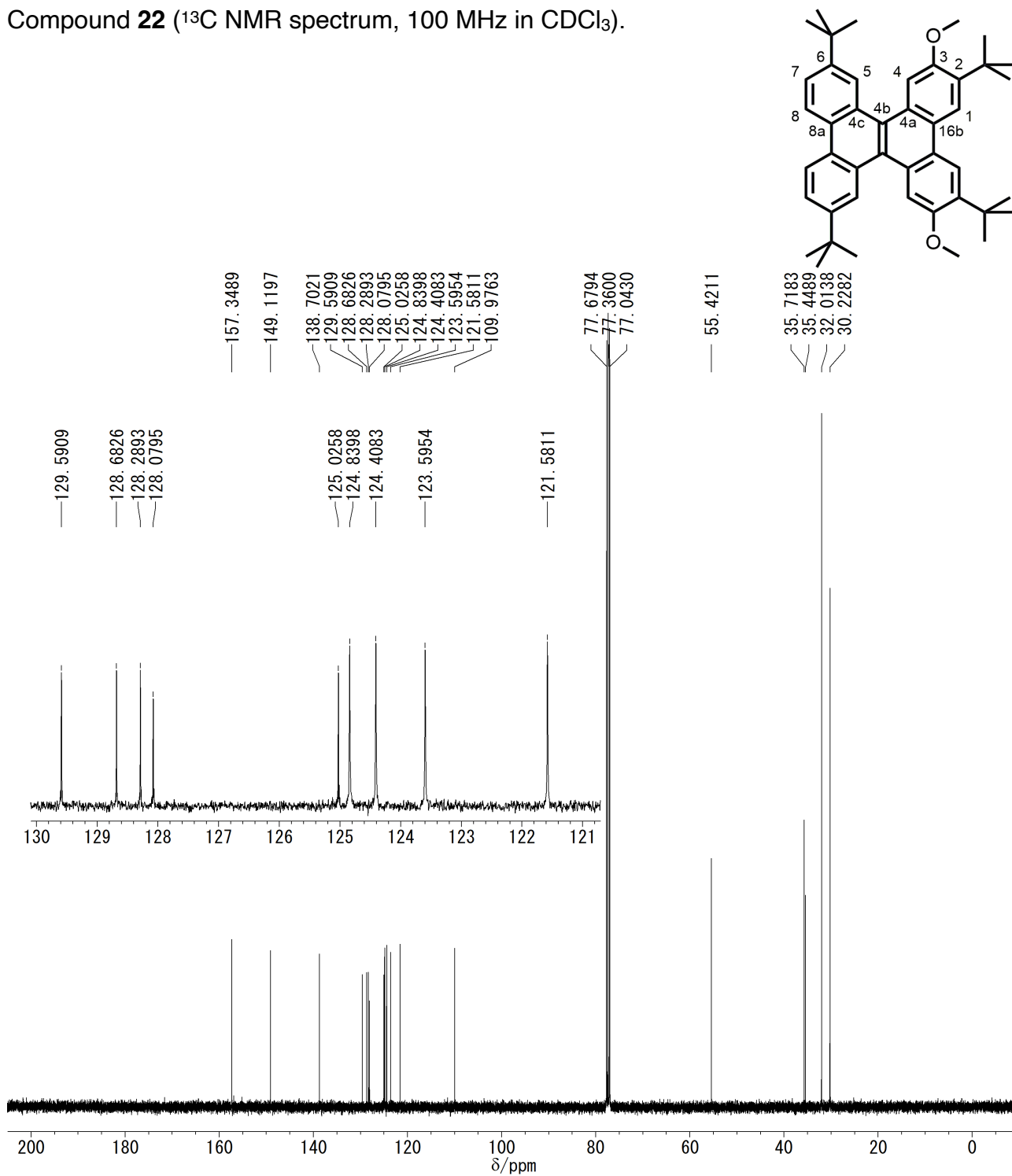
Compound **21** (^{13}C NMR spectrum, 100 MHz in $\text{DMSO-}d_6$).



