Supporting Information

C-Shaped Diastereomers Containing Cofacial Thiophene-Substituted Quinoxaline Rings: Synthesis, Photophysical Properties, and X-ray Crystallography.

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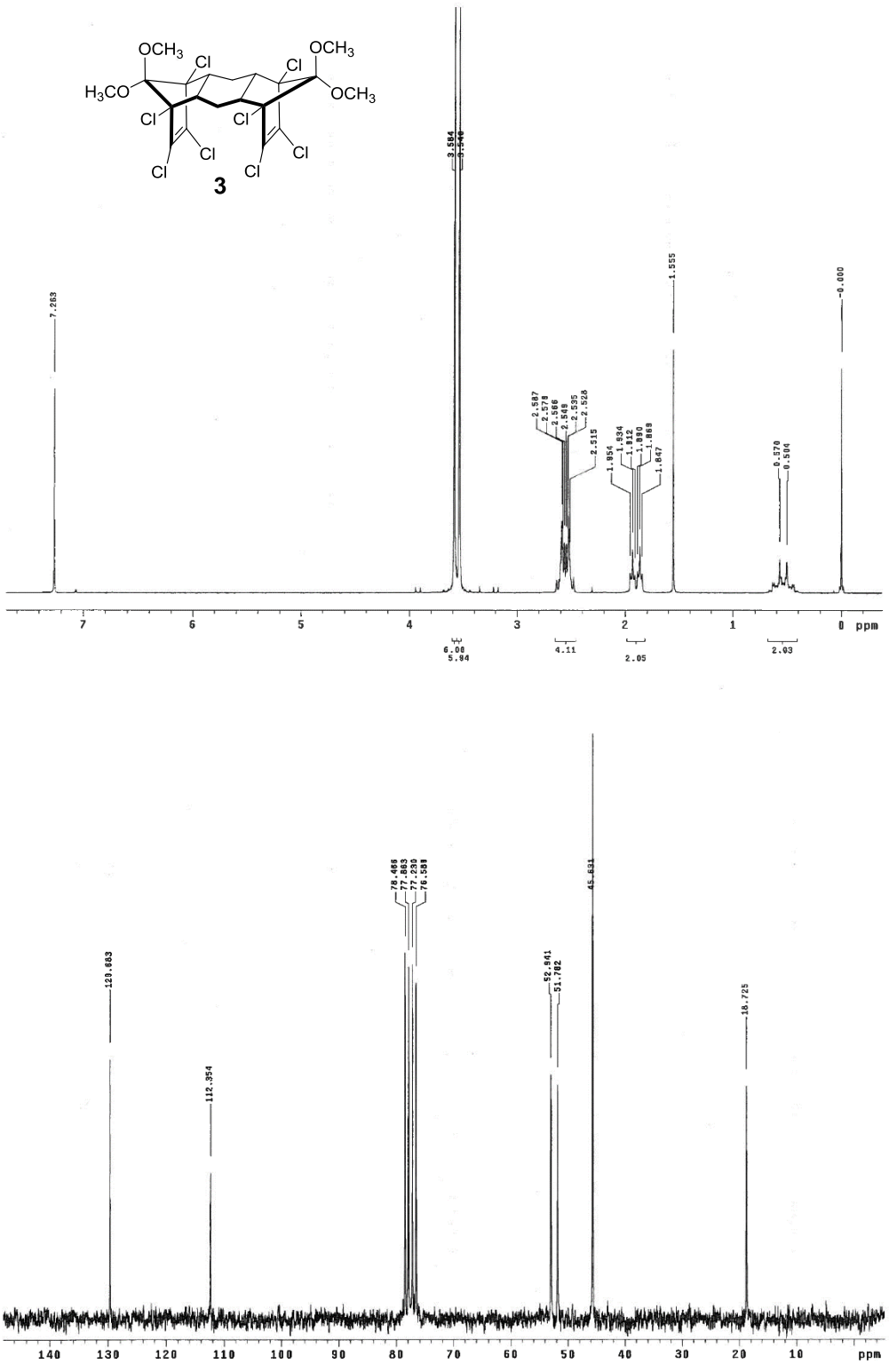


Figure S-1. ^{1}H (200 MHz, $CDCl_3$) and ^{13}C (50 MHz, $CDCl_3$) NMR spectra of **3**.

