*Supporting Information for*

# Isomerically pure anthra[2,3-*b*:6,7-*b*']-difuran (*anti*-ADF), -dithiophene (*anti*-ADT), and -diselenophene (*anti*-ADS): Selective synthesis, electronic structures, and application to organic field-effect transistors

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## 1. CV, PESA, UV-vis spectra of BDX, NDT, and ADX

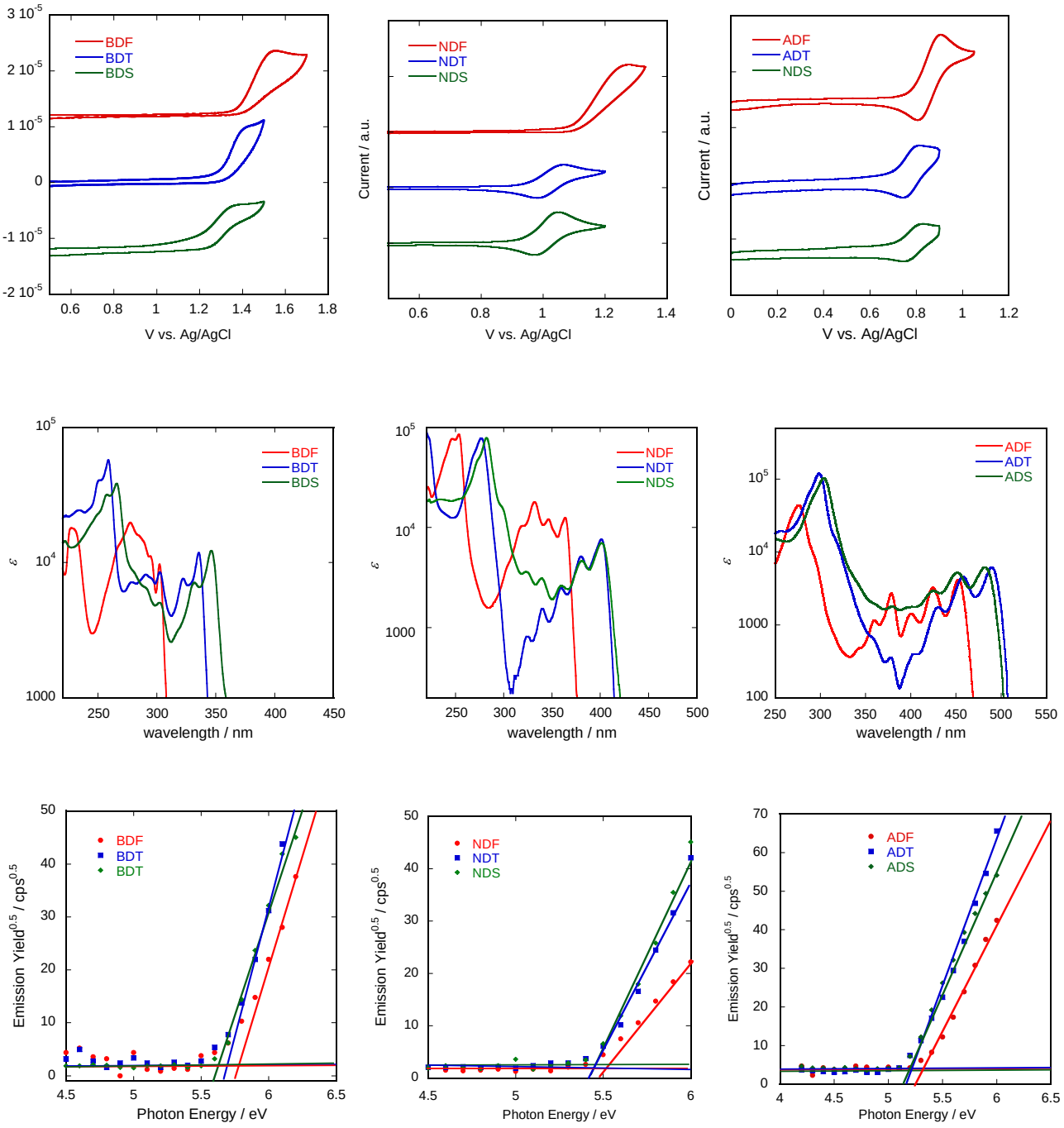



**Figure S1**. PESA, UV-vis spectra of BDXs, NDXs, and ADX.

## 2. XRDs of evaporated thin films

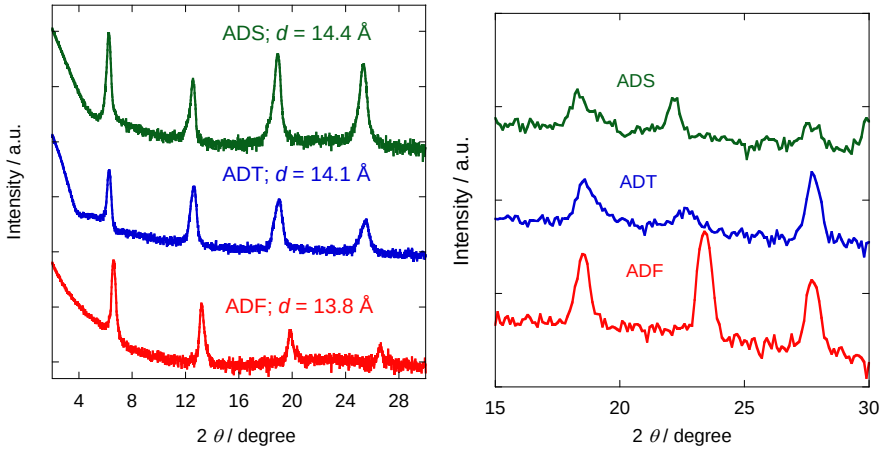



**Figure S2**. Out-of-plane and In-plane XRD patterns of ADX thin films on $Si/SiO_2$ substrates.

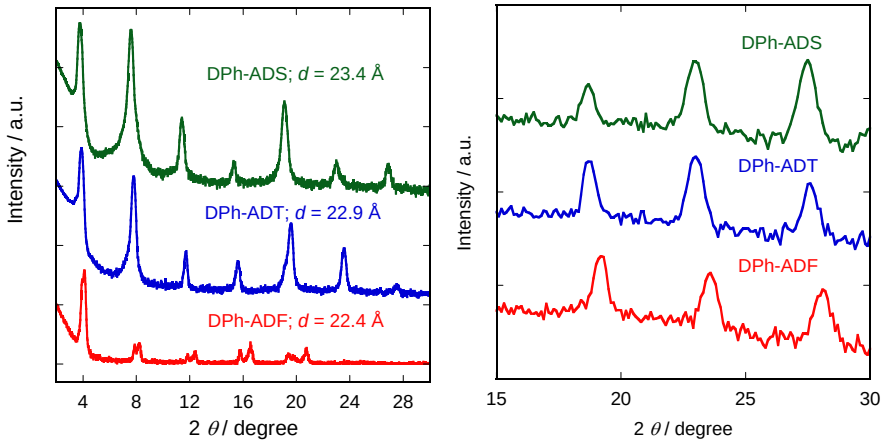



**Figure S3**. Out-of-plane and In-plane XRD patterns of DPh-NDX thin films on $Si/SiO_2$ substrates.

## 3. AFM images of evaporated thin films

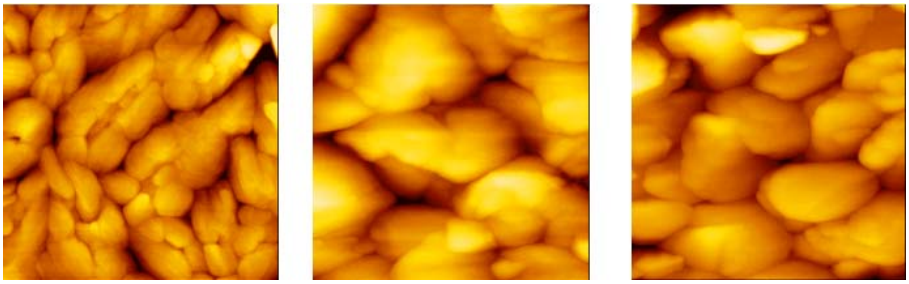


**Figure S4**. AFM imeges (2 ×2 μm) of evaporated thin film of ADF, ADT and ADS on $Si/SiO_2$ substrate.

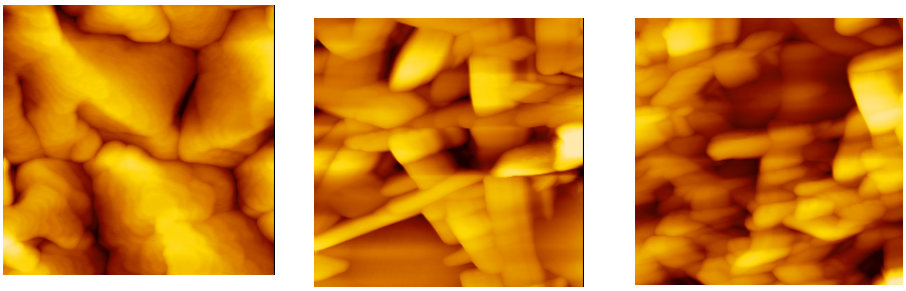


**Figure S5**. AFM imeges (2 ×2 μm) of evaporated thin film of DPh-ADF, DPh-ADT and DPh-ADS on $Si/SiO_2$ substrate.

## 4. FET characteristics of DPh-BDF

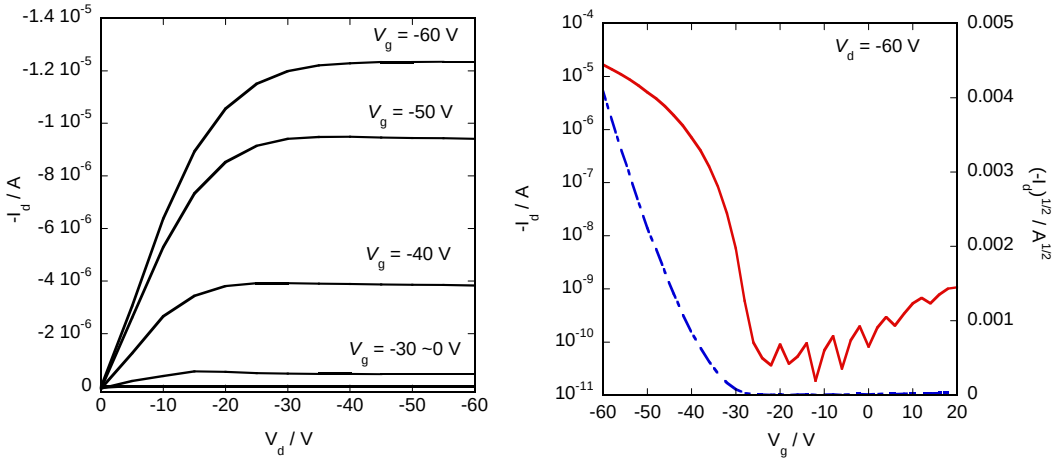


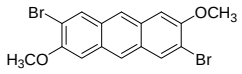

**Figure S5**. Output and transfer characteristics of DPh-BDF-based transistor

## 5. FET characteristics of ADXs and DPh-ADXs

**Table S1**. FET characteristics of ADX- and DPh-ADX-based OFETs

| *compound* | $T_{sub}$ | *SAM* | $\mu_{FET}$ | $I_{on}/I_{off}$ | $V_{th}$ |
|---|---|---|---|---|---|
| ADT | 60°C | ODTS | 0.16-0.22 | 1.80E+06 | +4.0 |
| | | HMDS | 0.11-0.29 | 2.40E+06 | +1.7 |
| | 85°C | ODTS | 0.20-0.30 | 2.80E+06 | -3.3 |
| | | HMDS | 0.11-0.18 | 5.50E+05 | -4.9 |
| ADS | 60°C | ODTS | 0.11-0.23 | 1.70E+06 | -4.6 |
| | | HMDS | 0.21-0.23 | 2.40E+06 | +1.7 |
| | 85°C | ODTS | 0.31-0.75 | 1.70E+06 | -9.8 |
| | | HMDS | 0.11-0.18 | 6.10E+08 | -3.0 |
| DPh-ADF | 150°C | ODTS | 0.50-0.60 | 6.53E+05 | +0.5 |
| | | HMDS | 0.35-0.46 | 1.56E+05 | -3.2 |
| DPh-ADT | 150°C | ODTS | 0.72-1.30 | 3.50E+06 | -4.9 |
| | | HMDS | 0.44-0.67 | 8.50E+05 | -6.7 |
| DPh-ADS | 150°C | ODTS | 0.38-0.53 | 1.20E+06 | -11 |
| | | HMDS | 0.25-0.37 | 1.70E+06 | -5.7 |

## 2,6-Dibromo-3,7-dimethoxyanthracene (2)

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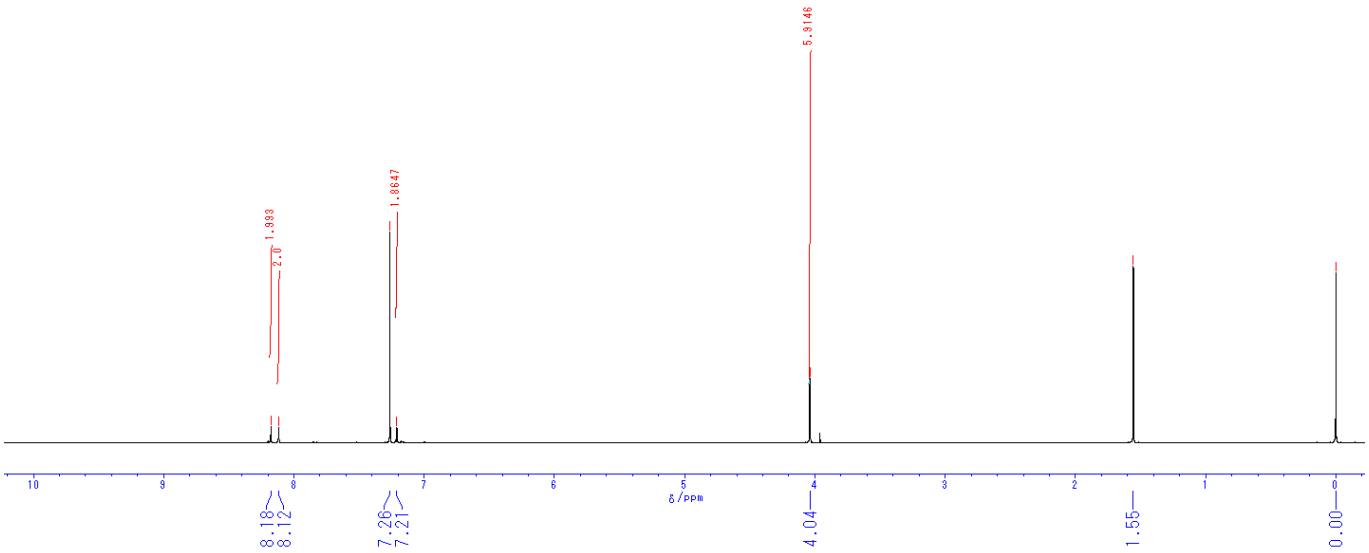


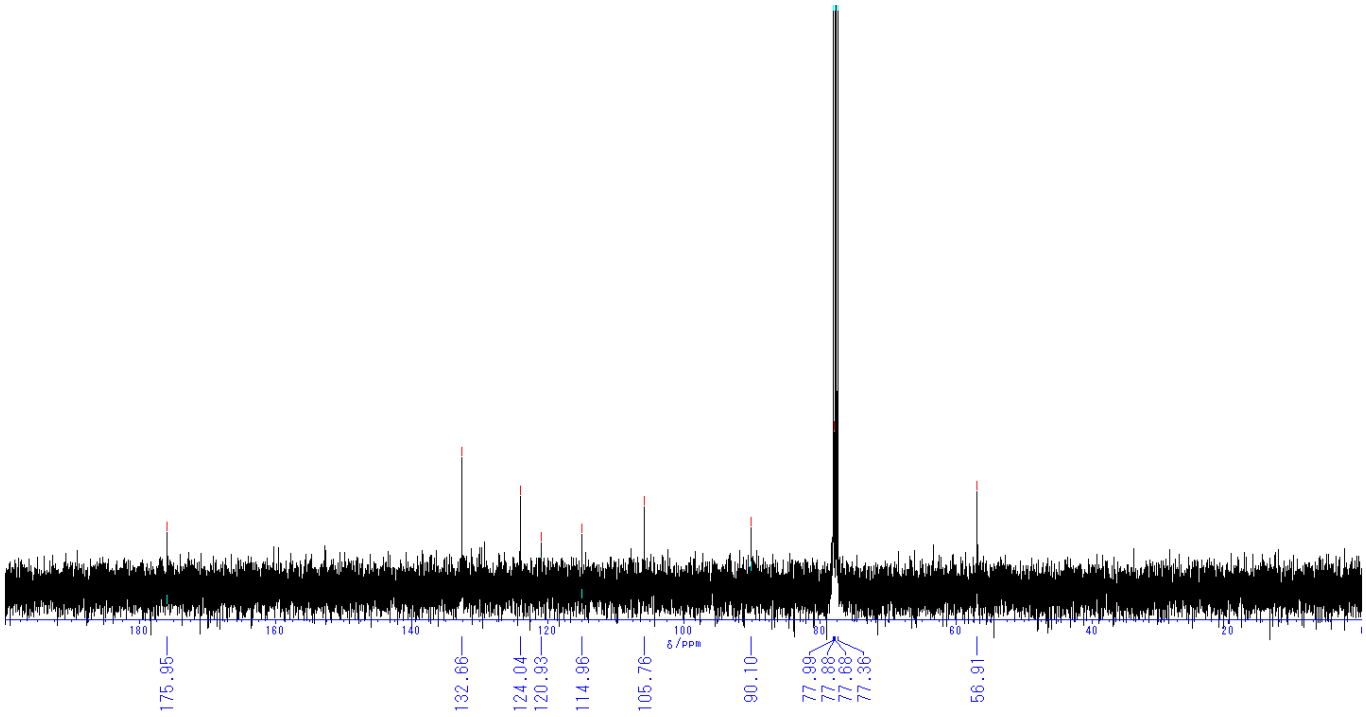

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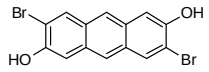


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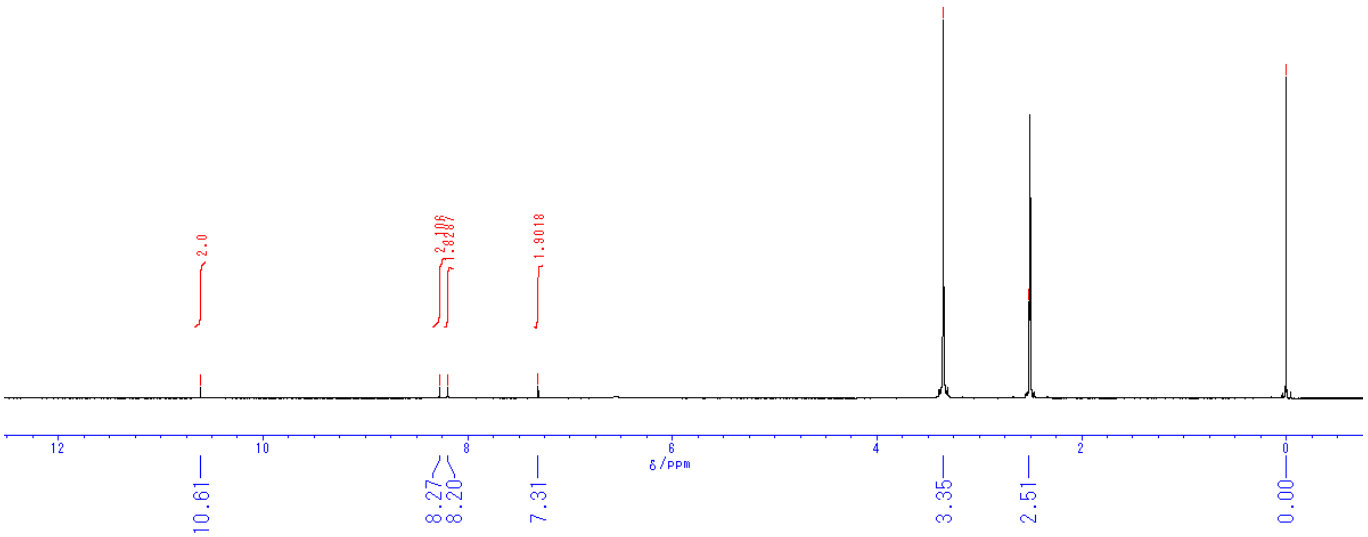


