

Electronic Supplementary Information (ESI)

Dimethylamine Substituted Bisbenzocoumarins: Solvatochromic, Mechanochromic and Acidochromic properties

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Table 1 Crystal data and structure refinement for DB-C2.

Empirical formula	C ₃₆ H ₃₂ N ₂ O ₈
Formula weight	620.63
Temperature/K	100.00(10)
Crystal system	monoclinic
Space group	C2/c
a/Å	29.9695(15)
b/Å	8.1566(5)
c/Å	12.1516(7)
α/°	90
β/°	90.466(5)
γ/°	90
Volume/Å ³	2970.3(3)
Z	4
ρ _{calc} g/cm ³	1.388
μ/mm ⁻¹	0.813
F(000)	1304.0
Crystal size/mm ³	0.14 × 0.13 × 0.12
Radiation	CuKα ($\lambda = 1.54184$)
2Θ range for data collection/°	5.898 to 146.762
Index ranges	-37 ≤ h ≤ 28, -9 ≤ k ≤ 10, -14 ≤ l ≤ 13
Reflections collected	5681
Independent reflections	2896 [R _{int} = 0.0489, R _{sigma} = 0.0520]
Data/restraints/parameters	2896/0/215
Goodness-of-fit on F ²	1.023
Final R indexes [I>=2σ (I)]	R ₁ = 0.0743, wR ₂ = 0.2221
Final R indexes [all data]	R ₁ = 0.0909, wR ₂ = 0.2329
Largest diff. peak/hole / e Å ⁻³	0.46/-0.40