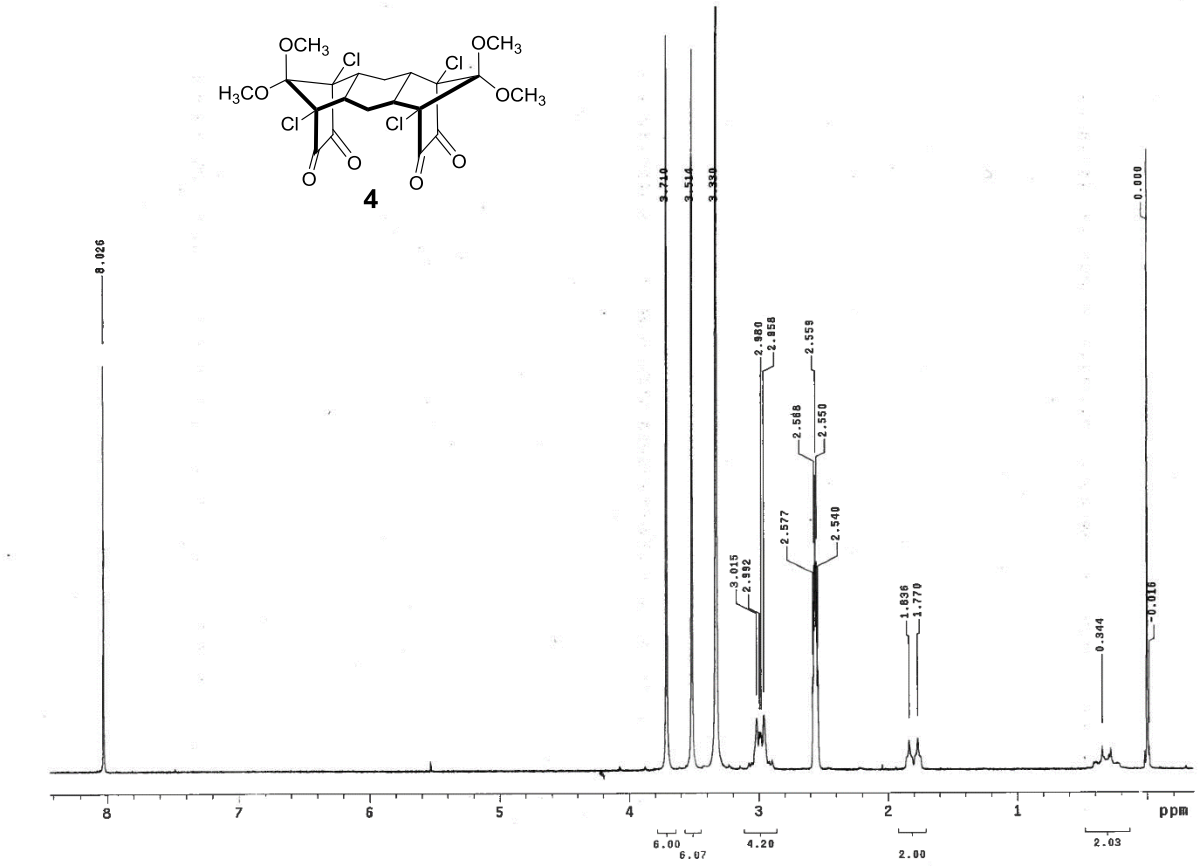


Figure S-2. ^{1}H NMR spectrum of **4** (200 MHz; 50:50 mixture of DMSO-d_6 and $CDCl_3$).

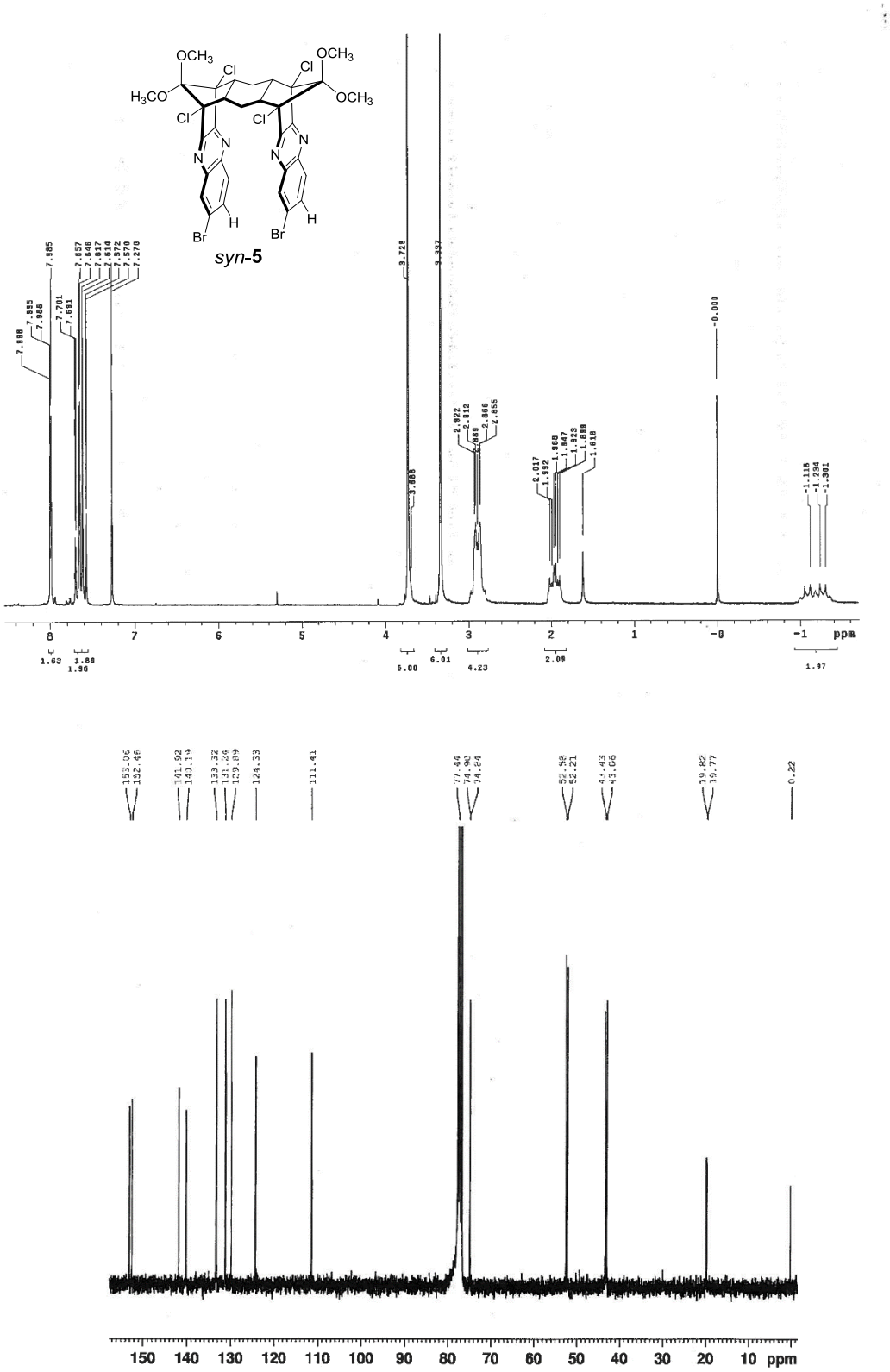


Figure S-3. ^{1}H (200 MHz, $CDCl_3$) and ^{13}C (75 MHz, $CDCl_3$) NMR spectra of *syn*-**5**.