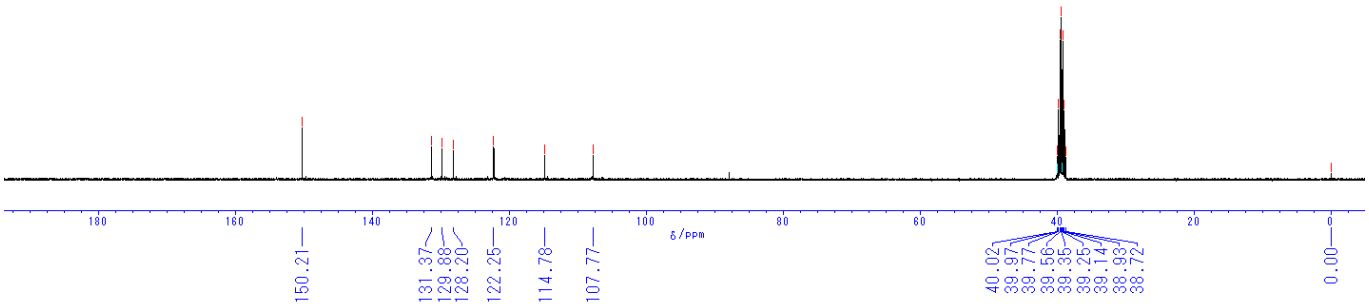

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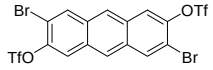


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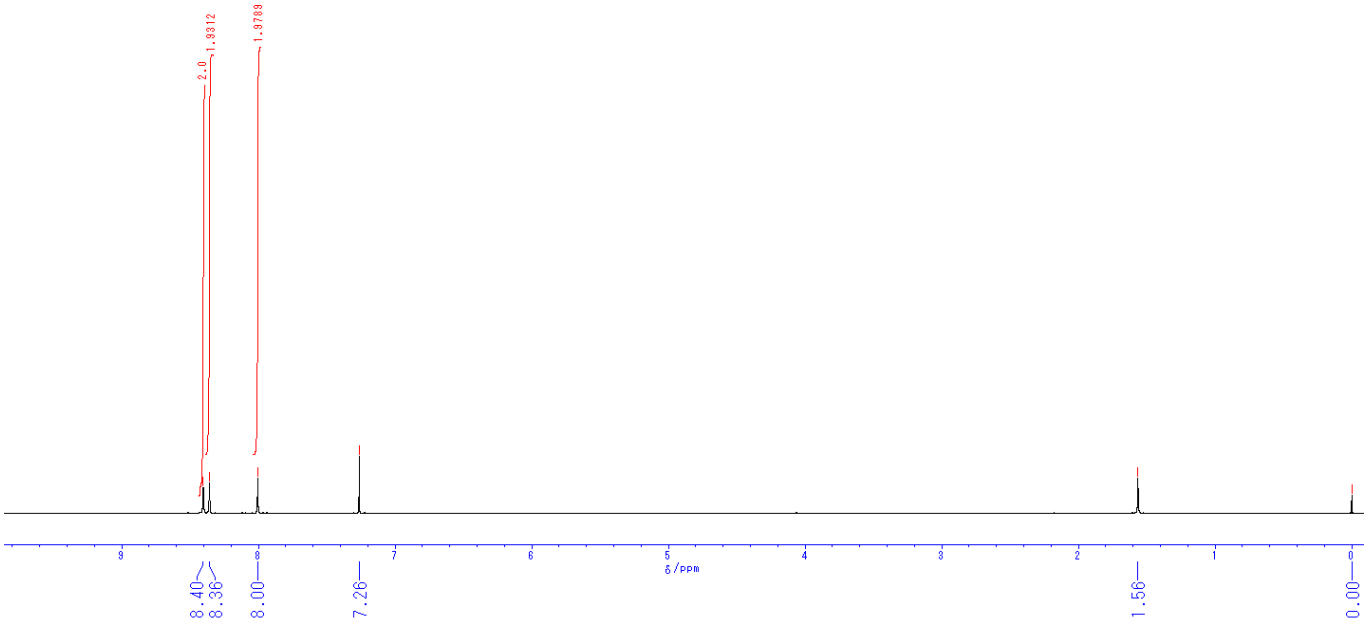
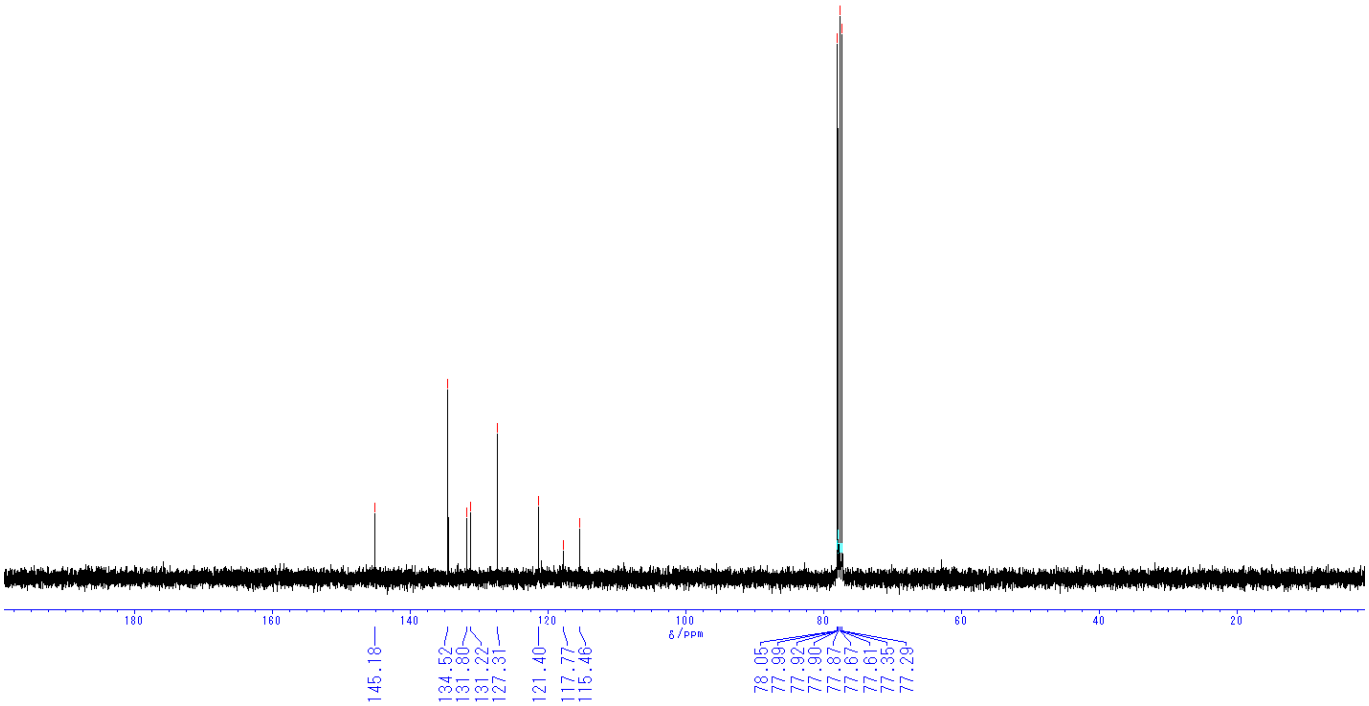
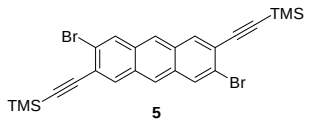


**3,7-Dibromo-2,6-bis(trimethylsilylethynyl)anthracene (5)**

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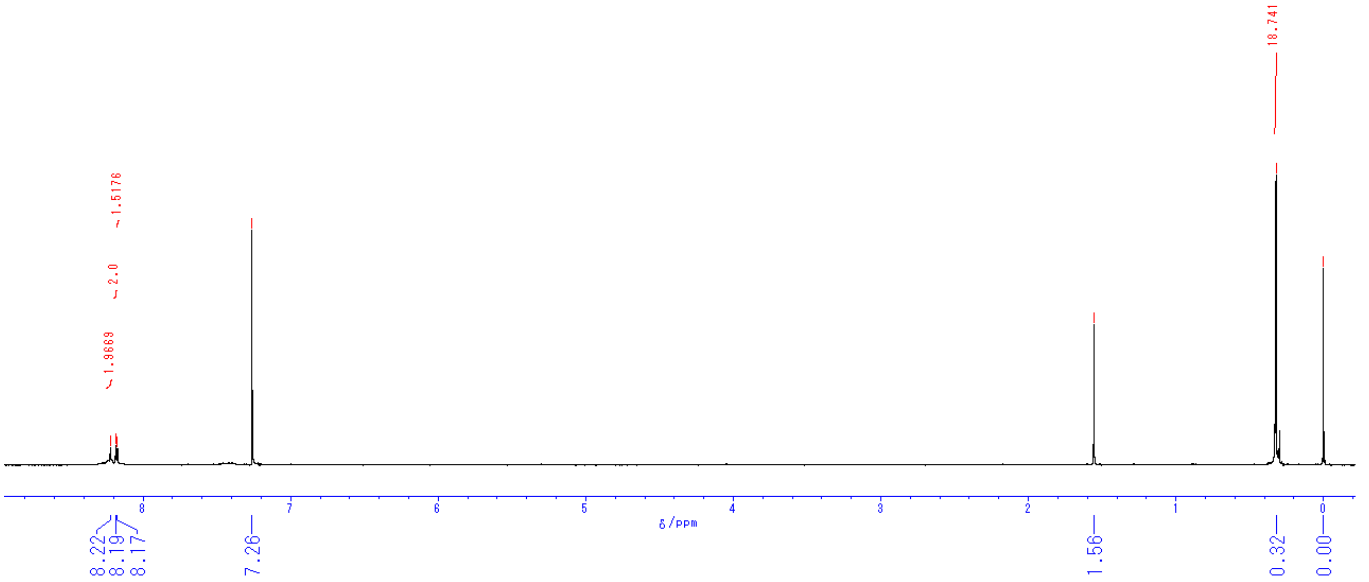


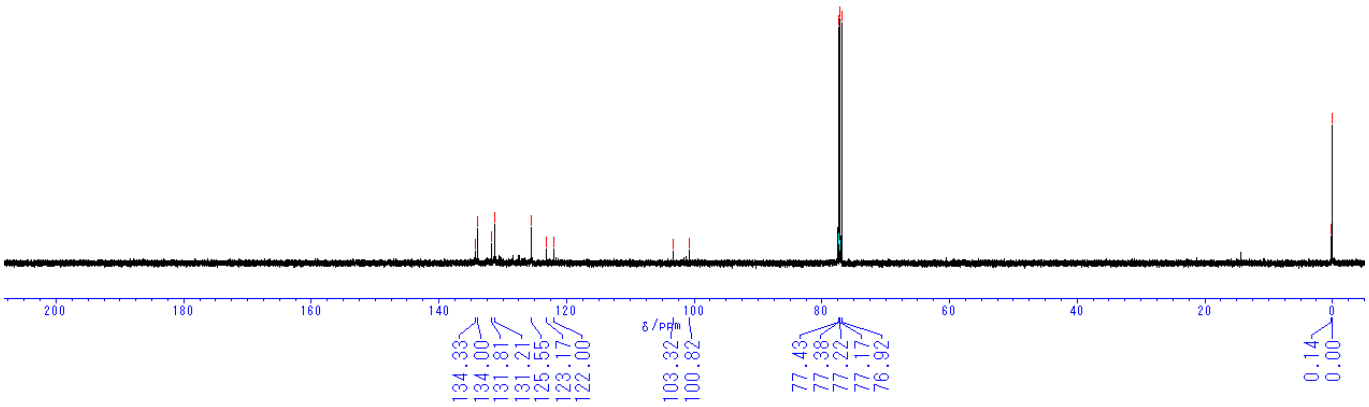

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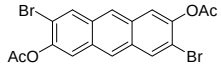


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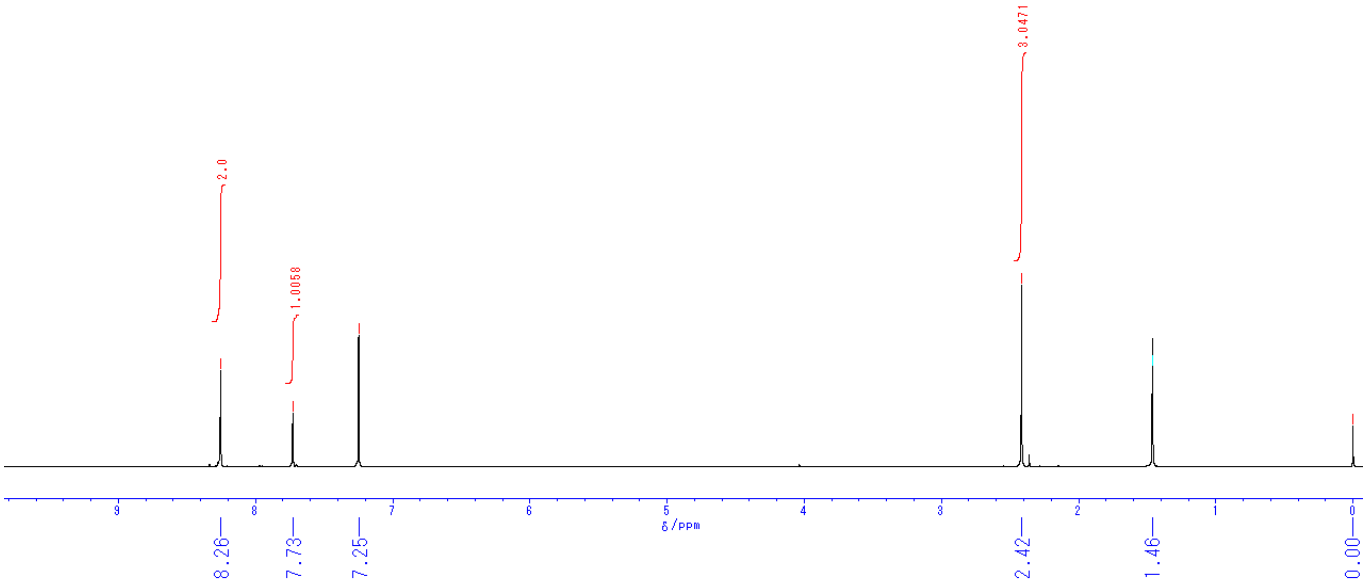


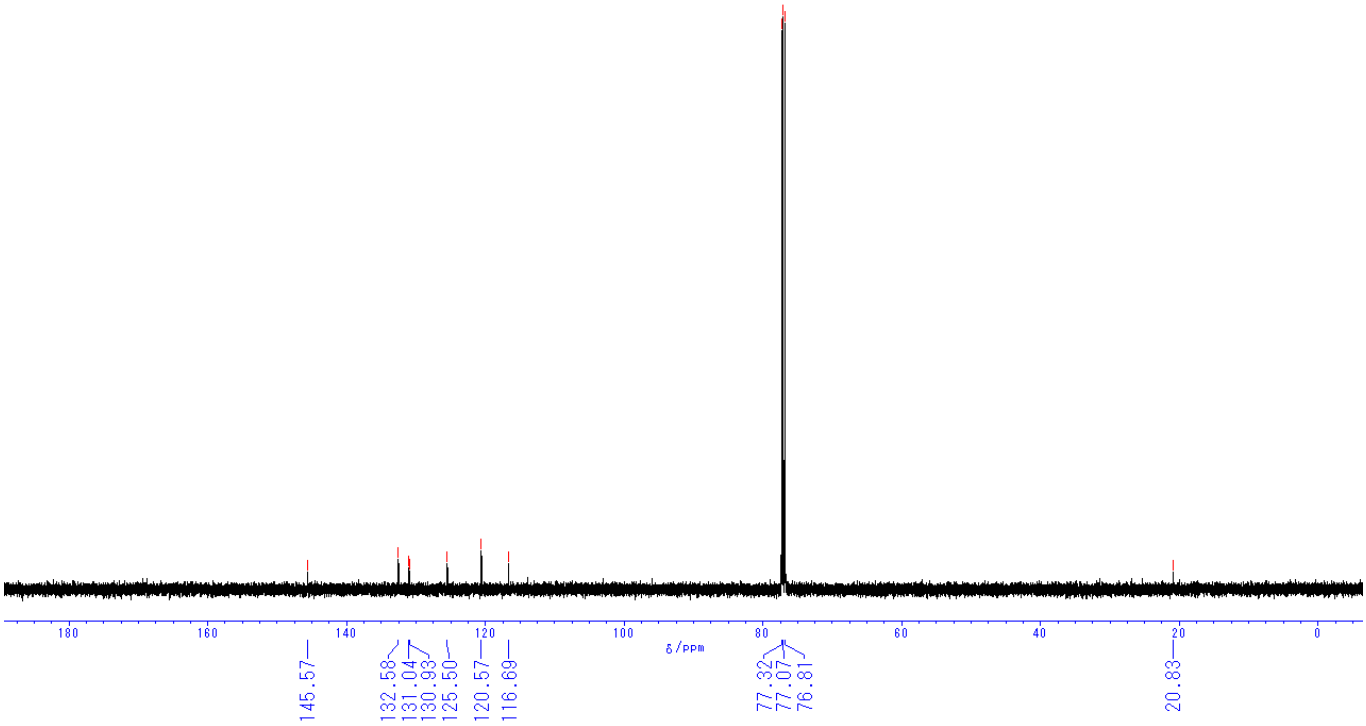

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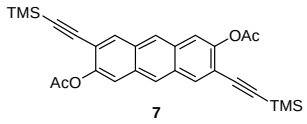


