# Electronic Supplementary Information

## Dialkoxybenzo[j]fluoranthenes: synthesis, structures, photophysical properties, and optical waveguide application

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## Contents

## I. $^{1}$H NMR and $^{13}$C NMR spectra of new compounds

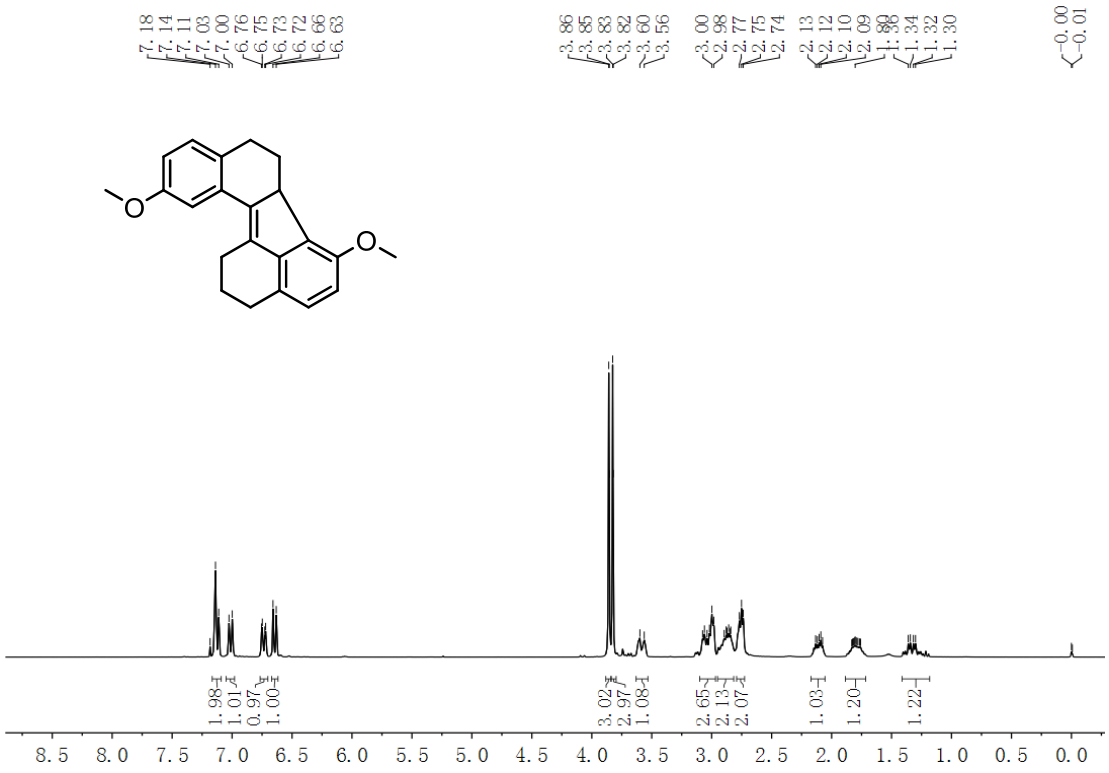


**Fig. S1** $^{1}$H NMR spectrum (400 MHz, $CDCl_3$) of **3a**.

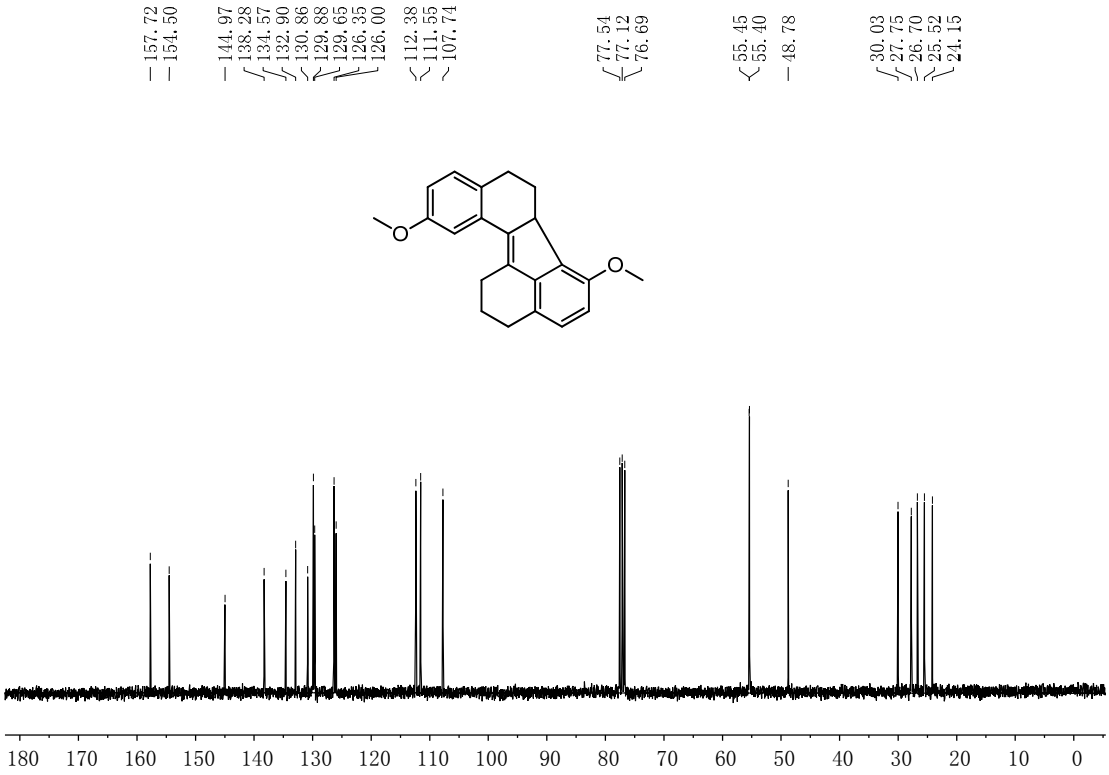


