

Supporting information for

**Ion induced cycle opening of a diarylethene and its application on visual detection
of Cu²⁺ and Hg²⁺ and keypad lock**

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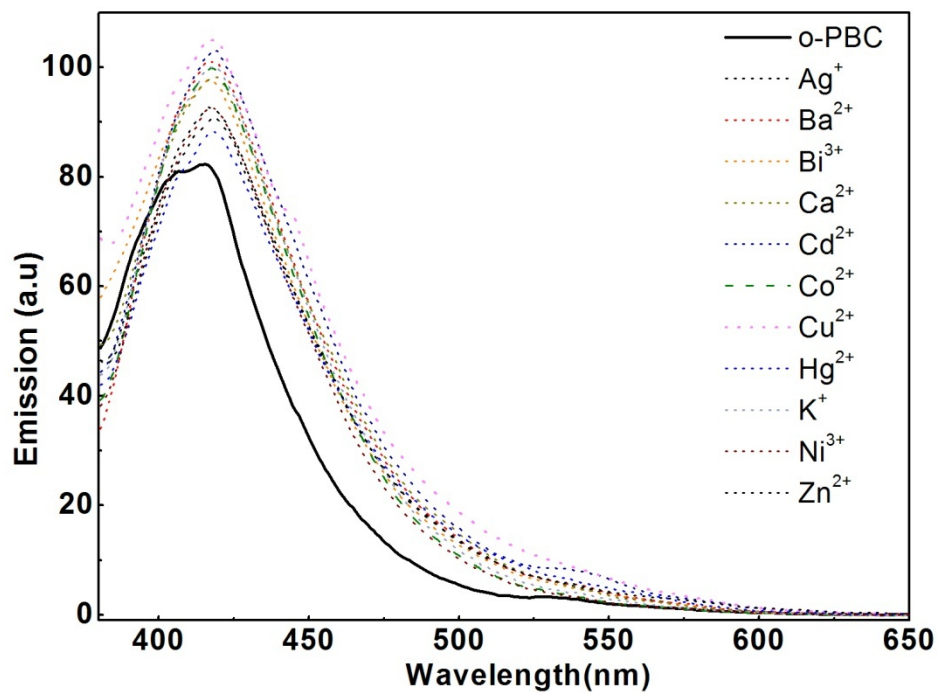


Fig. S 1 Fluorescence spectra of **o-PBC** solutions added different metal ions.

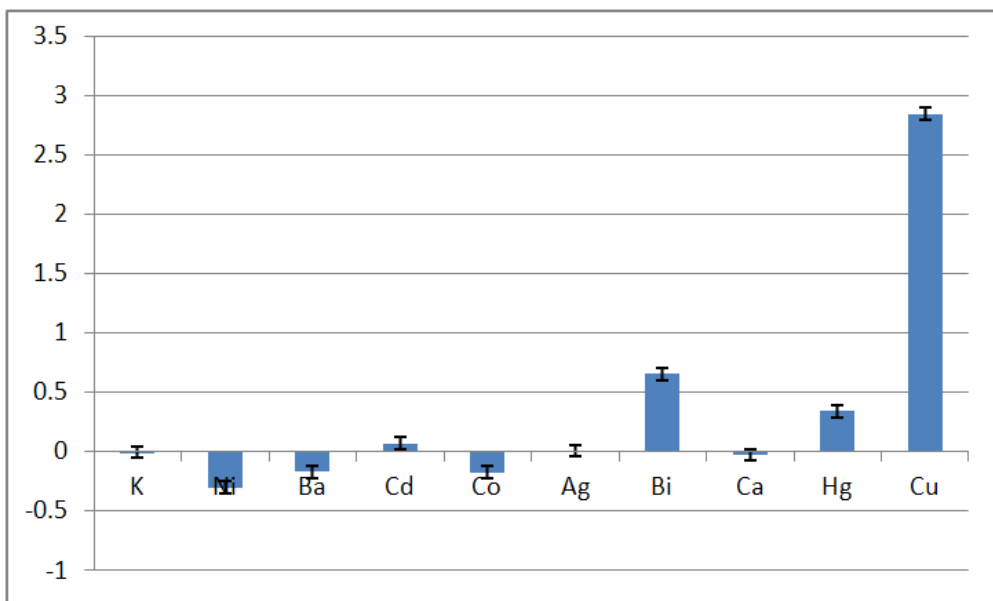


Fig. S 2 Emission intensity changes of **PBC** acetonitrile solution (1.0×10^{-5} mol L⁻¹) at 452 nm in PSS in the presence of respective metal ions (20 equiv.) at room temperature. F0: initial emission intensity of **PBC**; F: emission intensity of **PBC** in the presence of metal ions(20 equiv.).

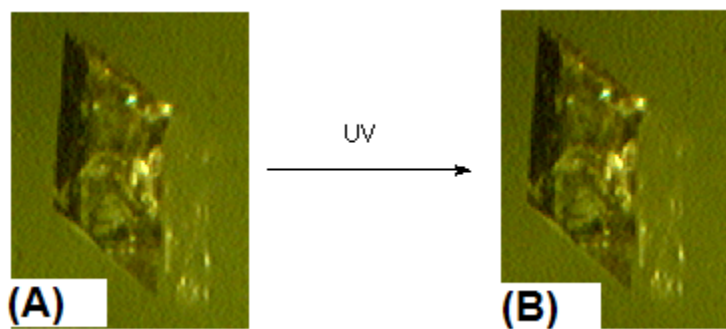


Fig. S 3 Color change of crystal **PBC** before(A) and after(B)UV light irradiation.

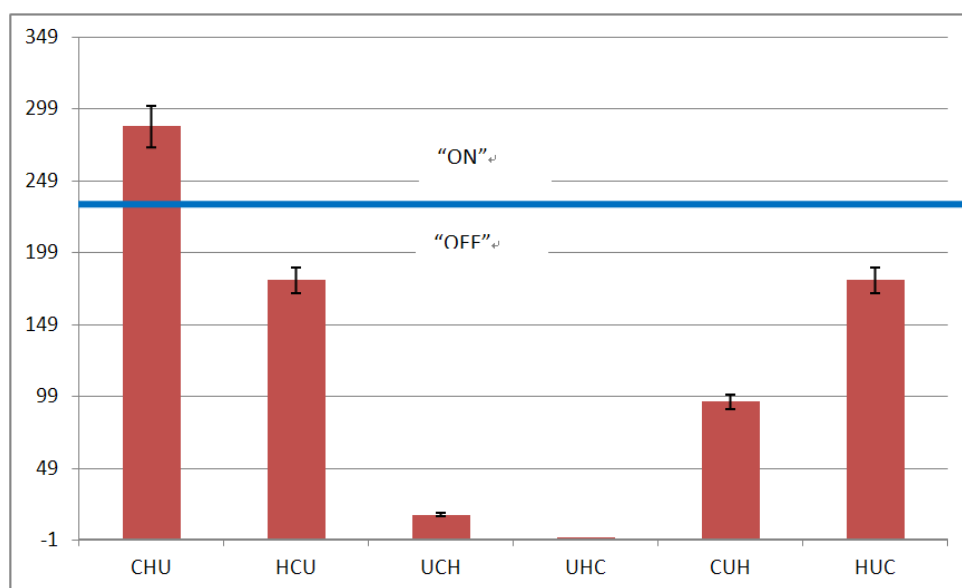


Fig. S 4 Fluorescence emission output of compound **PBC** corresponding to six possible input combinations at 480 nm