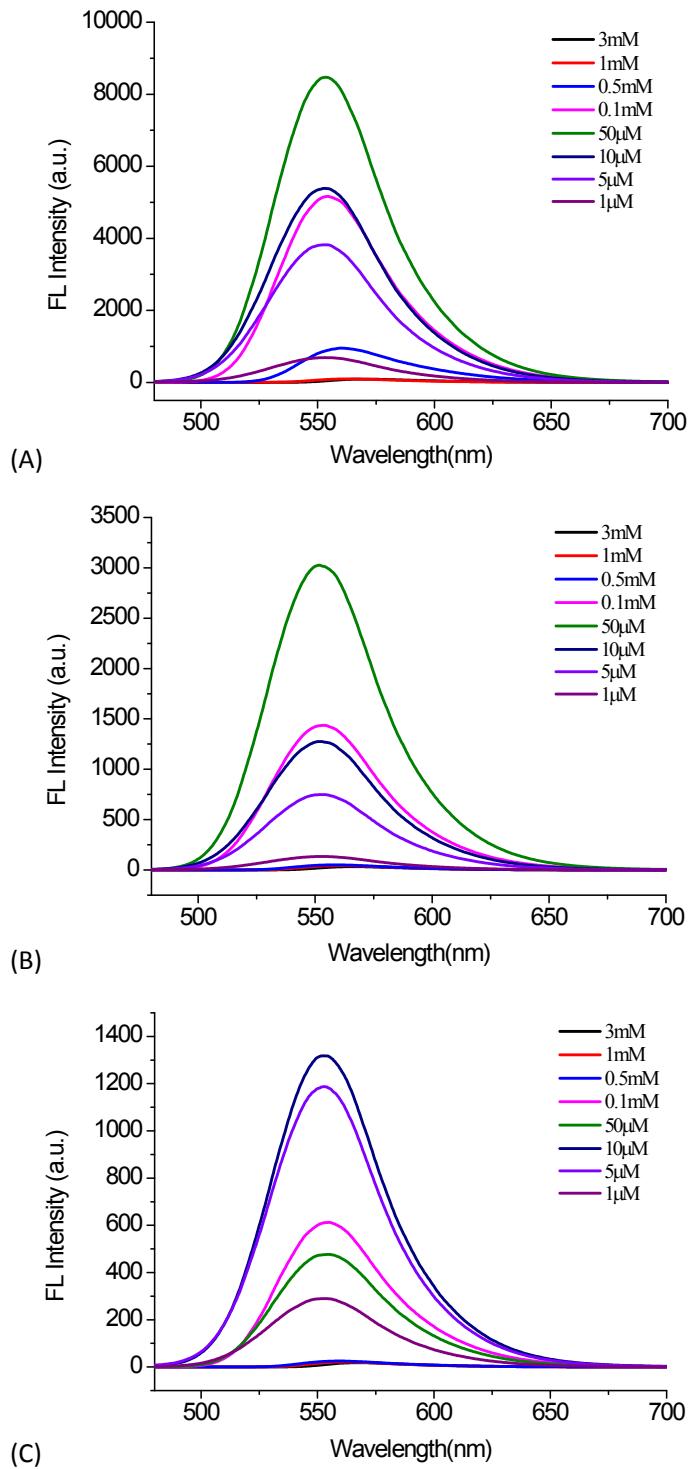


Figure S1 FL emission spectra in DCM with increasing concentrations.

(A) Spectra of **DB-C2**, (B) Spectra of **DB-C6**, (C) Spectra of **DB-C12**,
concentration range: 1 μ M – 3 mM, $\lambda_{\text{ex}} = 415$ nm.