**Fig. S2** $^{13}$C NMR spectrum (101 MHz, $CDCl_3$) of **3a**.

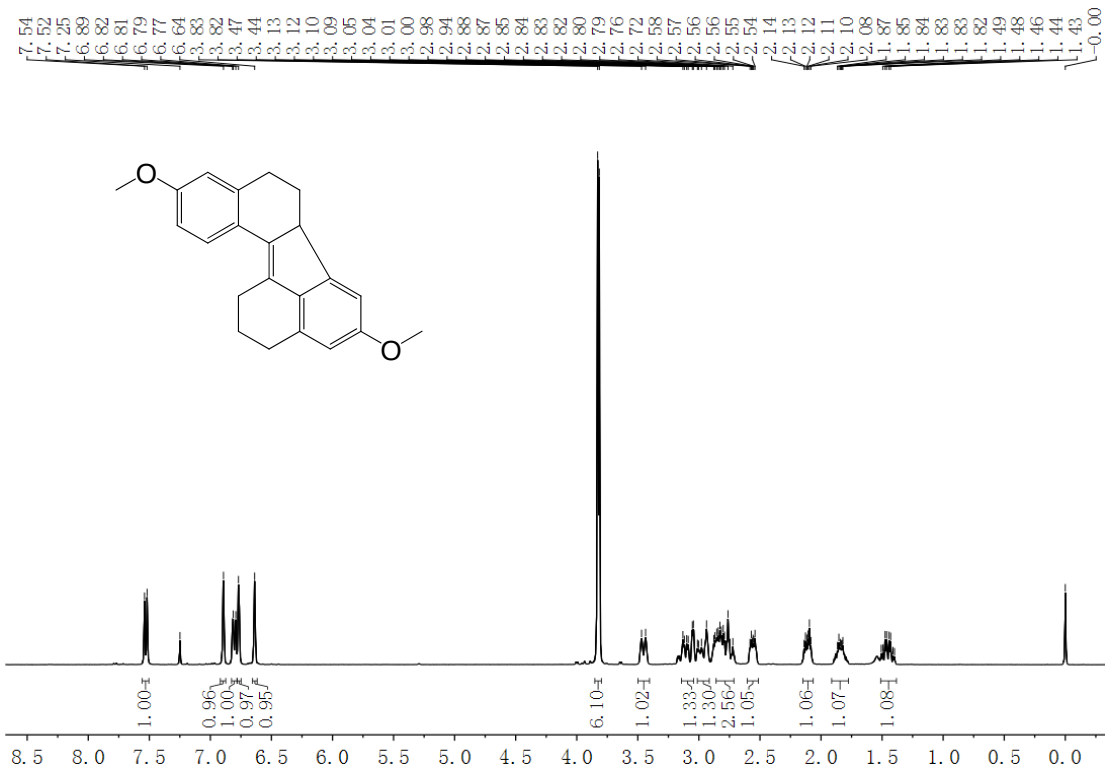

**Fig. S3** $^{1}$H NMR spectrum (400 MHz, $CDCl_3$) of **3b**.

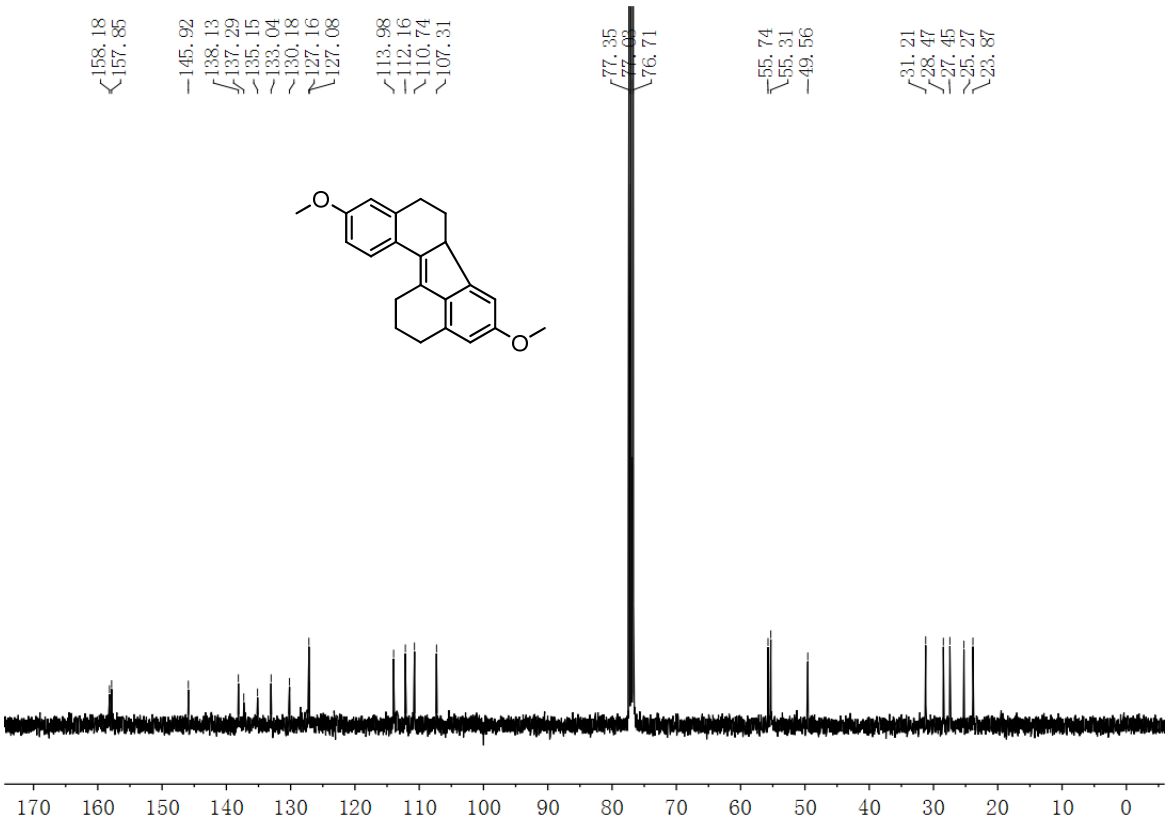

**Fig. S4** $^{13}$C NMR spectrum (101 MHz, $CDCl_3$) of **3b**.

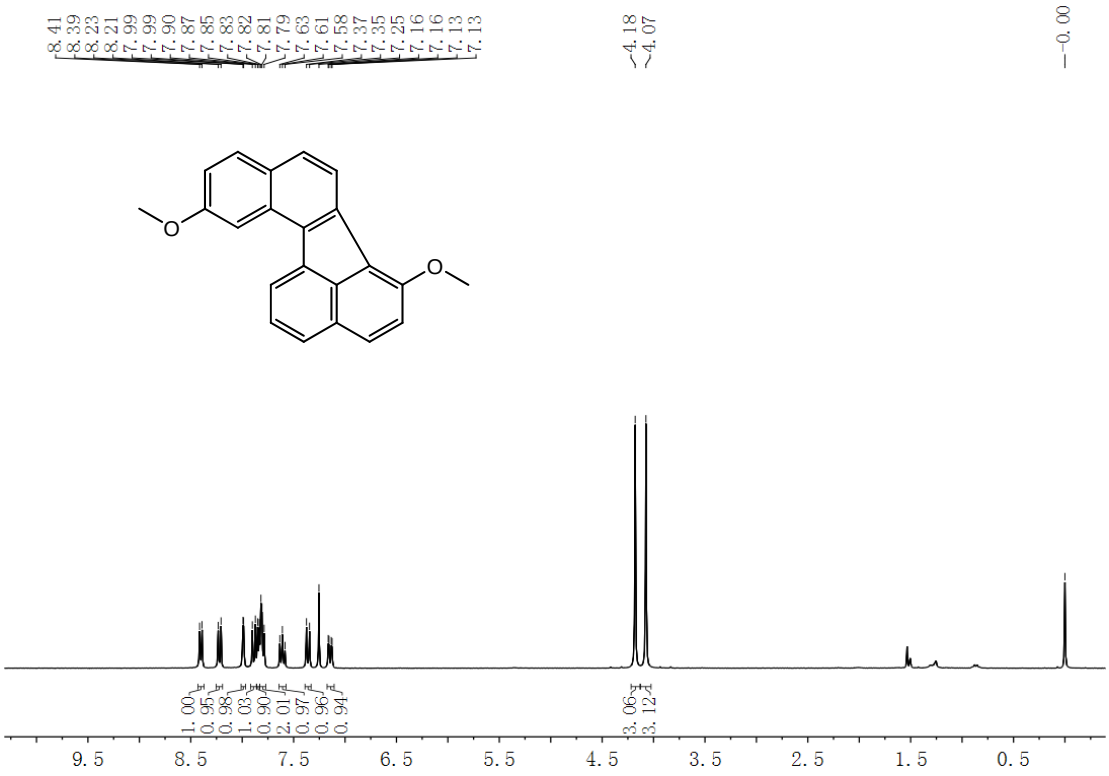