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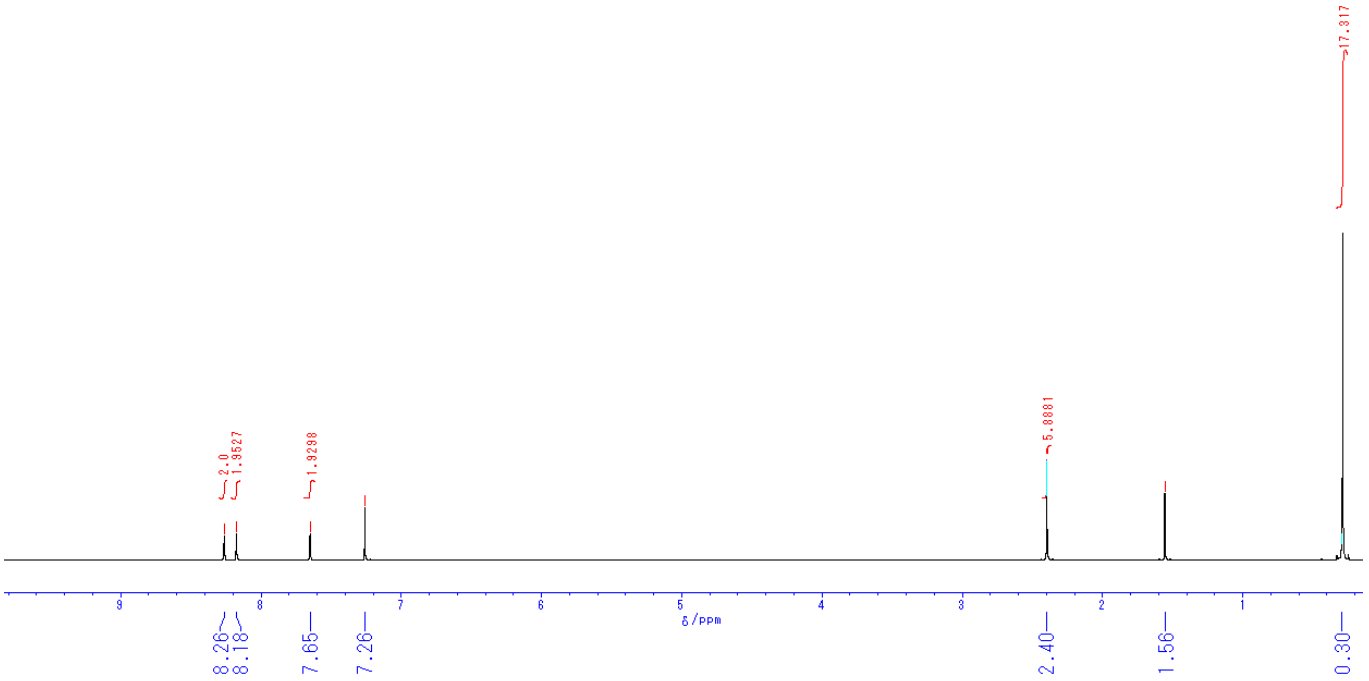
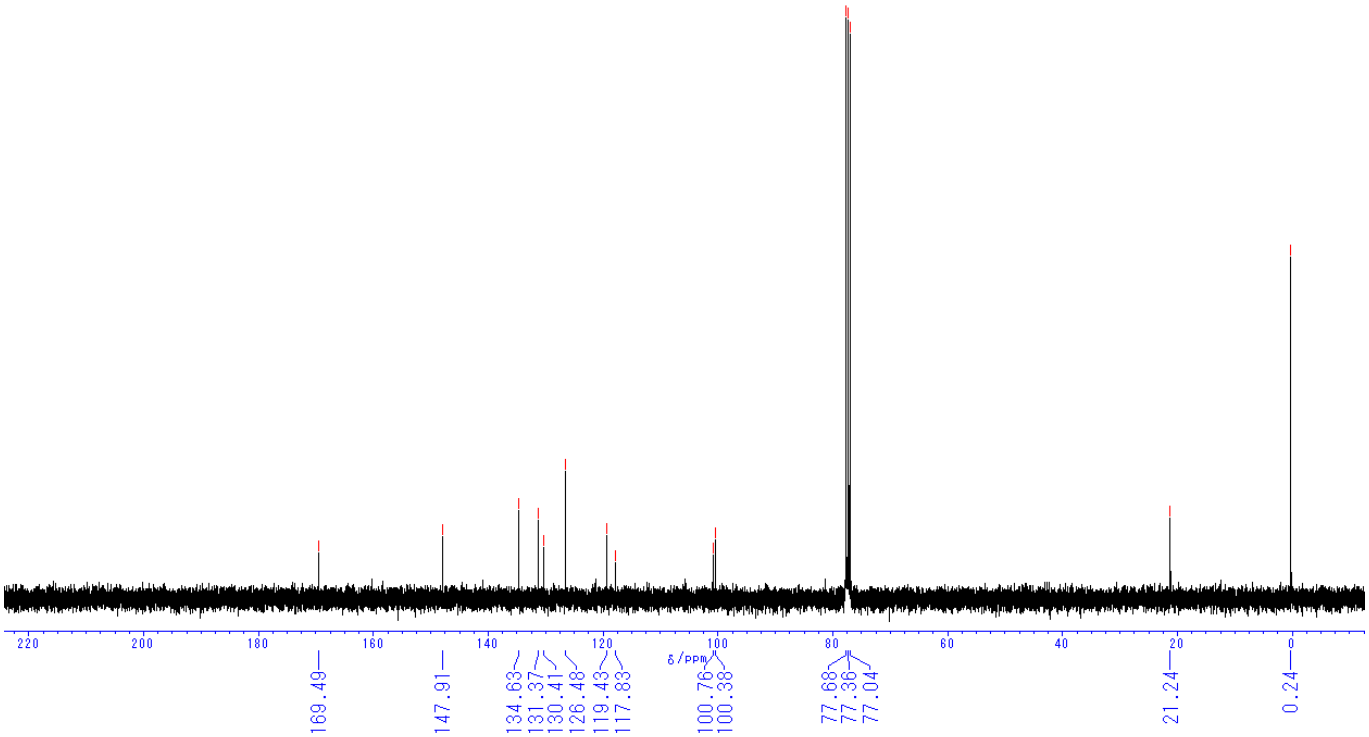
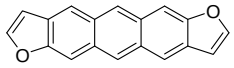
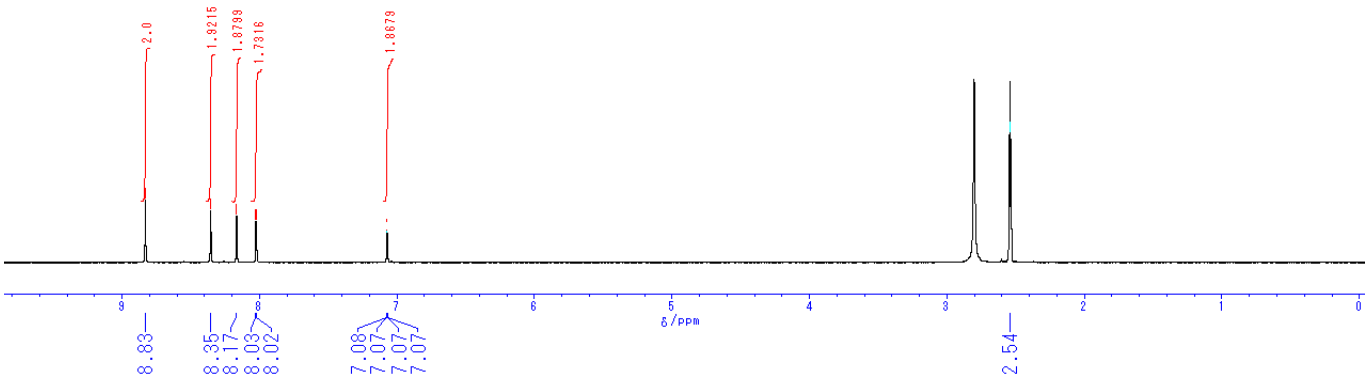


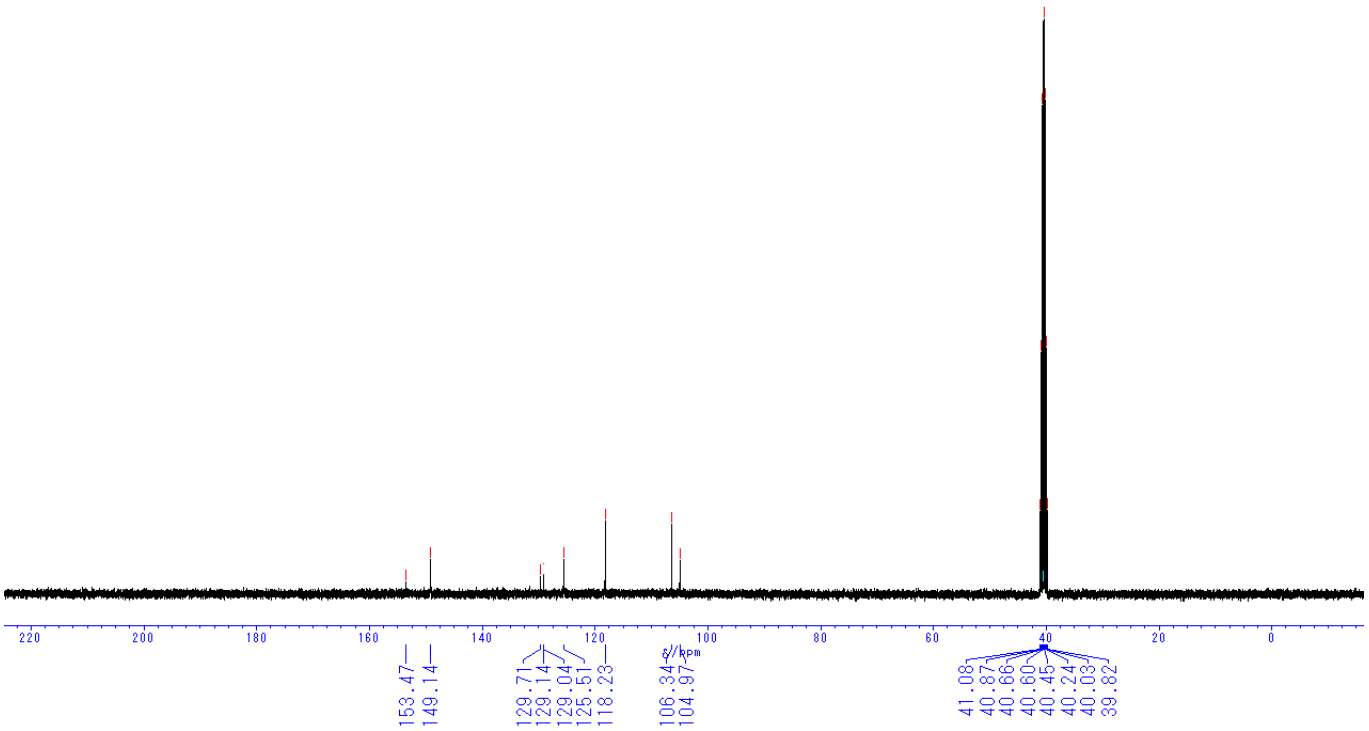



**Anthra[2,3-*b*:6,7-*b'*]difuran**

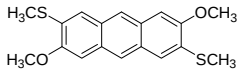


ADF



## 2,6-Dimethoxy-3,7-bis(methylthio)anthracene (8)

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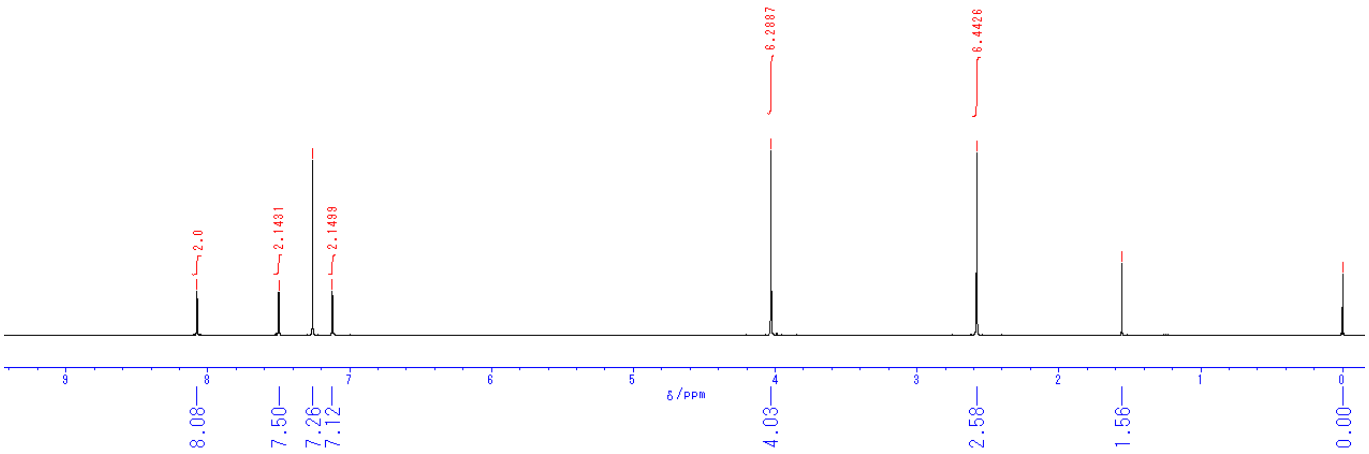
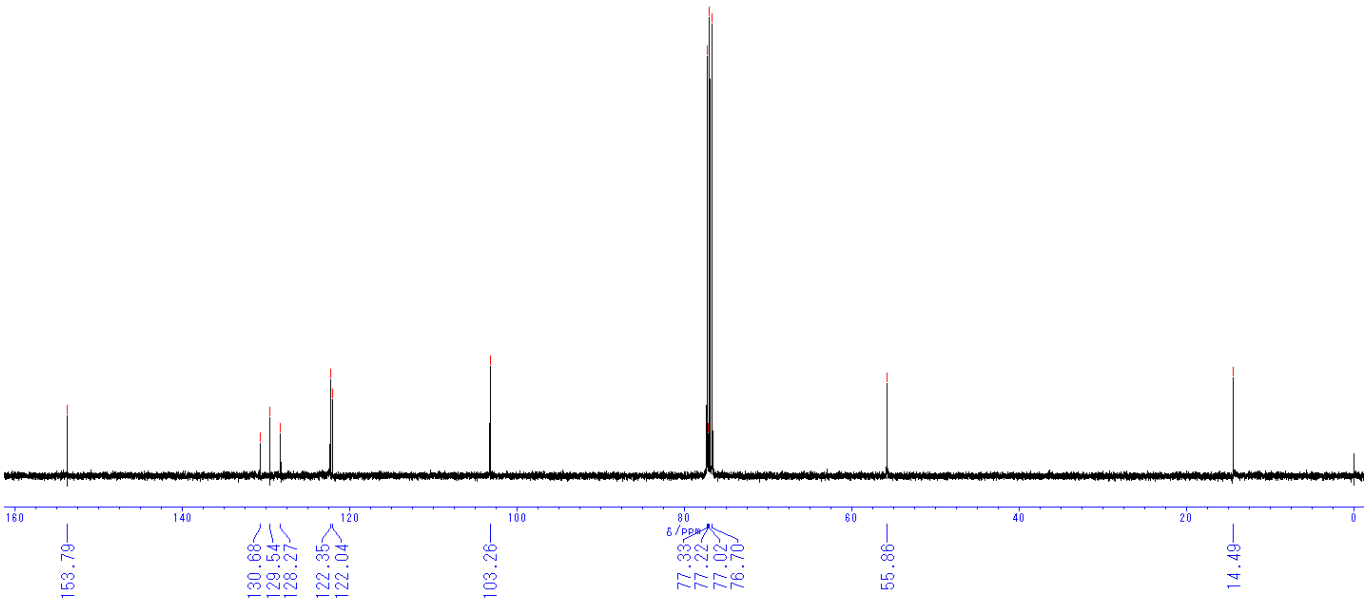
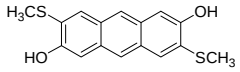


## 2,6-Dihydroxy-3,7-bis(methylthio)anthracene (9)

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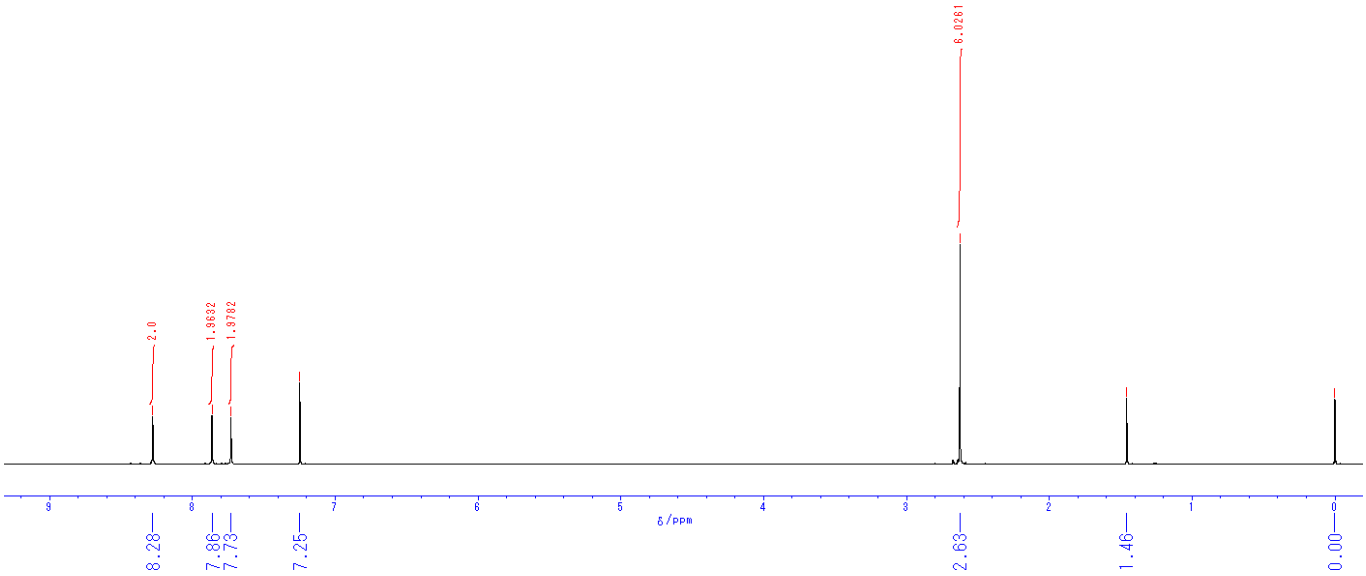
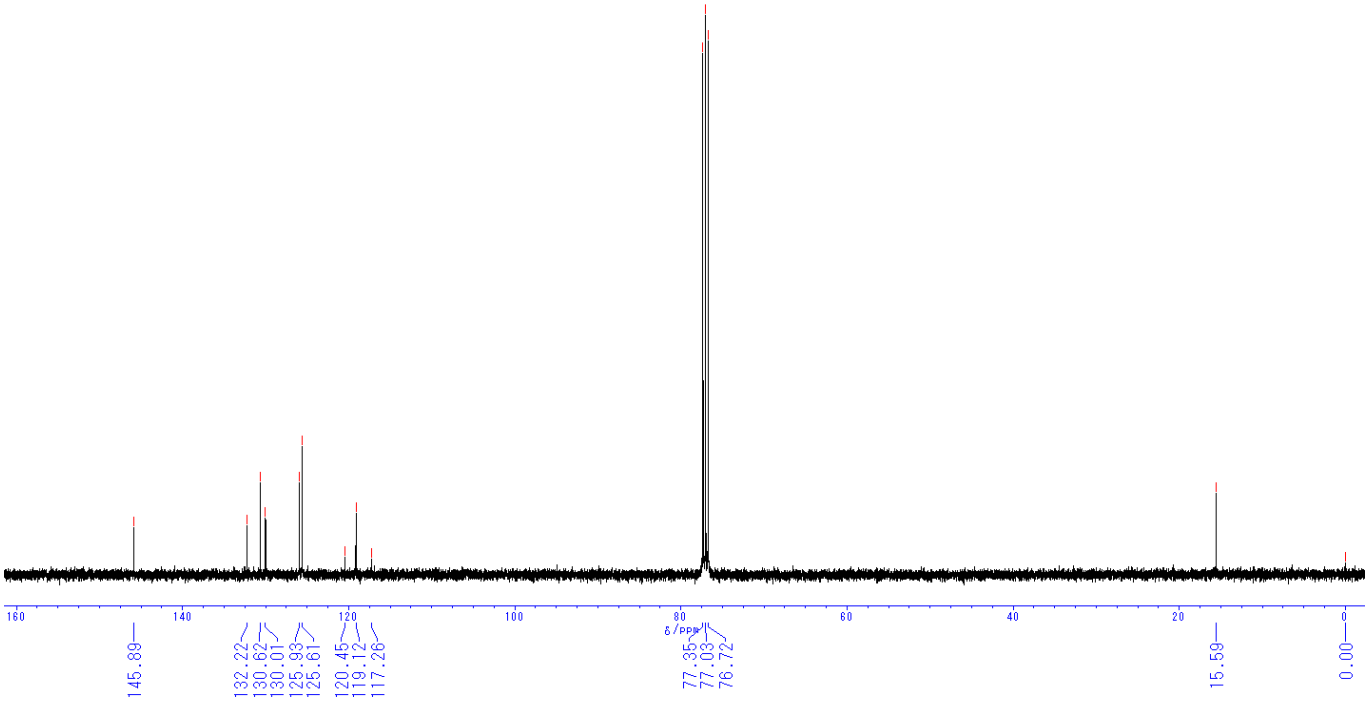
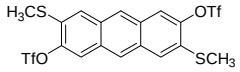