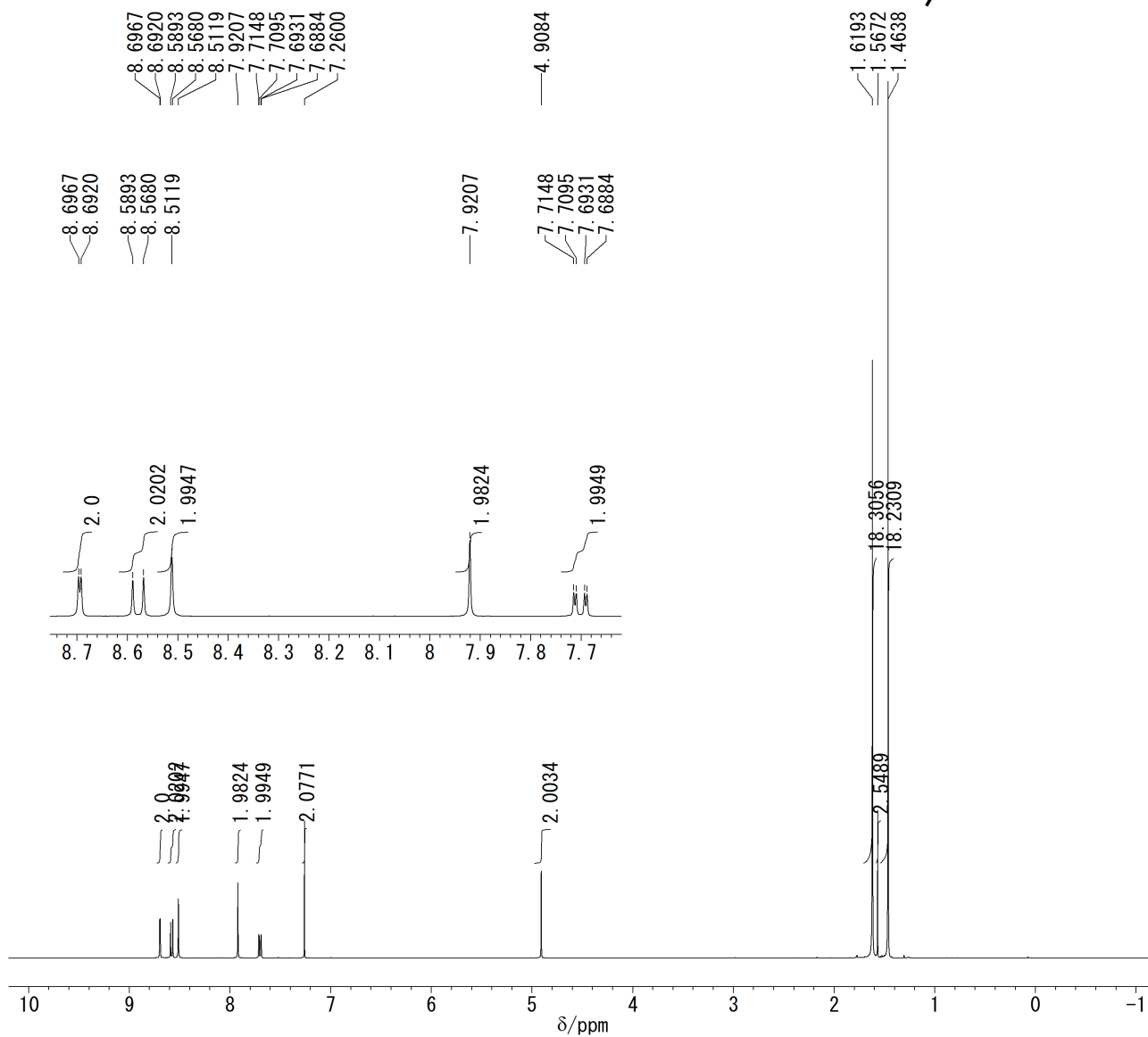
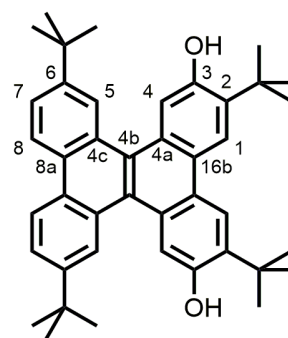
Compound **22** (¹H NMR spectrum, 400 MHz in CDCl₃).



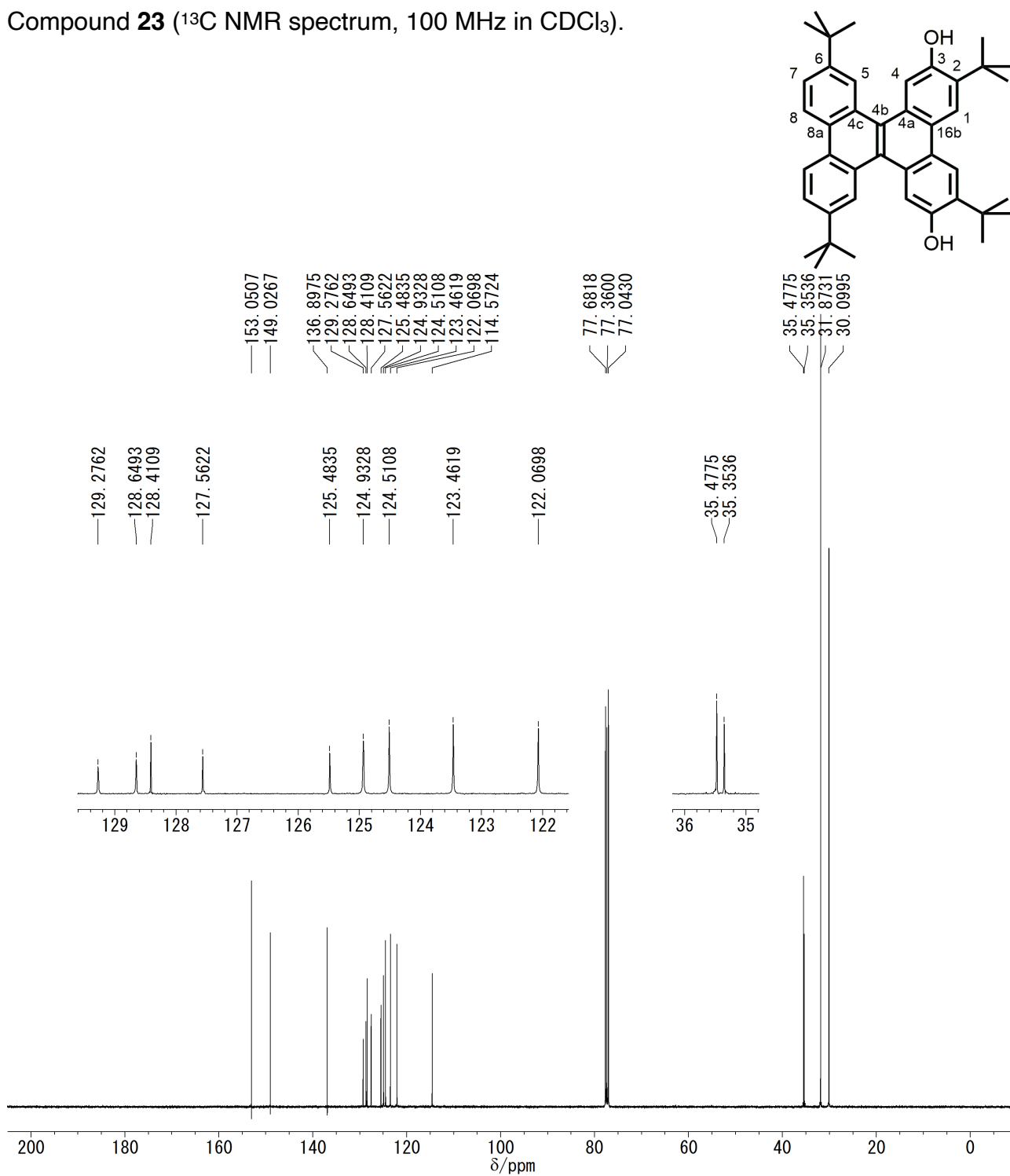
