

SUPPLEMENTARY MATERIAL

2-Chloro-4,6-bis{(E)-3-methoxy-4-[(4-methoxybenzyl)oxy]styryl}pyrimidine: Synthesis, Spectroscopic, and Computational Evaluation

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§ This work is dedicated to the memory of the honorable Brazilian scientist, teacher, friend, and human being Dr. Vitor Sueth-Santiago (1987–2021). A victim from Covid-19.

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INDEX

Figure S1. The ¹H-NMR spectra for the compound **7**. (A) Experimental and (B) Theoretical (DFT).
p.2

Figure S2. The ¹³C-NMR spectra for the compound **7**. (A) Experimental (DEPTQ) and (B) Theoretical (DFT).
p.3

Table S1. Comparison between experimental and theoretical (calculated - DFT) signals (δ) for ¹H- and ¹³C-NMR to the compound **7**.
p.4

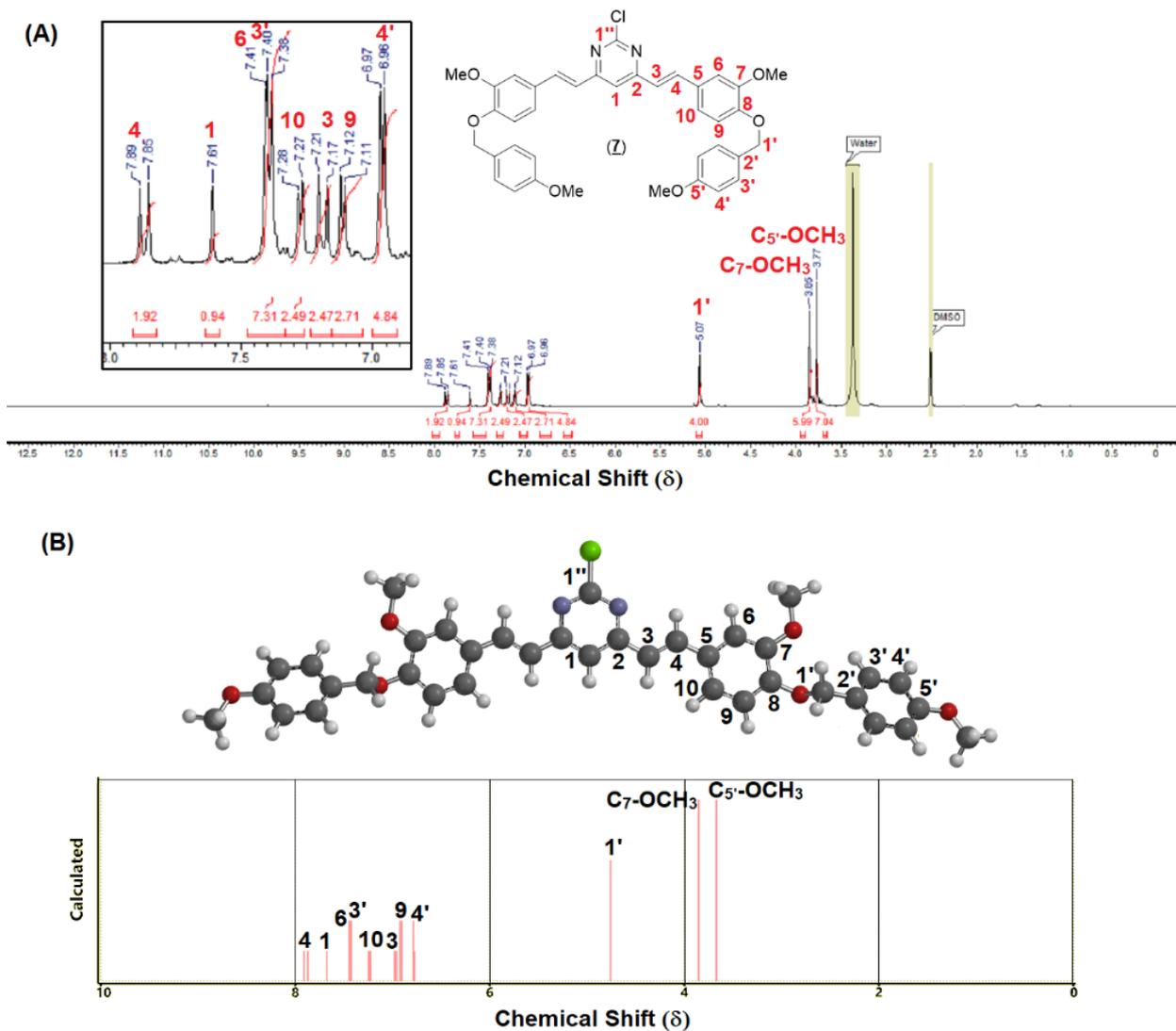


Figure S1. The ^1H -NMR spectra for the compound **7**. (A) Experimental and (B) Theoretical (DFT).