## 2,6-Bis(trifluoromethanesulfonyloxy)-3,7-bis(methylthio)anthracene (10)

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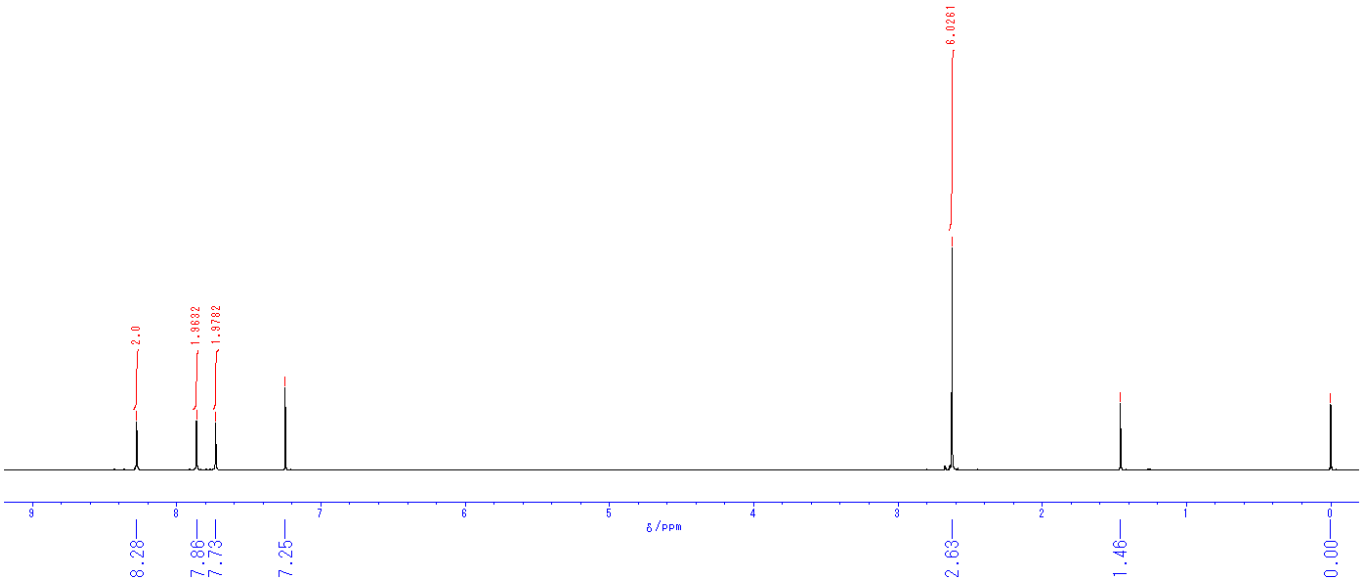


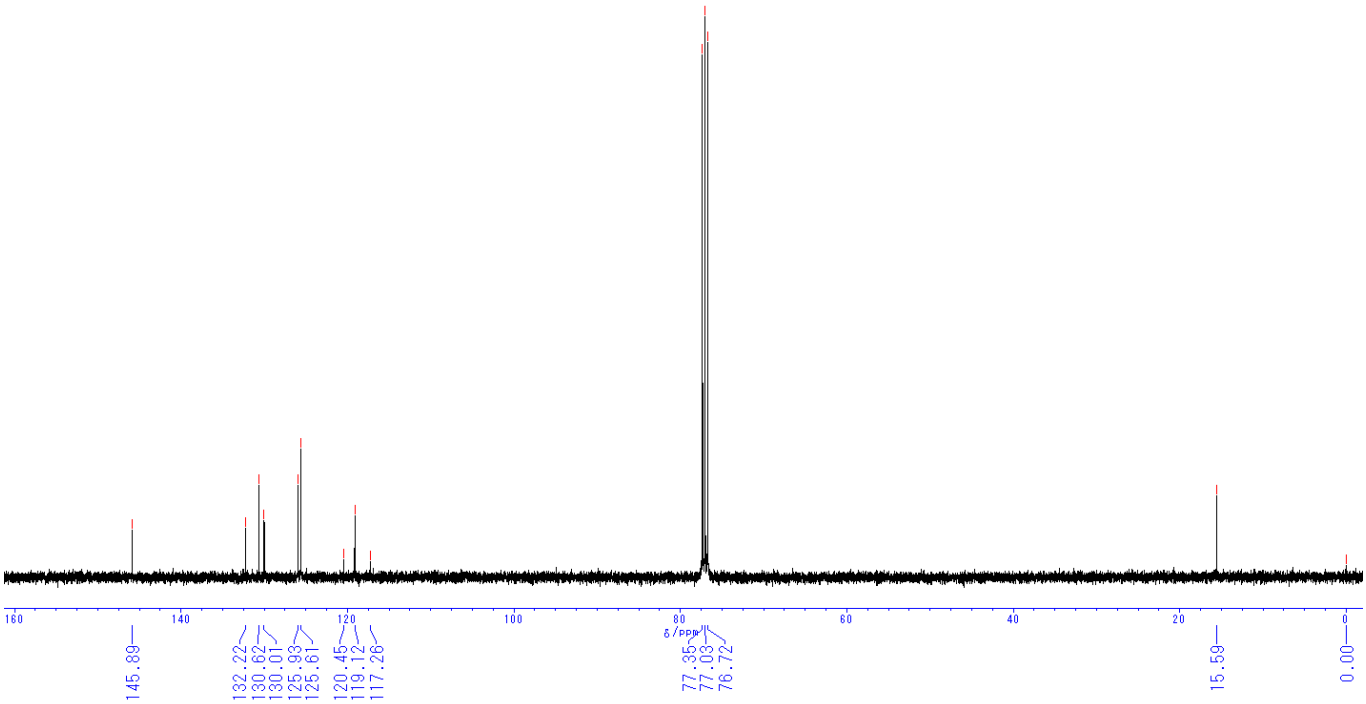

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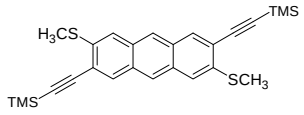


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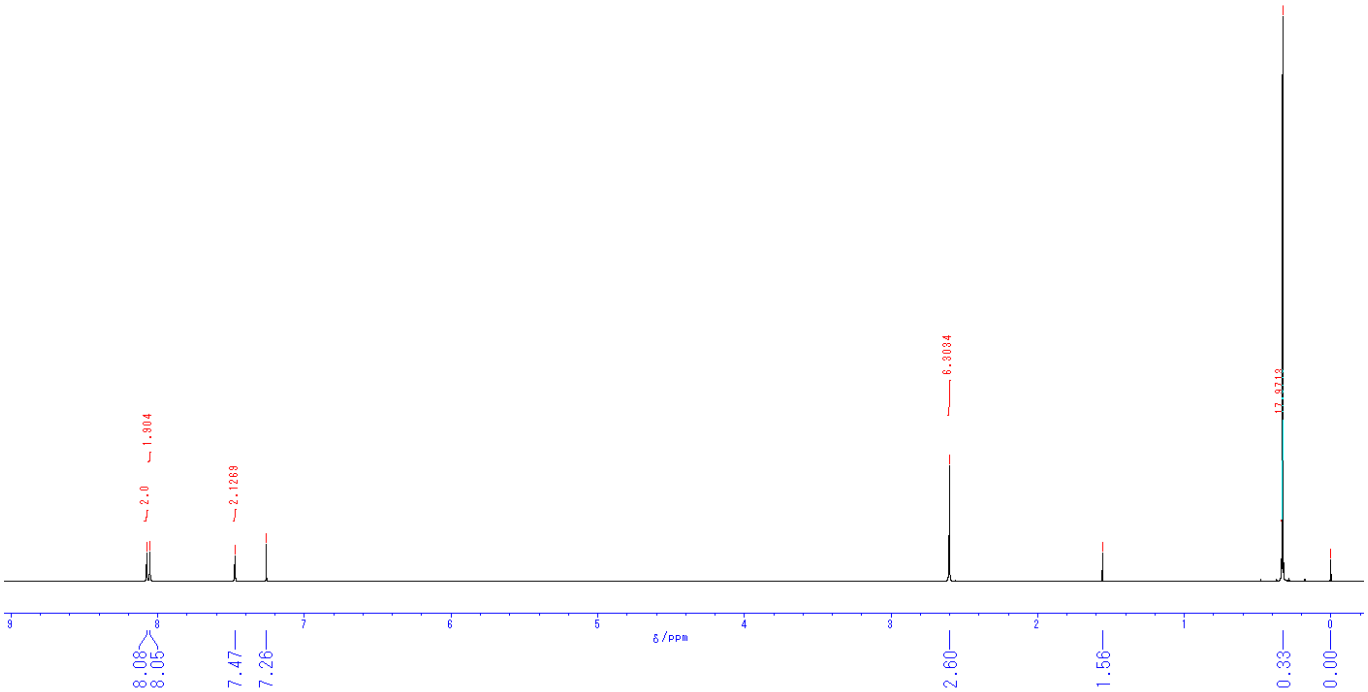


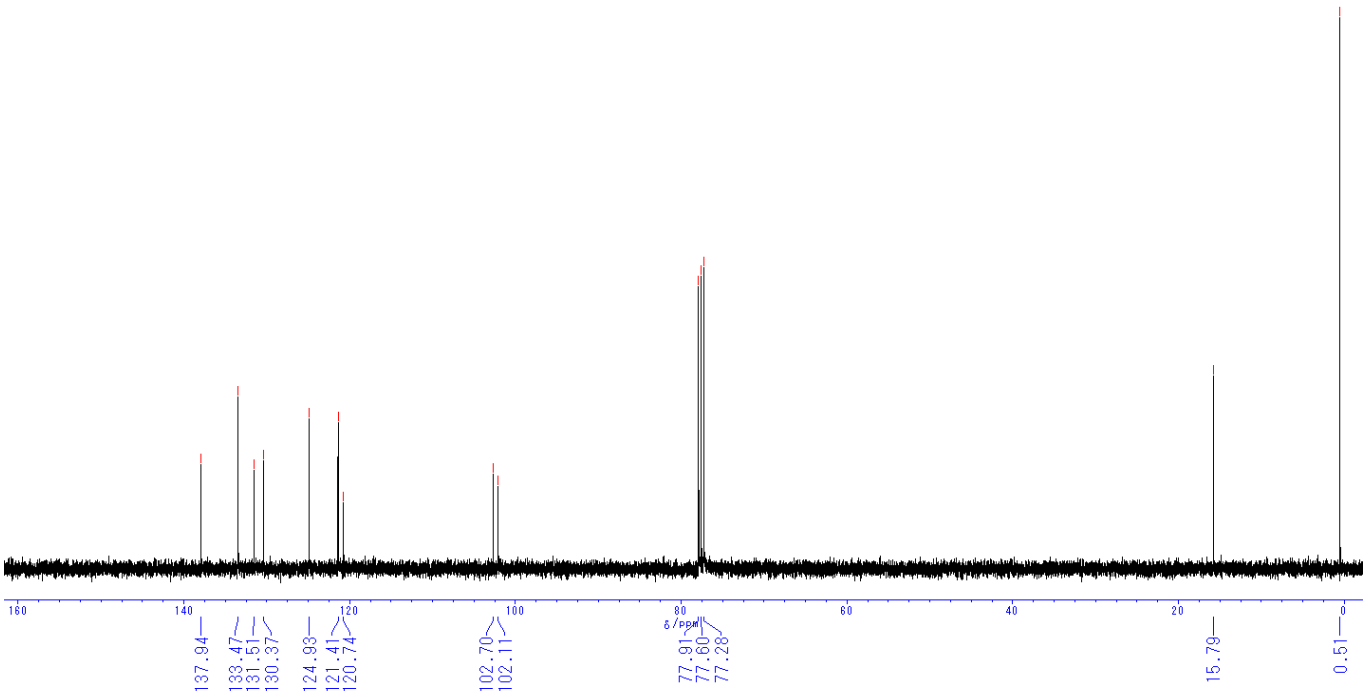

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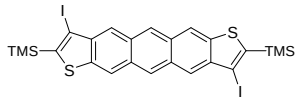


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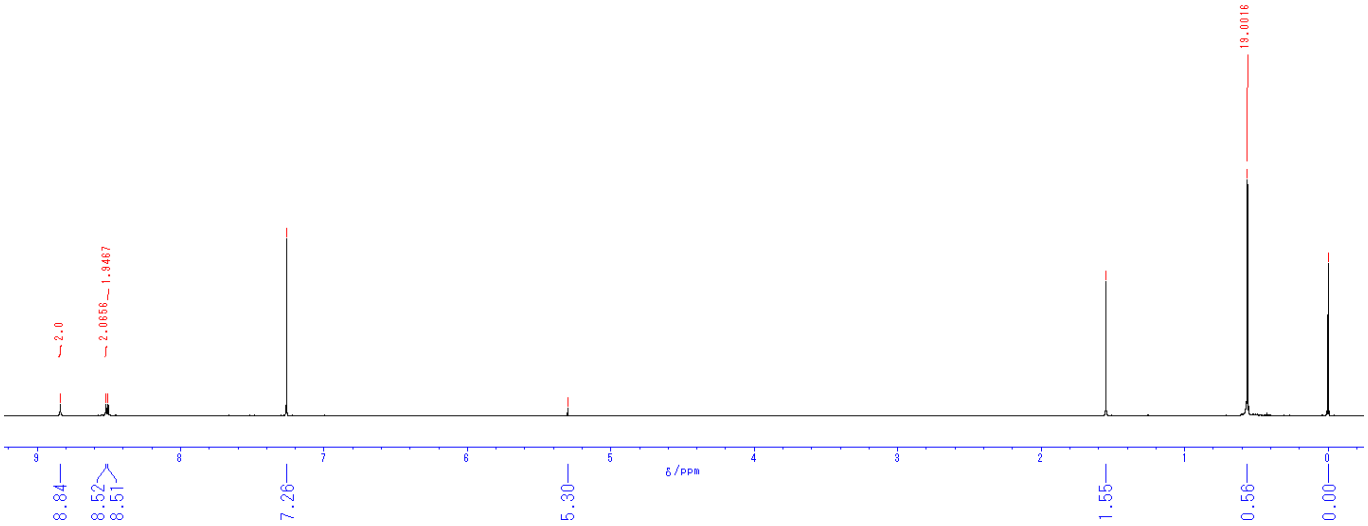
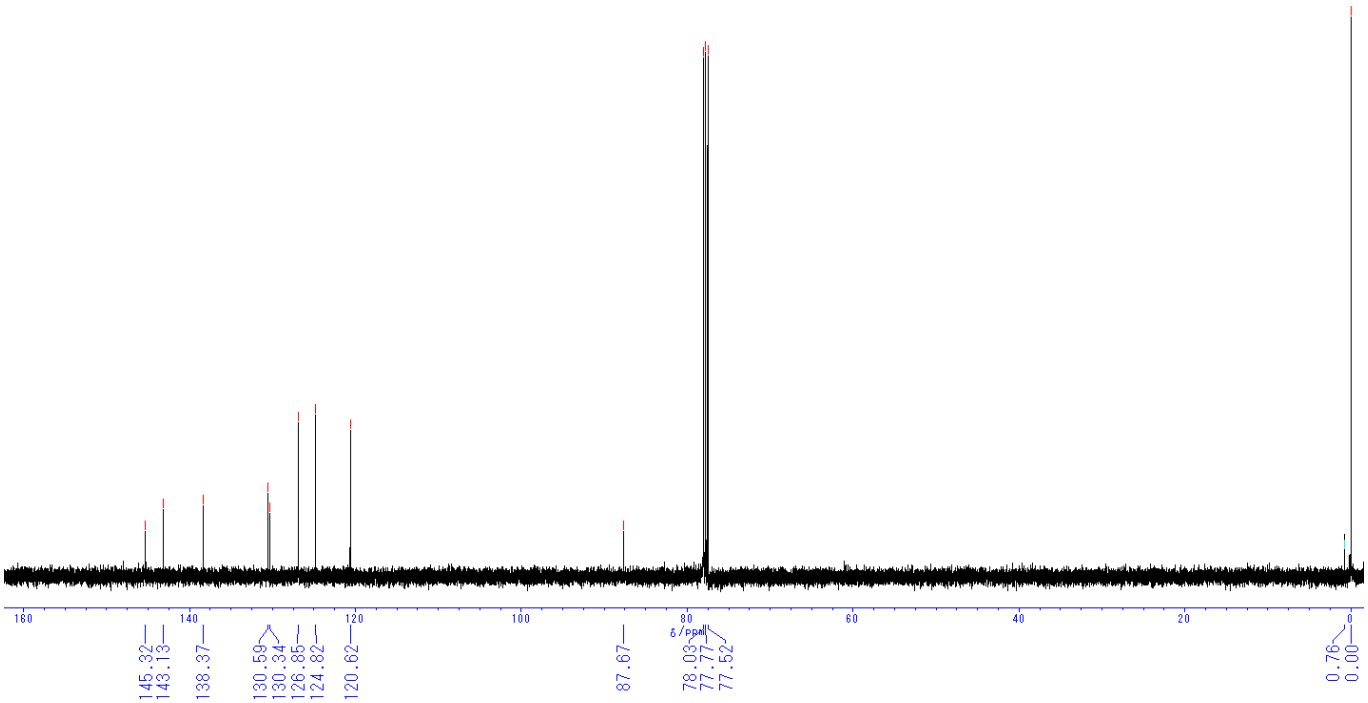
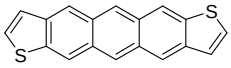


**Anthra[2,3-*b*:6,7-*b'*]dithiophene**

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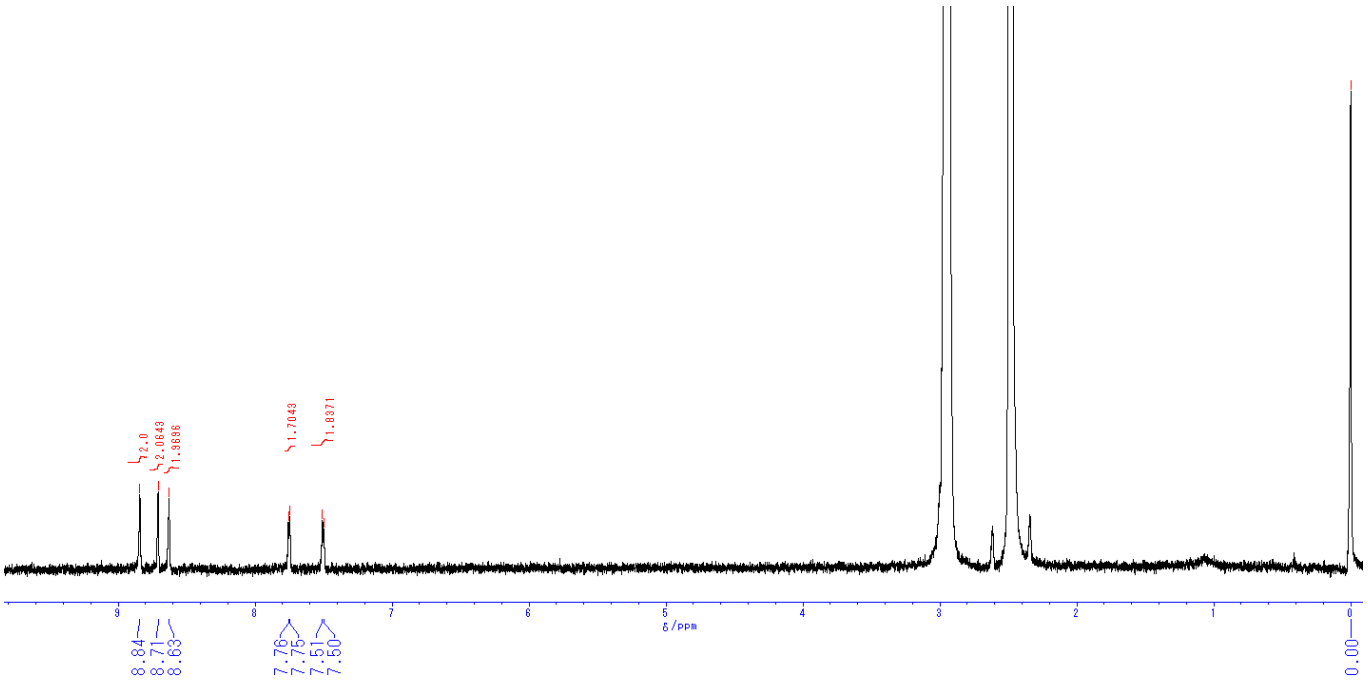