Compound **22** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



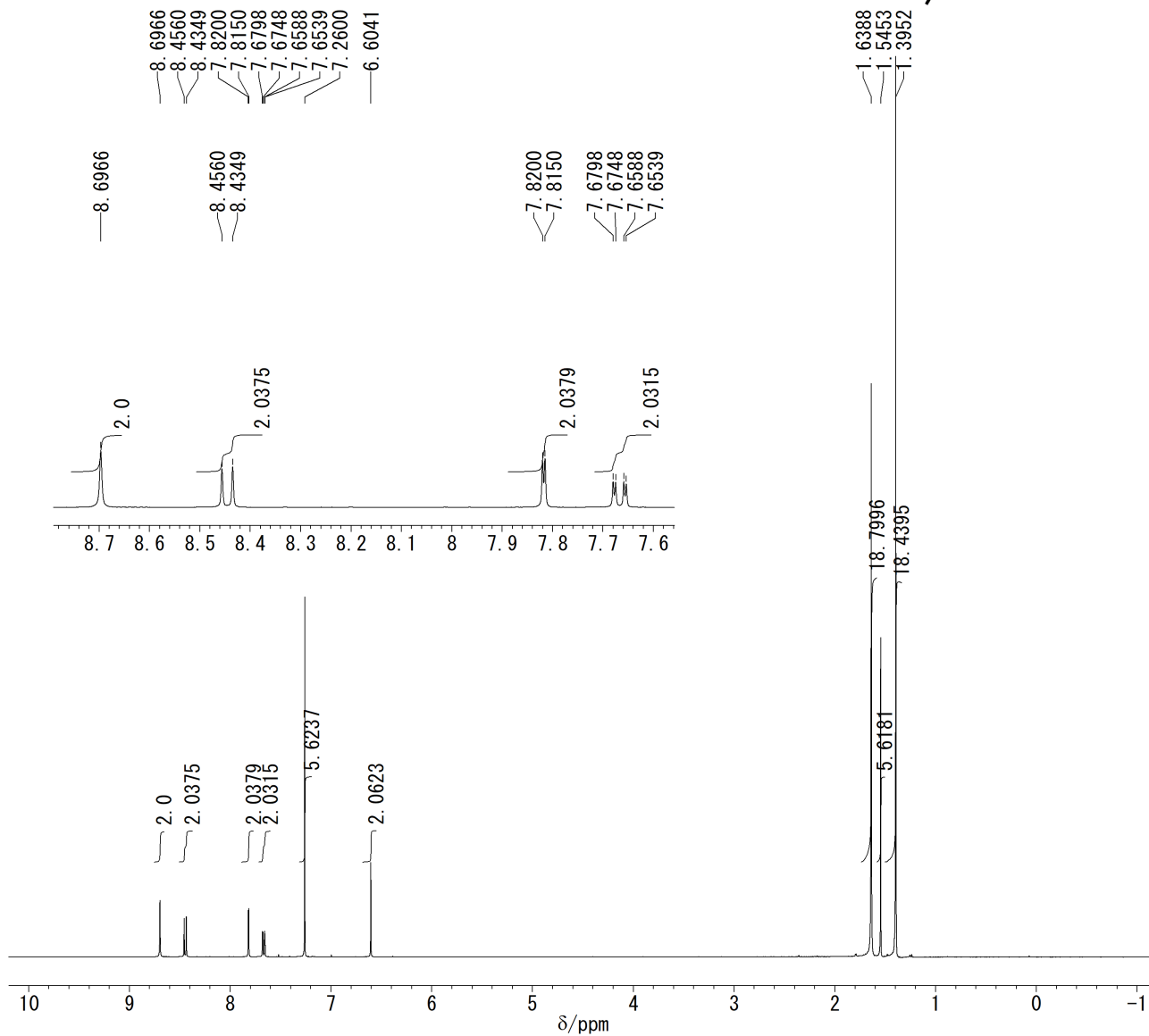
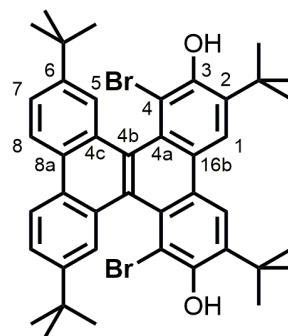
Compound **23** (¹H NMR spectrum, 400 MHz in CDCl₃).