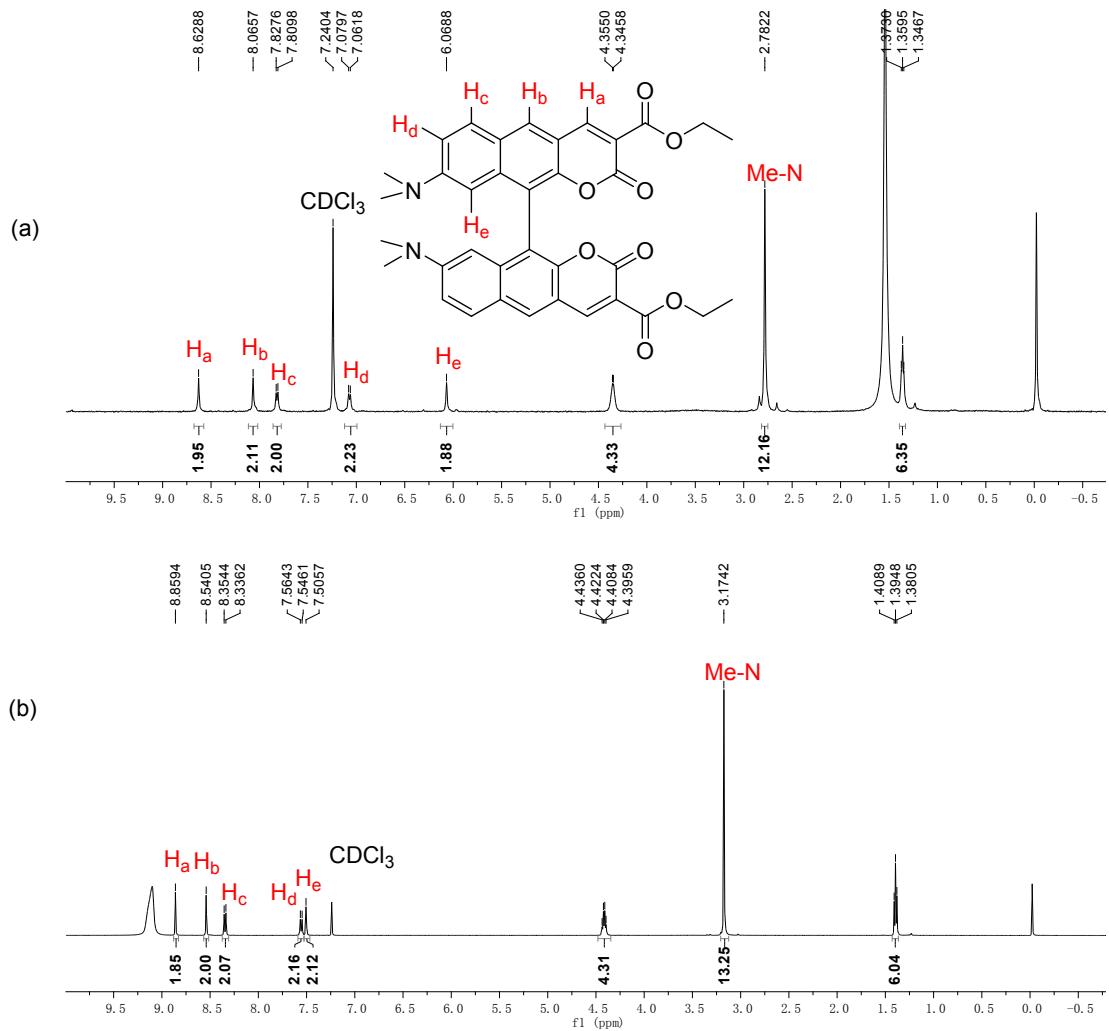


Figure S2 The control ^1H NMR experiment. (a) The ^1H NMR spectra of **DB-C2** in CDCl_3 . (b) The ^1H NMR spectra of **DB-C2** with trifluoroacetic acid (10 eq.) in CDCl_3 .

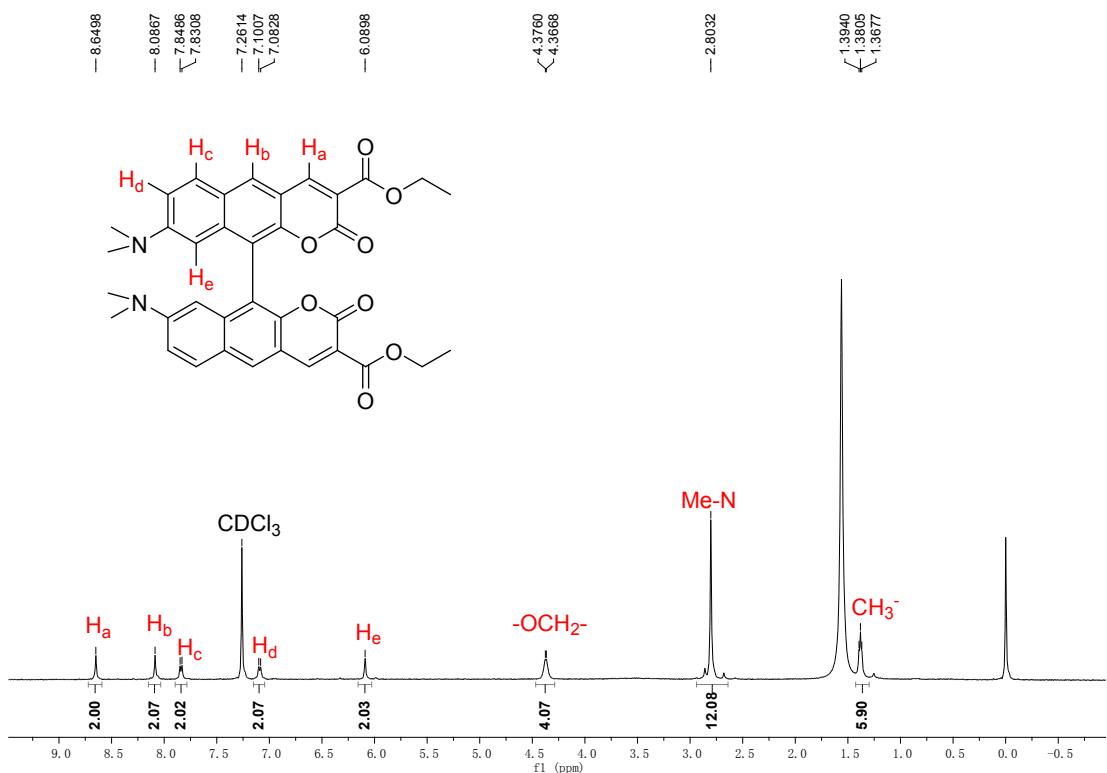


Figure S3 ^1H NMR of **DB-C2** in CDCl_3 .