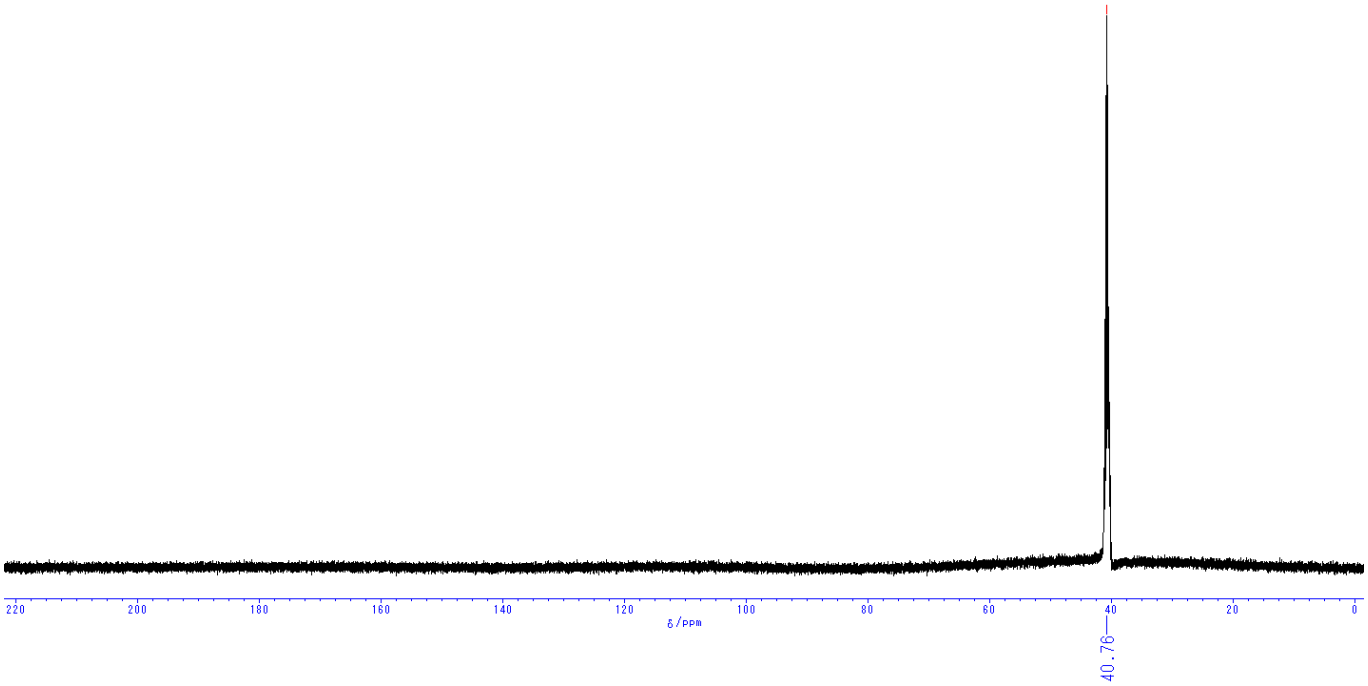

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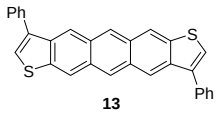


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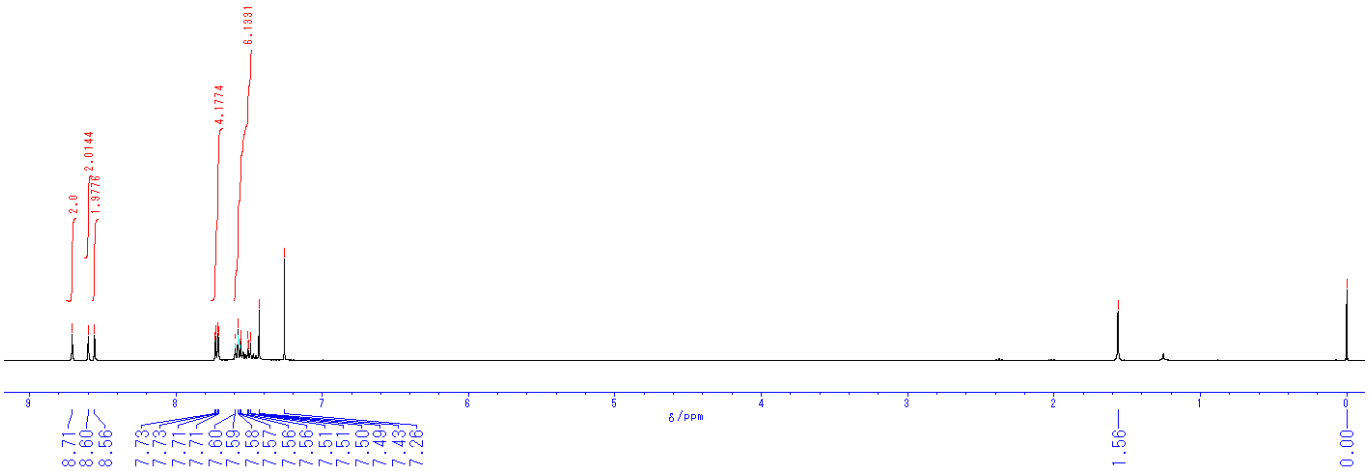
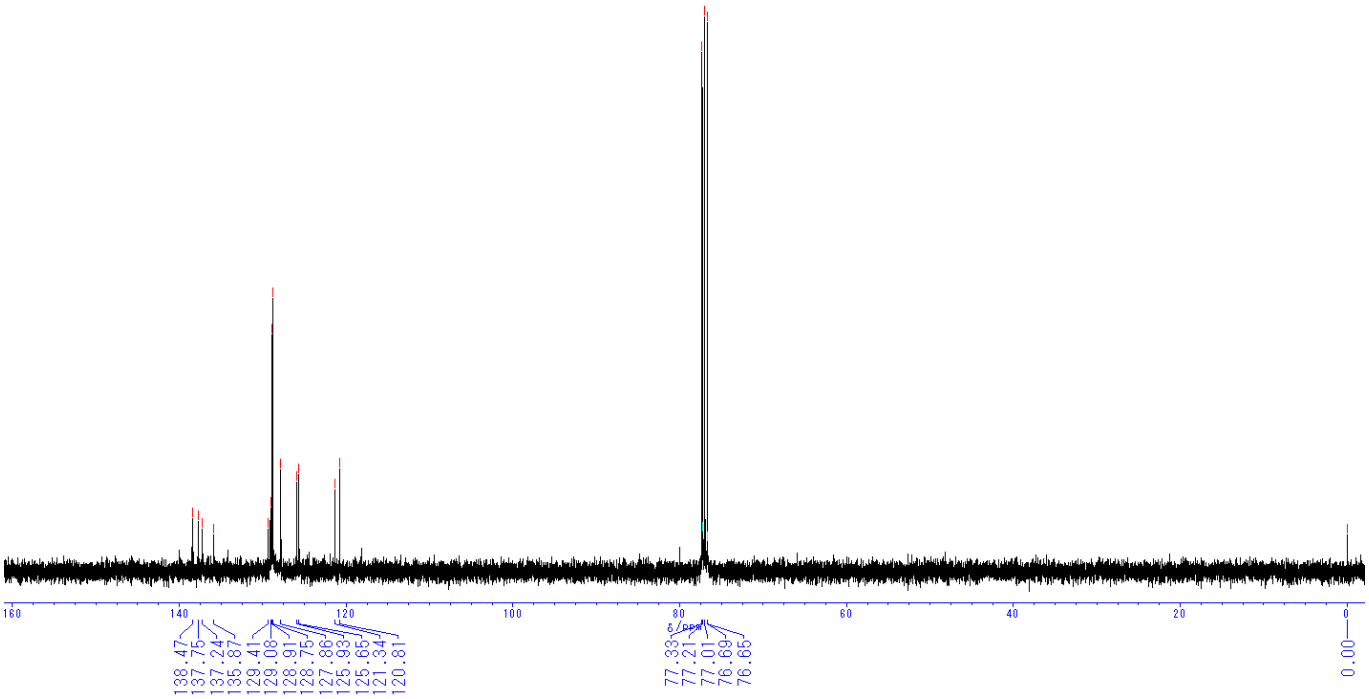
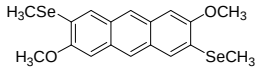


## 2,6-Dimethoxy-3,7-bis(methylseleno)anthracene (14)

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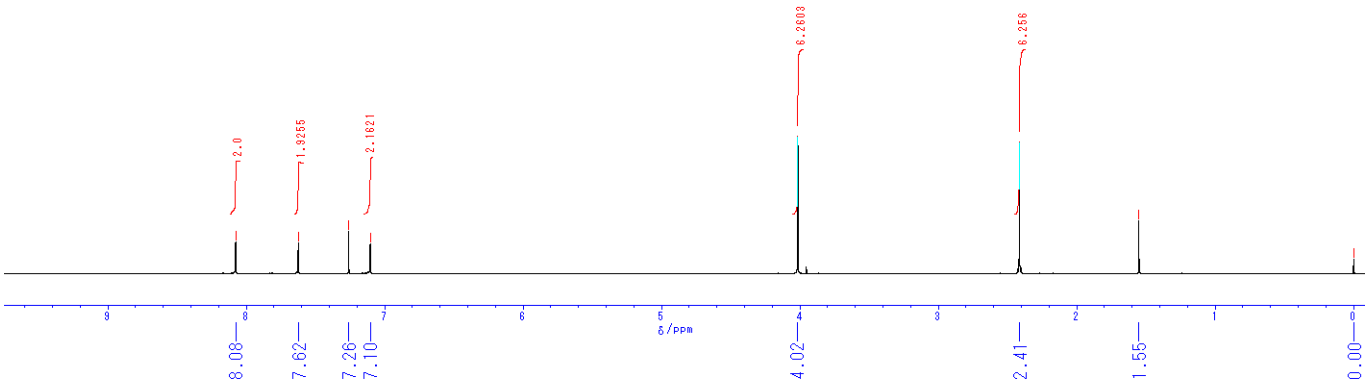
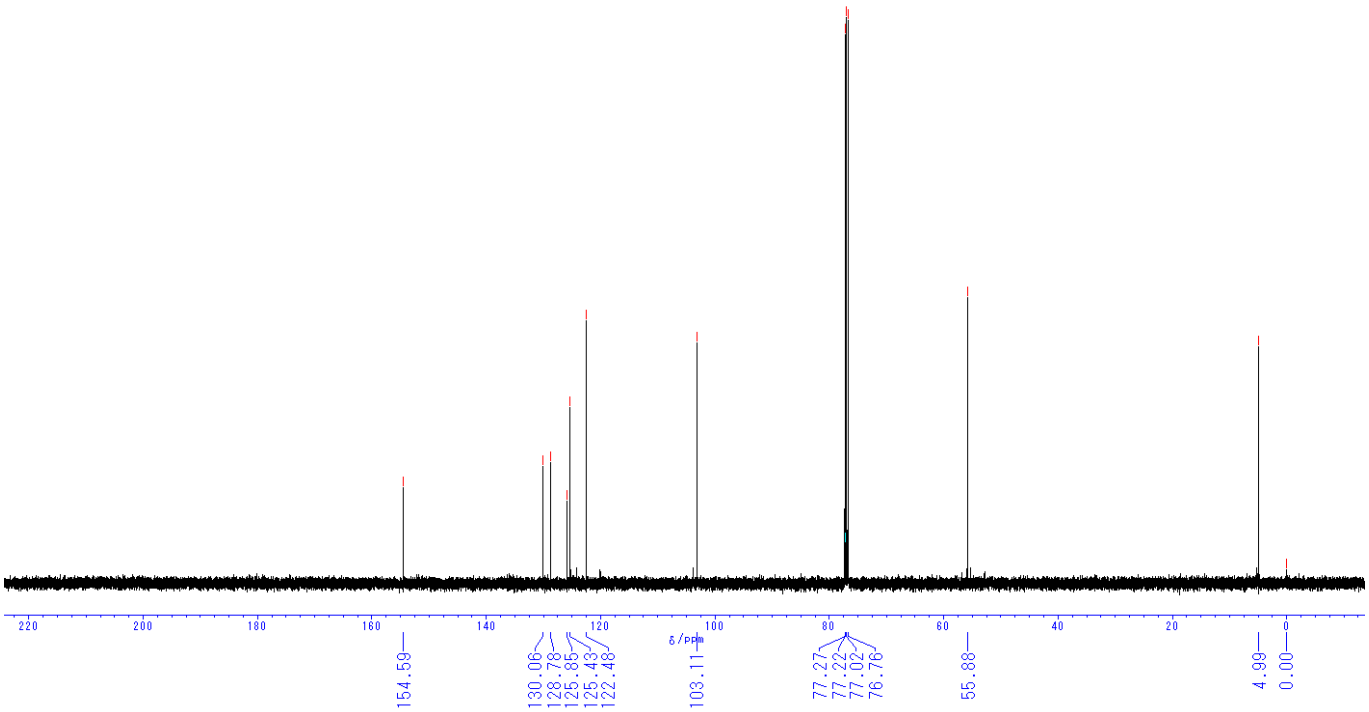
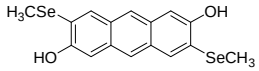
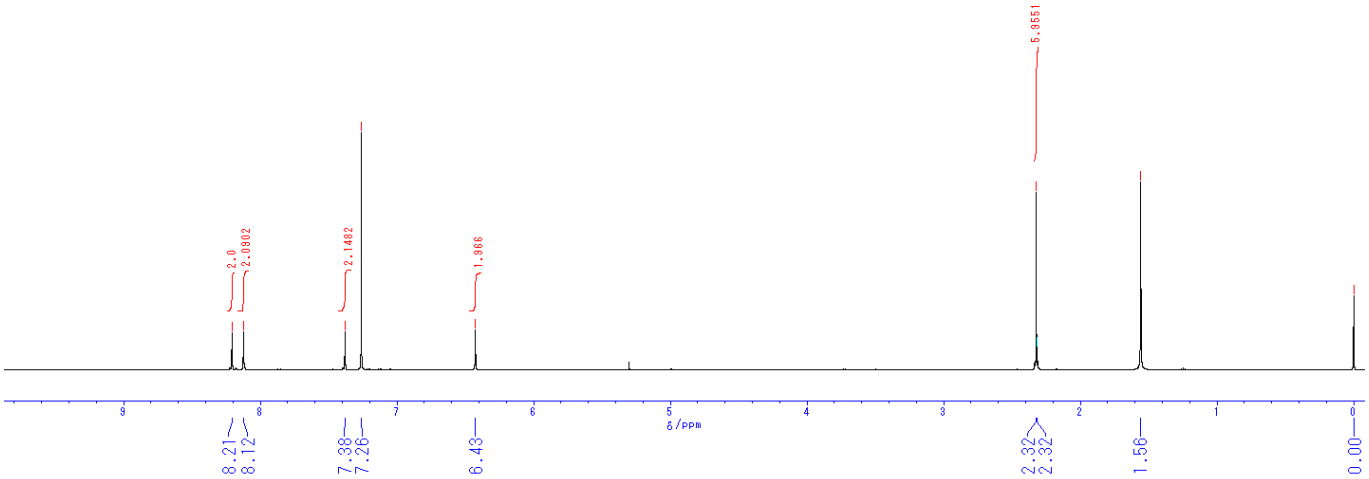