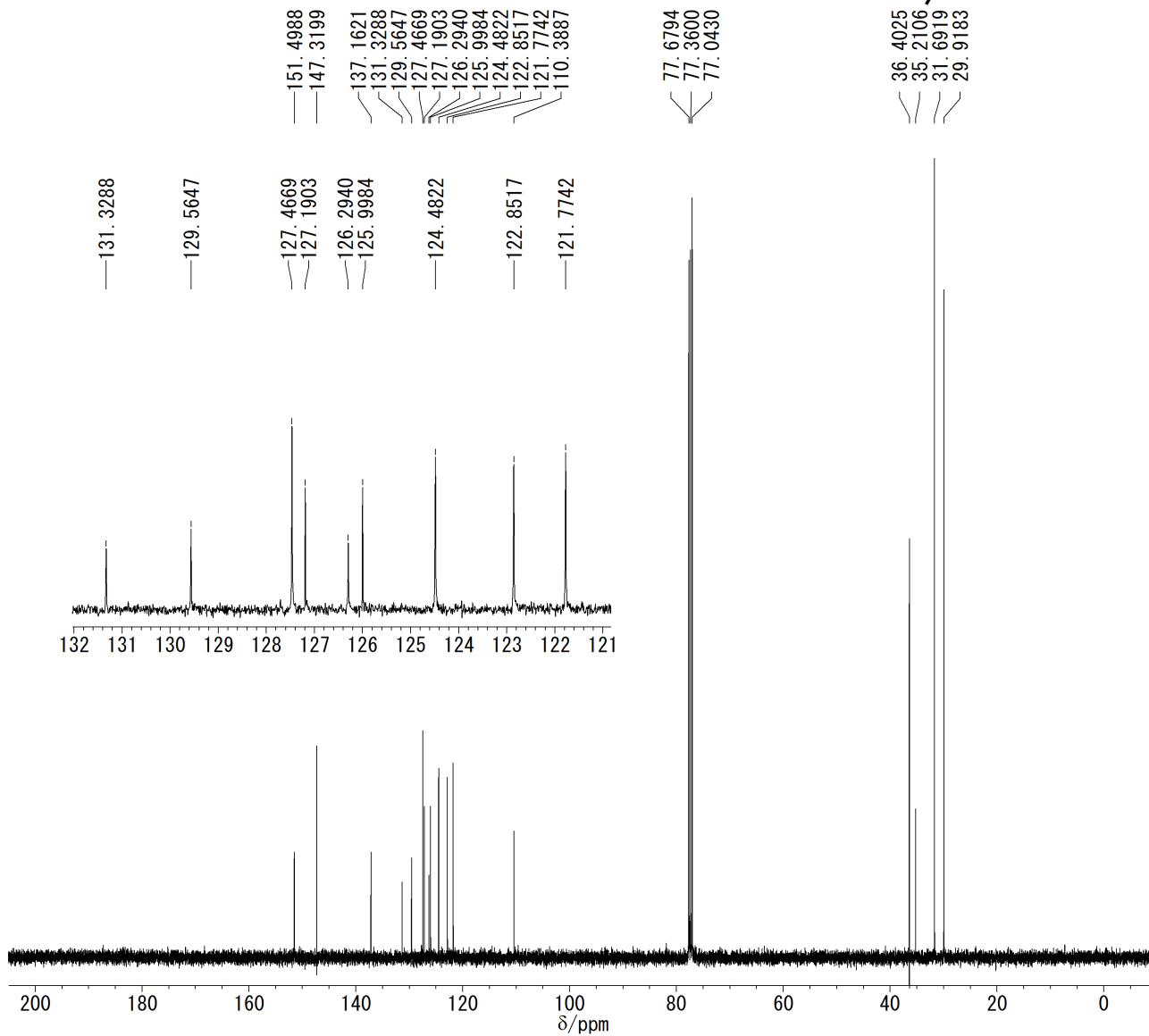
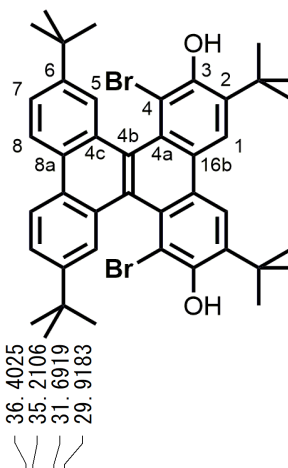
Compound **23** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