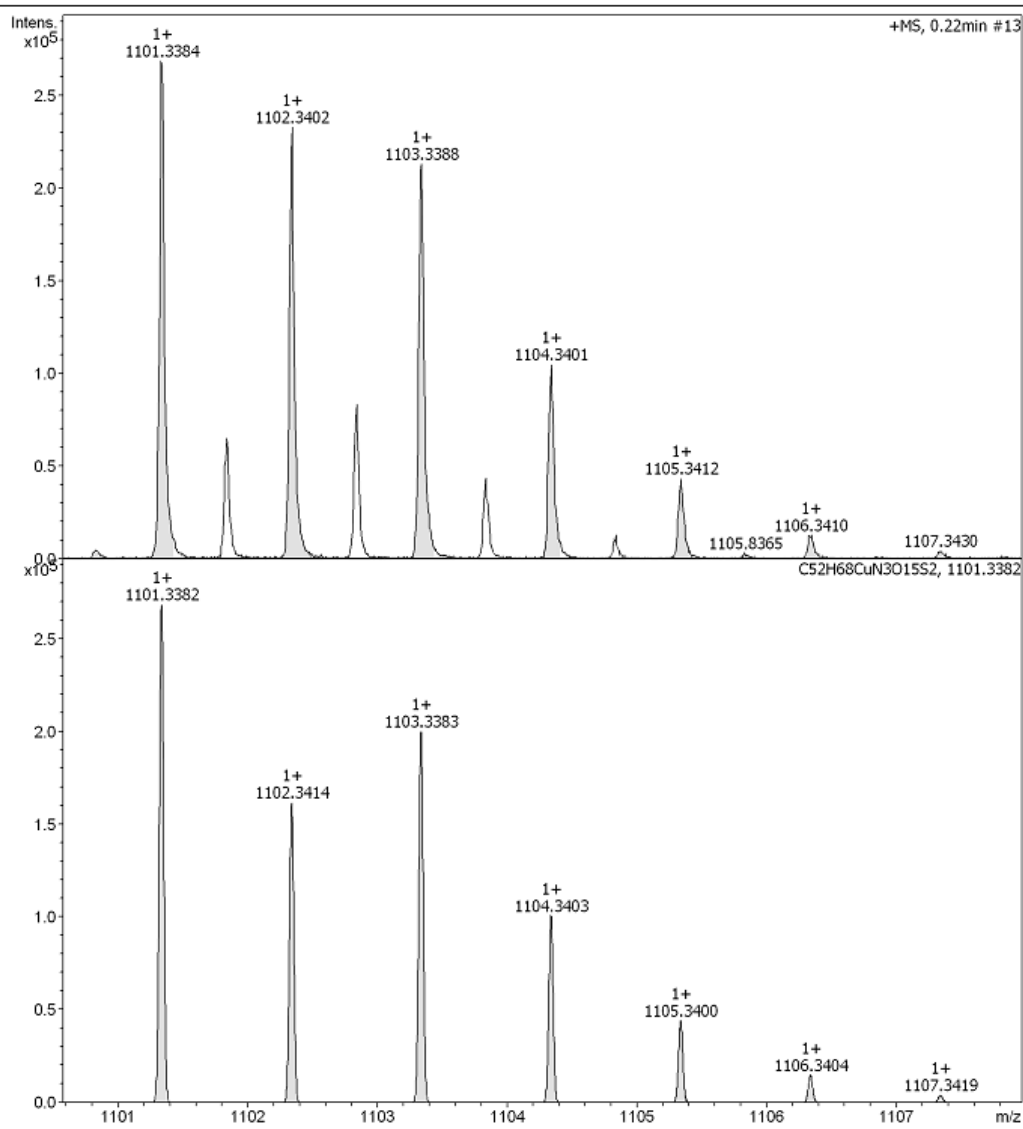


Fig. S 5 Generic display report of HRMS for **PBC-Cu-NO₃**

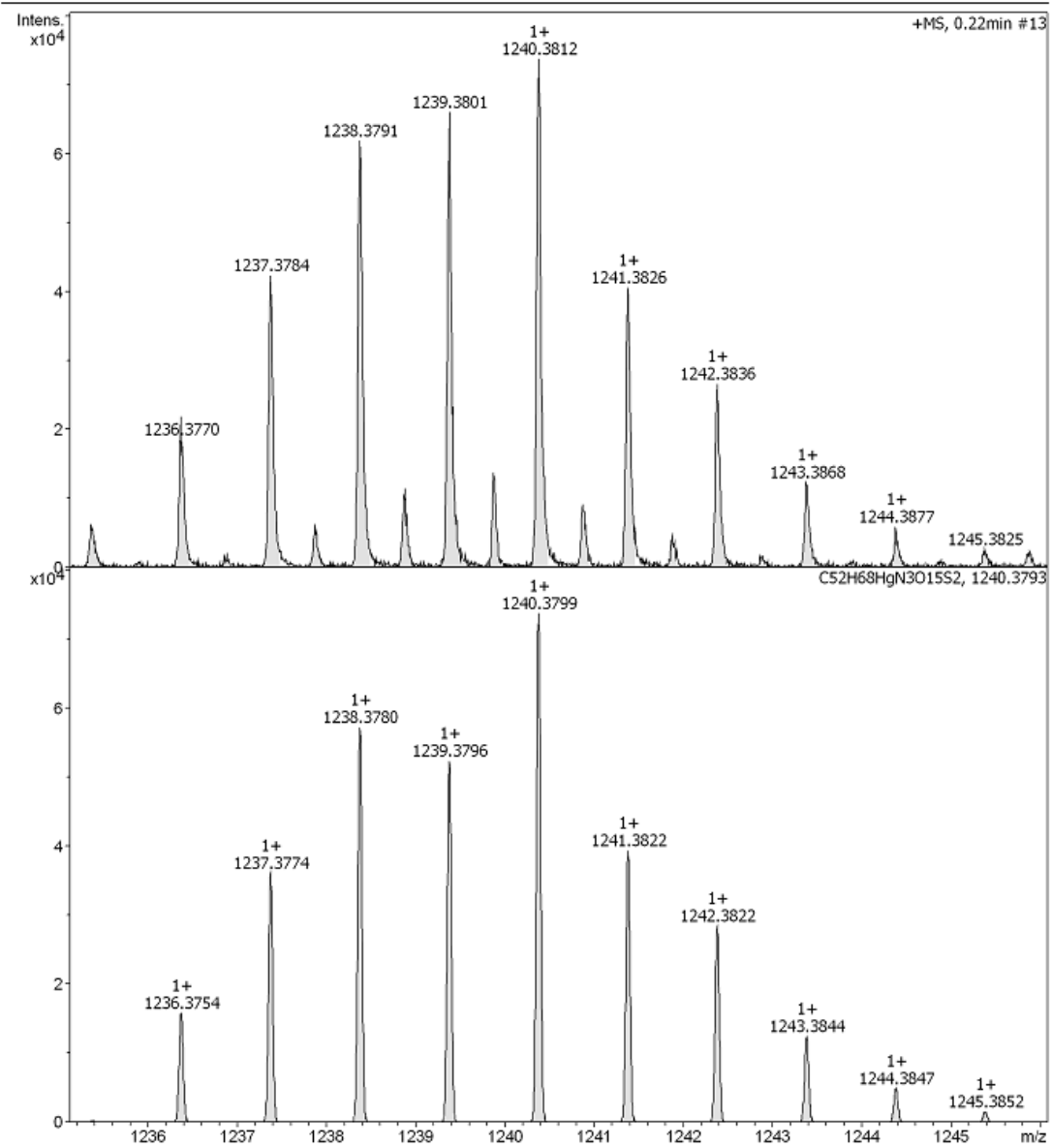


Fig. S 6 Generic display report of HRMS for **PBC-Hg-NO₃**

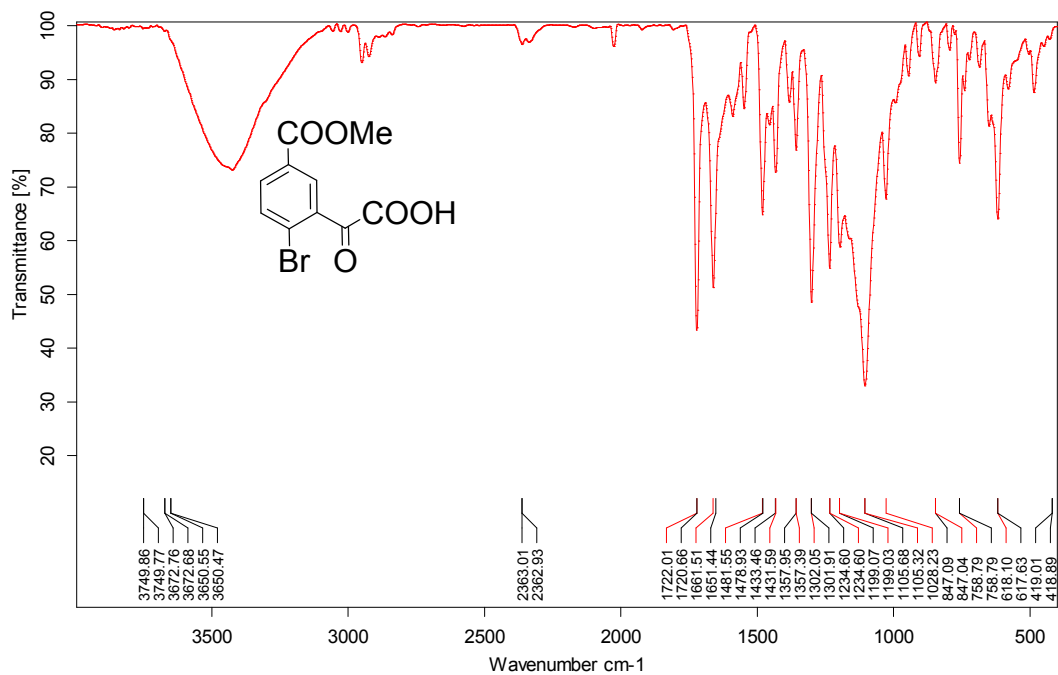


Fig. S 7 IR spectrum of 2-bromo-5-(methoxycarbonyl)benzoic acid(2)

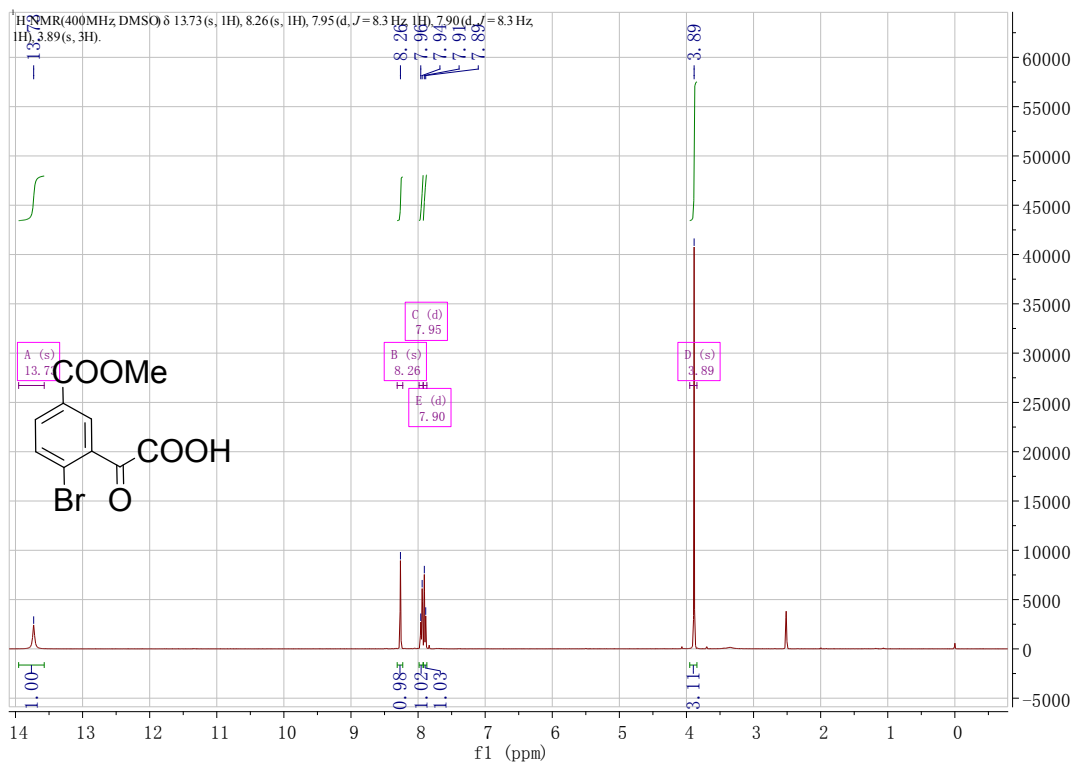


Fig. S 8 ^1H NMR spectrum of 2-bromo-5-(methoxycarbonyl)benzoic acid(2)