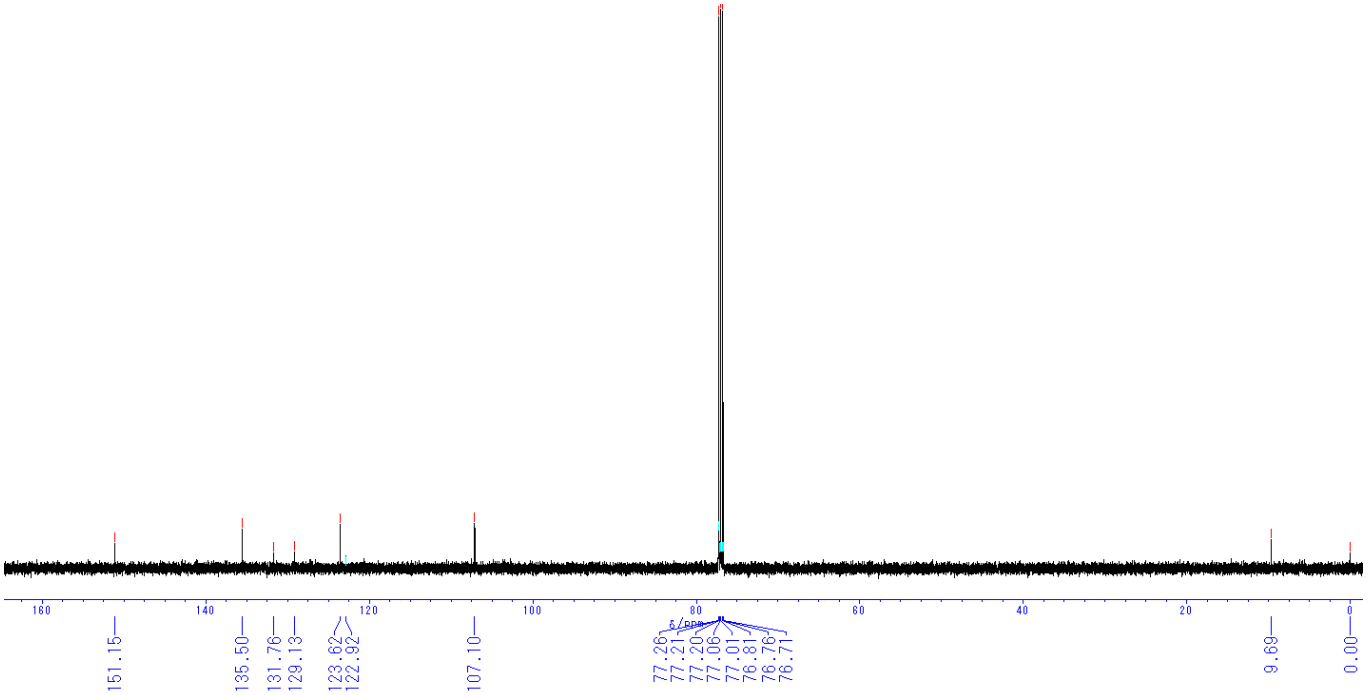



## 2,6-Dihydroxy-3,7-bis(methylseleno)anthracene (15)

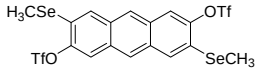



**15**

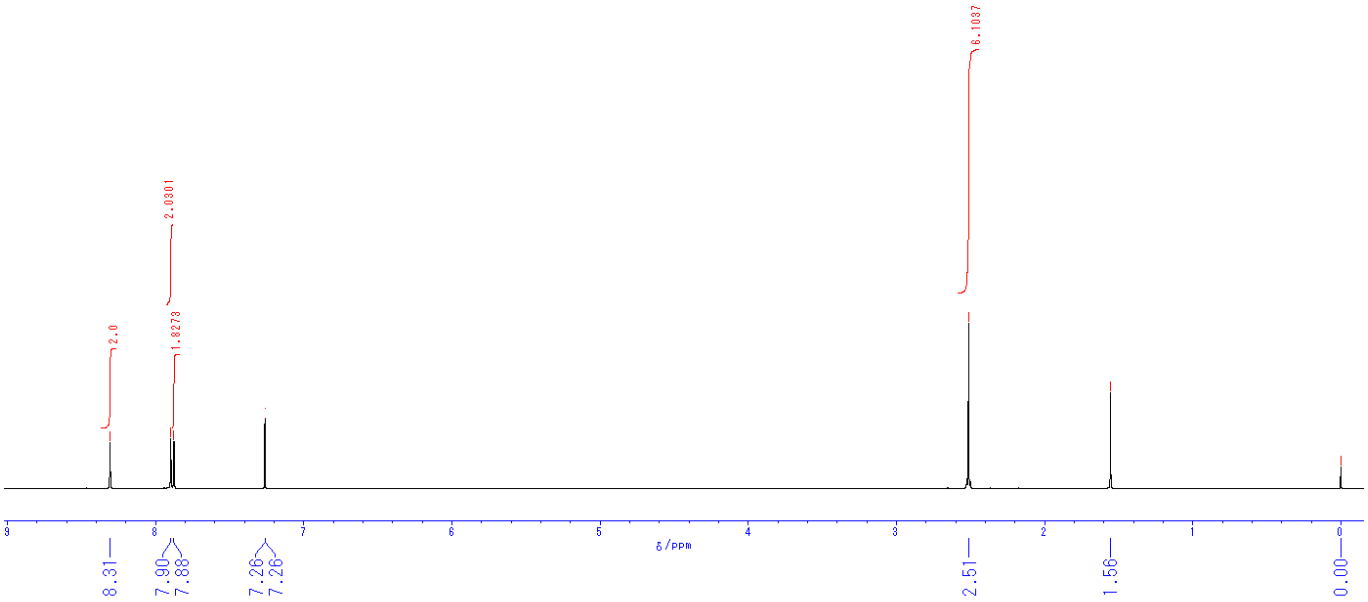


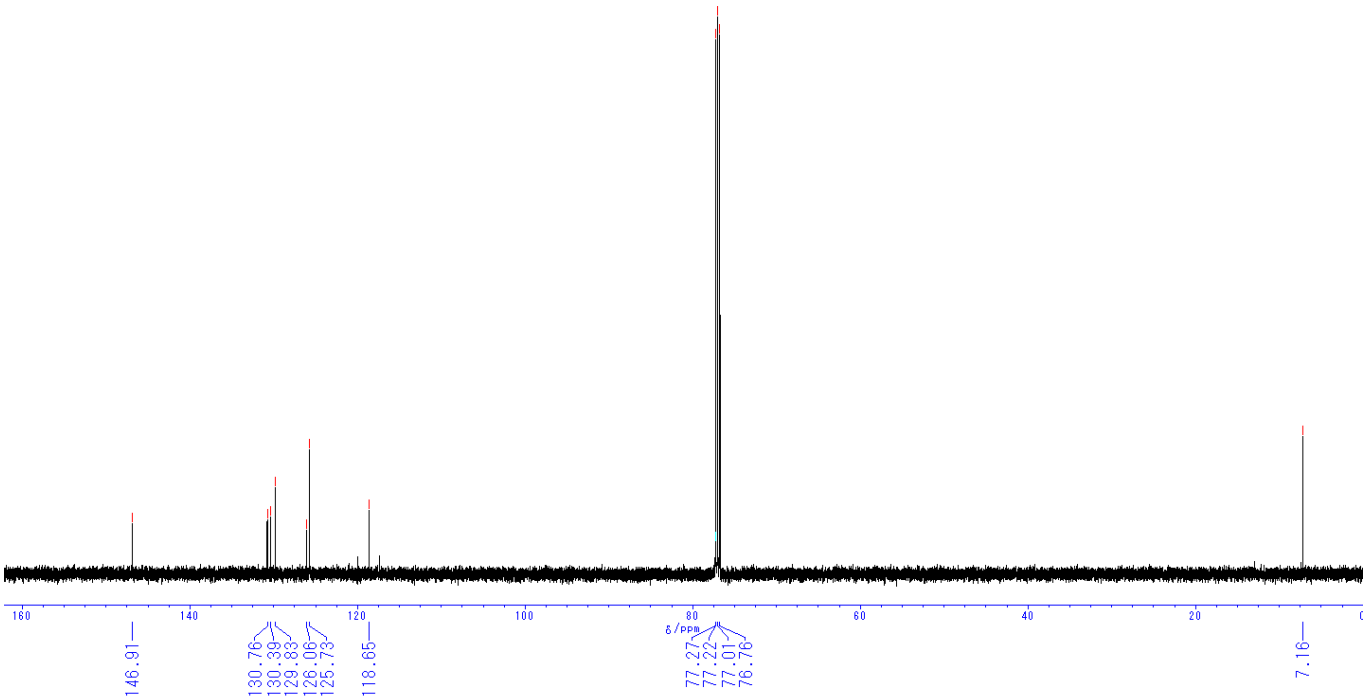



## 2,6-Bis(trifluoromethanesulfonyloxy)-3,7-bis(methylseleno)anthracene (16)

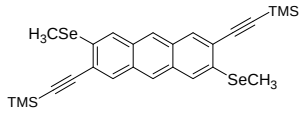



**16**

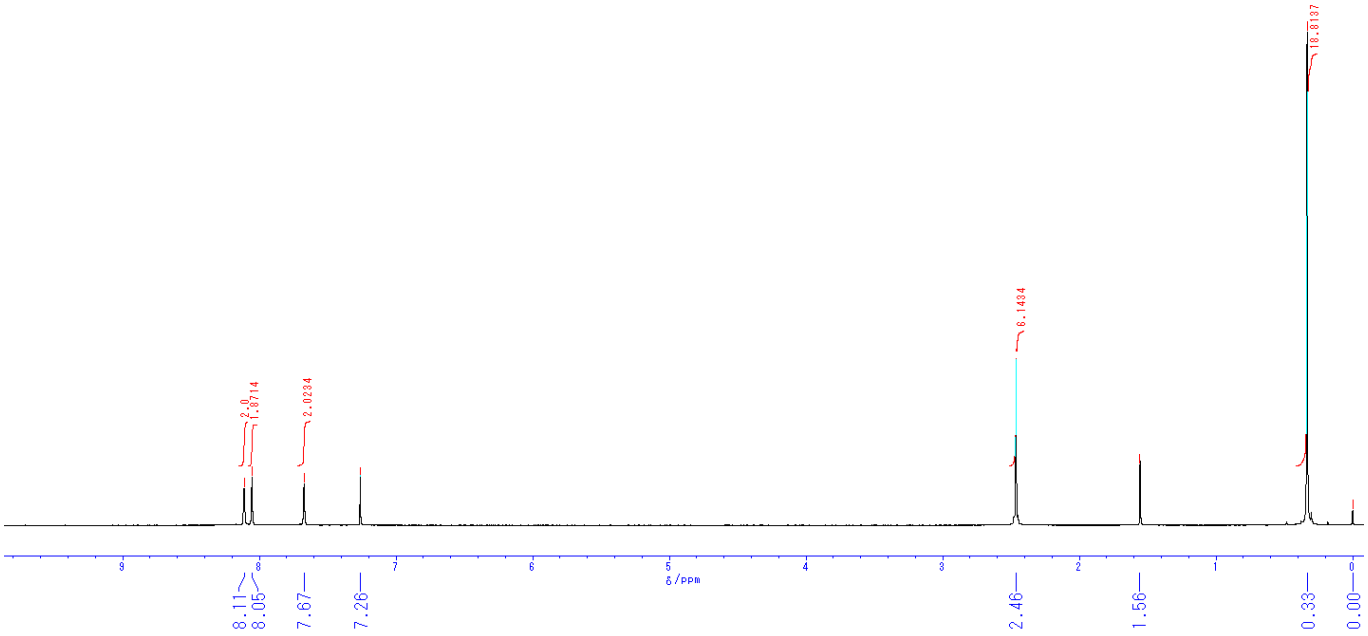


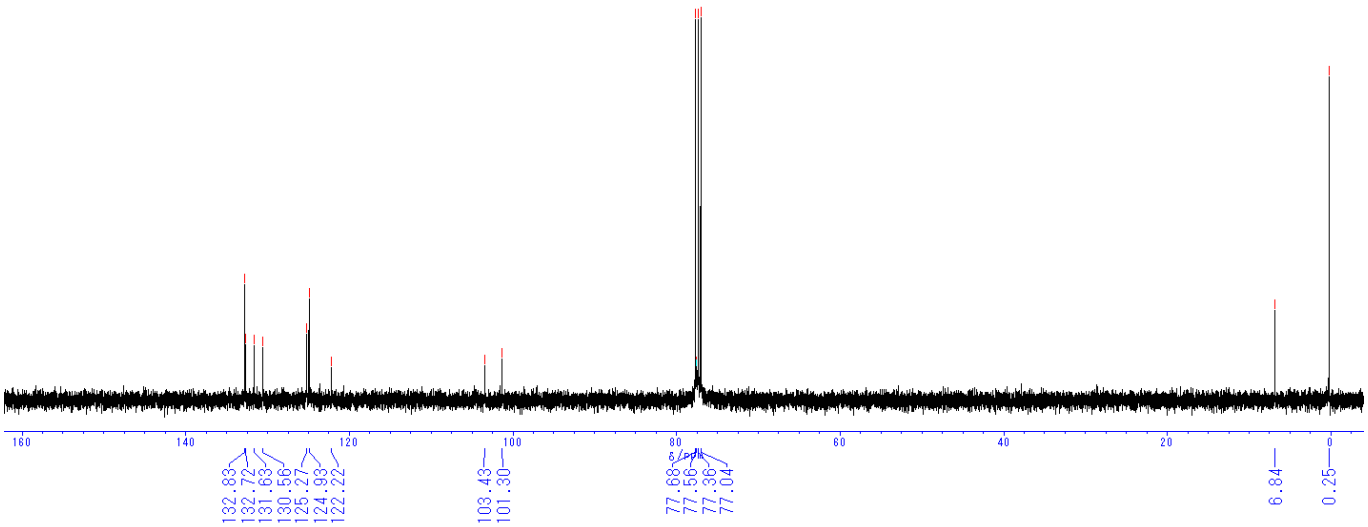



## 2,6-Bis(trimethylsilylethynyl)-3,7-bis(methylseleno)anthracene (17)

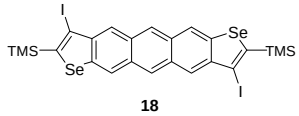



**17**

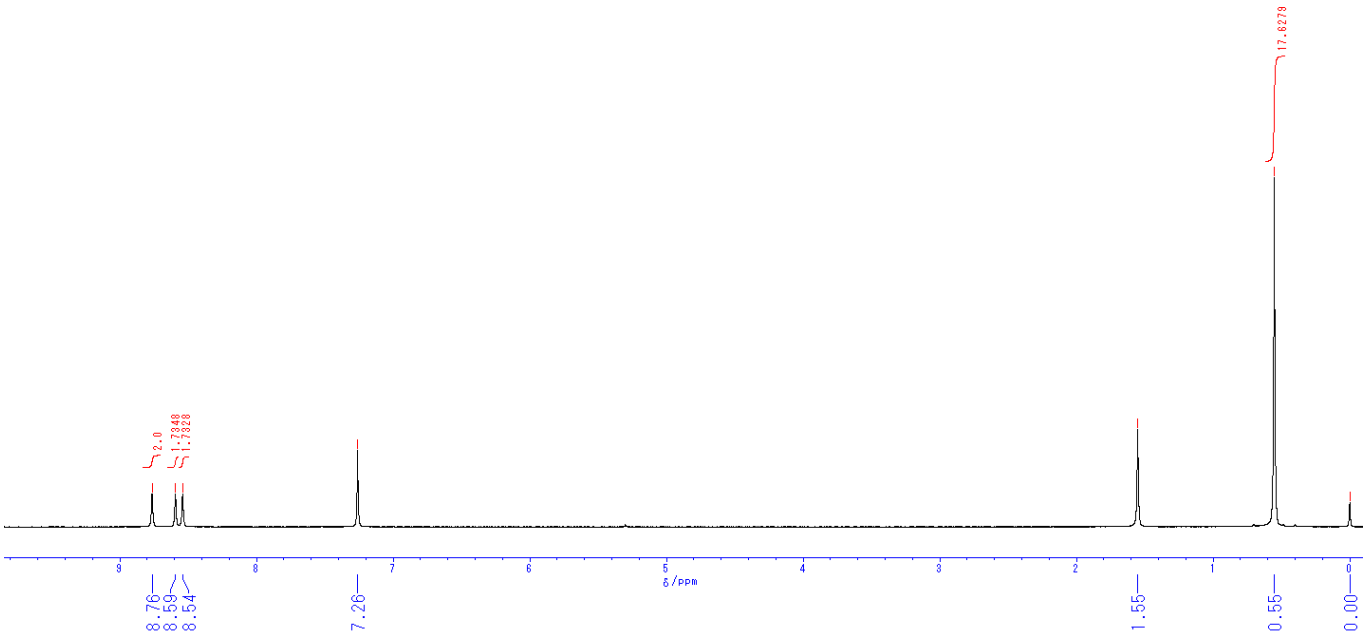


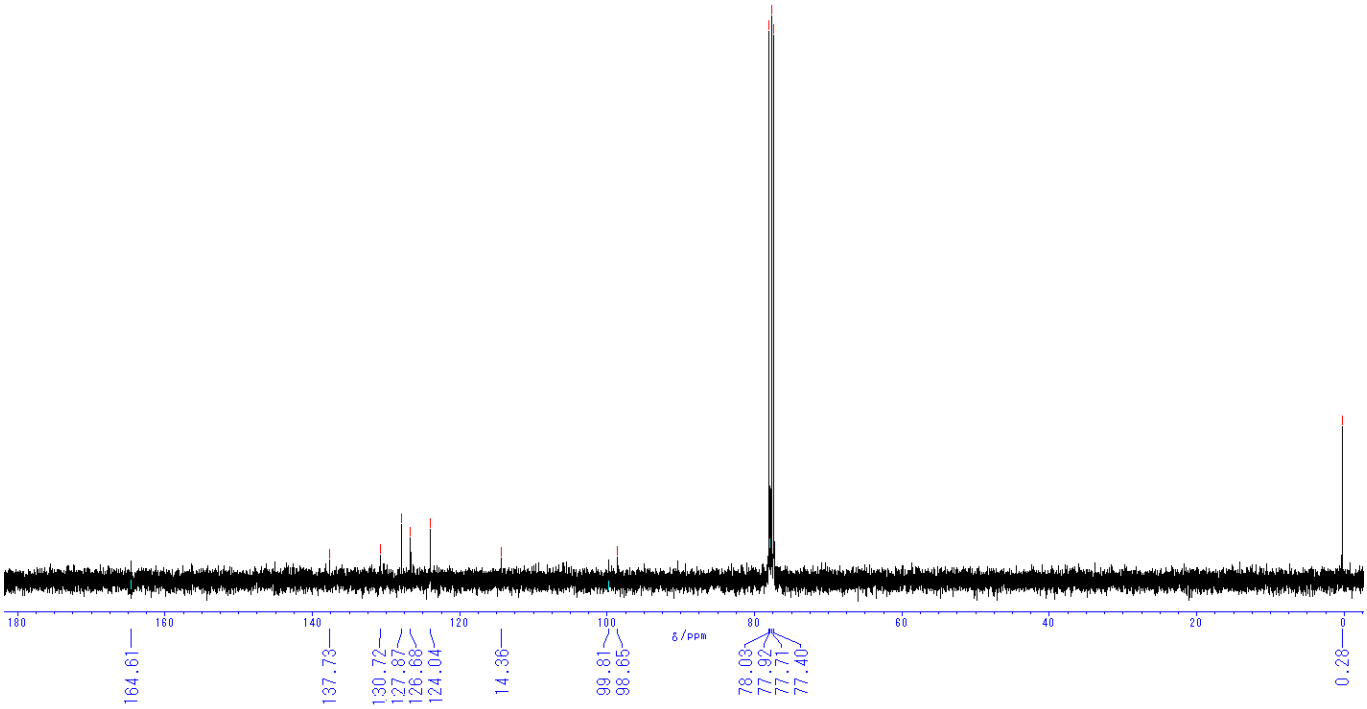



**3,9-Diiodo-2,8-bis(trimethylsilyl)anthra[2,3-*b*:6,7-*b*']diselenophene (18)**

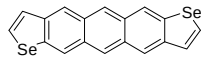


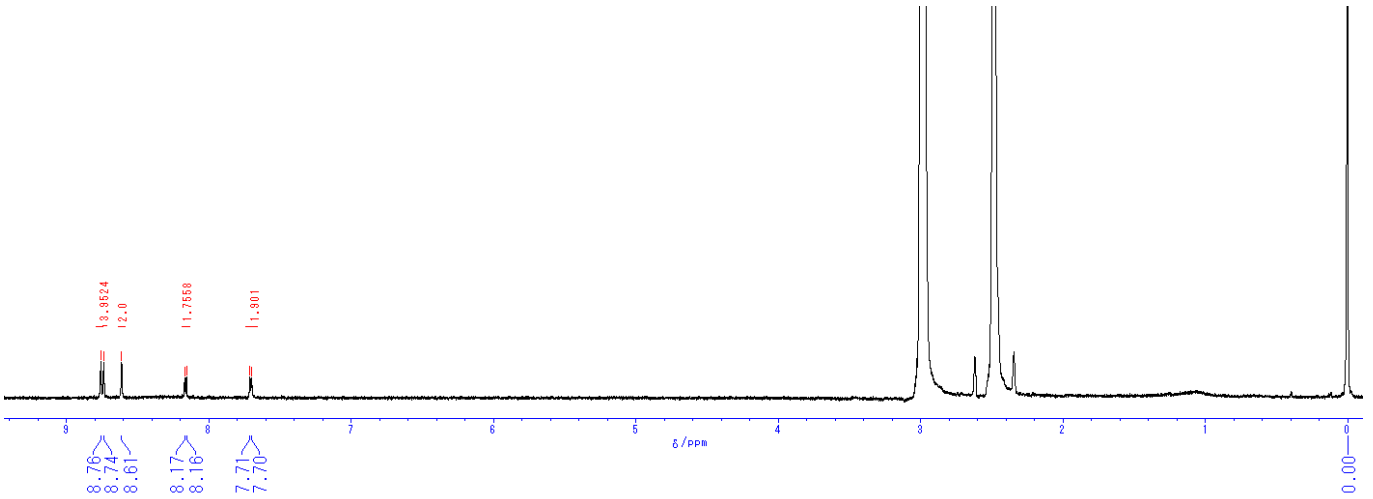

**18**

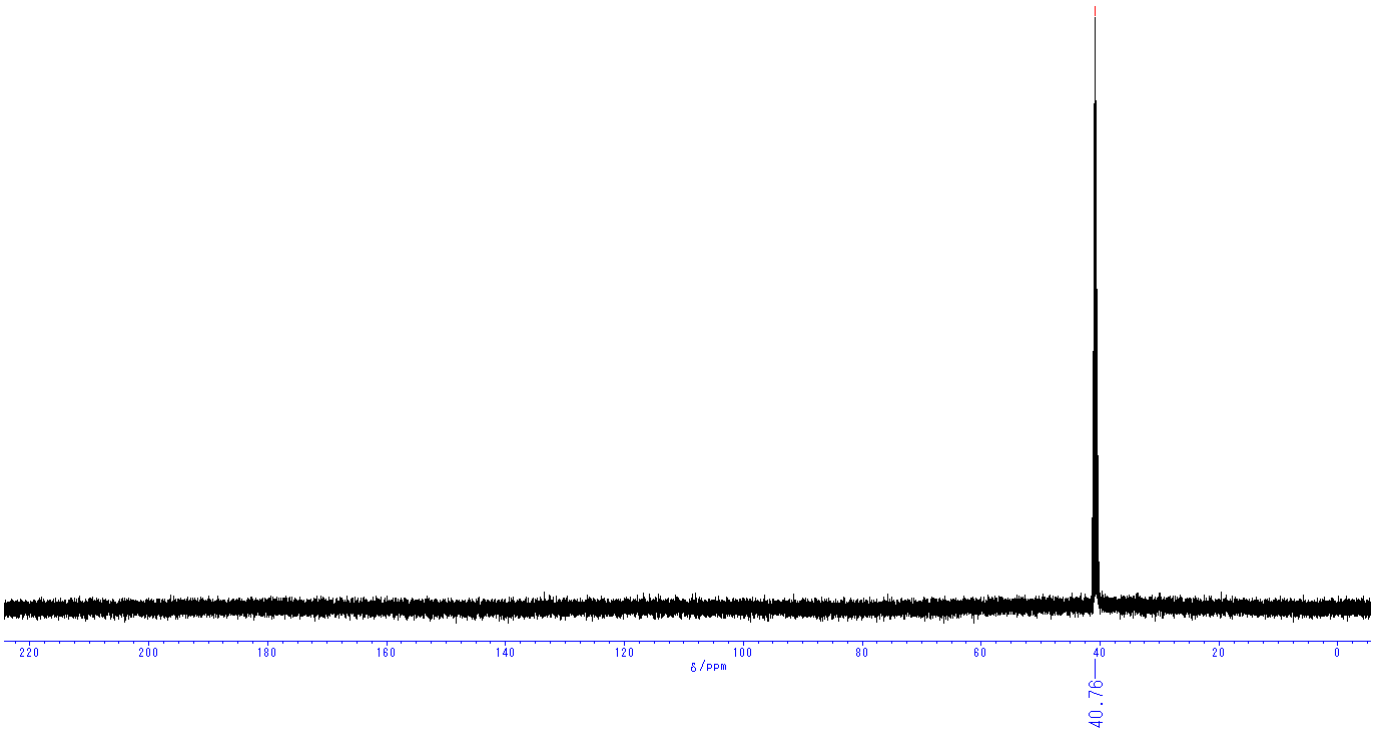


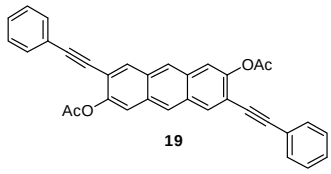
**Anthra[2,3-*b*:6,7-*b'*]diselenophene**