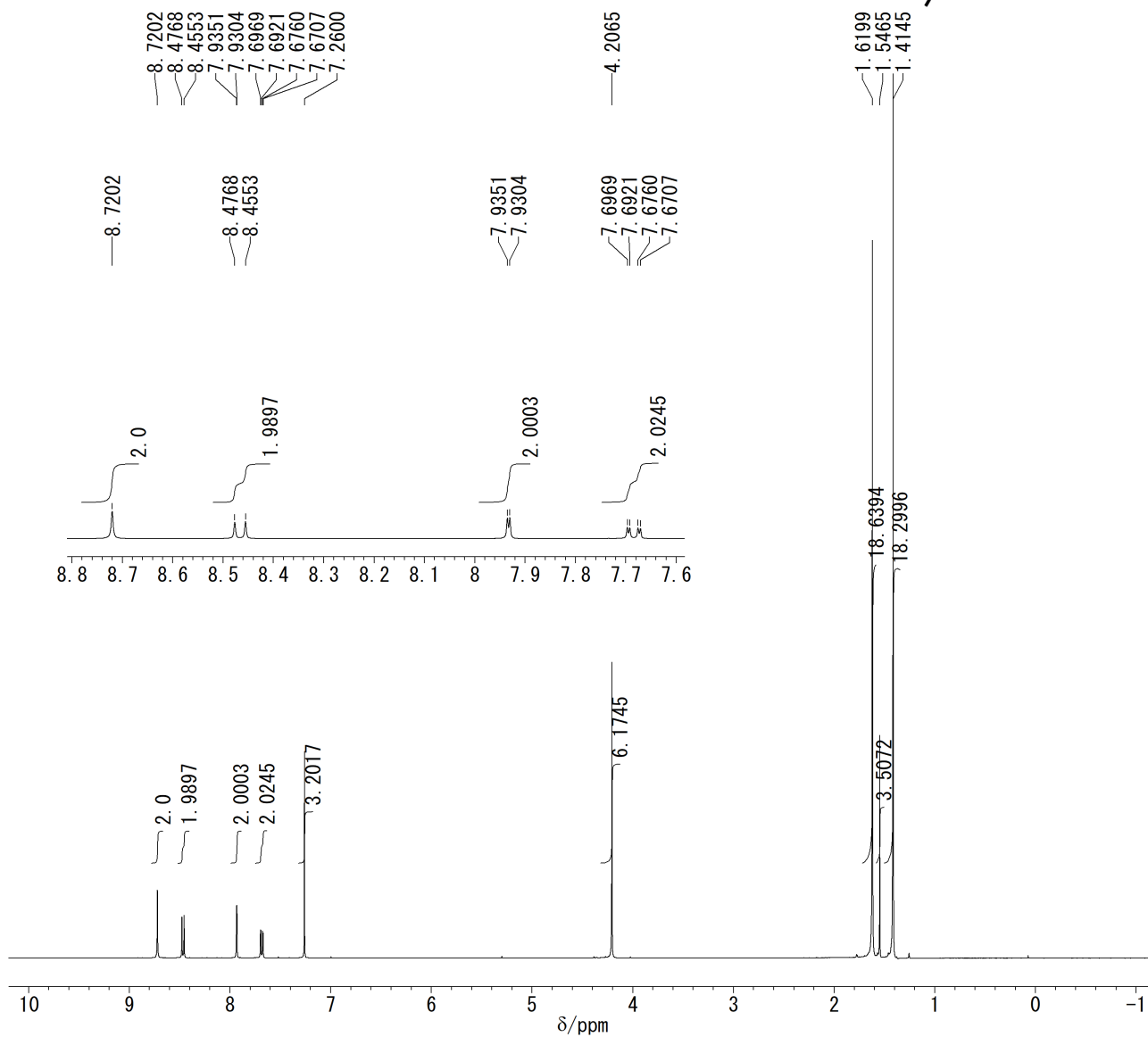
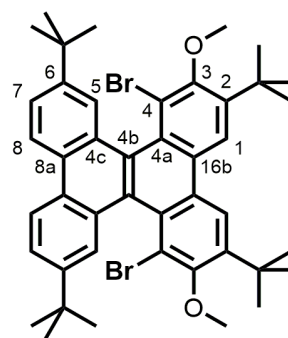
Compound **24** (¹H NMR spectrum, 400 MHz in CDCl₃).