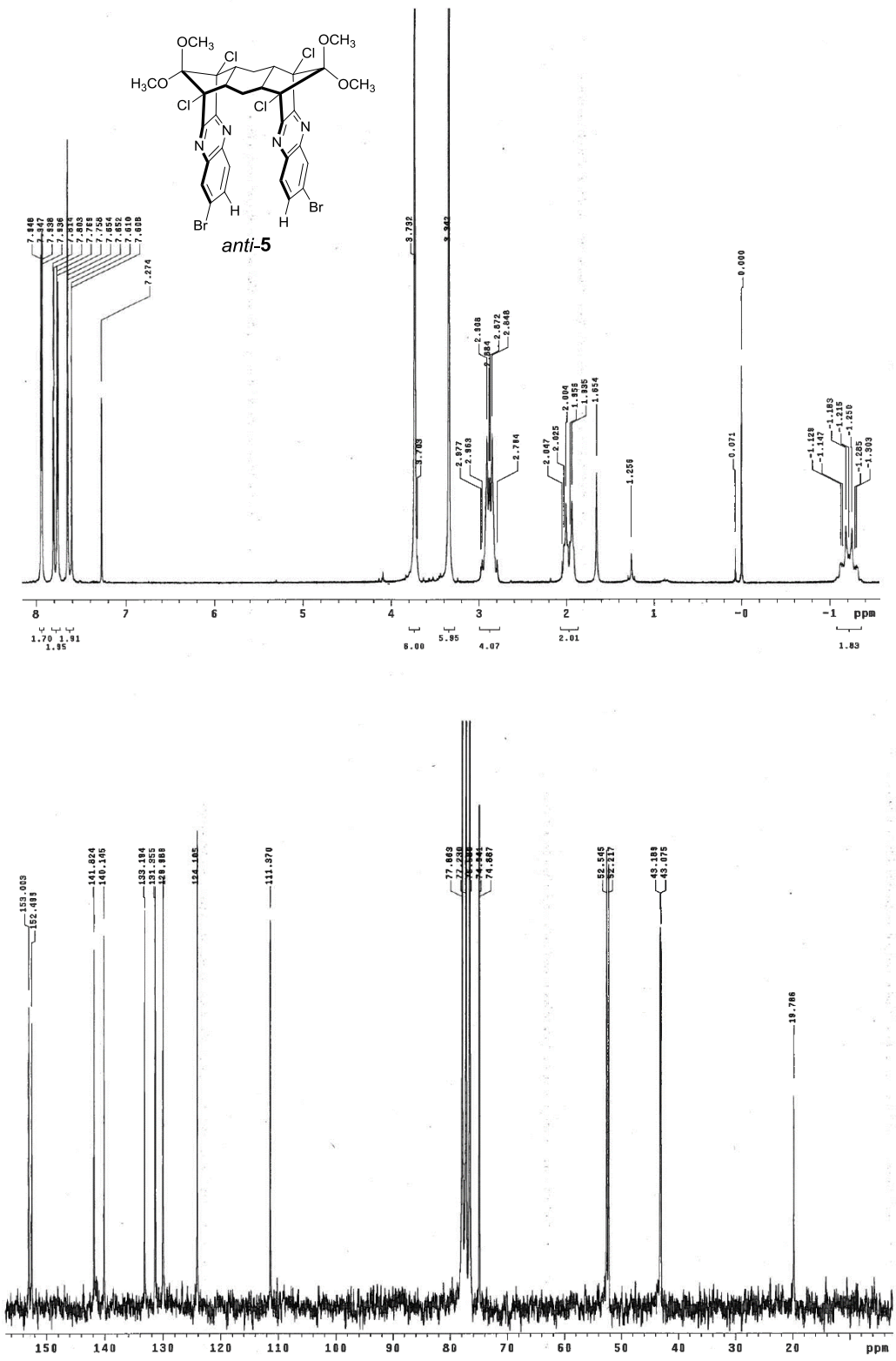
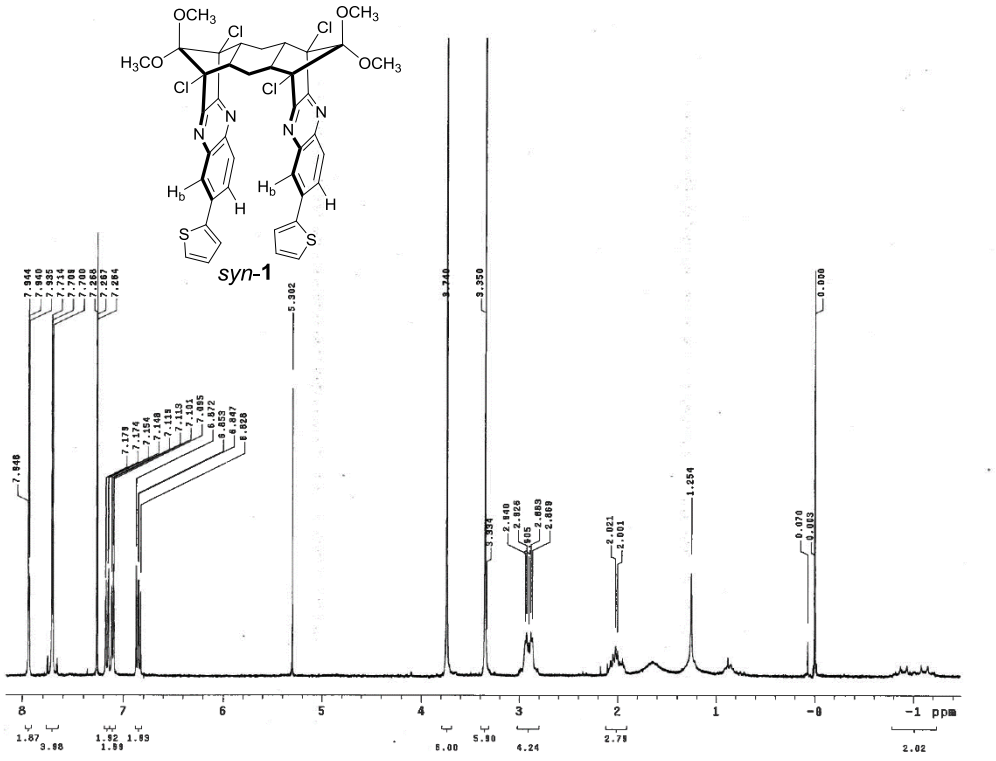


Figure S-4. ^{1}H (200 MHz, $CDCl_3$) and ^{13}C (50 MHz, $CDCl_3$) NMR spectra of *anti*-**5**.