**Fig. S5** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **4a**.

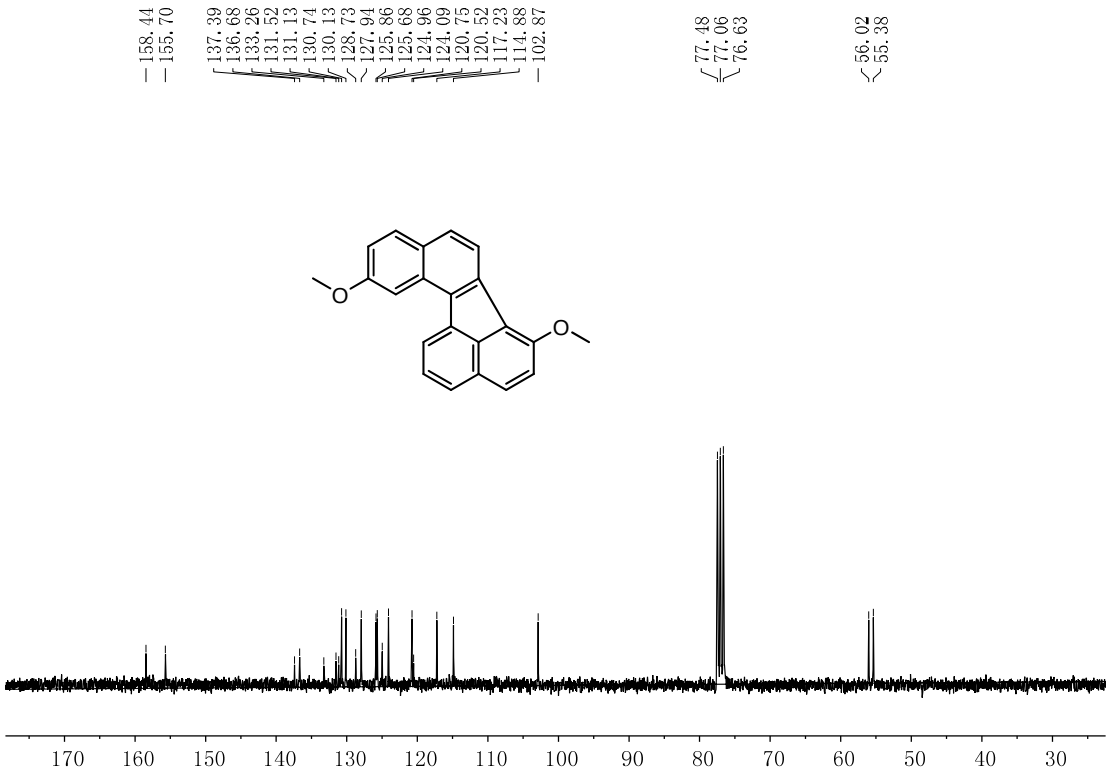


**Fig. S6** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **4a**.

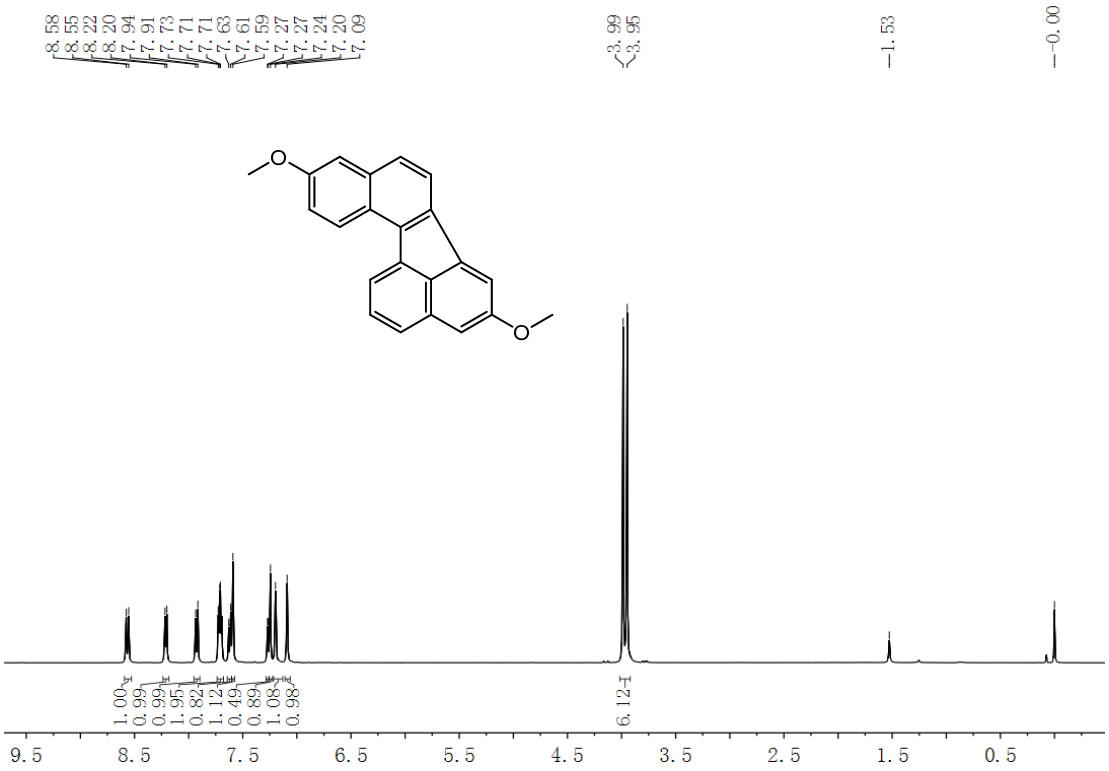


**Fig. S7** $^{1}$H NMR spectrum (400 MHz, $CDCl_3$) of **4b**.

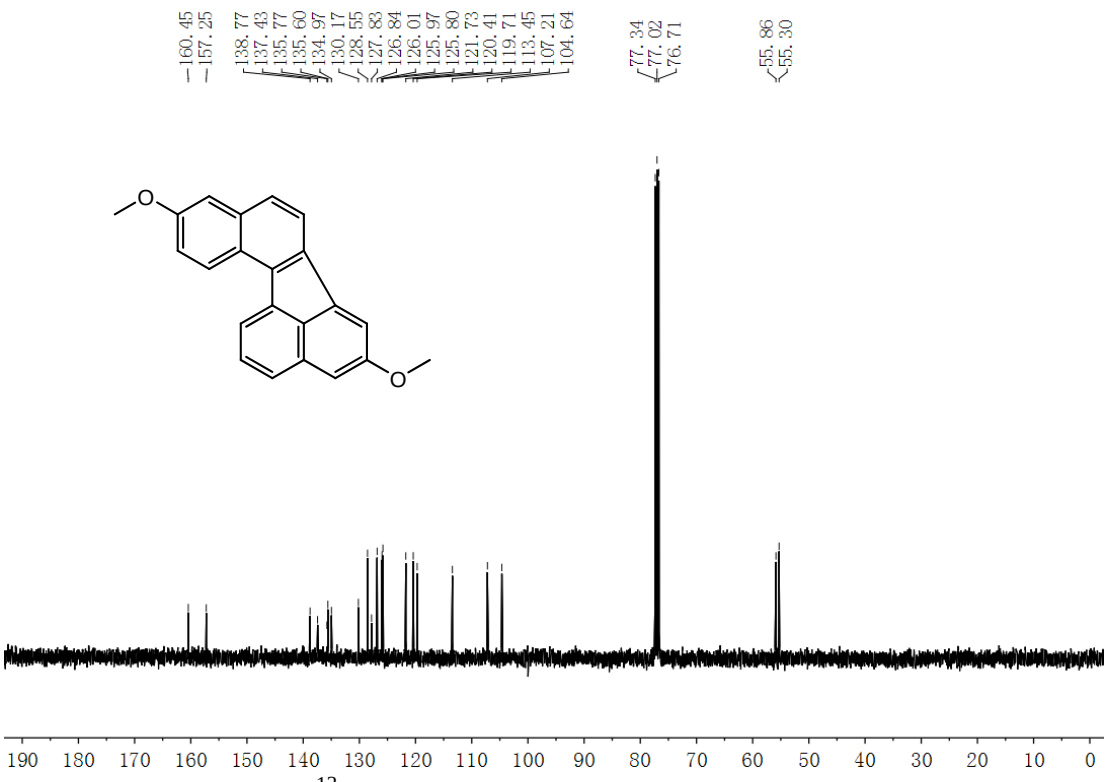