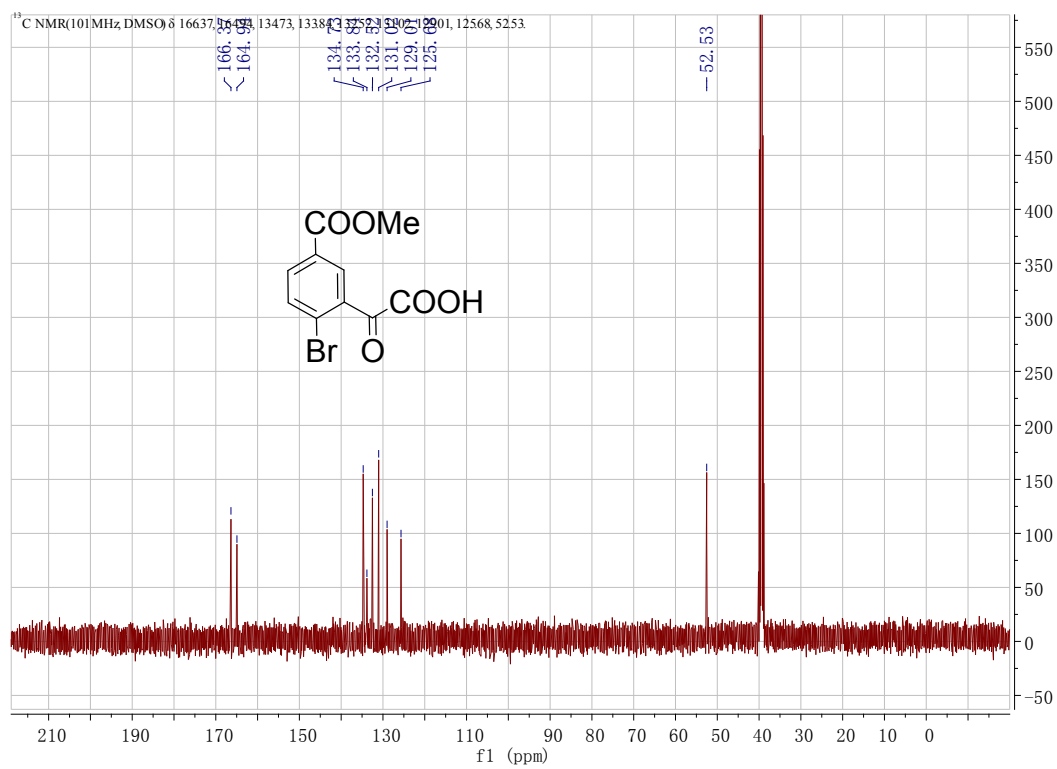


Fig. S 9 ^{13}C NMR spectrum of 2-bromo-5-(methoxycarbonyl)benzoic acid(2)

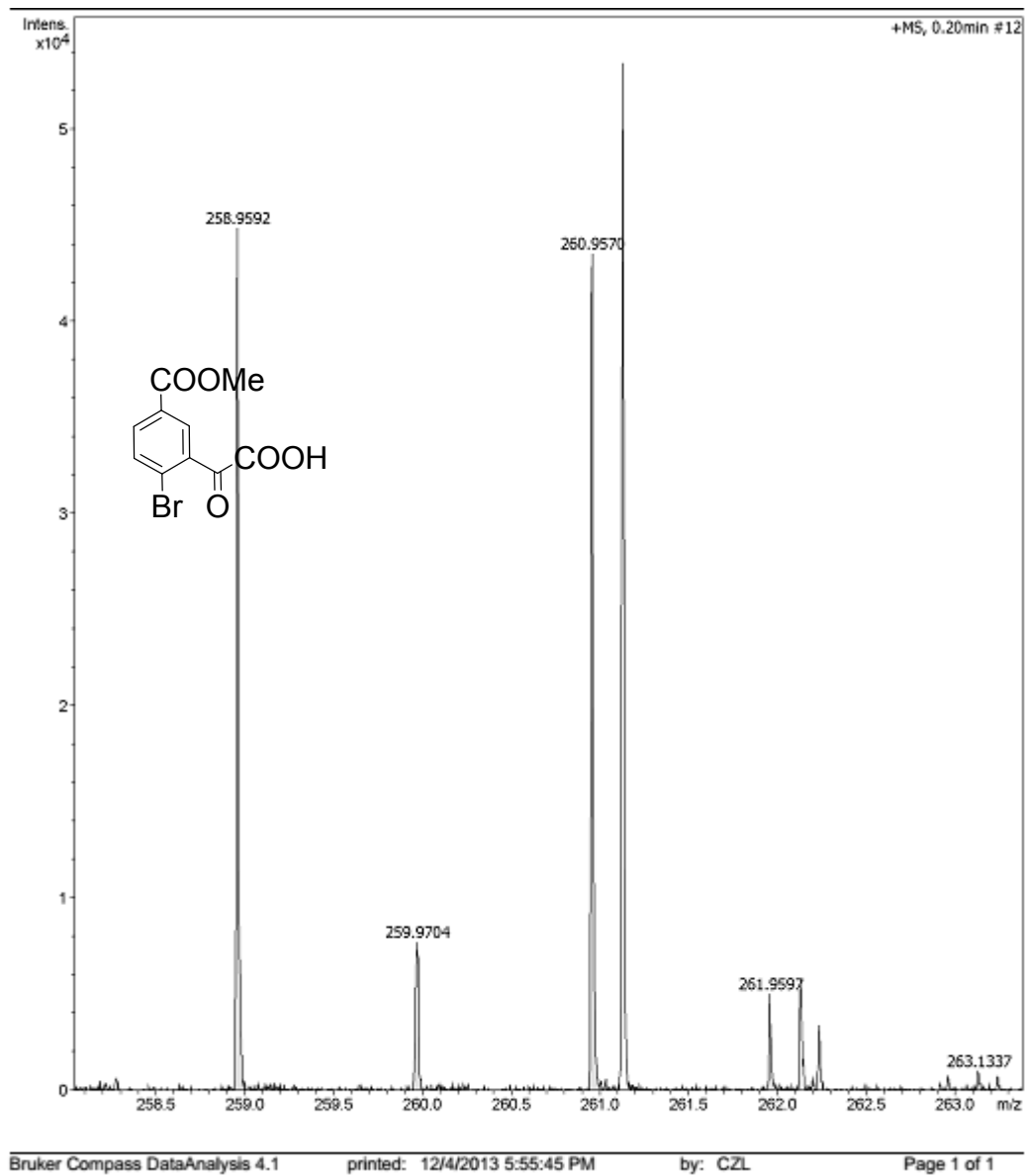


Fig. S 10 HRMS spectrum of 2-bromo-5-(methoxycarbonyl)benzoic acid(2)

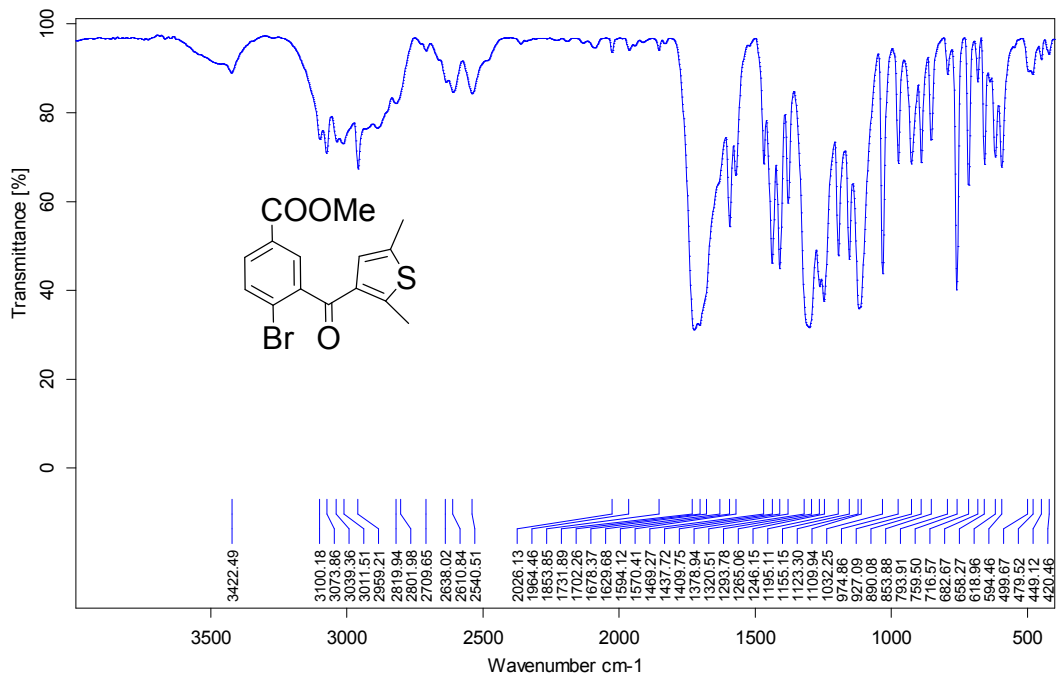


Fig. S 11 IR spectrum of methyl 4-bromo-3-(2,5-dimethylthiophene-3-carbonyl)benzoate(3)