(a)



(b)

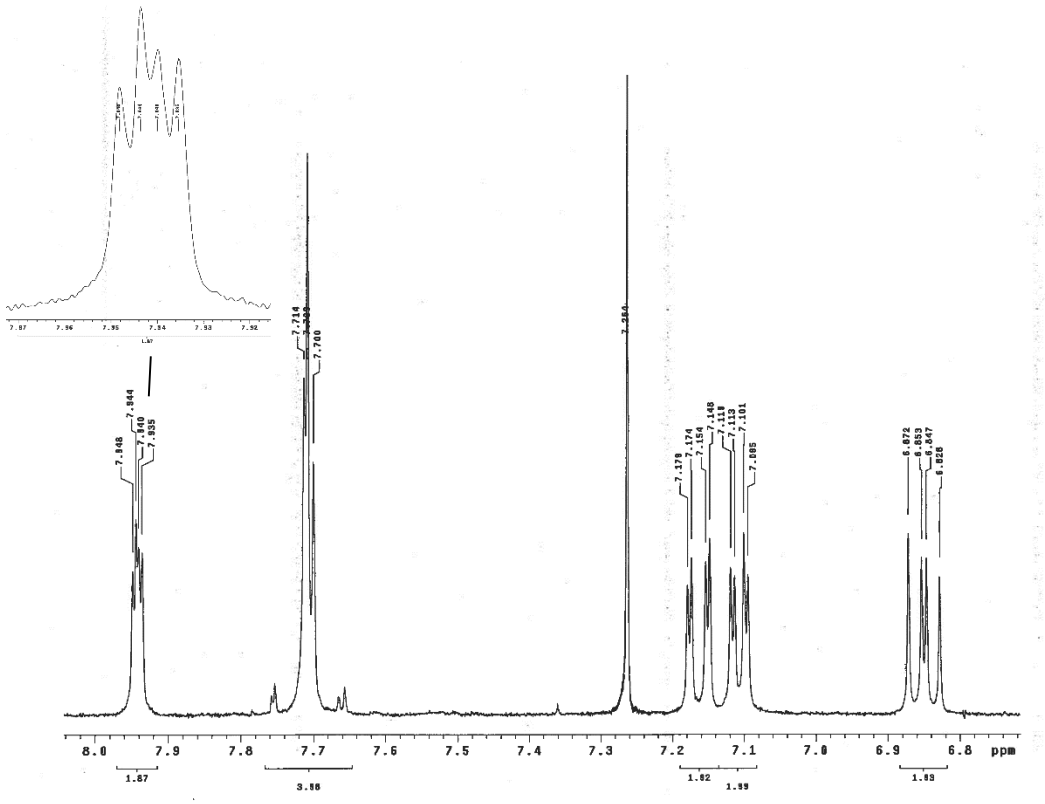


Figure S-5. ^{1}H (200 MHz; $CDCl_3$) NMR spectrum of *syn*-**1** (a) full spectrum, (b) aromatic region with expanded multiplet inset.

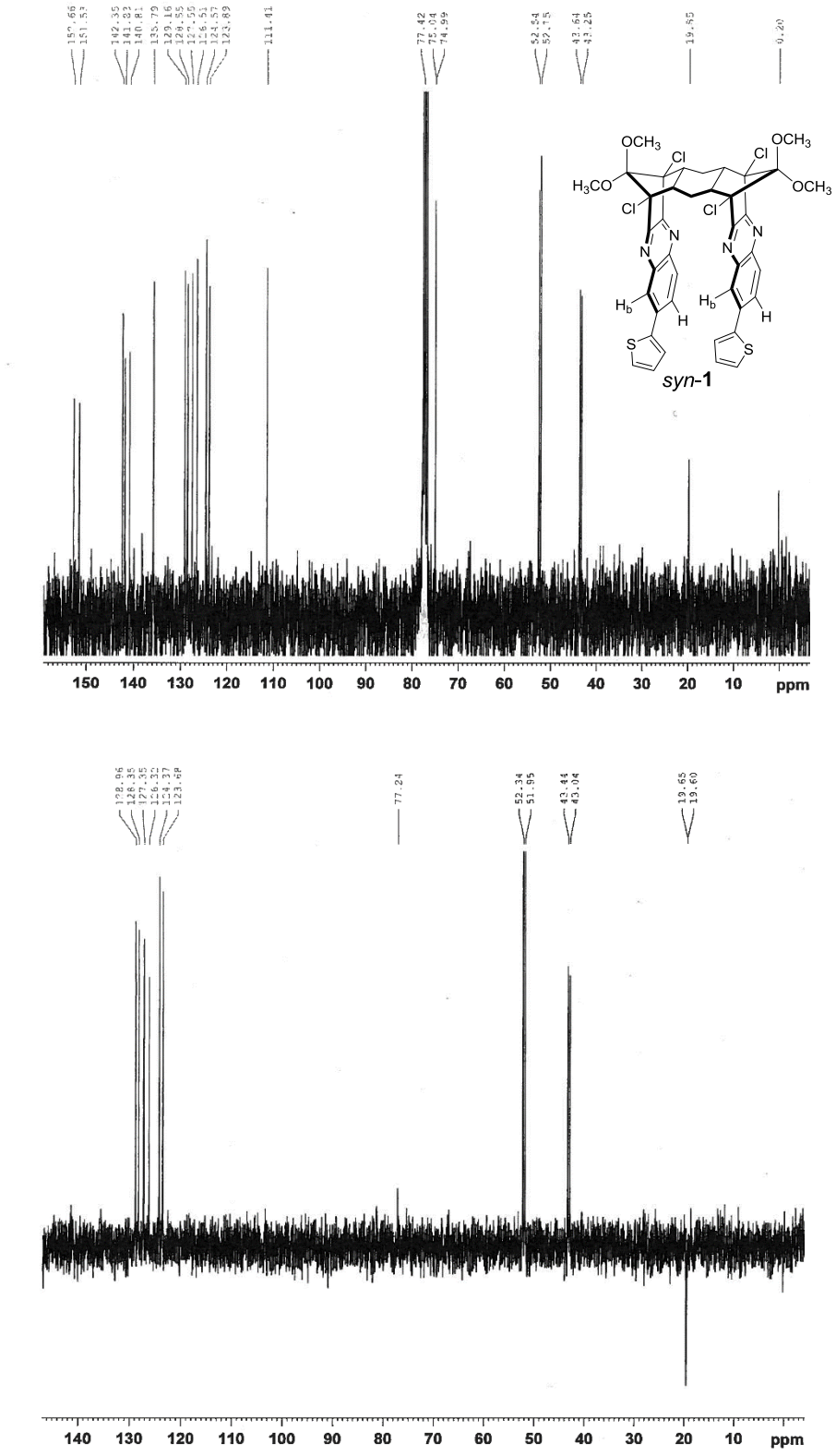


Figure S-6. ^{13}C NMR and DEPT 135 (75 MHz; $CDCl_3$) spectra of *syn*-**1**.