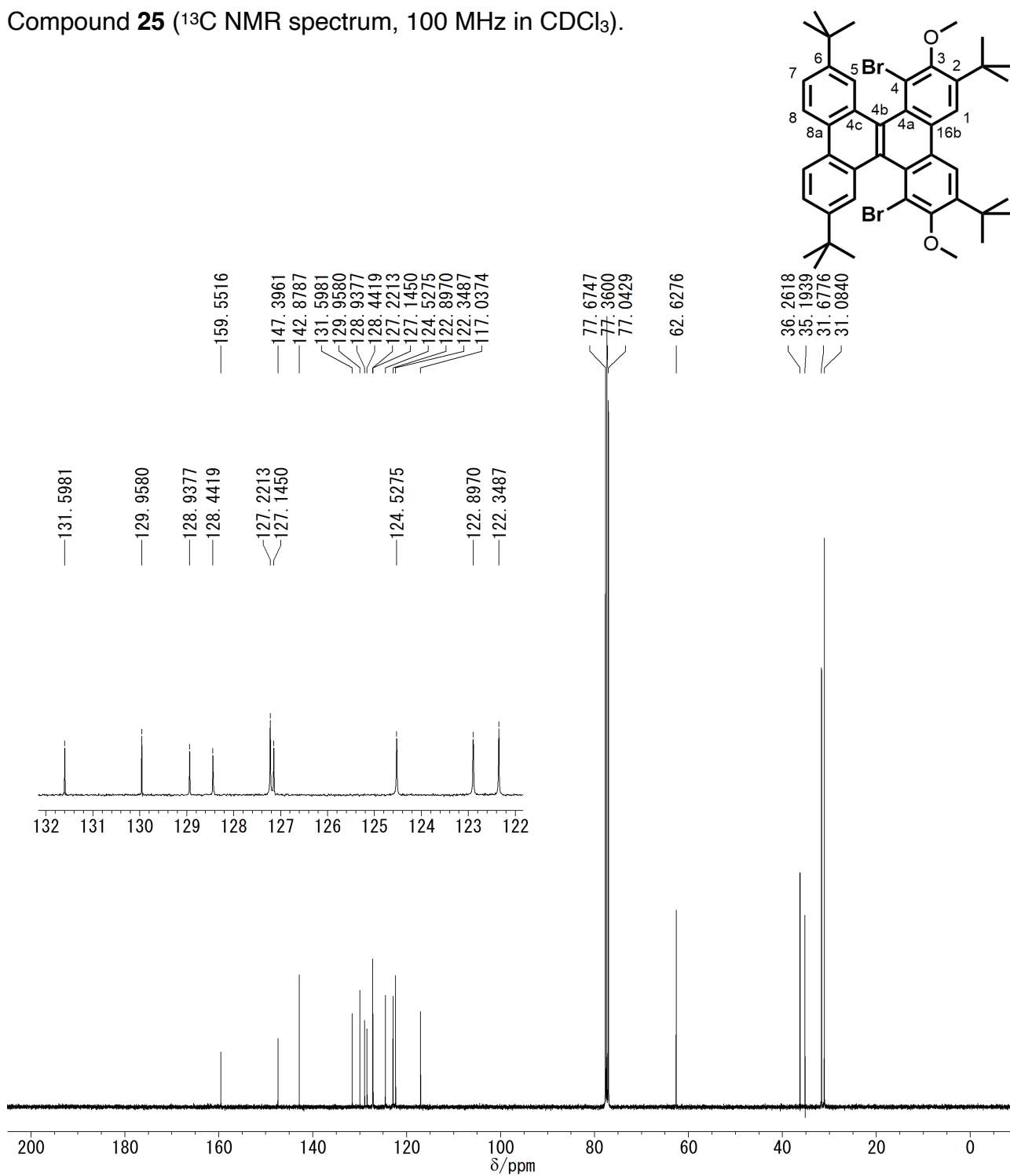
Compound **24** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



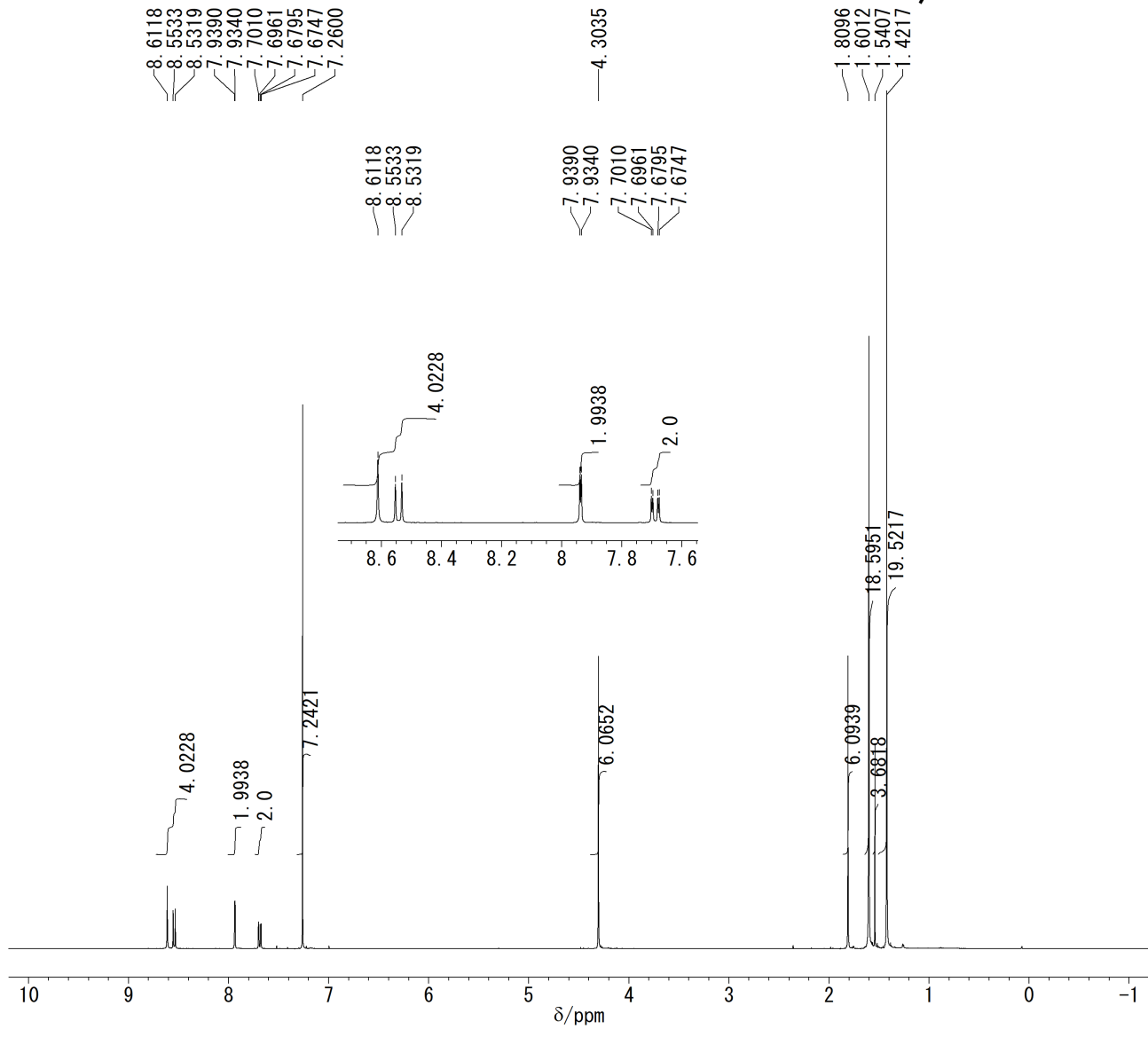
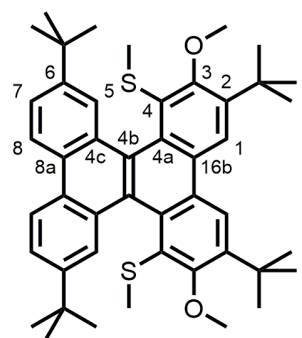
Compound **25** (¹H NMR spectrum, 400 MHz in CDCl₃).