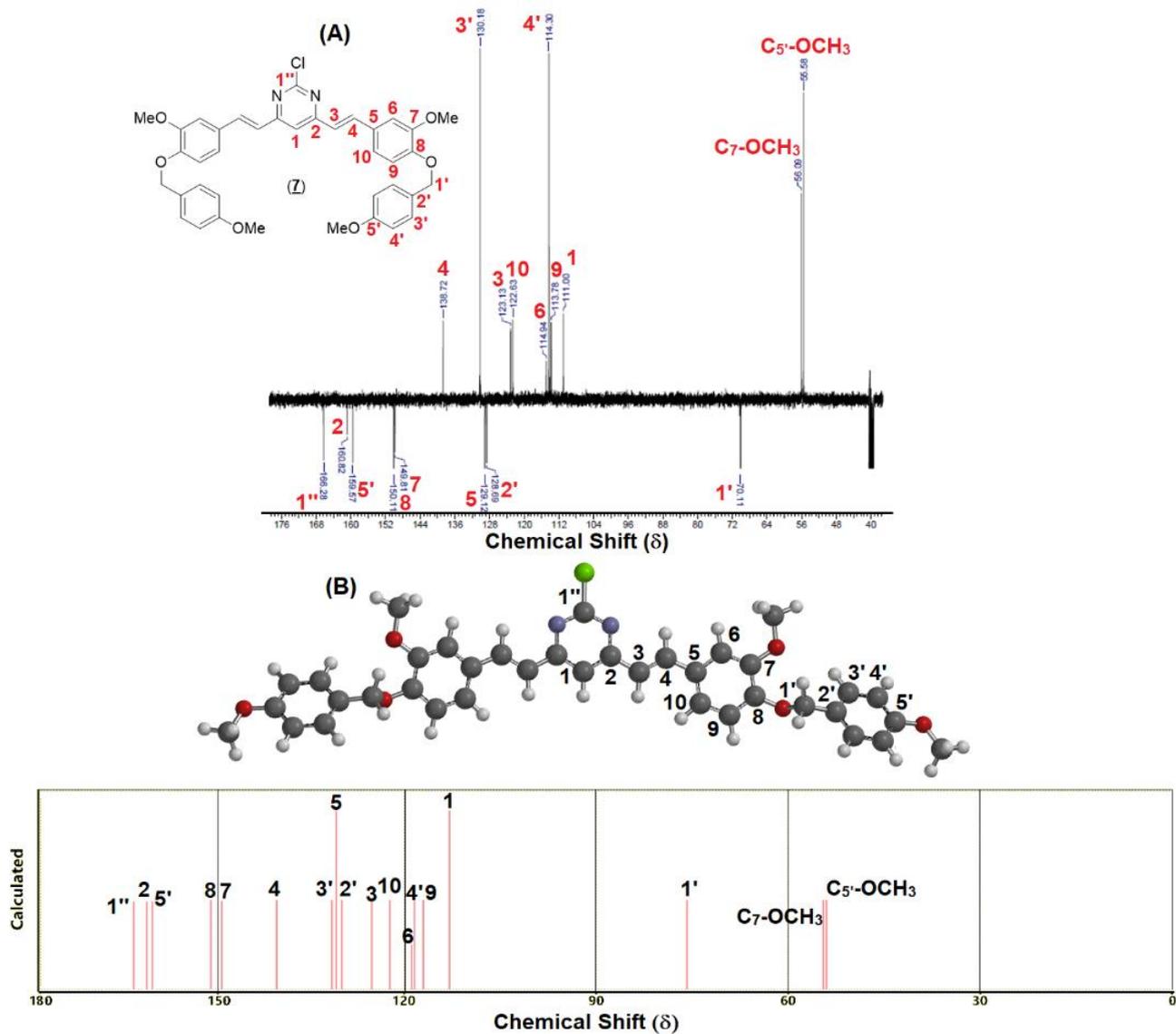


Figure S2. The ^{13}C -NMR spectra for the compound **7**. (A) Experimental (DEPTQ) and (B) Theoretical (DFT).

Table S1. Comparison between experimental and theoretical (calculated - DFT) signals (δ) for ^1H - and ^{13}C -NMR to the compound **7**.

Position	$\delta_{\text{H(exp)}}$	$\delta_{\text{H(calc)}}$	$\delta_{\text{C(exp)}}$	$\delta_{\text{C(calc)}}$
1	7.61	7.66	111.00	112.90
2	-	-	160.82	161.00
3	7.19	6.98	123.13	125.20
4	7.87	7.87	138.72	139.90
5	-	-	129.12	130.60
6	7.41	7.45	114.94	117.00
7	-	-	149.81	149.90
8	-	-	150.11	151.00
9	7.12	6.93	113.78	115.50
10	7.27	7.24	122.63	123.00
1'	5.07	4.86	70.11	75.80
2'	-	-	128.69	129.80
3'	7.40	7.43	130.18	131.30
4'	6.96	6.89	114.30	116.50
5'	-	-	159.57	160.10
1''	-	-	166.28	167.00
C ₇ -OCH ₃	3.85	3.85	56.09	54.50
C _{5'} -OCH ₃	3.77	3.67	55.58	54.00