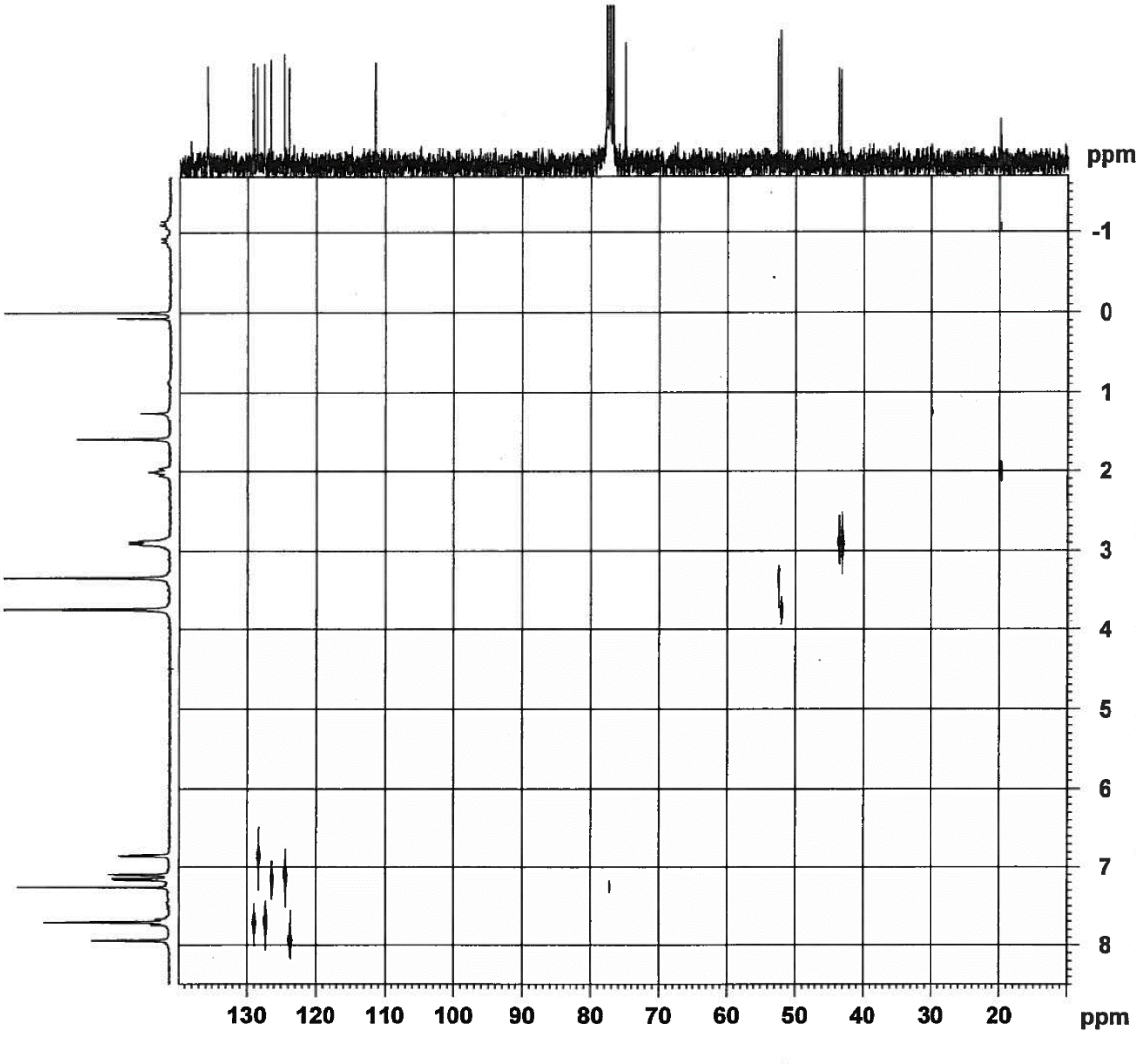


Figure S-7. HETCOR spectrum of *syn*-**1** (75 MHz; $CDCl_3$).