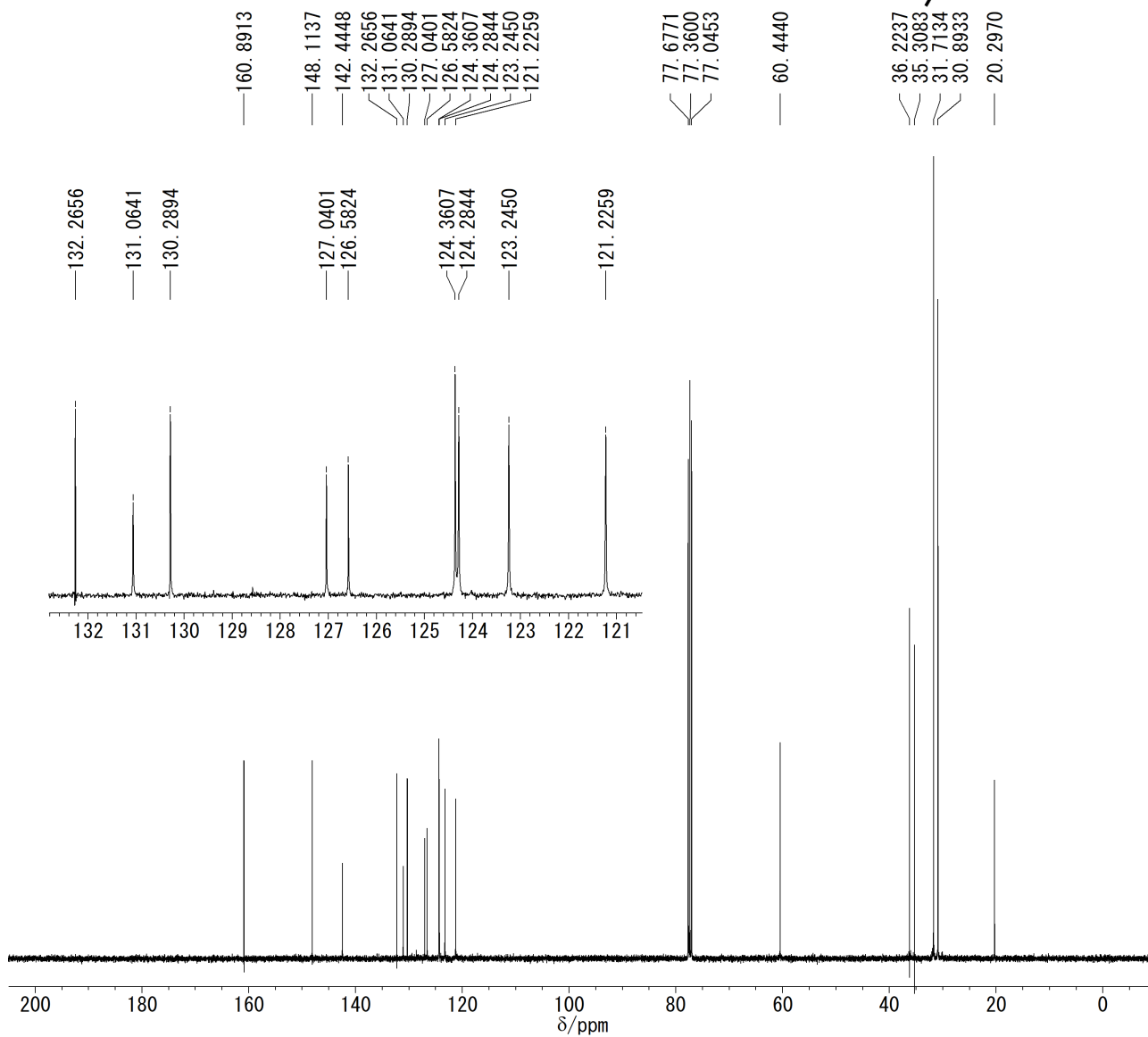
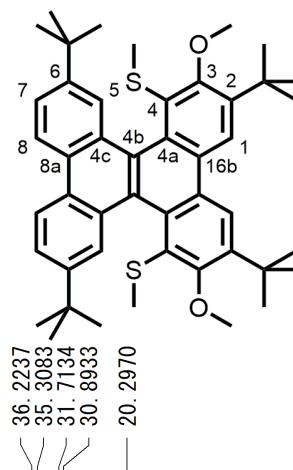
Compound **25** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



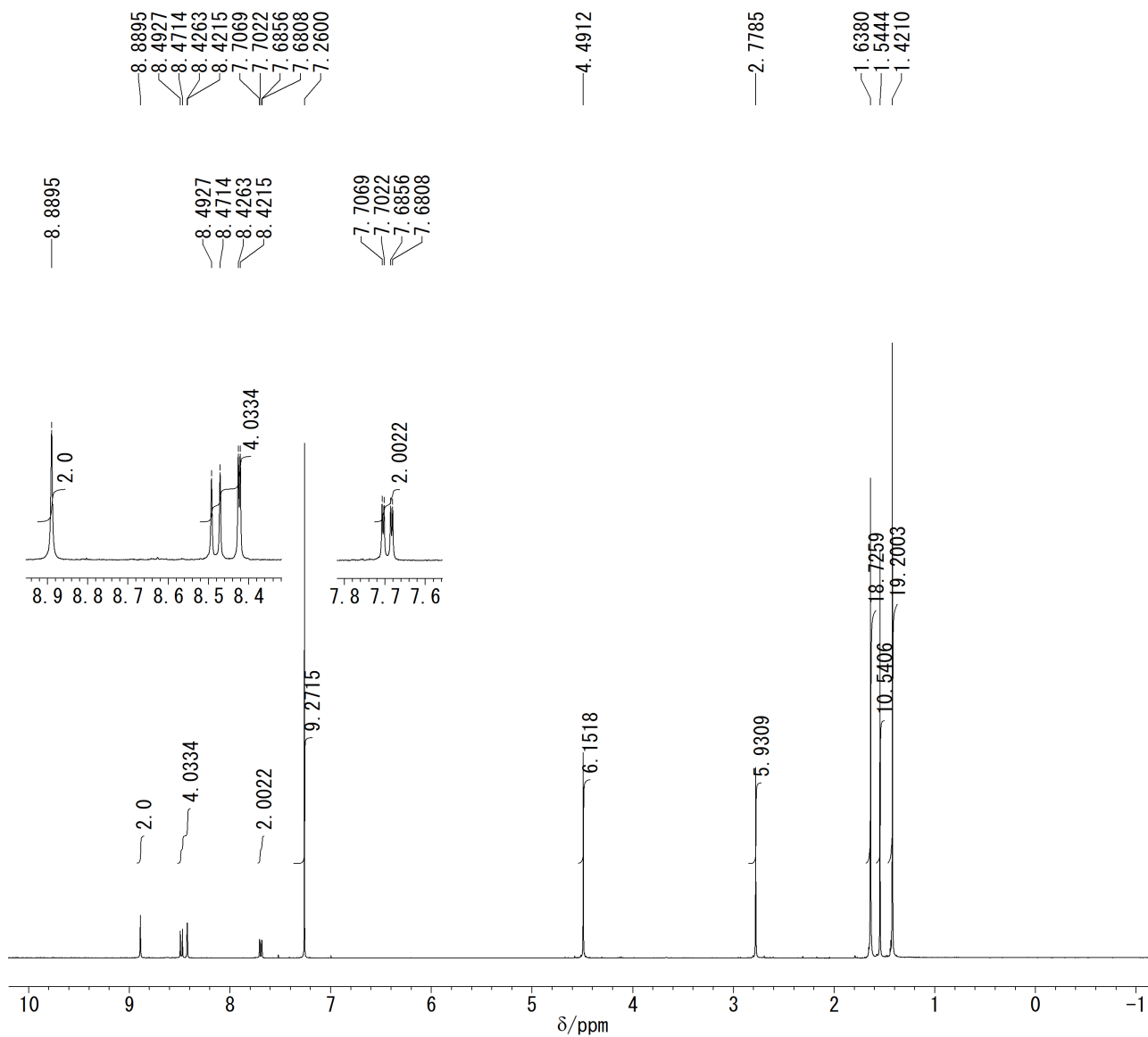
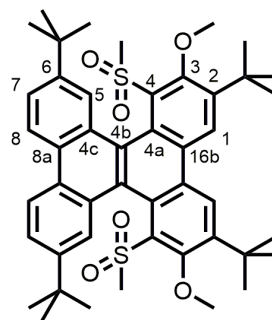
Compound **26** (¹H NMR spectrum, 400 MHz in CDCl₃).



Compound **26** (^{13}C NMR spectrum, 100 MHz in CDCl_3).



Compound **27** (¹H NMR spectrum, 400 MHz in CDCl₃).



Compound **27** (^{13}C NMR spectrum, 100 MHz in CDCl_3).