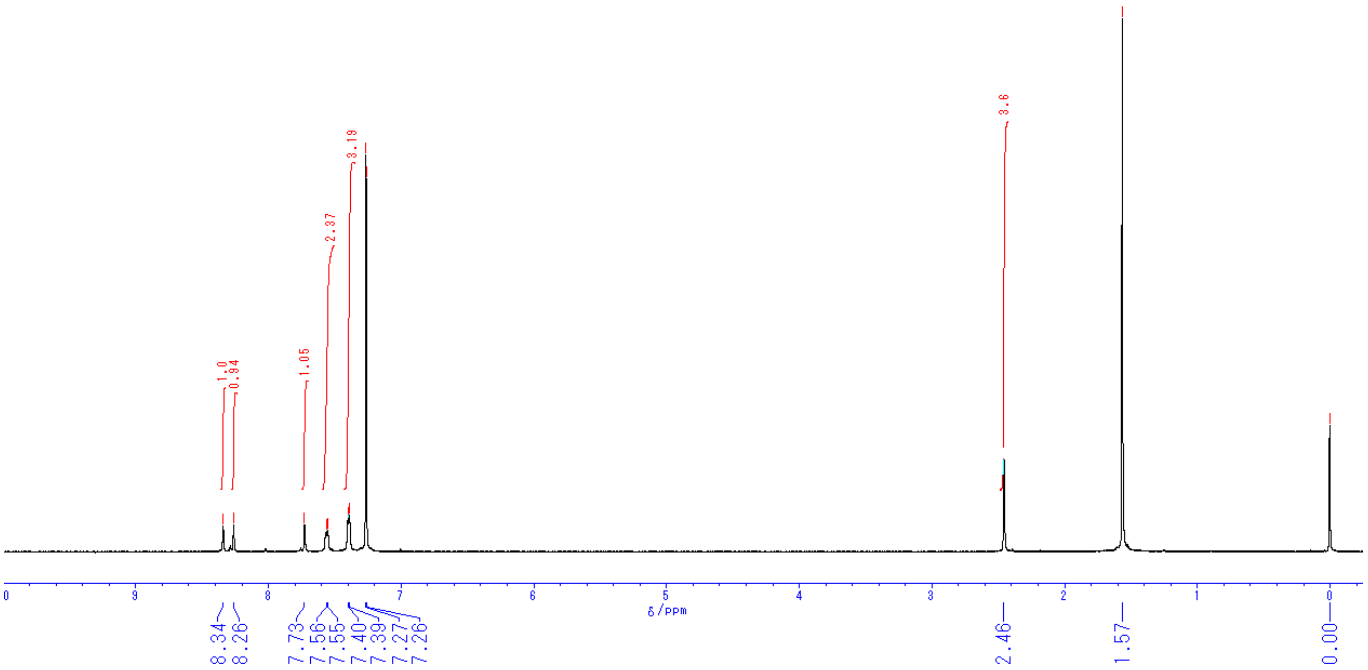



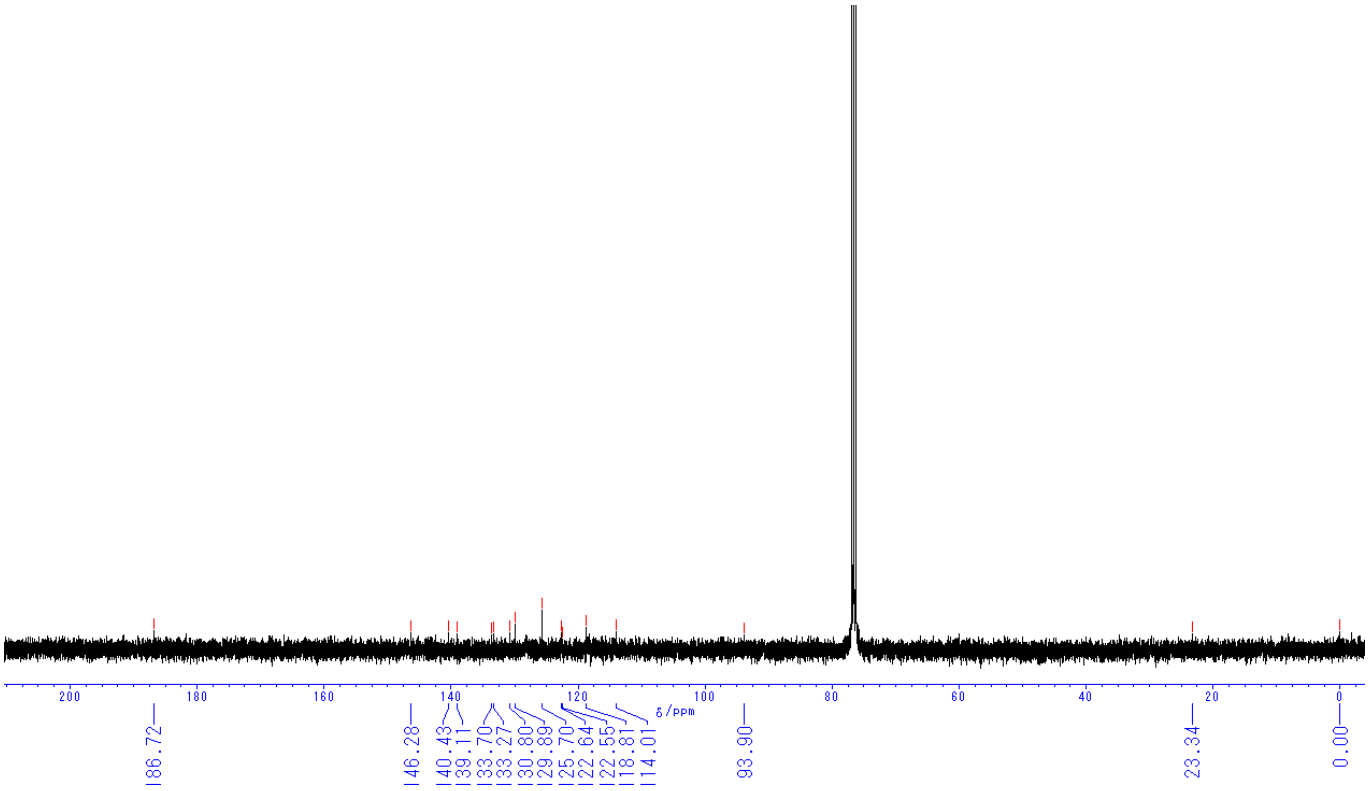



**2,6-Diacetoxy-3,7-bis(phenylethynyl)anthracene (19)**

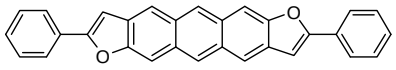



**19**

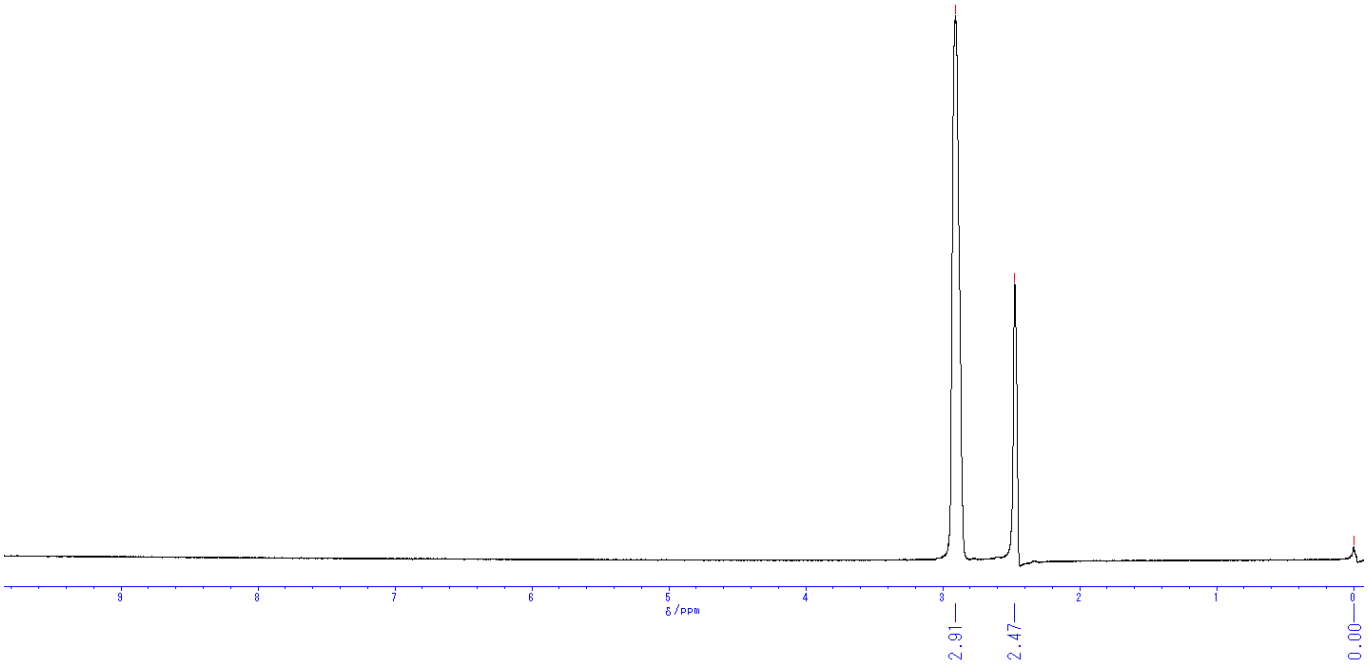


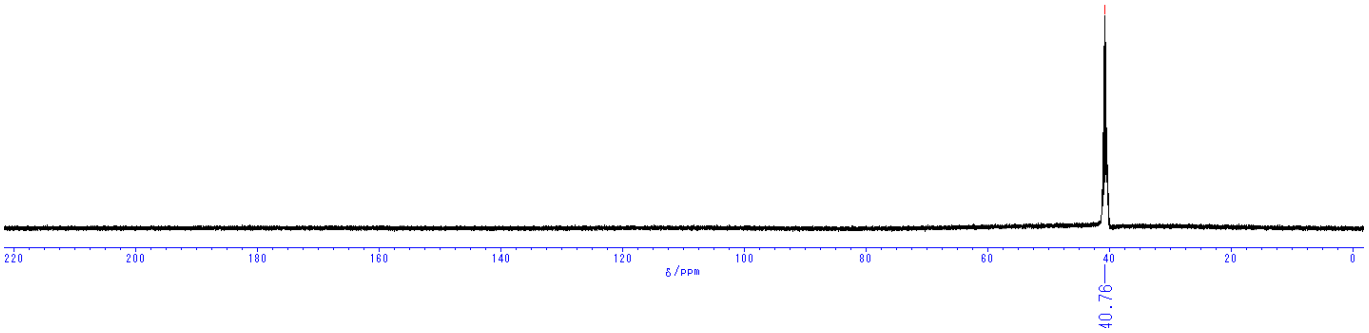



**2,8-Diphenylanthra[2,3-*b*:6,7-*b*']difuran**

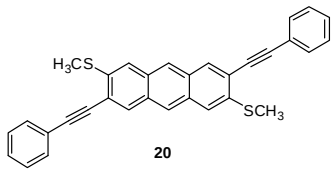


DPh-ADF

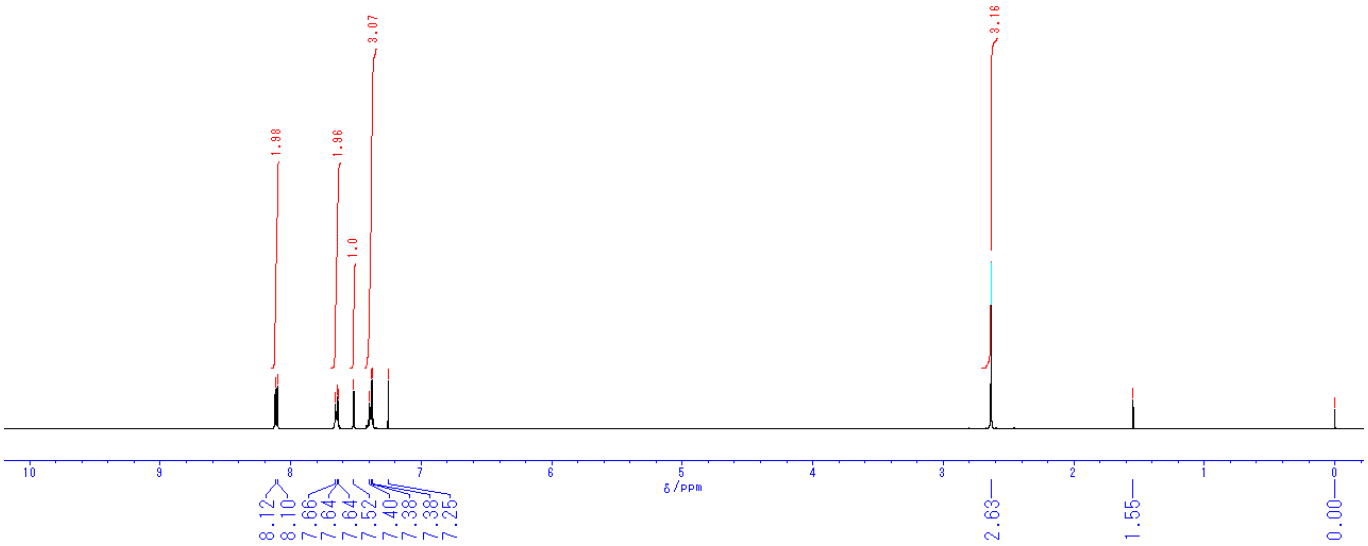


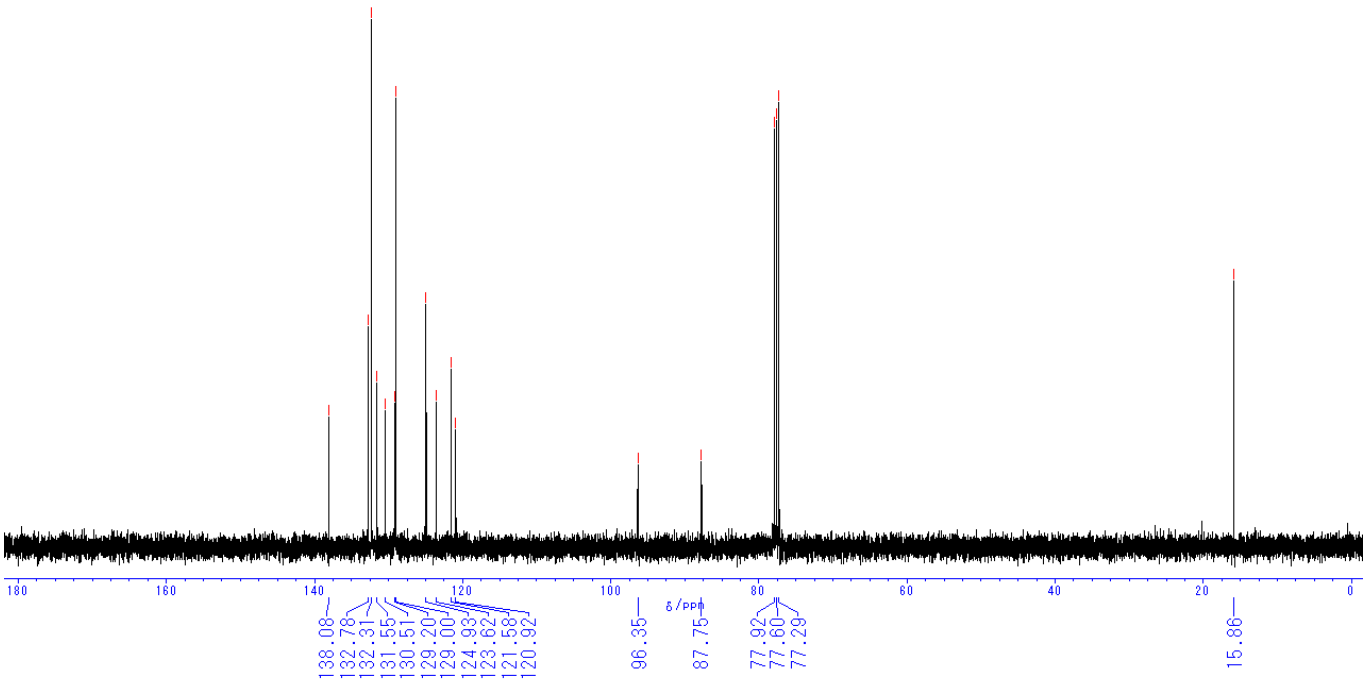



**2,6-Bis(phenylethynyl)-3,7-bis(methylthio)anthracene (20)**

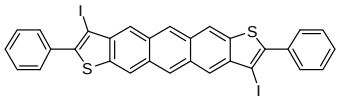



**20**

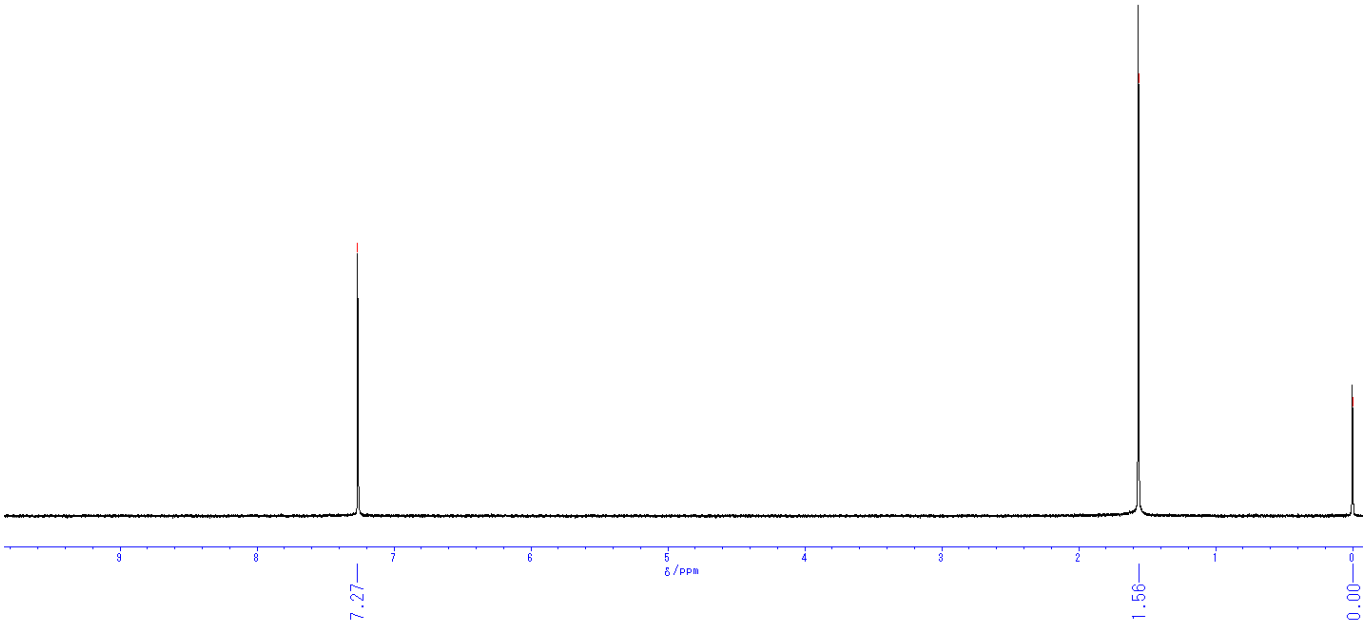


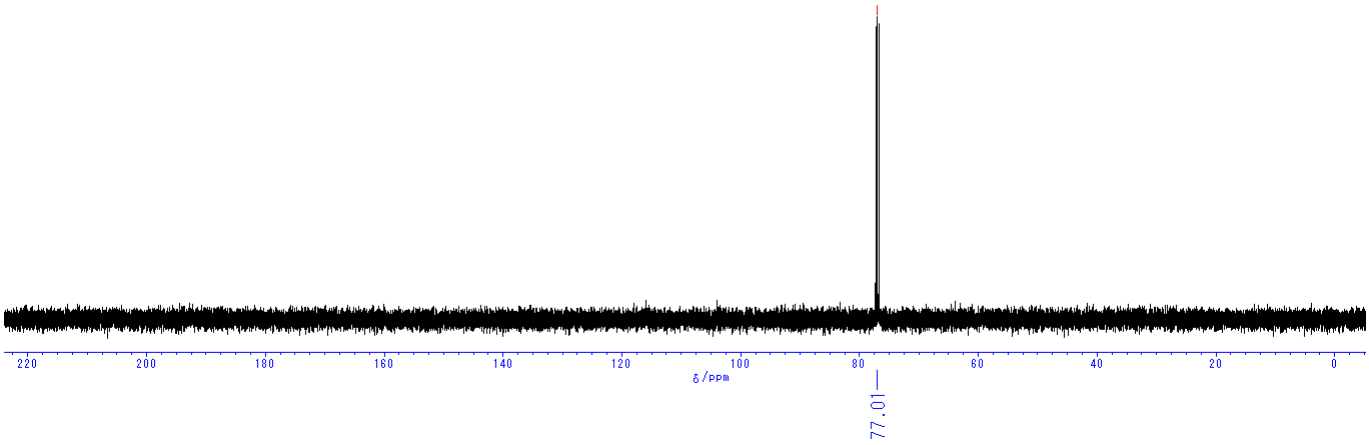



**3,9-Diiodo-2,8-diphenylanthra[2,3-*b*:6,7-*b'*]dithiophene (21)**

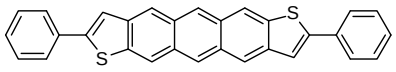