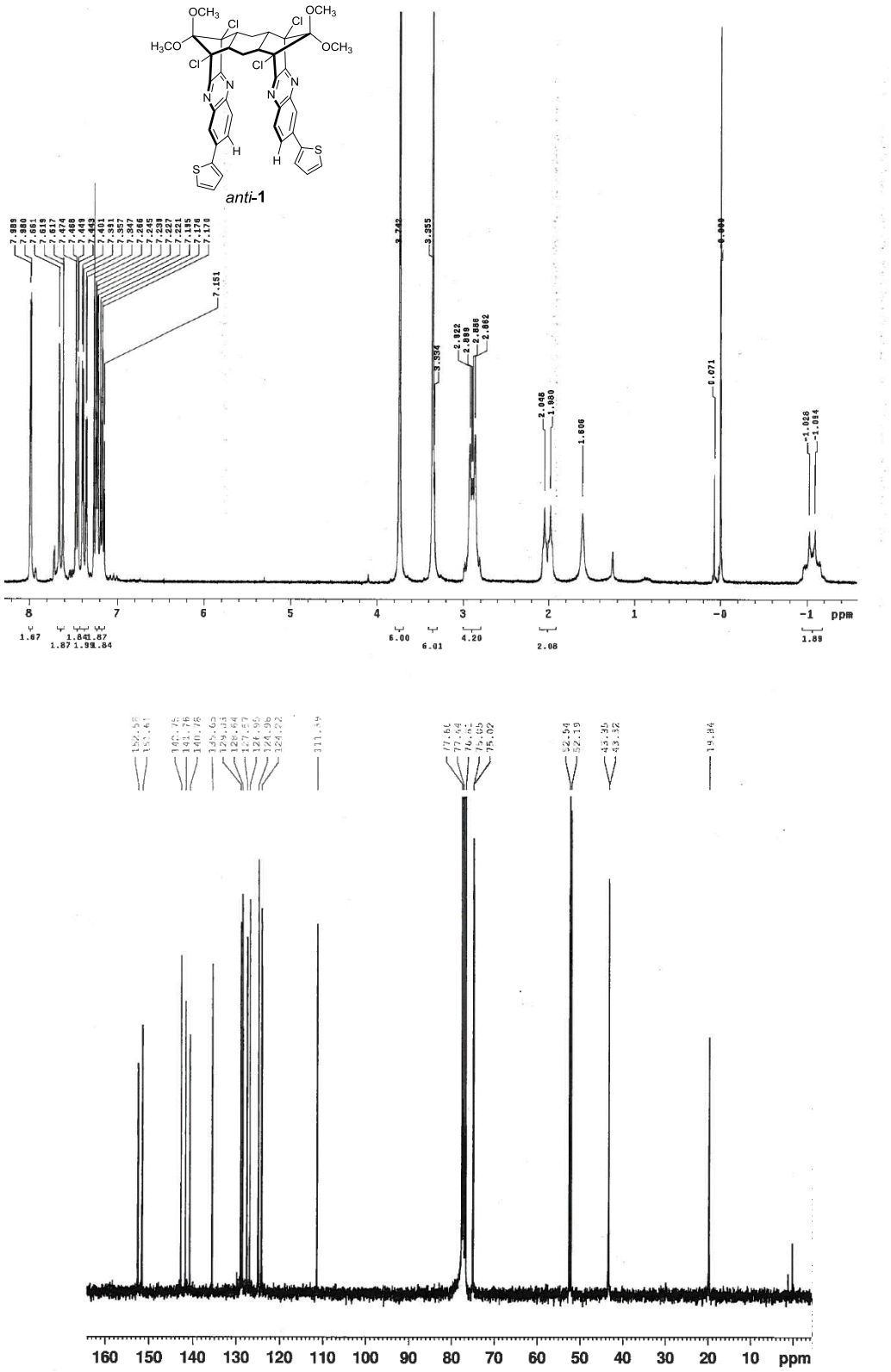


Figure S-8. ^{1}H (200 MHz; $CDCl_3$) and ^{13}C (75 MHz; $CDCl_3$) NMR spectra of *anti*-**1**.

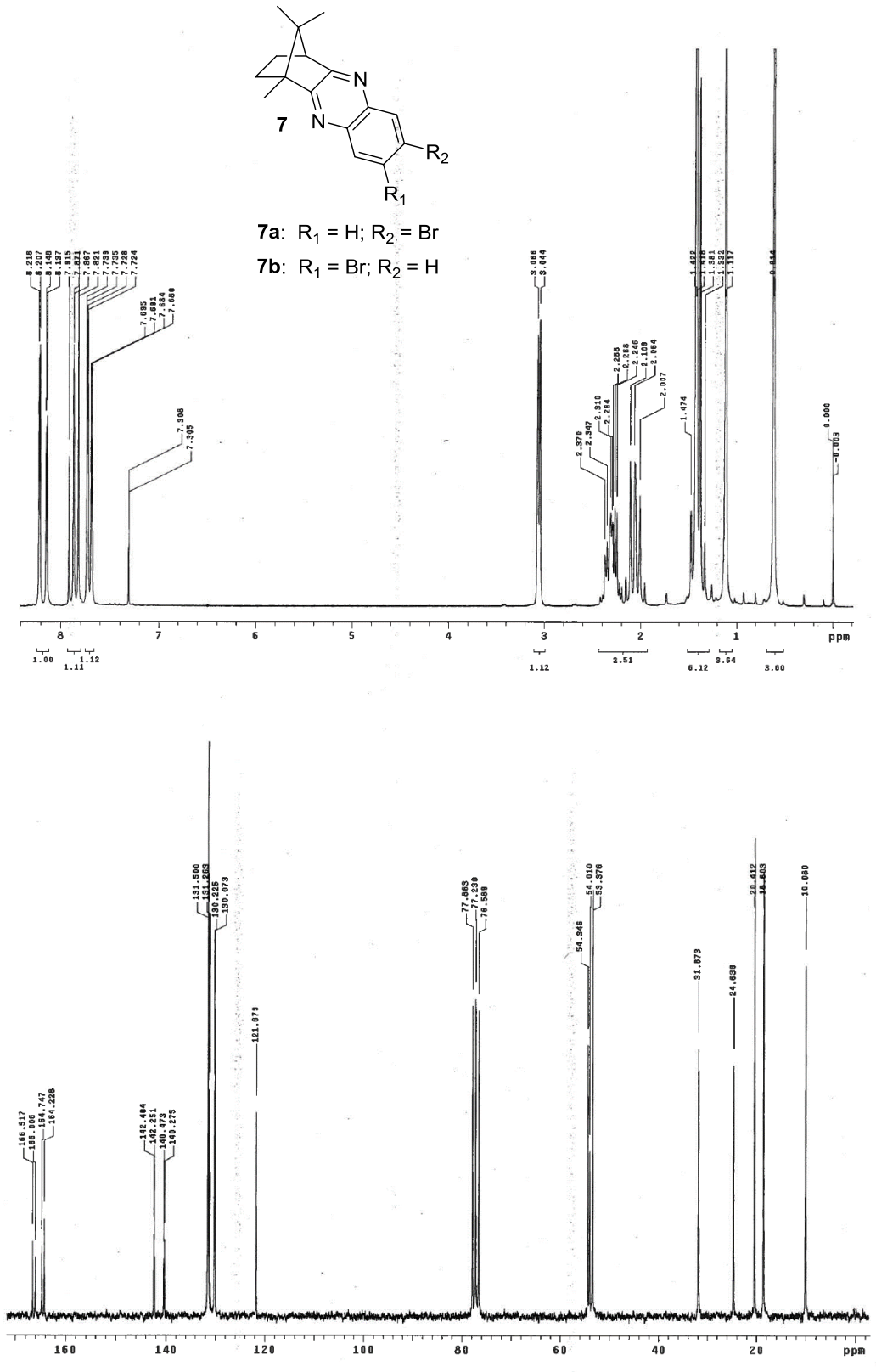


Figure S-9. ^{1}H (200 MHz; $CDCl_3$) and ^{13}C (50 MHz; $CDCl_3$) NMR spectra of **7**.