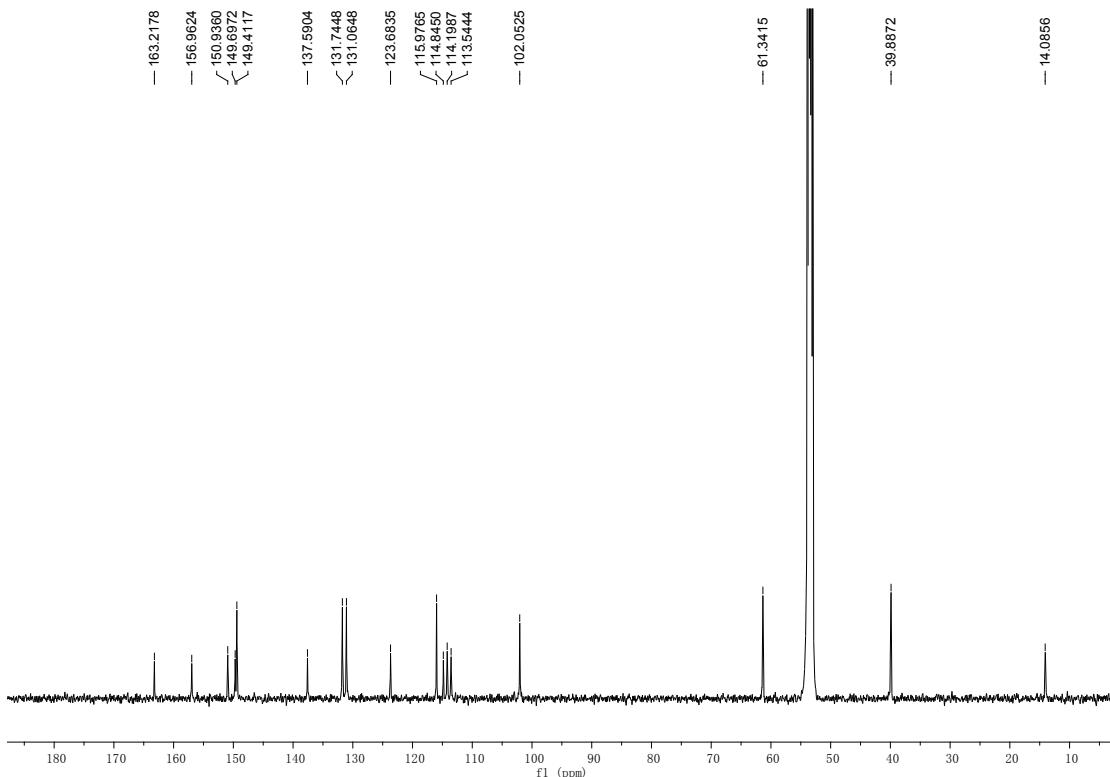


Figure S4 ^{13}C NMR of **DB-C2** in CD_2Cl_2 .