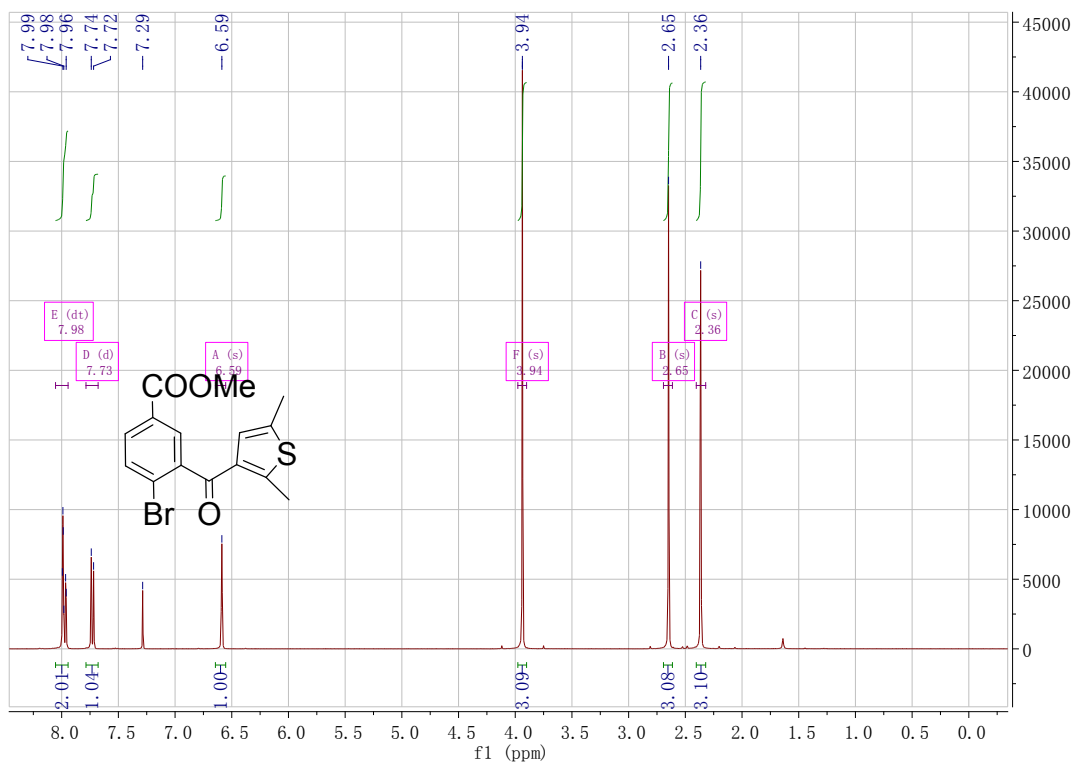


Fig. S 12 ¹H NMR spectrum of methyl 4-bromo-3-(2,5-dimethylthiophene-3-carbonyl)benzoate(3)

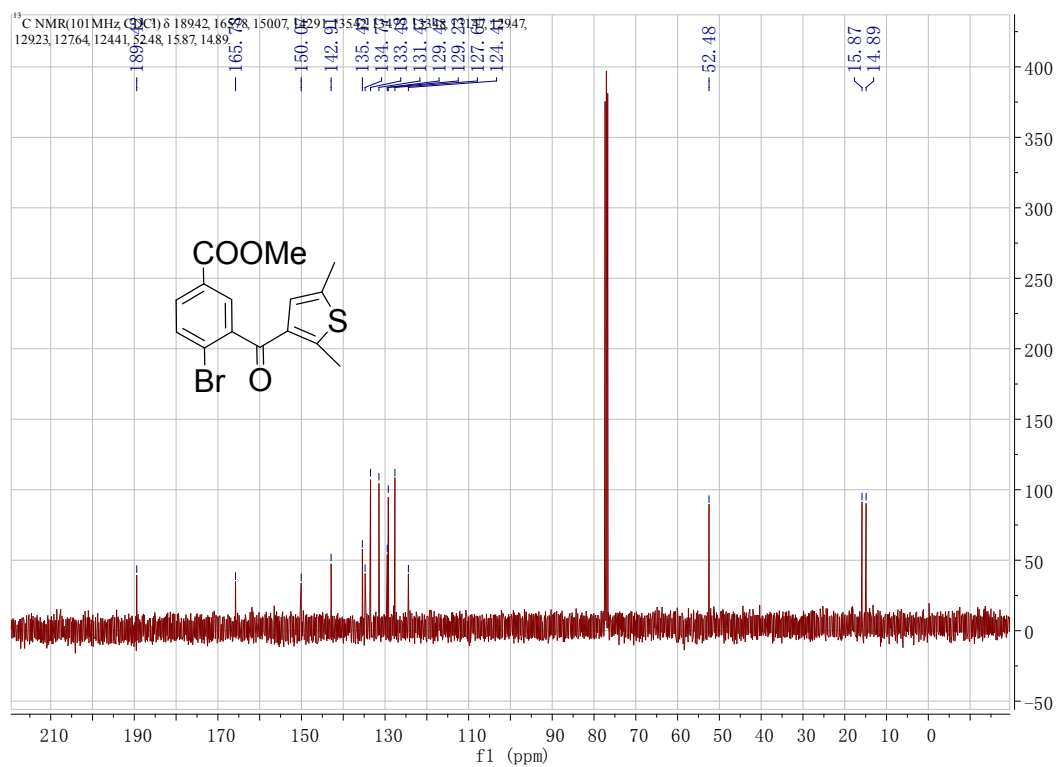


Fig. S 13 ^{13}C NMR spectrum of methyl 4-bromo-3-(2,5-dimethylthiophene-3-carbonyl)benzoate(3)

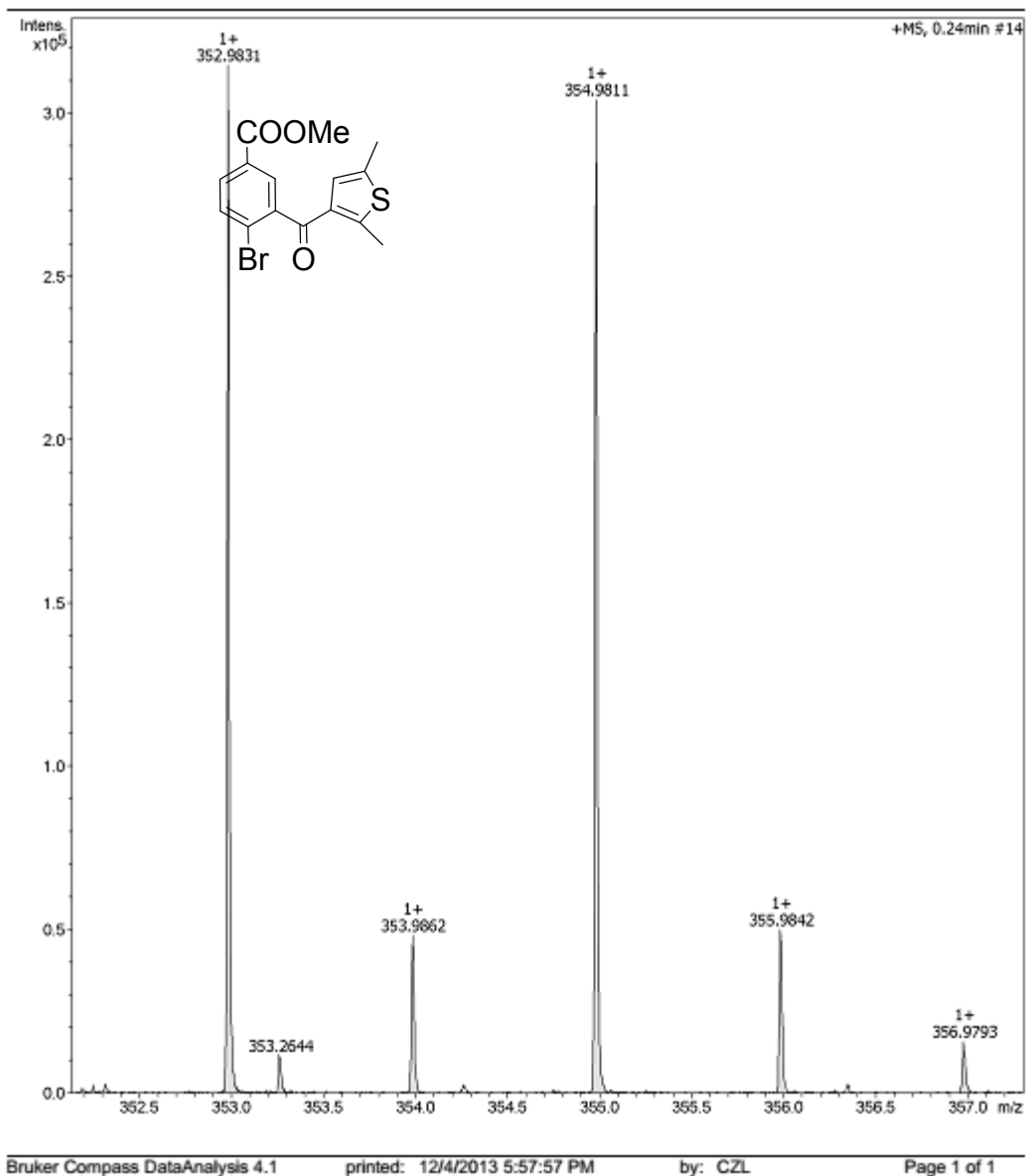


Fig. S 14 MS spectrum of methyl 4-bromo-3-(2,5-dimethylthiophene-3-carbonyl)benzoate(3)