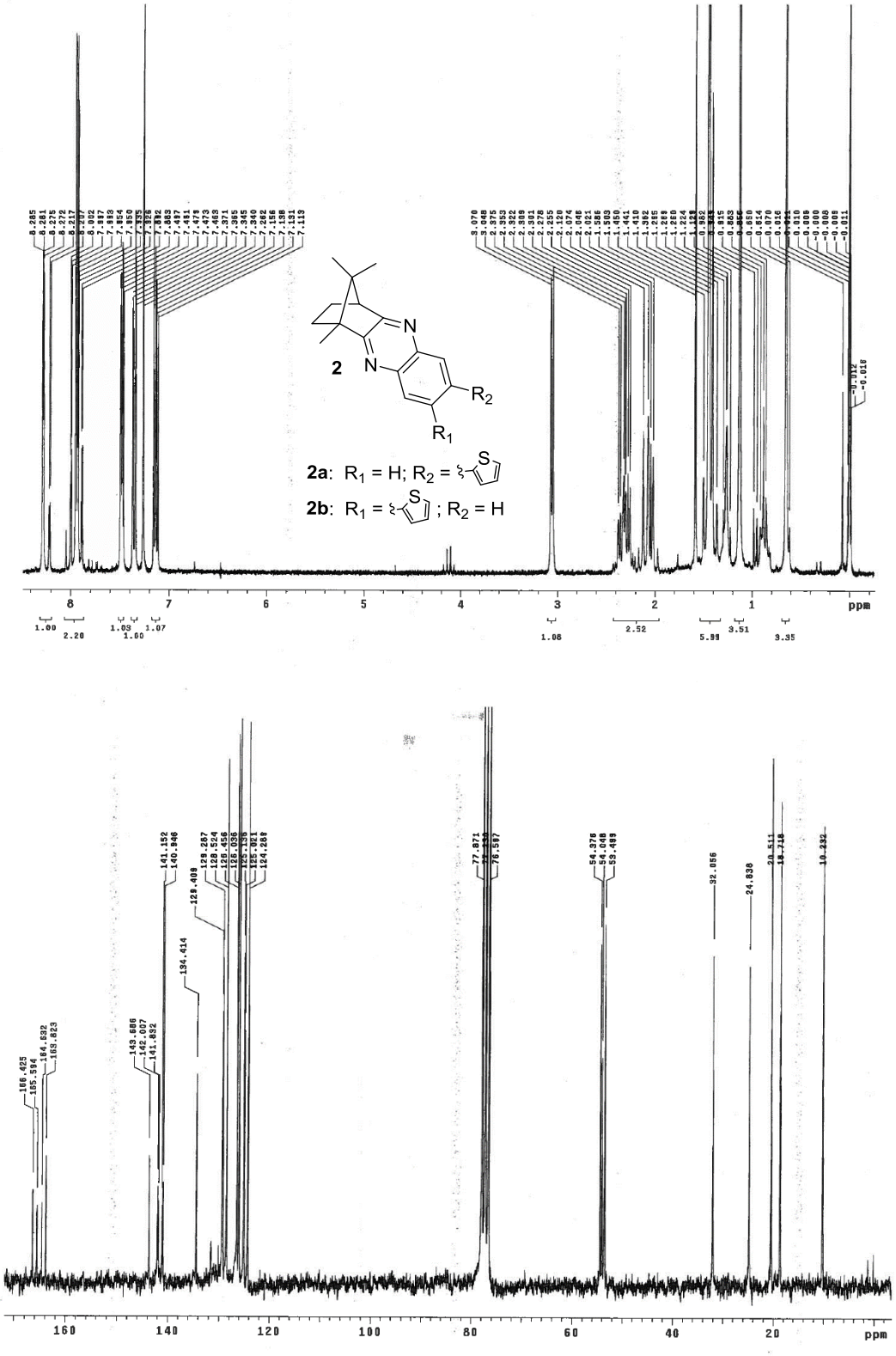


Figure S-10. ^{1}H (200 MHz; $CDCl_3$) and ^{13}C (50 MHz; $CDCl_3$) NMR spectra of **2**.

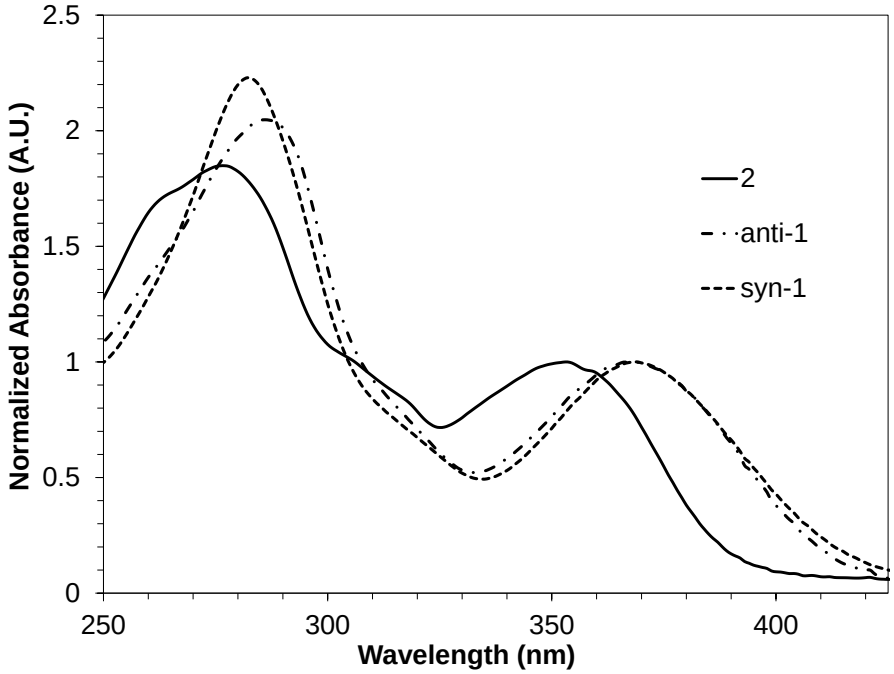


Figure S-11. UV-vis spectra of **2**, *anti*-**1**, and *syn*-**1** in methanol.