**Fig. S8** $^{13}$C NMR spectrum (101 MHz, $CDCl_3$) of **4b**.

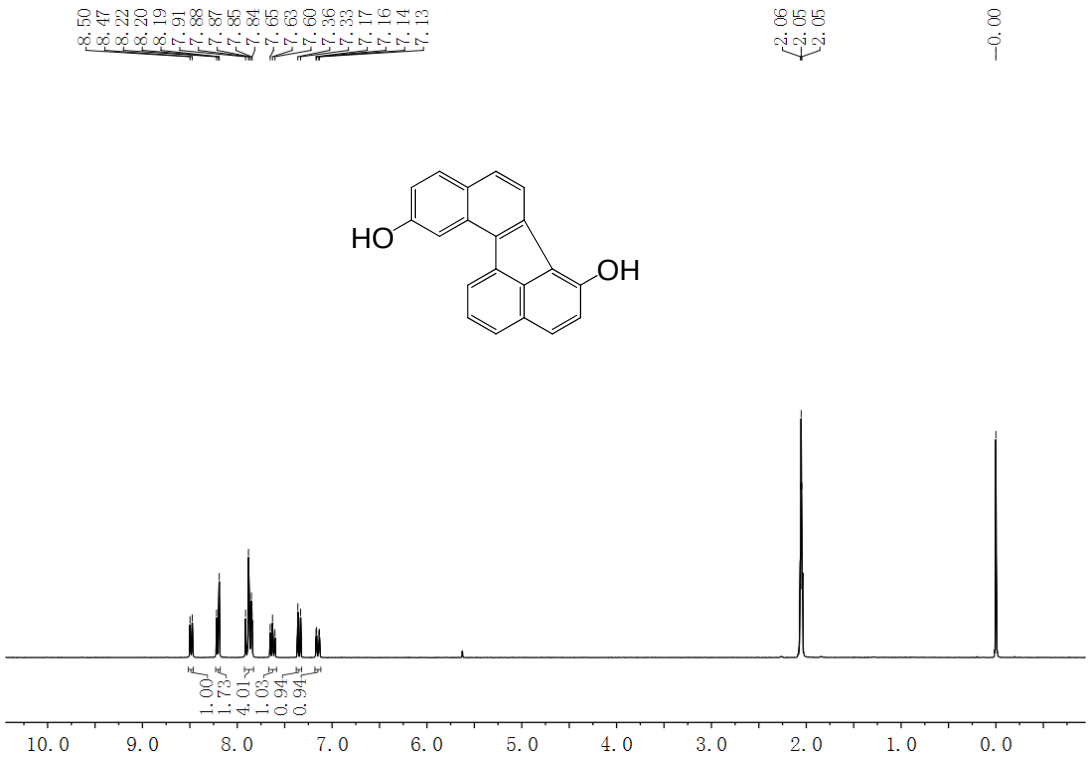


**Fig. S9** $^{1}$H NMR spectrum (300 MHz, acetone-$d_6$) of **5**.

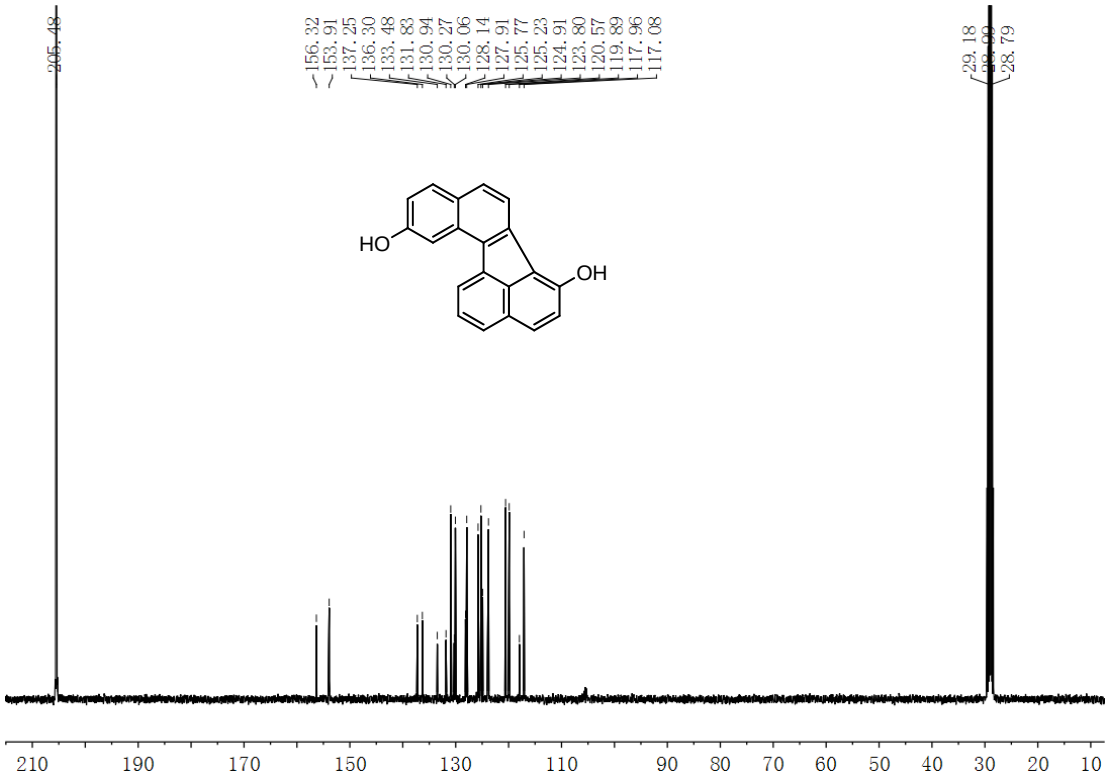


**Fig. S10** $^{13}$C NMR spectrum (101 MHz, acetone-$d_6$) of **5**.

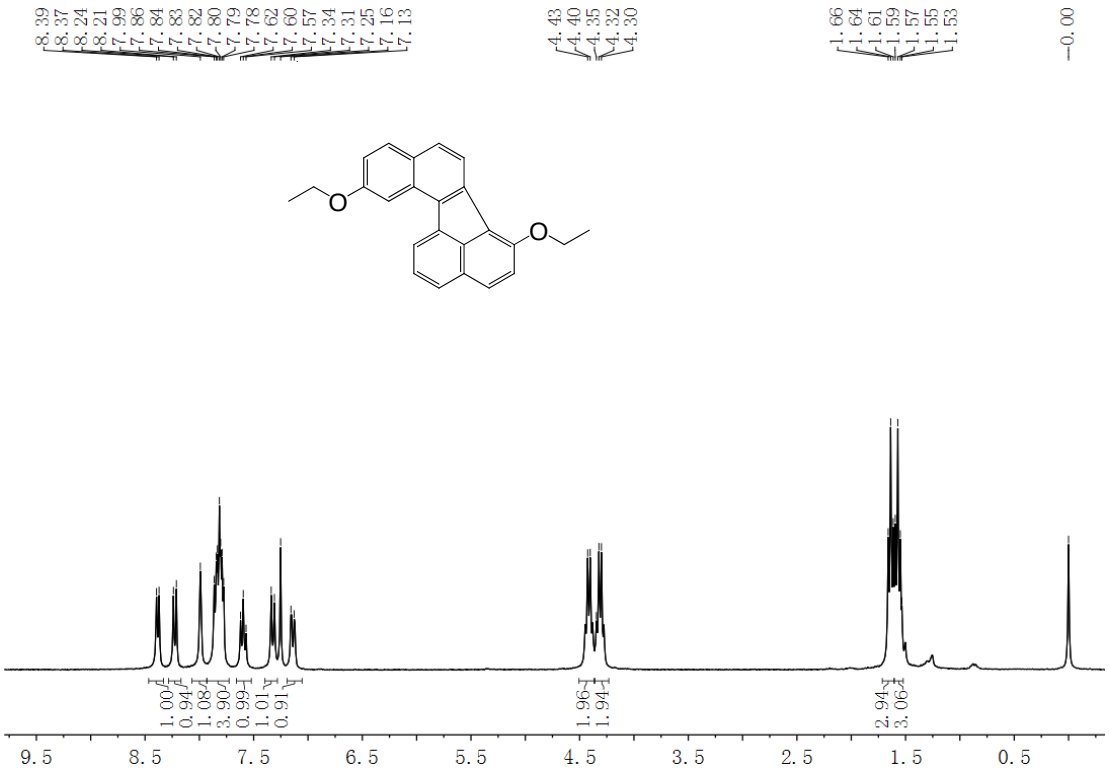


**Fig. S11** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **4c**.

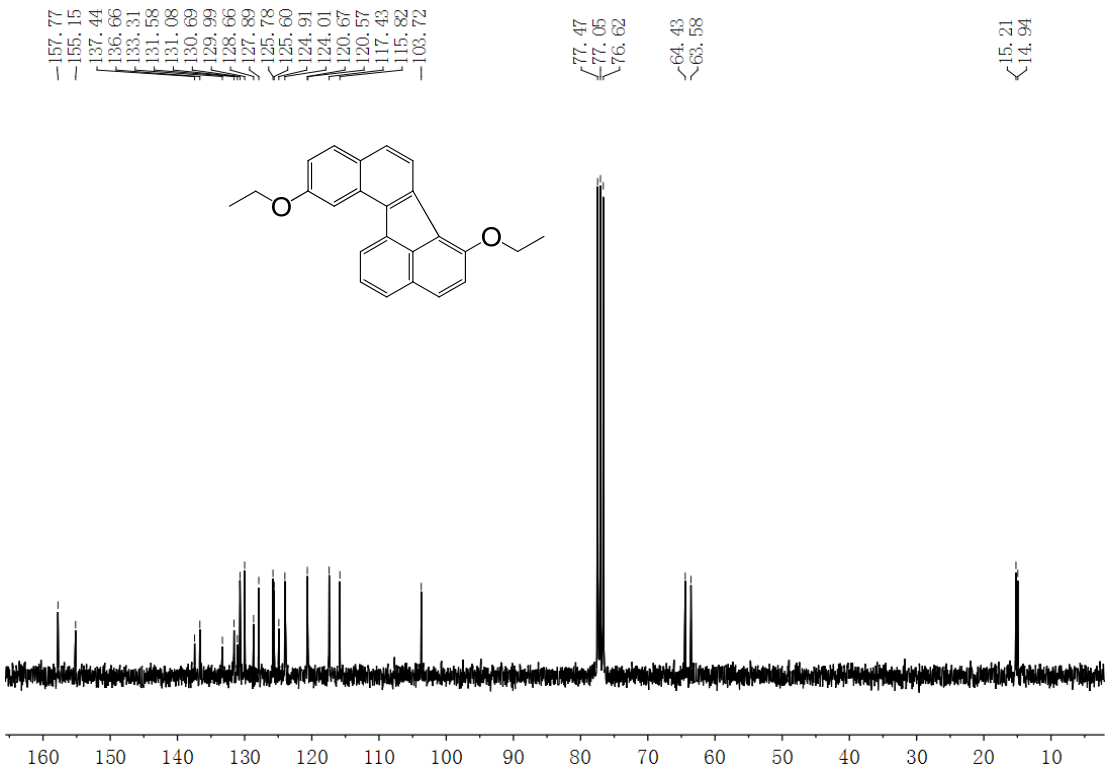