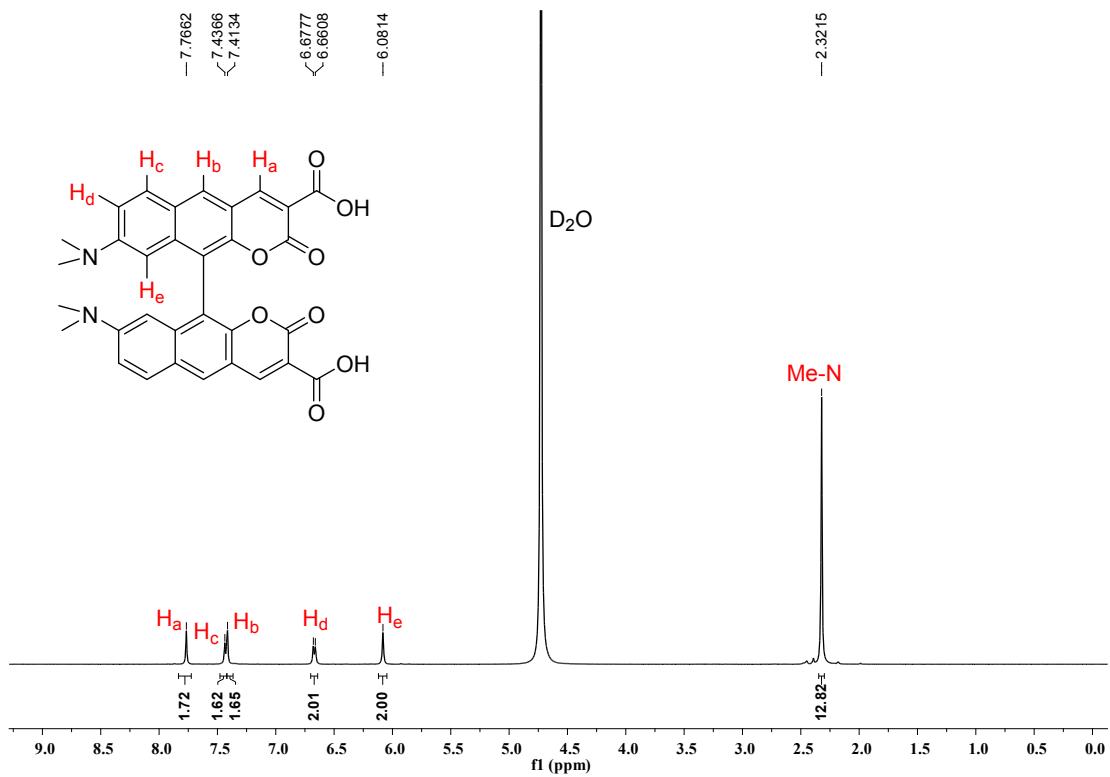


Figure S5 ¹H NMR of **2** in D₂O.

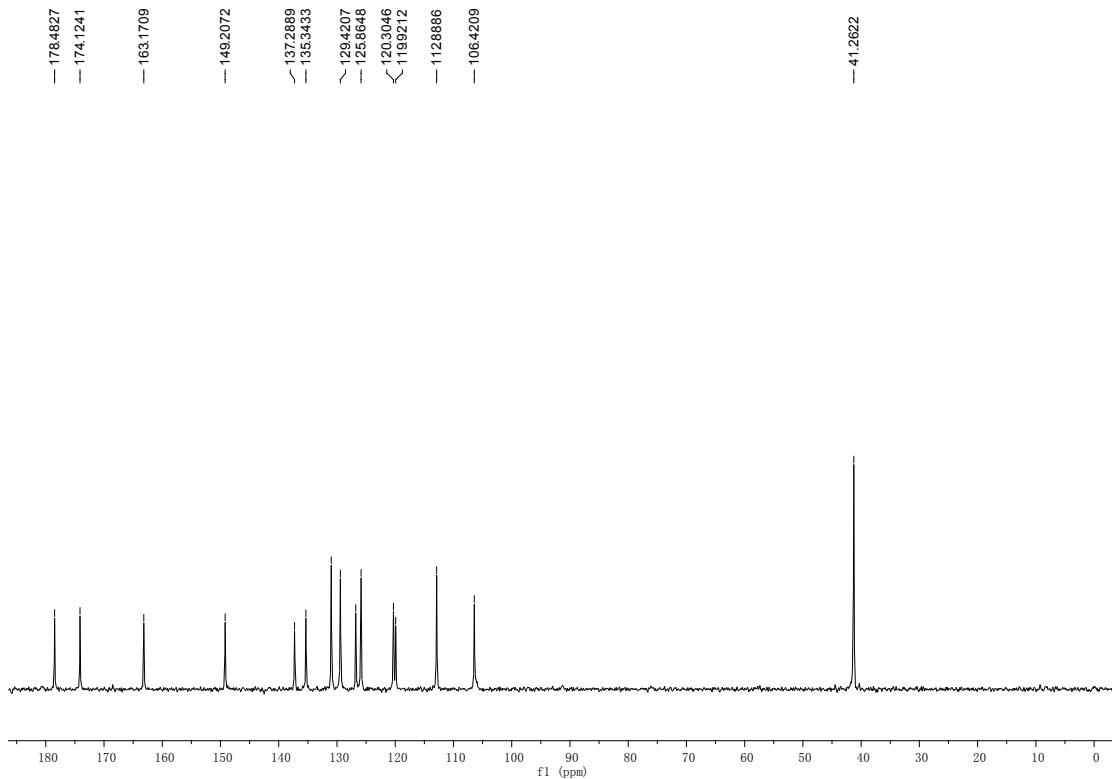


Figure S6 ¹³C NMR of **2** in D₂O.