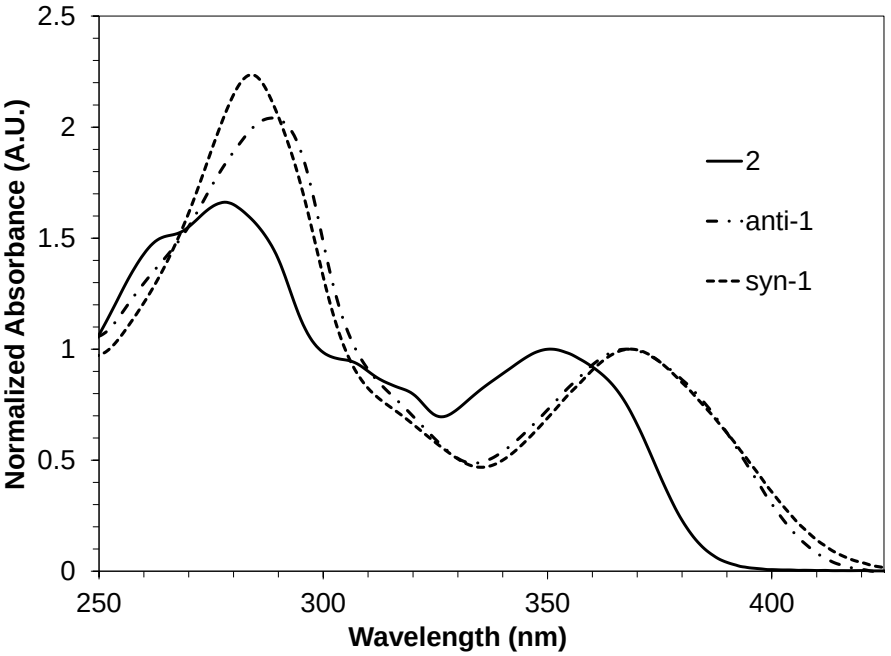


Figure S-12. UV-vis spectra of **2**, *anti*-**1**, and *syn*-**1** in chloroform.

Table S-1. Crystal, intensity collection, and refinement data for *syn*-**5**, *syn*-**1**, and *anti*-**1**.

	syn-**5**	*syn*-**1**	*anti*-**1**
formula	$C_{32}H_{26}Br_2Cl_4N_4O_4 \bullet C_6H_{14}$	$C_{40}H_{32}Cl_4N_4O_4S_2 \bullet CHCl_3$	$C_{40}H_{32}Cl_4N_4O_4S_2 \bullet 2\ (CH_2Cl_2)$
formula weight	918.36	957.98	1008.47
lattice	monoclinic	monoclinic	triclinic
space group	*P2₁/c*	*P2₁/n*	*P-1*
a/Å	12.7758(6)	11.1490(4)	10.5303(8)
b/Å	12.4749(6)	32.773(1)	11.5381(9)
c/Å	24.701(1)	11.5886(5)	18.581(2)
α/°	90	90	86.903(1)
β/°	96.782(1)	98.527(1)	74.816(1)
γ/°	90	90	77.042(1)
V/Å^3	3909.2(3)	4187.5(3)	2123.3(3)
Z	4	4	2
temperature (K)	125(2)	125(2)	125(2)
radiation (λ, Å)	0.71073	0.71073	0.71073
crystal size, mm	0.17 x 0.06 x 0.04	0.33 x 0.17 x 0.10	0.32 x 0.24 x 0.19
color, habit	colorless, block	yellow, plate	yellow, block
ρ (calcd.), g cm^{-3}	1.560	1.520	1.577
μ (Mo Kα), mm^{-1}	2.393	0.622	0.678
max., min. trans.	0.6865, 0.9104	0.8211, 0.9404	0.8122, 0.8819
θ range, deg.	1.61 – 29.57	1.88 – 30.53	2.05 – 30.56
completeness to θ max, %	29.57°, 99.8	30.53°, 99.8	30.56°, 96.5
reflections collected	59292	67690	23563
unique reflections	10958	12782	12559
R_{int} , R_σ	0.0749, 0.0648	0.061, 0.0504	0.0549, 0.1116
data, restraints, params.	10958/0/419	12782/123/567	12572/0/546
R_1, wR_2 (F^2, $I > 2\sigma(I)$) [a,b]	0.0577, 0.1409	0.0781, 0.2076	0.0648, 0.1810
R_1, wR_2 (F^2, *all data*) [a,b]	0.0957, 0.1544	0.1190, 0.2373	0.0964, 0.1978
weighting scheme *a*, *b* [a,b]	0.0790, 0	0.1106, 9.1246	0.1187, 0
GOF [c]	1.054	1.023	1.029
largest diff. peak, hole, e/Å^{-3}	2.653, -1.338	1.648, -1.410	1.583, -1.179

[a] $R_1 = \Sigma||F_o| - |F_c||/\Sigma|F_o|$, $wR_2 = \{\Sigma[w(F_o^2 - F_c^2)^2]/\Sigma[w(F_o^2)^2]\}^{1/2}$.

[b] $w = 1/[\sigma^2(F_o)^2 + (aP)^2 + bP]$, where $P = [1/3]\ \max(0, F_o^2) + [2/3]\ F_c^2$.

[c] GOF $= S = [\Sigma w(F_o^2 - F_c^2)^2/(N_R\text{-}N_P)]^{1/2}$, where N_R is the number of reflections and N_P is the number of parameters.