**Fig. S12** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **4c**.

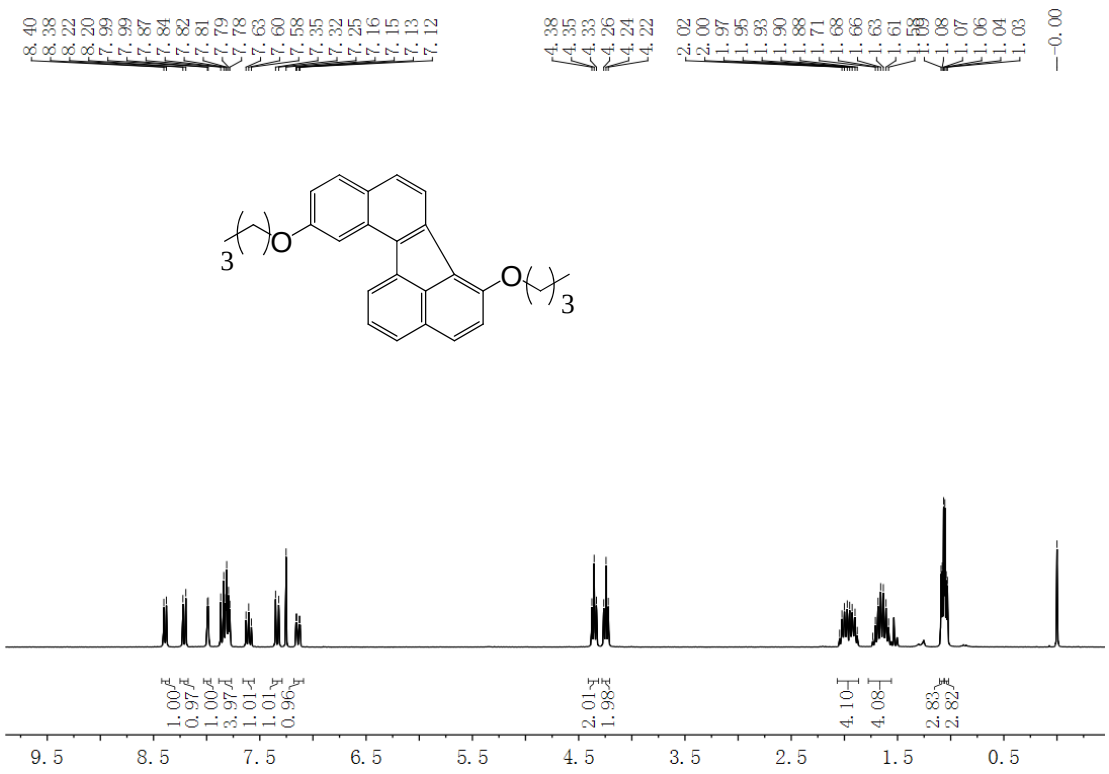

**Fig. S13** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **4d**.

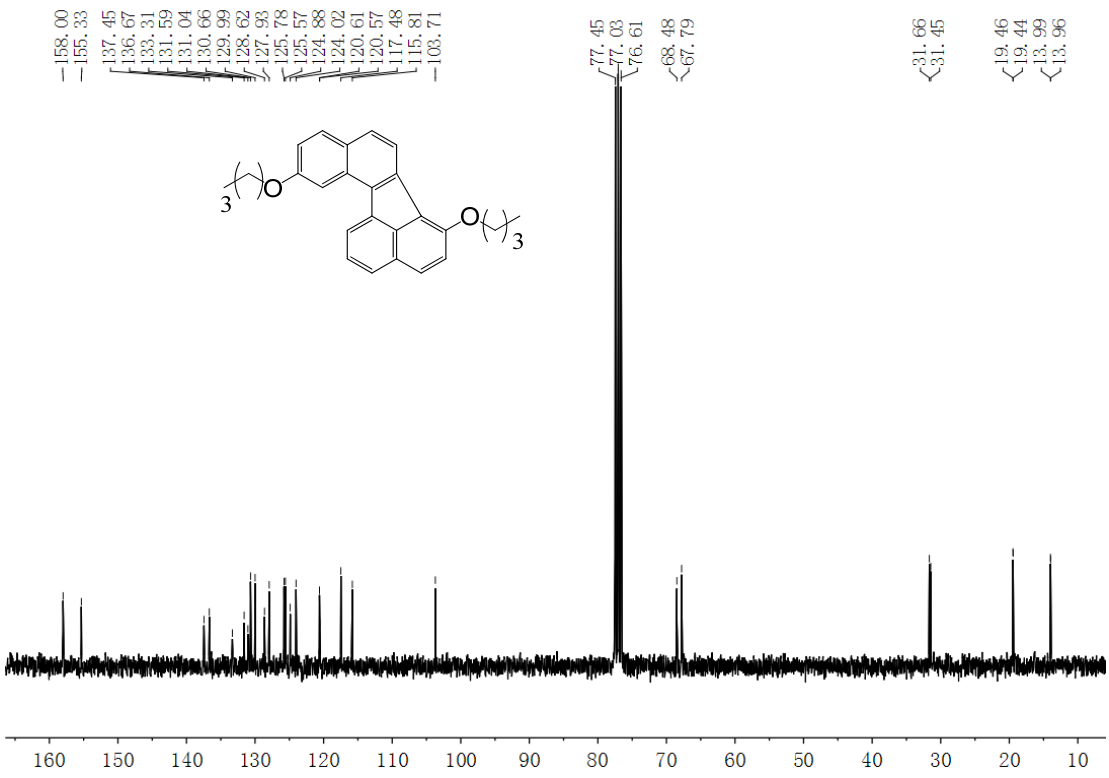

**Fig. S14** $^{13}$C NMR spectrum (75 MHz, $CDCl_3$) of **4d**.

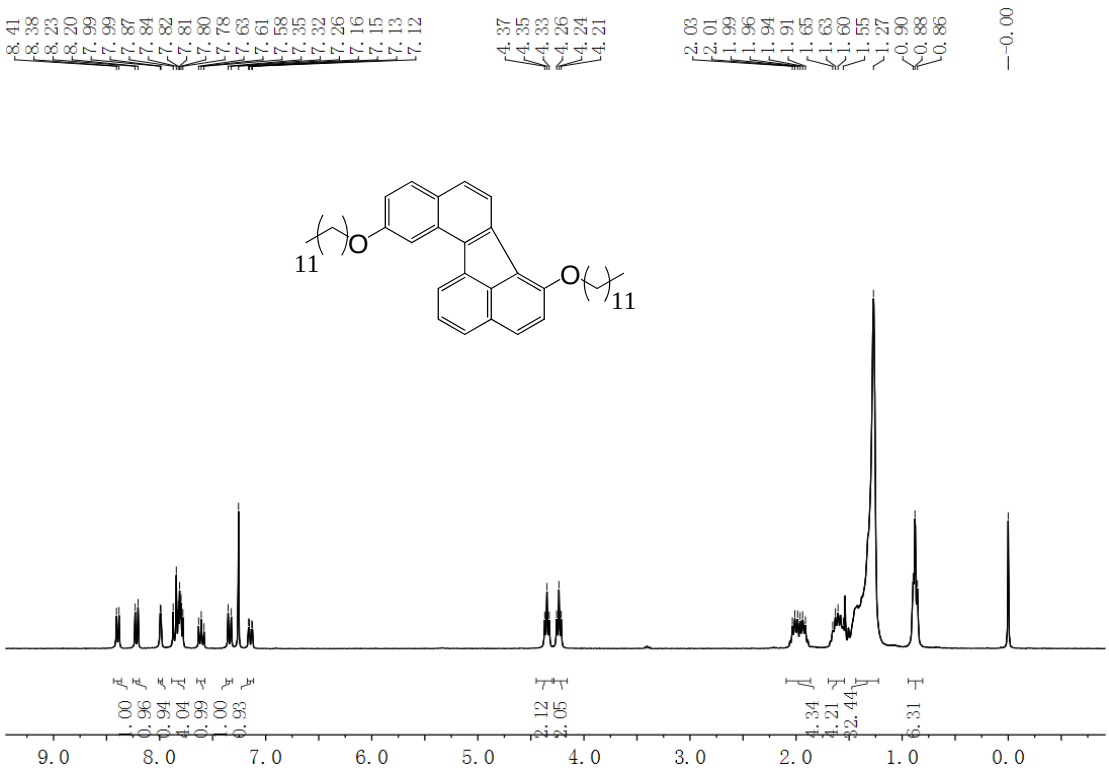