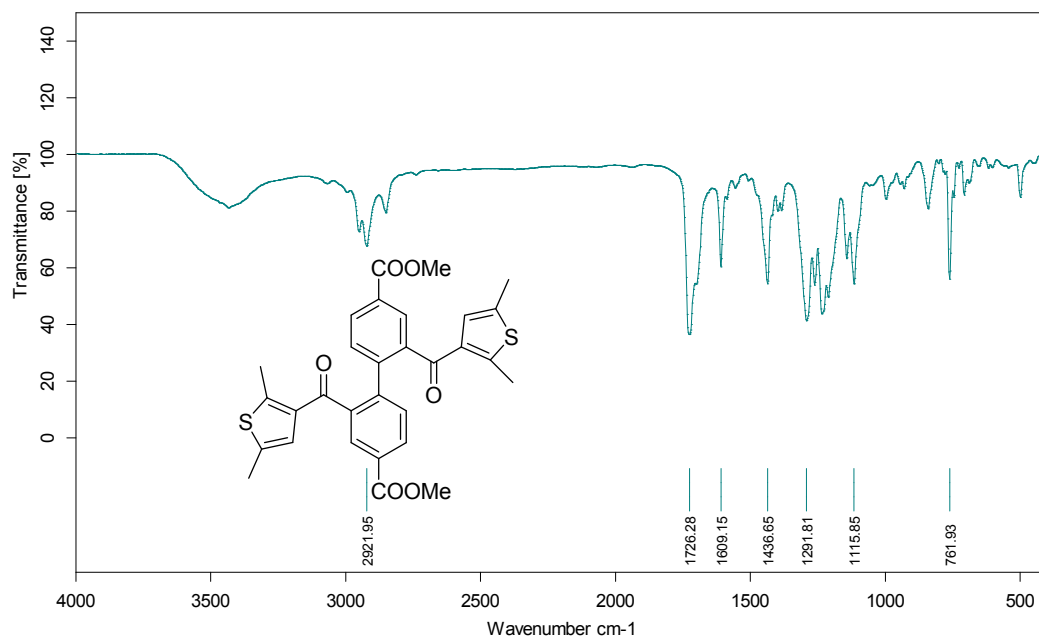


Fig. S15 IR spectrum of 2,2'-bis(2,5-dimethylthiophene-3-carbonyl) biphenyl-4,4'-dicarboxylate(4).

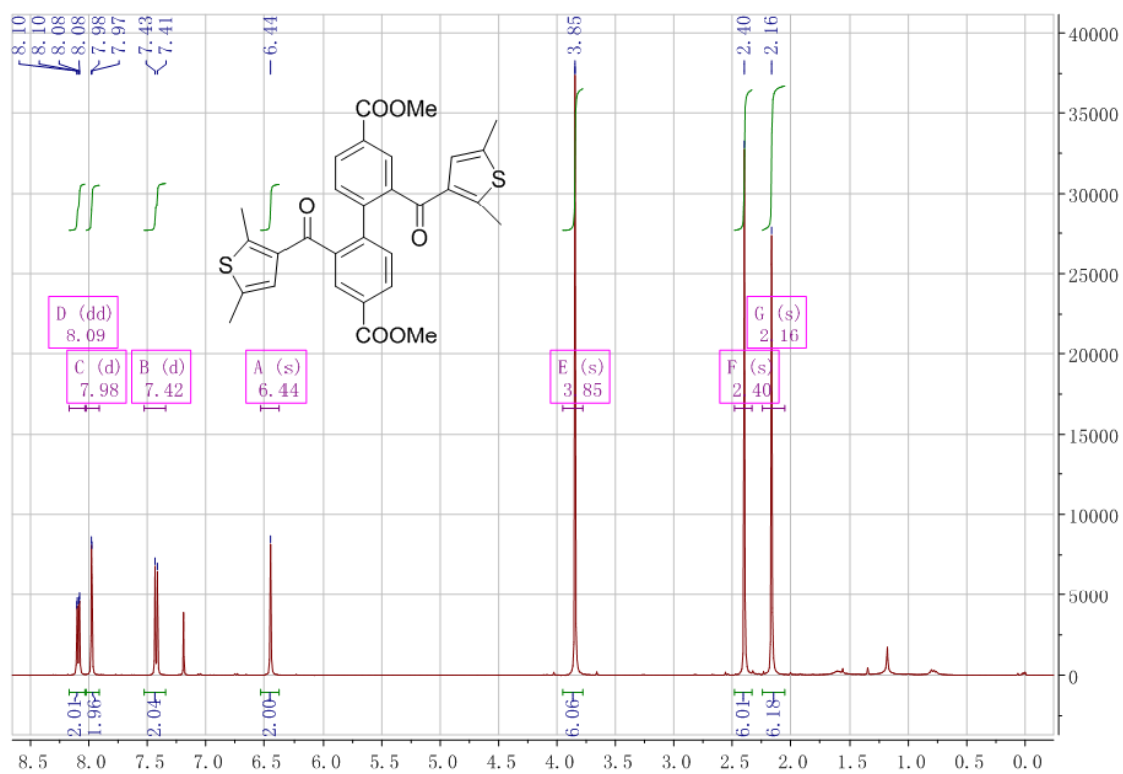


Fig. S16 ^1H NMR spectrum of 2,2'-bis(2,5-dimethylthiophene-3-carbonyl) biphenyl-4,4'-dicarboxylate(4).

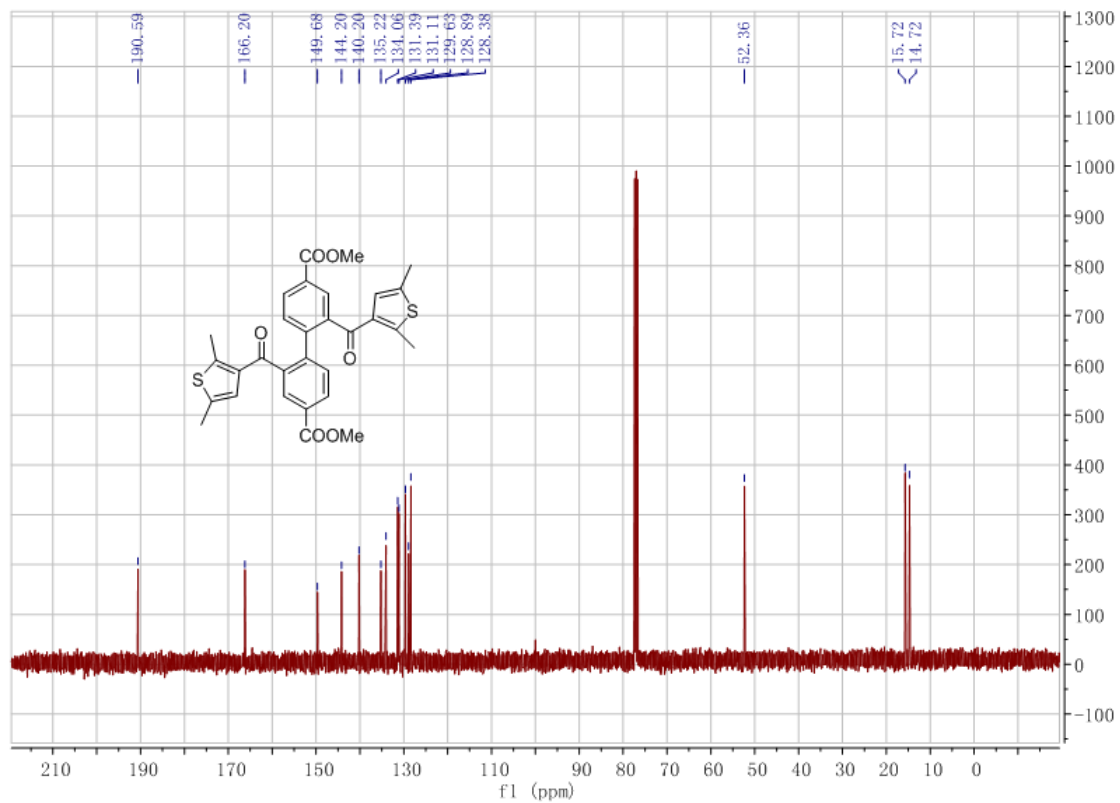


Fig. S17 ^{13}C NMR spectrum of 2,2'-bis(2,5-dimethylthiophene-3-carbonyl) biphenyl-4,4'-dicarboxylate(4).

Mass Spectrum List Report

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 Comment

Acquisition Date 5/30/2011 11:33:36 AM

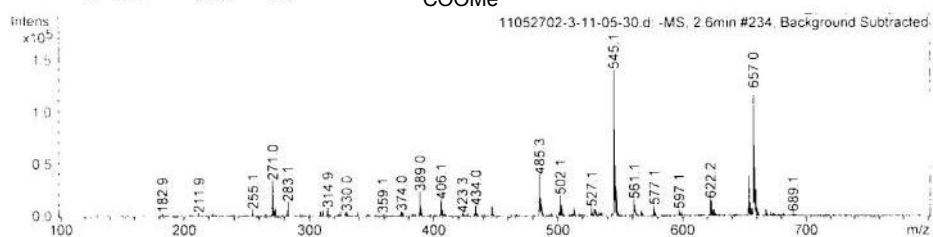
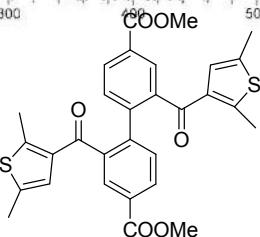
Operator xxr
 Instrument HCTplus

Acquisition Parameter

Ion Source Type ESI Ion Polarity Positive Alternating Ion Polarity on
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 Capillary Exit 129.6 Volt Skim 1 40.0 Volt Trap Drive 57.3
 Accumulation Time 132 μ s Averages 5 Spectra Auto MS/MS off



#	m/z	I	I%
1	230.2	108197	0.6
2	569.1	17514922	100.0
3	569.9	6132173	35.0
4	571.0	2788805	15.9
5	572.0	795052	4.5
6	573.0	110066	0.6
7	609.0	249412	1.4
8	637.2	103954	0.6
9	669.3	95651	0.5
10	682.1	93321	0.5



#	m/z	I	I%
1	271.0	34188	24.4
2	389.0	23741	16.9
3	485.3	39973	28.5
4	545.1	140360	100.0
5	546.0	48134	34.3
6	547.0	24527	17.5
7	653.2	39148	27.9
8	657.0	122247	87.1
9	658.0	46341	33.0
10	659.0	25375	18.1

Fig. S18 Mass spectrum of 2,2'-bis(2,5-dimethylthiophene-3-carbonyl) biphenyl-4,4'-dicarboxylate(4).