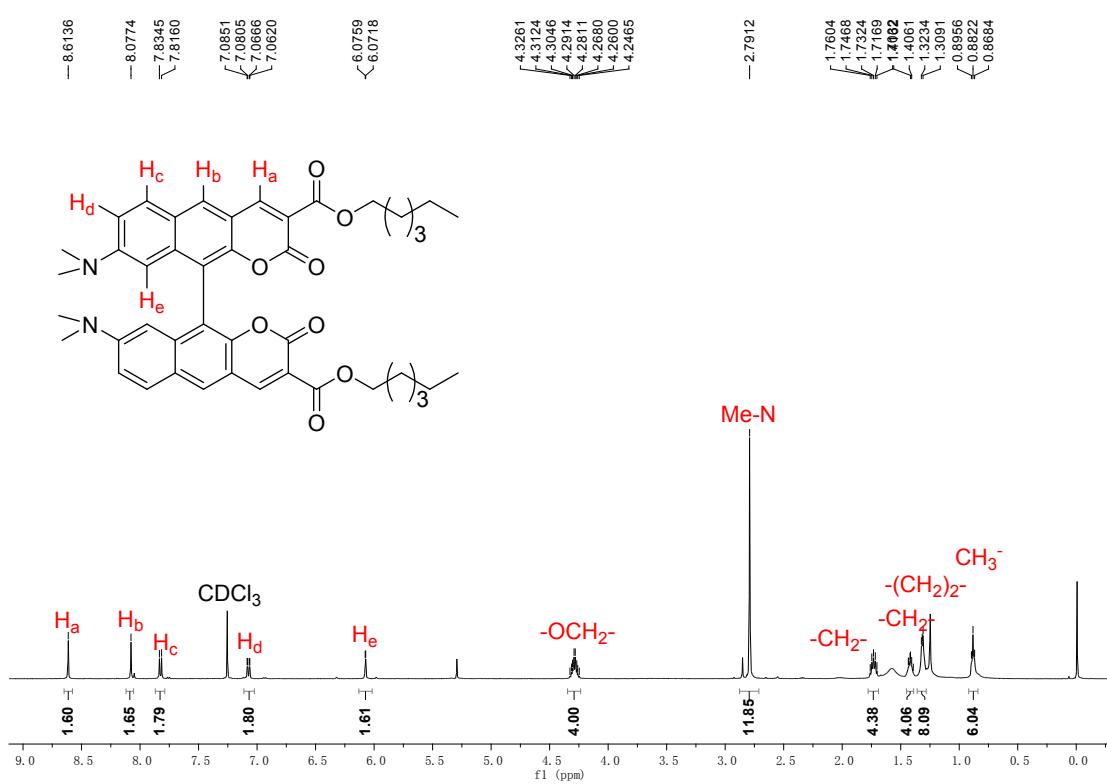


Figure S7 ^1H NMR of DB-C6 in CDCl₃.