**Fig. S15** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **4e**.

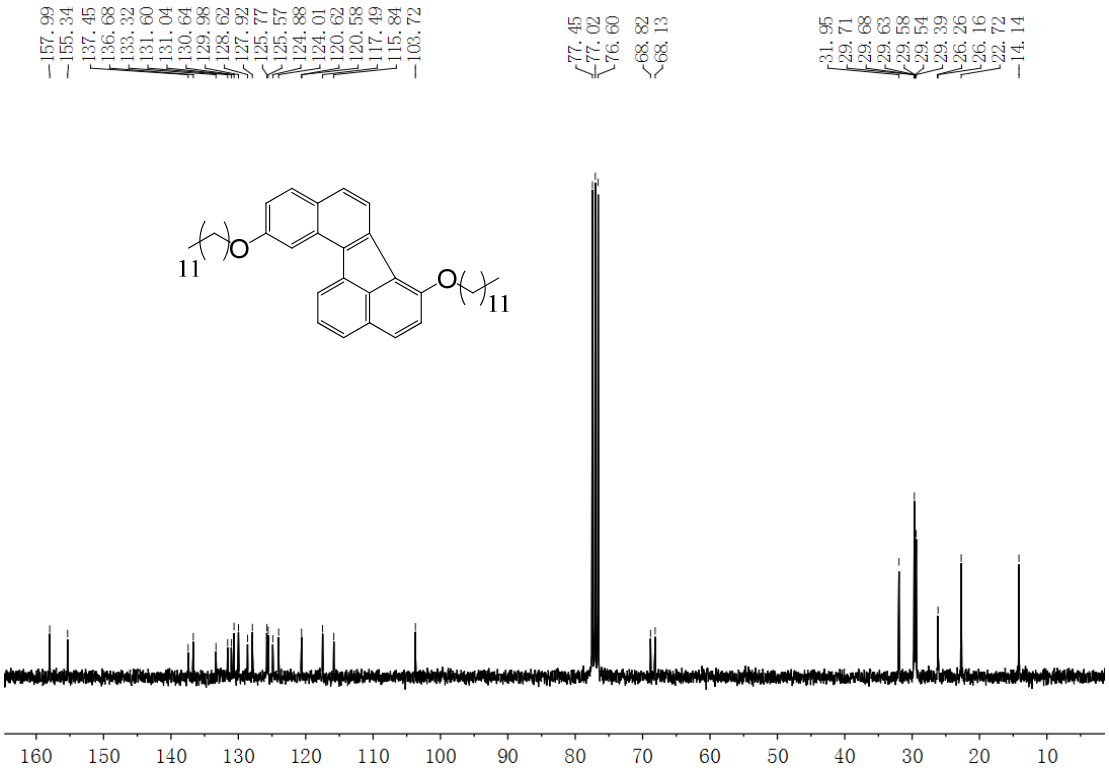

**Fig. S16** $^{1}$H NMR spectrum (300 MHz, $CDCl_3$) of **4e**.

## II. Absorption spectra of 4a-e in the spin-coated films

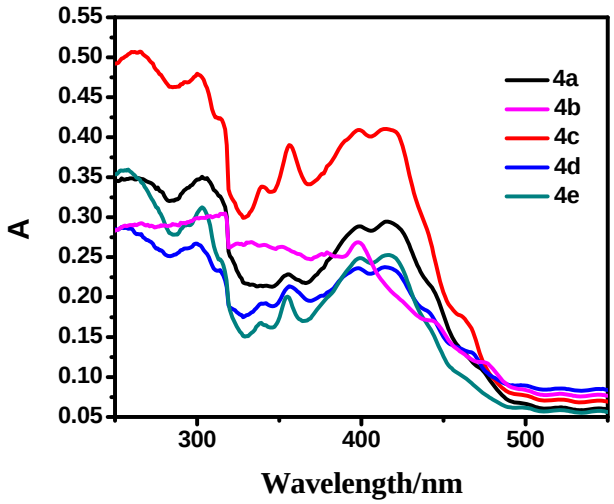


**Fig. S17** UV-Vis spectra of **4a-e** in the spin-coated films at room temperature.