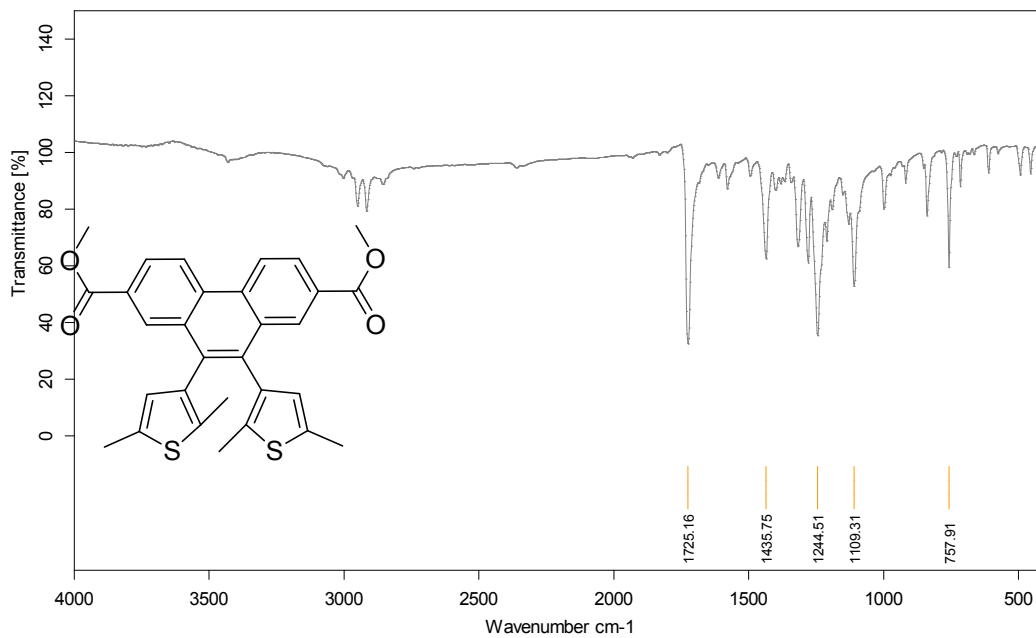


Fig. S19 IR spectrum of dimethyl 9, 10-bis(2,5-dimethylthiophen-3-yl)phenanthrene-2,7-dicarboxylate(5).

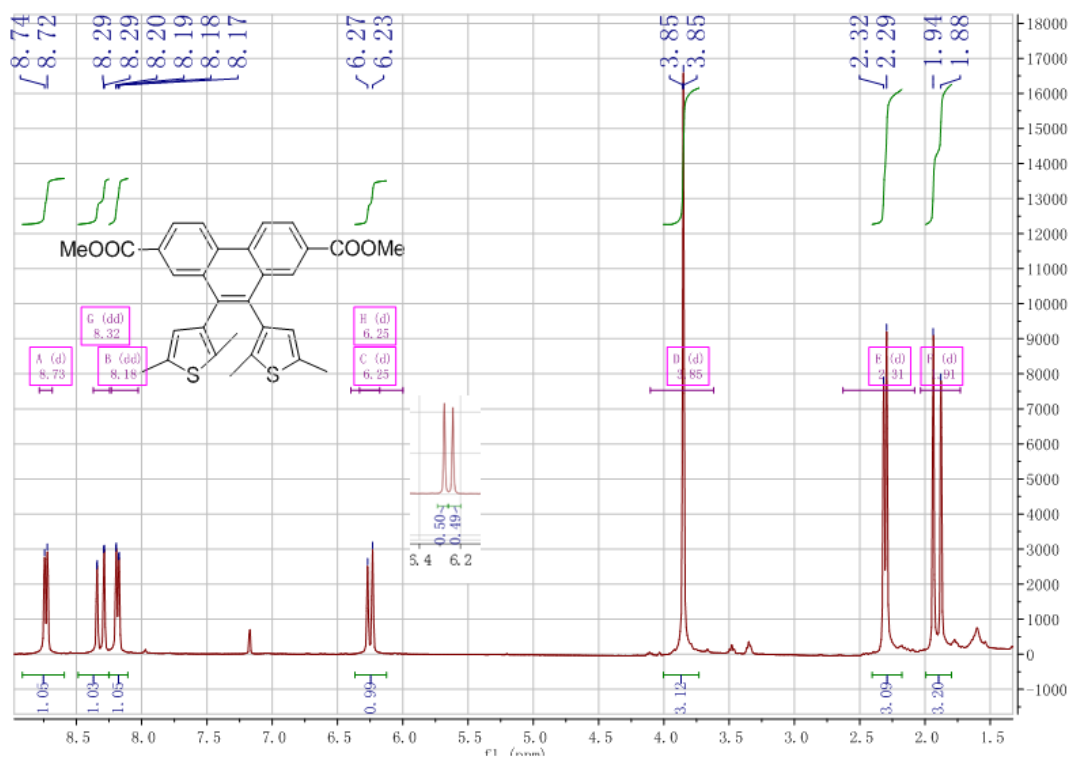


Fig. S20 ¹H NMR spectrum of dimethyl 9, 10-bis(2,5-dimethylthiophen-3-yl)phenanthrene-2,7-dicarboxylate(5). As the parallel and anti-parallel

form couldn't be isolated, the proton of thiophene shows two peaks at 6.2 -6.4 ppm and the integral is almost equal. It indicated that the quantity

of parallel form is equal to anti- parallel form.

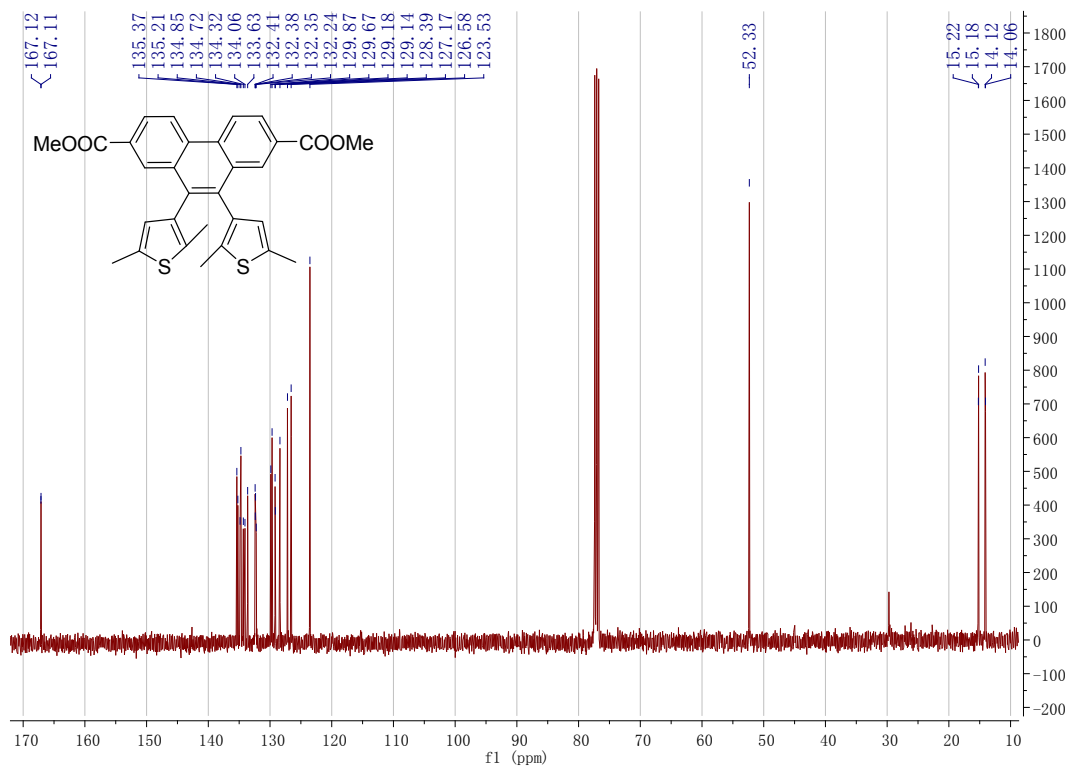


Fig. S21 ^{13}C NMR of dimethyl 9, 10-bis(2,5-dimethylthiophen-3-yl)phenanthrene-2,7-dicarboxylate(5).

Mass Spectrum List Report

Analysis Info

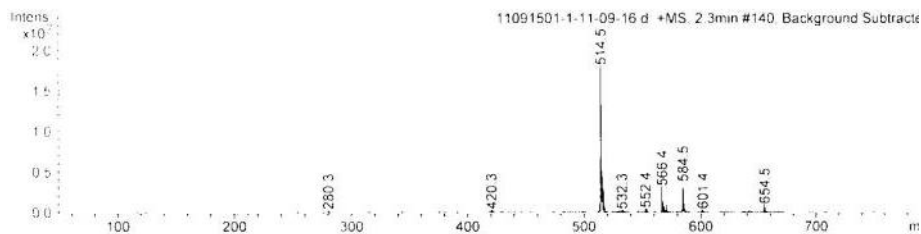
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 Sample Name 514
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Acquisition Date 9/16/2011 4:10:14 PM

Operator xxr
 Instrument HCTplus

Acquisition Parameter

Ion Source Type	APCI	Ion Polarity	Positive	Alternating Ion Polarity	on
Mass Range Mode	Ultra Scan	Scan Begin	50 m/z	Scan End	800 m/z
Capillary Exit	121.8 Volt	Skim 1	40.0 Volt	Trap Drive	62.7
Accumulation Time	6168 μ s	Averages	5 Spectra	Auto MS/MS	off



#	m/z	I	I%
1	513.4	1044814	5.8
2	514.5	18120532	100.0
3	515.4	5062228	27.9
4	516.4	2892374	16.0
5	566.4	3214742	17.7
6	567.4	1207509	6.7
7	570.3	962097	5.3
8	584.5	3756736	20.7
9	585.5	1068531	5.9
10	654.5	1016406	5.6

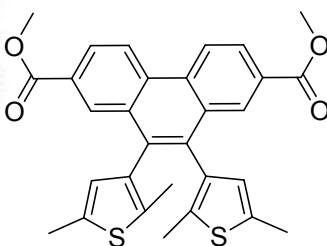


Fig. S22 Mass spectrum of dimethyl 9, 10-bis(2,5-dimethylthiophen-3-yl)phenanthrene-2,7-dicarboxylate(5)..