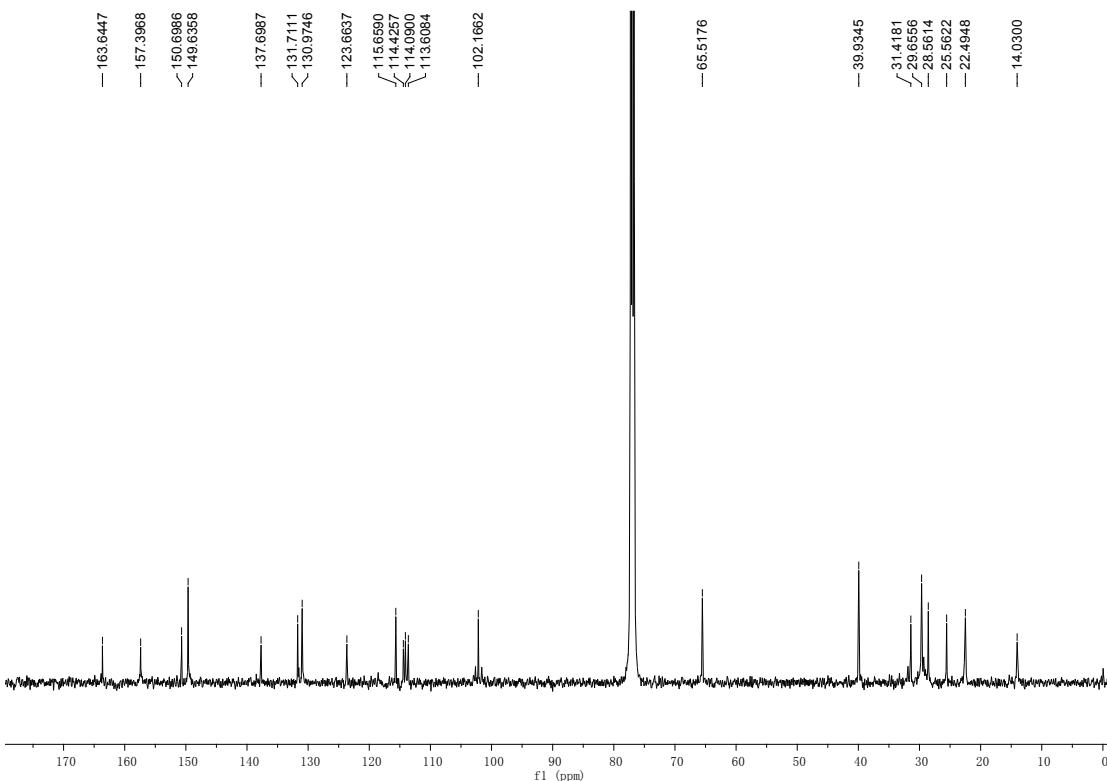


Figure S8 ^{13}C NMR of DB-C6 in CDCl₃.