## III. Fluorescence spectra of 4e in the spin-coated films

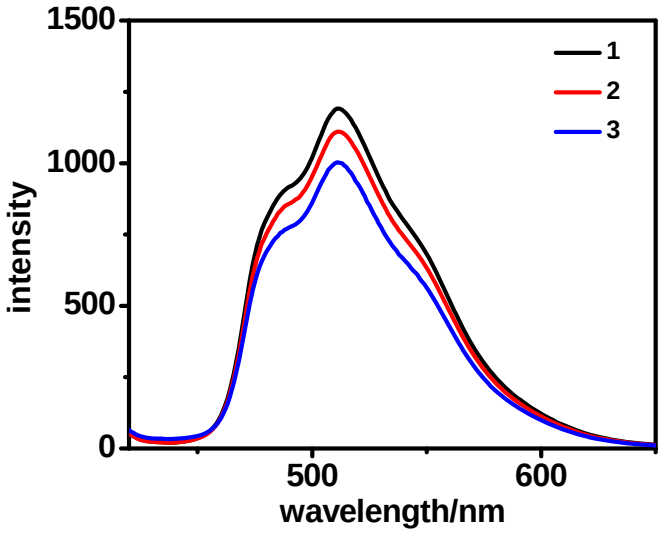


**Fig. S18** Fluorescence spectra of **4e** in the spin-coated films prepared from the different concentrations of the stock solutions in $CH_2Cl_2$ at room temperature and same rotate speed. The concentrations of the stock solutions were 10 mg/mL (1), 12 mg/mL (2), and 15 mg/mL (3), respectively. $\lambda_{ex}$ = 407 nm.