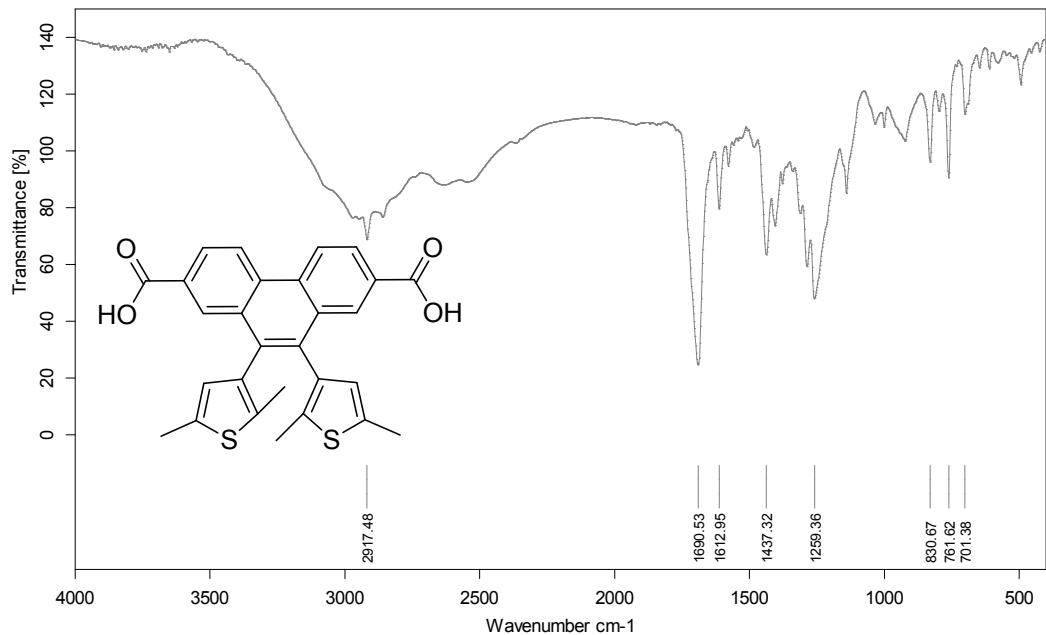


Fig. S23 IR spectrum of 9, 10-bis(2,5-dimethylthiophen-3-yl)phenanthrene-2,7-dicarboxylic acid(6).

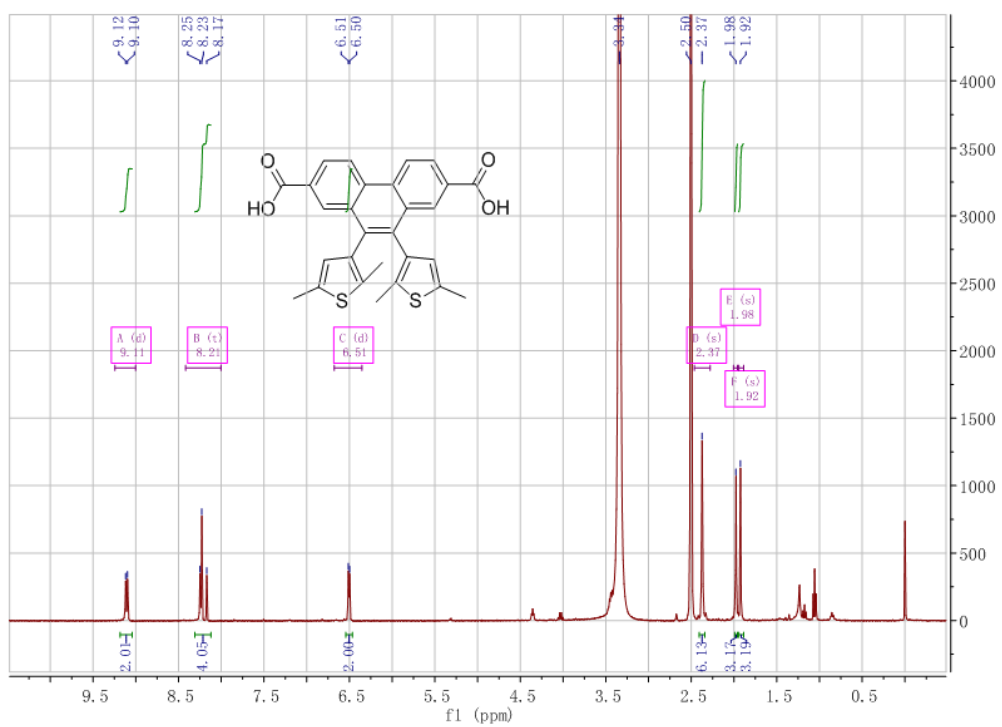


Fig. S24 ¹H NMR spectrum of 9, 10-bis(2,5-dimethylthiophen-3-yl)phenanthrene-2,7-dicarboxylic acid(6).

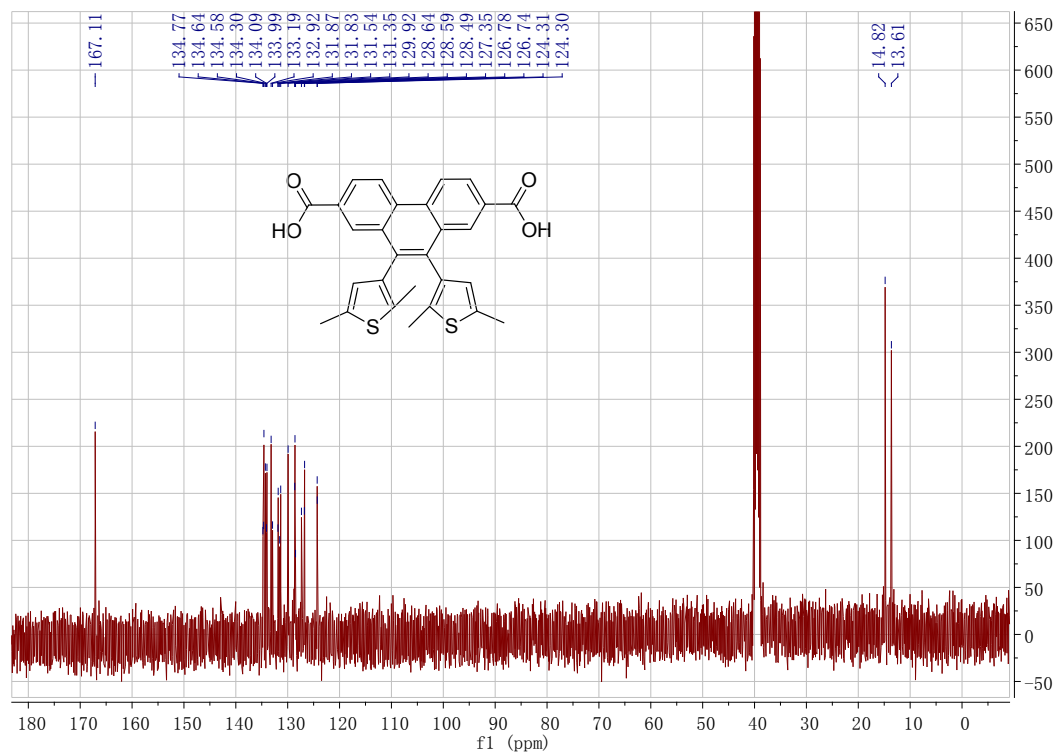


Fig. S25 ^{13}C NMR spectrum of 9, 10-bis(2,5-dimethylthiophen-3-yl)phenanthrene-2,7-dicarboxylic acid(6).

Mass Spectrum List Report

Analysis Info

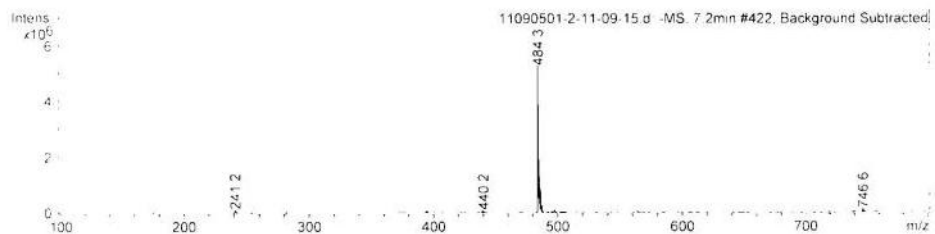
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Method 11090901.M
Sample Name 486
Comment

Acquisition Date 9/15/2011 4:02:07 PM

Operator xxr
Instrument HCTplus

Acquisition Parameter

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Mass Range Mode	Ultra Scan	Scan Begin	100 m/z	Scan End	800 m/z
Capillary Exit	-120.2 Volt	Skim 1	-40.0 Volt	Trap Drive	67.3
Accumulation Time	58030 μ s	Averages	5 Spectra	Auto MS/MS	off



#	m/z	I	I%
1	241.2	115617	2.2
2	439.2	72052	1.4
3	440.2	91756	1.7
4	484.3	5265583	100.0
5	485.2	1871755	35.5
6	486.3	850121	16.1
7	487.3	254777	4.8
8	497.4	110717	2.1
9	746.6	131679	2.5
10	747.8	67325	1.3

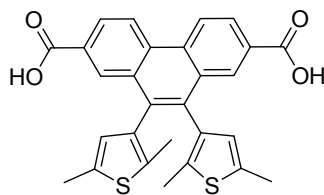


Fig. S26 Mass spectrum of 9,10-bis(2,5-dimethylthiophen-3-yl)phenanthrene-2,7-dicarboxylic acid(6).