**21**

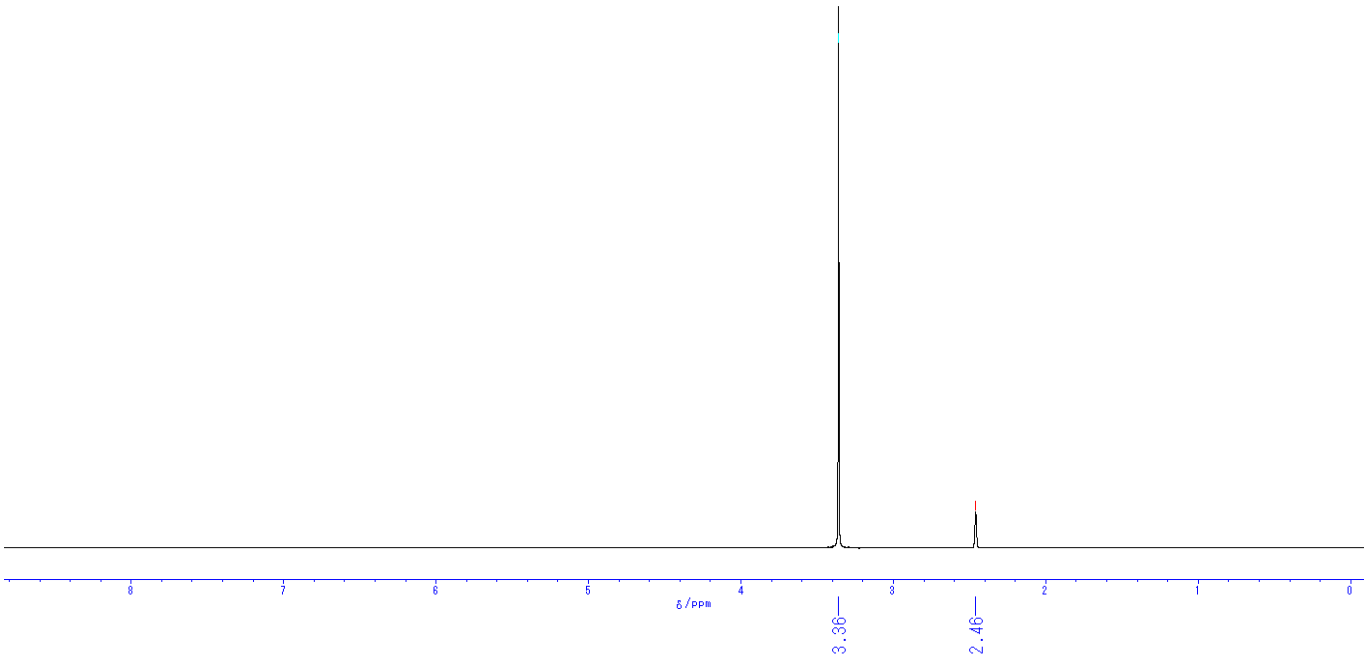


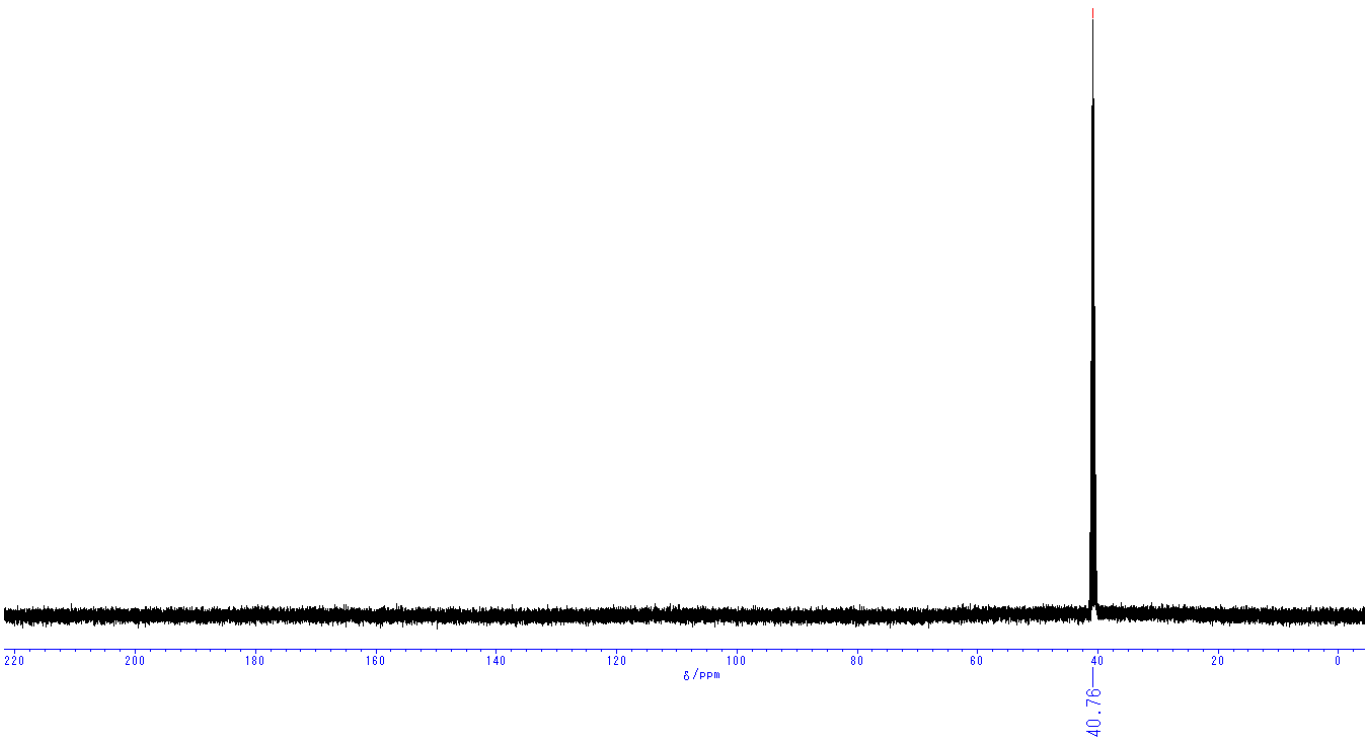



**2,8-DiphenylAnthra[2,3-*b*:6,7-*b'*]dithiophene**

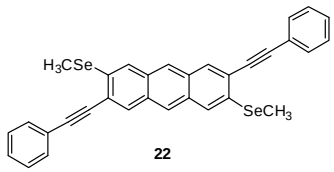



DPh-ADT

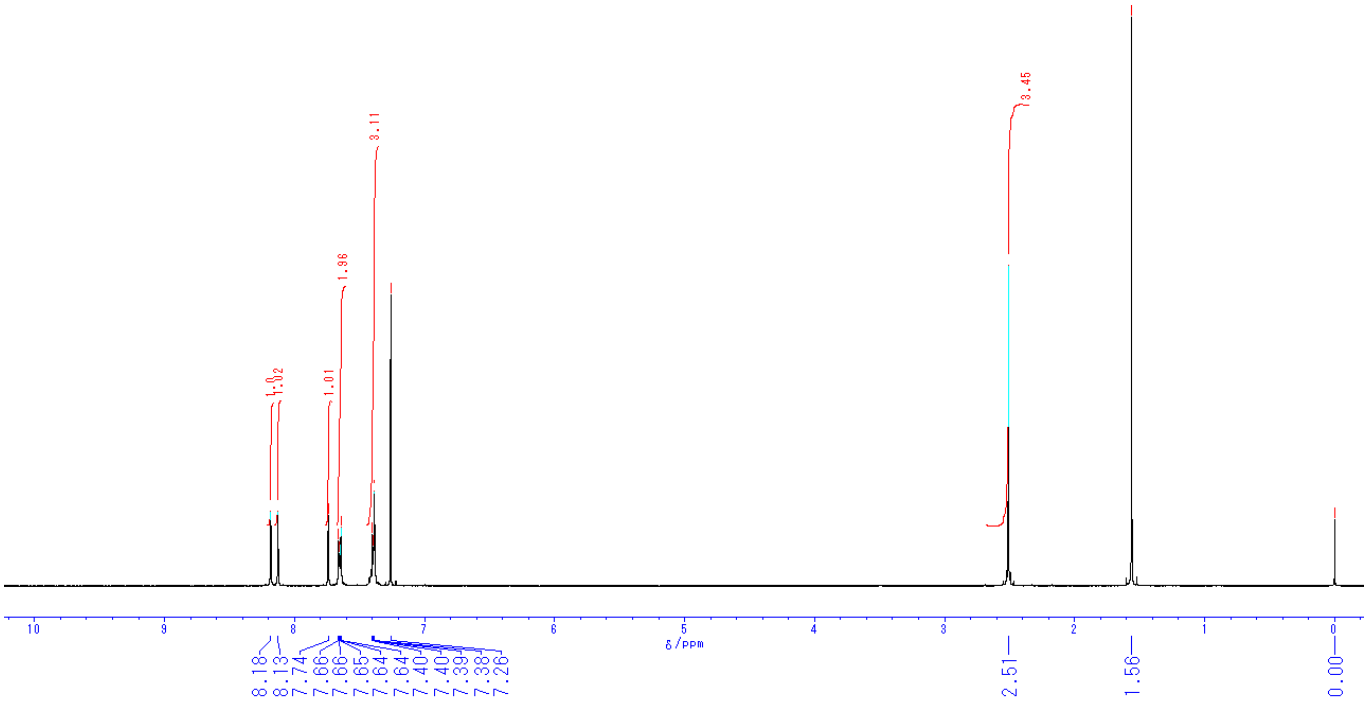


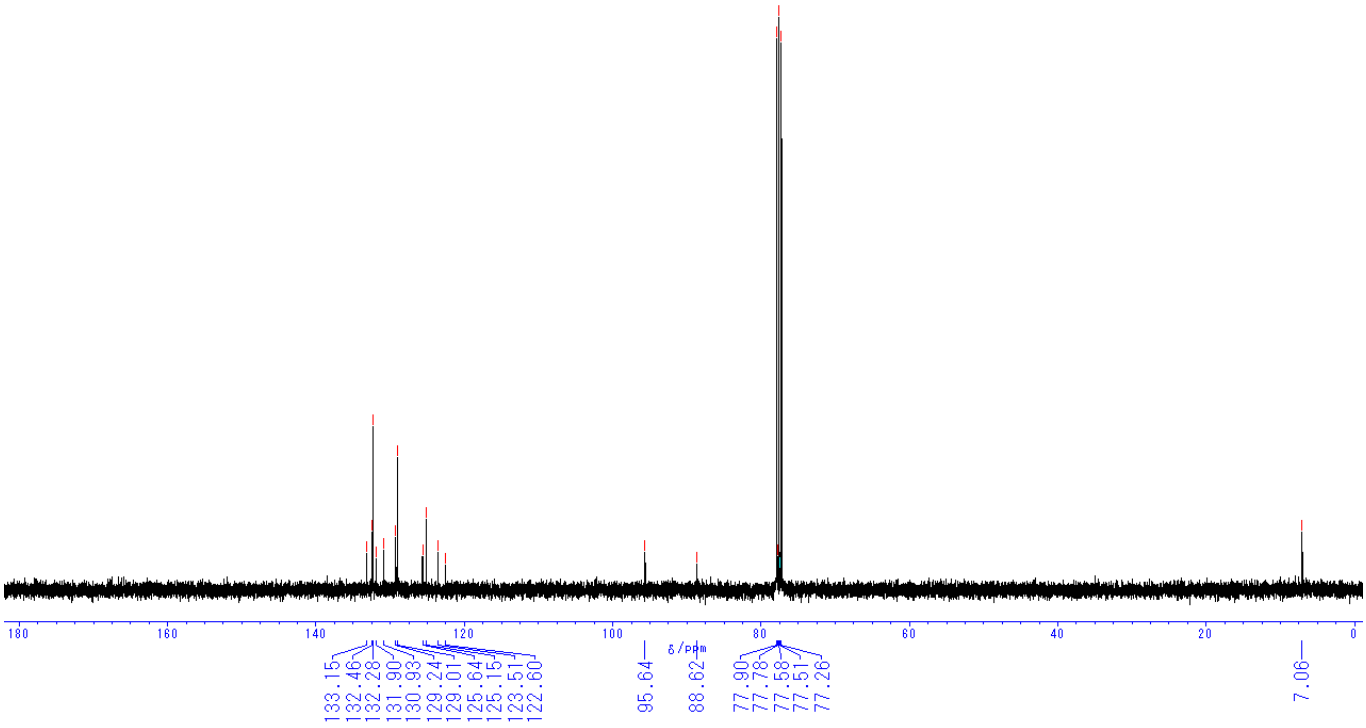



**2,6-Bis(phenylethynyl)-3,7-bis(methylseleno)anthracene (22)**

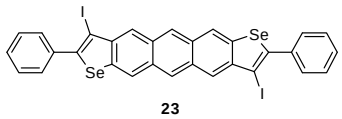



22

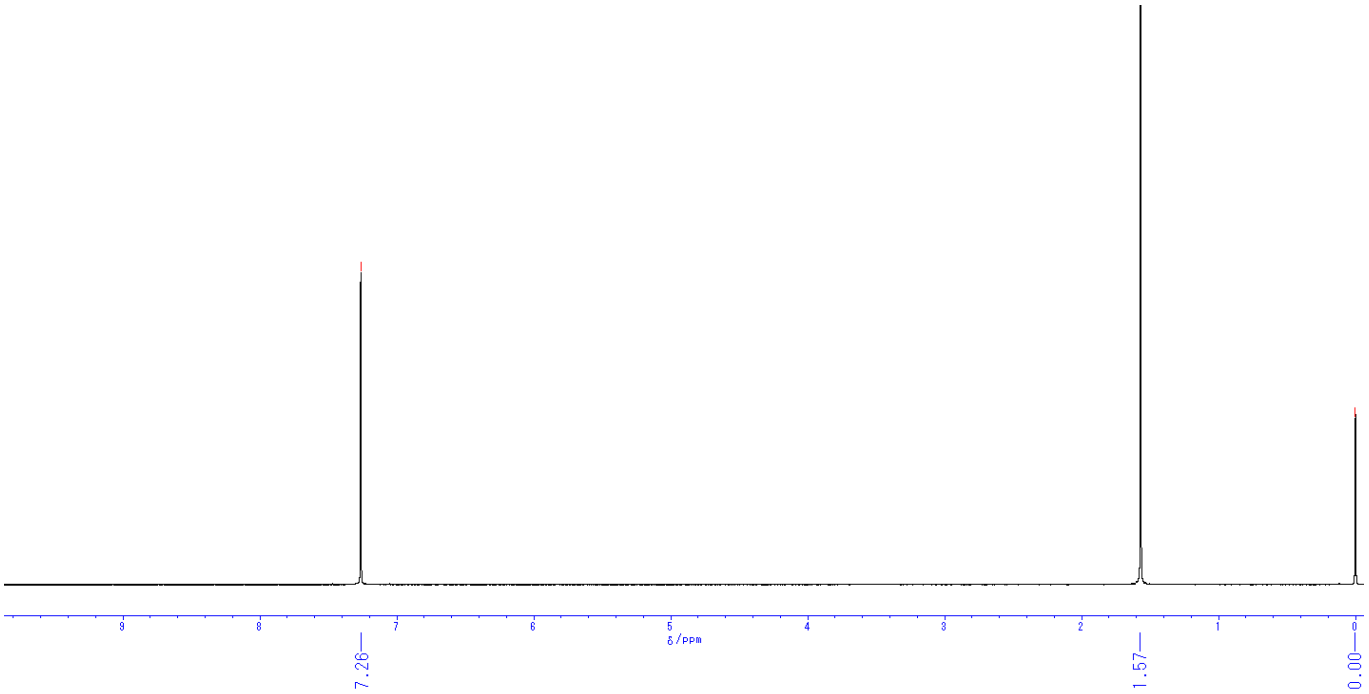


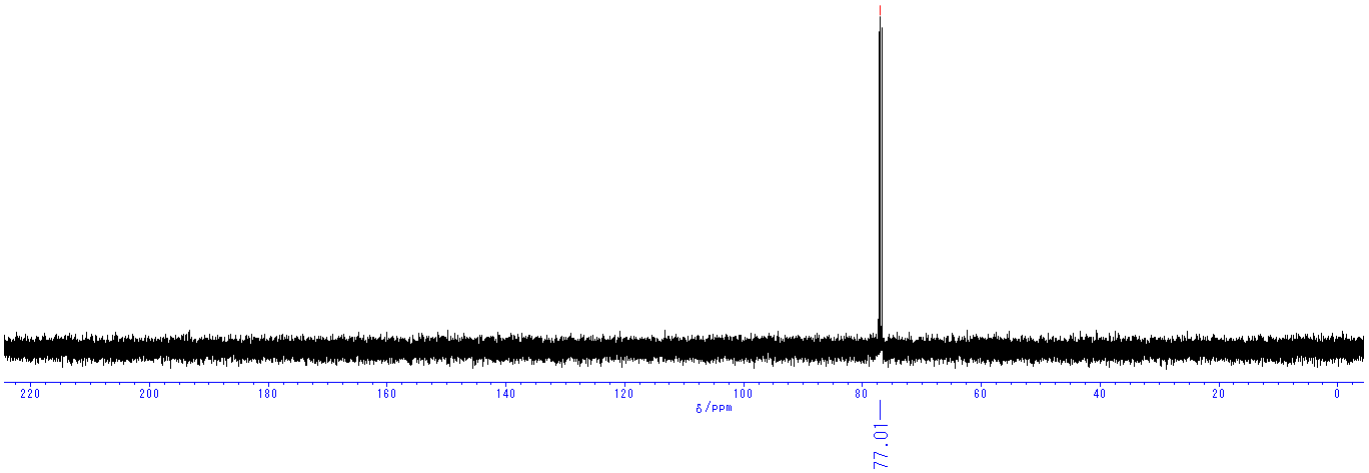



**3,9-Diiodo-2,8-diphenylanthra[2,3-*b*:6,7-*b'*]diselenophene (23)**

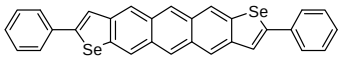



**23**



**2,8-Diphenylanthra[2,3-*b*:6,7-*b'*]diselenophene (DPh-ADS)**




DPh-ADS