## IV. AFM topography image of spin-coated film of 4e

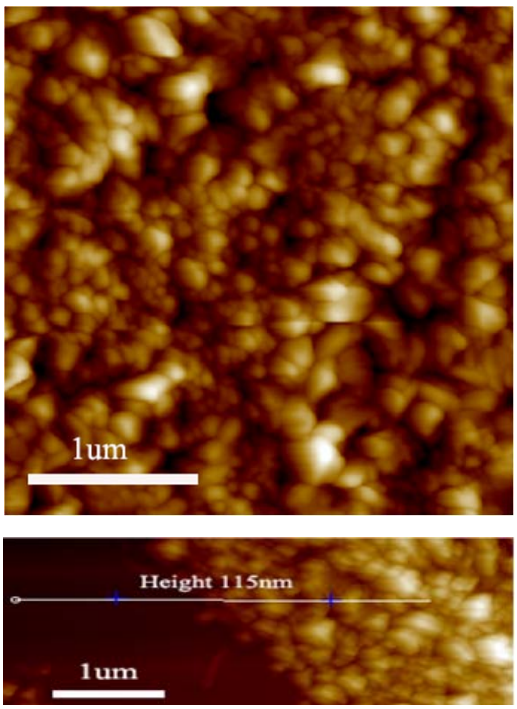


**Fig. S19** AFM topography image of spin-coated film of **4e** on OTS-modified $SiO_2$/Si substrates. The concentration of the stock solution in $CH_2Cl_2$ was 12 mg/mL.

## V. Crystal data

**Table S1. Crystal data of 3a, 4a, 4b, and 4d.**

| Compound | **3a** | **4a** | **4b** | **4d** |
|---|---|---|---|---|
| CCDC number | 1037207 | 1037219 | 1038631 | 1037208 |
| Empirical formula | $C_{22}$ $H_{22}$ $O_2$ | $C_{22}$ $H_{16}$ $O_2$ | $C_{22}$ $H_{16}$ $O_2$ | $C_{28}$ $H_{28}$ $O_2$ |
| Formula weight | 318.39 | 312.35 | 312.35 | 396.50 |
| Temperature | 173.1500 K | 173.1500 K | 173.1500 K | 173.1500 K |
| Wavelength | 0.71073 Å | 0.71073 Å | 0.71073 Å | 0.71073 Å |
| Crystal system | Orthorhombic | Orthorhombic | Triclinic | Triclinic |
| Space group | P b c a | P b c a | P -1 | P -1 |
| Unit cell dimensions | a = 11.935(3) Å α= 90° b = 12.812(3) Å β= 90° c = 20.795(5) Å γ = 90°. | a = 10.361(2) Å α= 90° b = 14.6319(7) Å β= 90° c = 20.1158(9) Å γ = 90°. | a = 6.3011(13) Å α= 90° b = 15.399(3) Å β= 90° c = 16.736(3) Å γ = 90°. | a = 8.1661(16) Å α= 90° b = 13.473(3) Å β= 90° c = 20.342(4) Å γ = 90°. |

| | | | | |
|---|---|---|---|---|
| Volume | 3179.6(12) $Å^3$ | 3049.4(7) $Å^3$ | 1554.3(6) $Å^3$ | 2170.1(8) $Å^3$ |
| Z | 8 | 8 | 4 | 4 |
| Density (calculated) | 1.330 $Mg/m^3$ | 1.361 $Mg/m^3$ | 1.335 $Mg/m^3$ | 1.214 $Mg/m^3$ |
| Absorption coefficient | 0.083 $mm^{-1}$ | 0.086 $mm^{-1}$ | 0.084 $mm^{-1}$ | 0.075 $mm^{-1}$ |
| F(000) | 1360 | 1312 | 656 | 848 |
| Crystal size | 0.38 x 0.17 x 0.13 $mm^3$ | 0.46 x 0.3 x 0.26 $mm^3$ | 0.42 x 0.12 x 0.07 $mm^3$ | 0.265 x 0.231 x 0.146 $mm^3$ |
| Theta range for data collection | 3.180 to 27.476° | 2.823 to 27.483°. | 1.263 to 25.199°. | 2.844 to 27.485°. |
| Index ranges | -12<=h<=15, -16<=k<=16, 15<=l<=26 | -13<=h<=13, -18<=k<=18, 11<=l<=26 | -7<=h<=7, -17<=k<=18, -20<=l<=19 | -10<=h<=10, -17<=k<=17, -26<=l<=22 |
| Reflections collected | 11691 | 11528 | 11770 | 21365 |
| Independent reflections | 3627 [R(int) = 0.0442] | 3474 [R(int) = 0.0406] | 5567 [R(int) = 0.0541] | 9810 [R(int) = 0.0694] |
| Completeness to theta = 26.000° | 99.4 % | 99.7 % | 98.8 % | 99.3 % |
| Absorption correction | Semi-empirical from equivalents | Semi-empirical from equivalents | Semi-empirical from equivalents | Semi-empirical from equivalents |
| Max. and min. transmission | 1.0000 and 0.8517 | 1.0000 and 0.6449 | 1.0000 and 0.6053 | 1.0000 and 0.4113 |
| Refinement method | Full-matrix least-squares on $F^2$ | Full-matrix least-squares on $F^2$ | Full-matrix least-squares on $F^2$ | Full-matrix least-squares on $F^2$ |
| Data / restraints / parameters | 3627 / 0 / 219 | 3474 / 0 / 219 | 5567 / 0 / 437 | 9810 / 0 / 545 |
| Goodness-of-fit on $F^2$ | 1.255 | 1.224 | 1.177 | 1.157 |
| Final R indices [I>2sigma(I)] | R1 = 0.0744, wR2 = 0.1259 | R1 = 0.0625, wR2 = 0.1224 | R1 = 0.0848, wR2 = 0.1539 | R1 = 0.1046, wR2 = 0.2319 |
| R indices (all data) | R1 = 0.0849, wR2 = 0.1343 | R1 = 0.0680, wR2 = 0.1250 | R1 = 0.1171, wR2 = 0.1769 | R1 = 0.1327, wR2 = 0.2511 |
| Extinction coefficient | n/a | n/a | n/a | n/a |
| Largest diff. peak and hole | 0.262 and -0.202 $e.Å^{-3}$ | 0.193 and -0.153 $e.Å^{-3}$ | 0.248 and -0.220 $e.Å^{-3}$ | 1.353 and -0.218 $e.Å^{-3}$ |