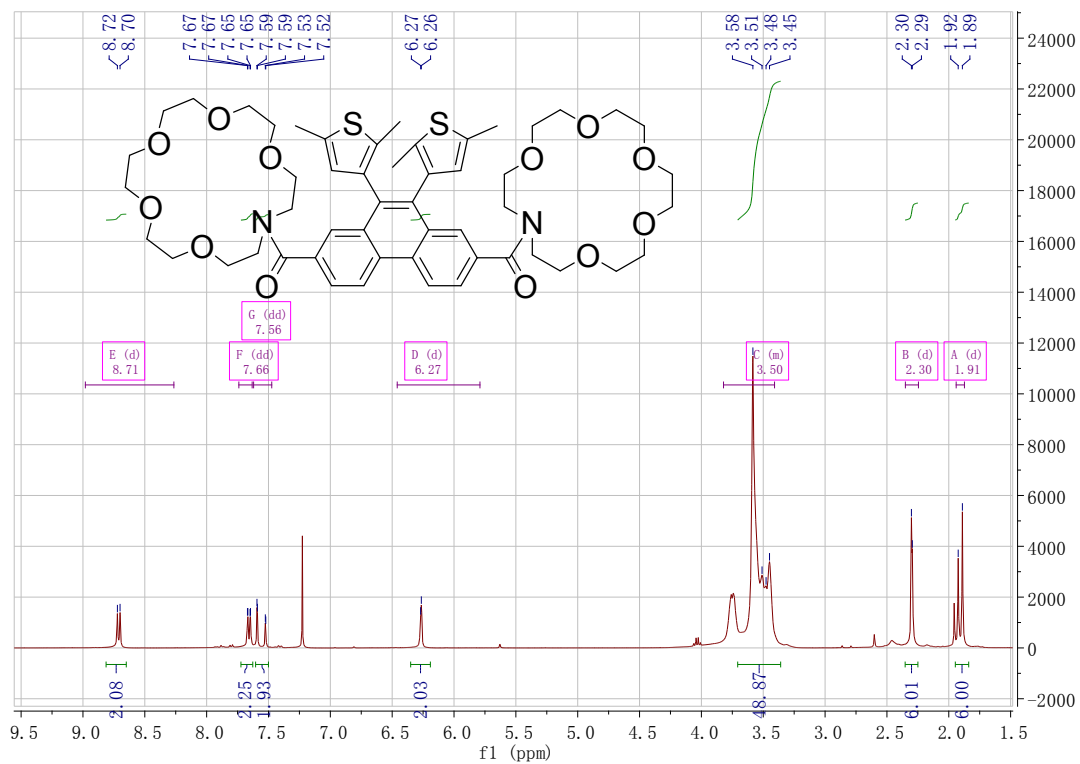


Fig. S 27 ¹H NMR spectrum of **PBC**

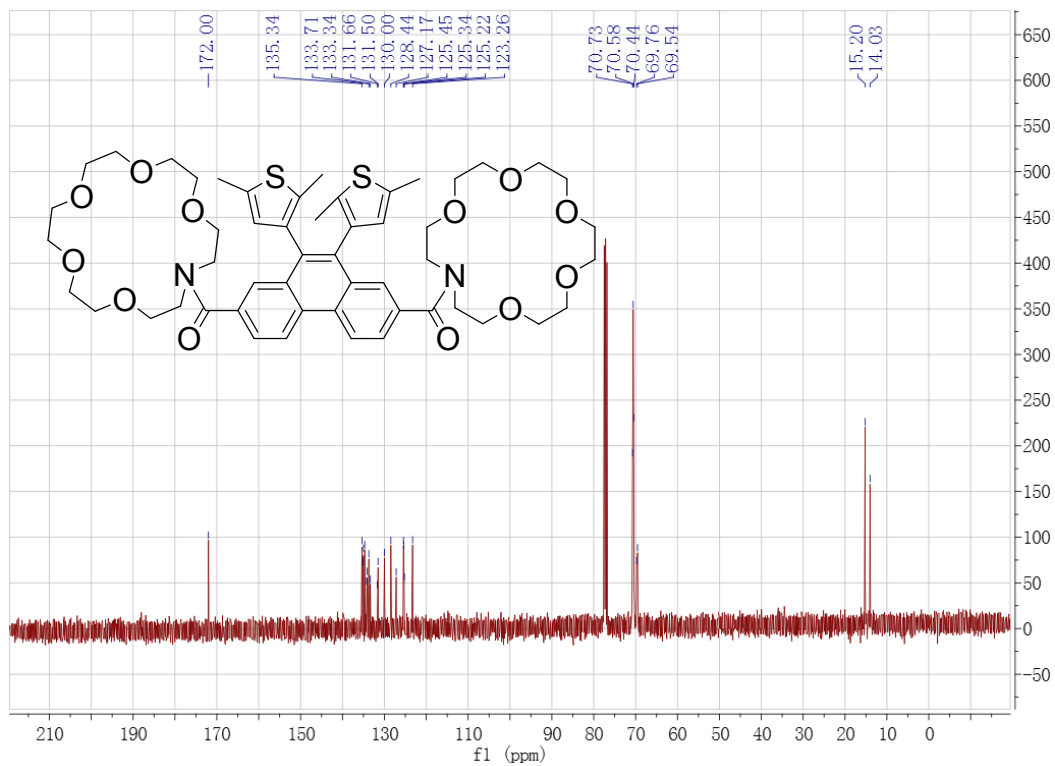


Fig. S 28 ¹³C NMR spectrum of PBC

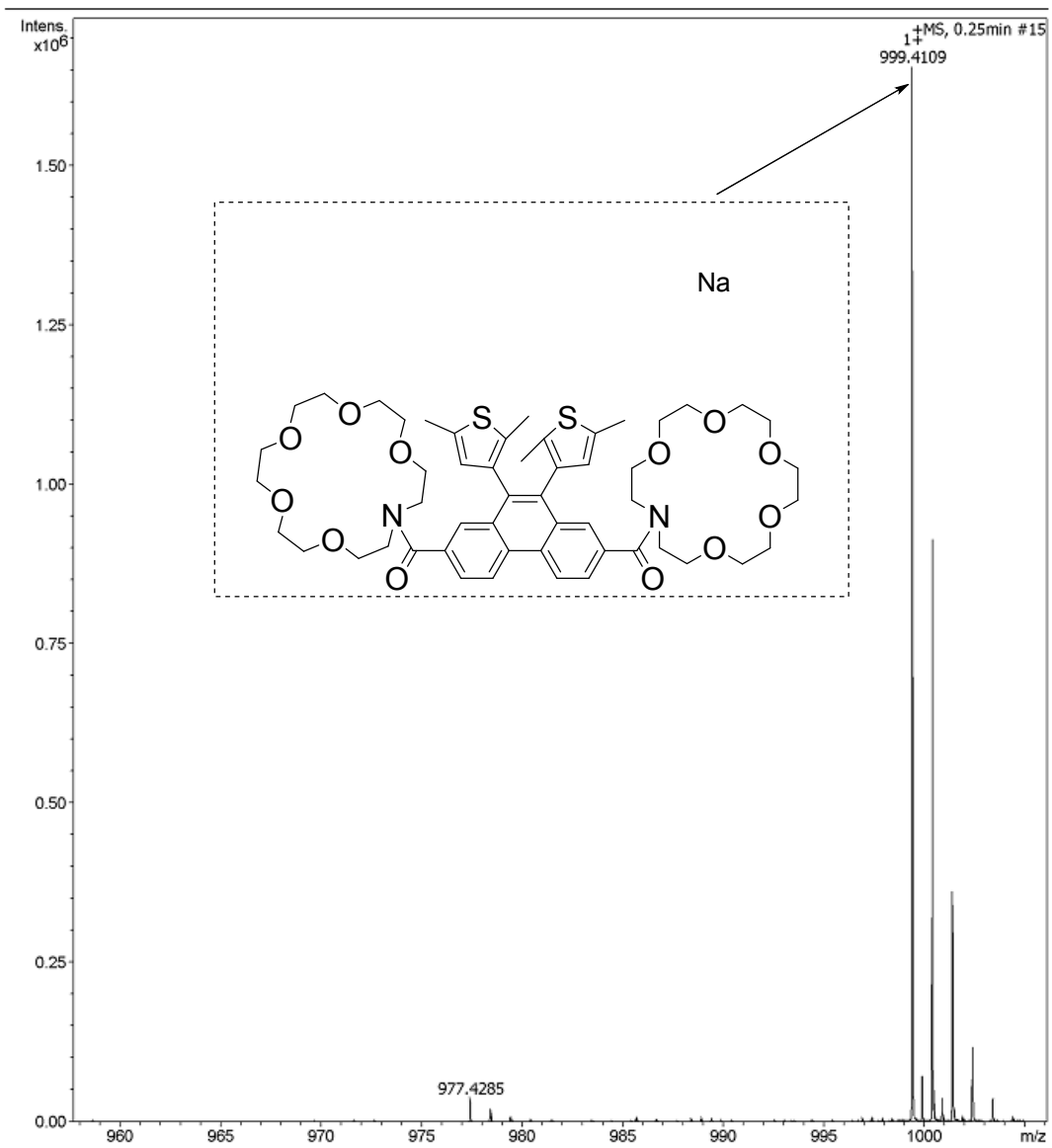


Fig. S 29 HRMS spectrum of **PBC**