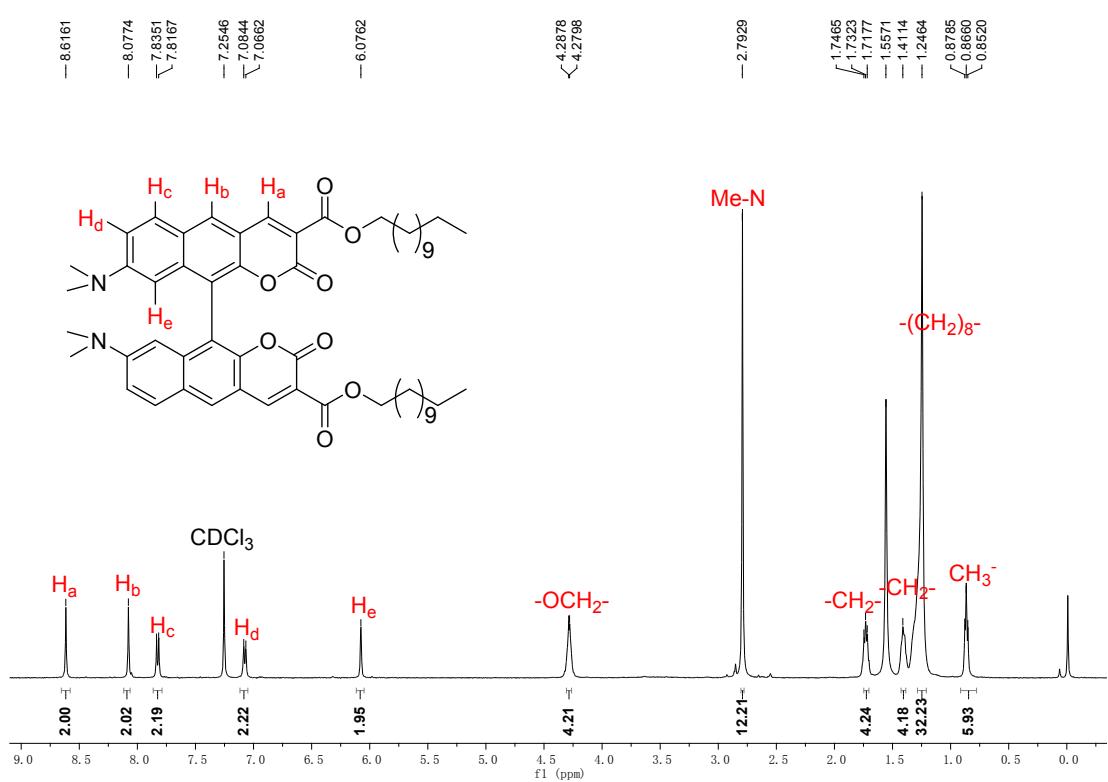


Figure S9 ^1H NMR of **DB-C12** in CDCl₃.

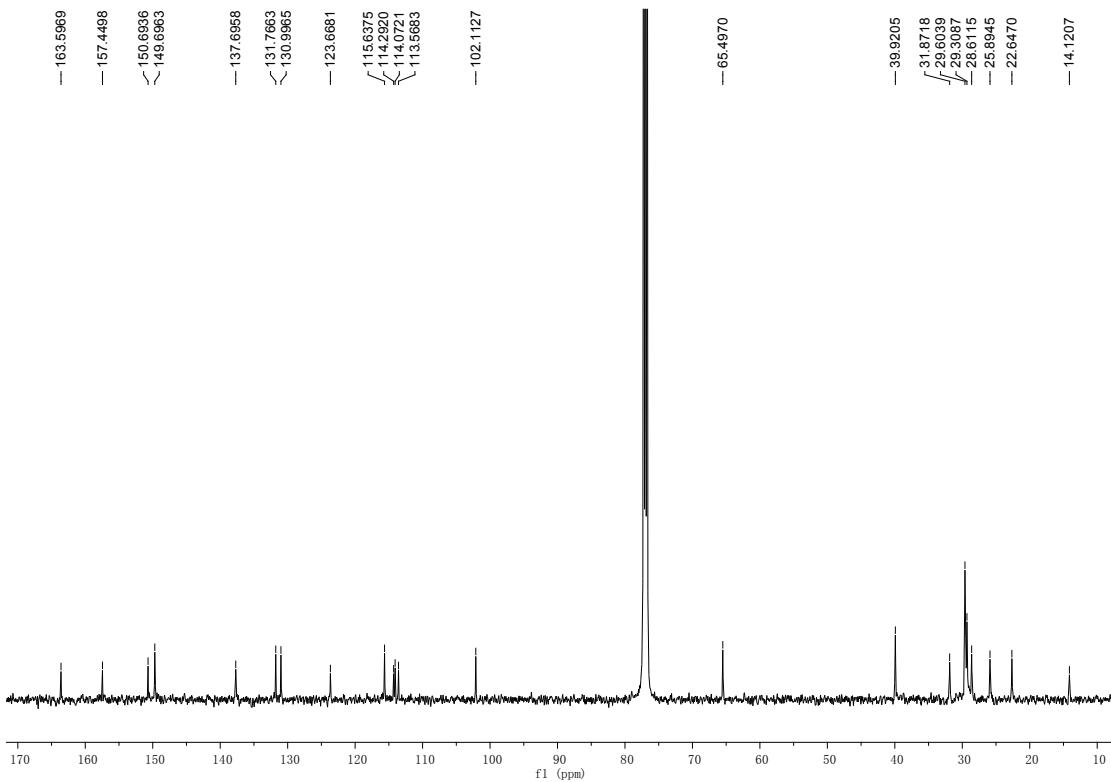


Figure S10 ^{13}C NMR of **DB-C12** in CDCl₃