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Supporting Information

Aggregation-Induced Enhanced Emission of a Dimethylacridan Substituted Pyrimidine Derivative

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SUPPORTING INFORMATION

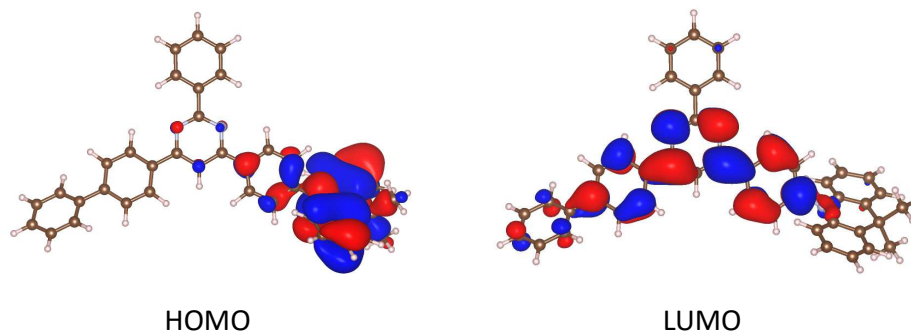


Figure S1. HOMO and LUMO orbitals (isovalue of 0.02 a.u.) of 1 in a constrained conformation with a 45° between the donor and the acceptor.

Table S1. Computed absorption and emission profiles of **1** with different DFT functionals.

DFT functional	λ_{abs} (nm)	f	S_n	λ_{em} (nm)	f
ω B97xD	306	0.00	S ₁	382	0.67
	283	1.02	S ₃		
	267	0.33	S ₇		
	258	0.41	S ₈		
	255	0.62	S ₉		
M062X	335	0.00	S ₁	405	0.38
	290	0.29	S ₂		
	289	0.87	S ₃		
	275	0.16	S ₆		
	269	0.20	S ₇		
B3LYP	469	0.00	S ₁	562	0.00
	338	0.80	S ₃		
	311	0.25	S ₇		
	305	0.12	S ₉		
	299	0.27	S ₁₁		

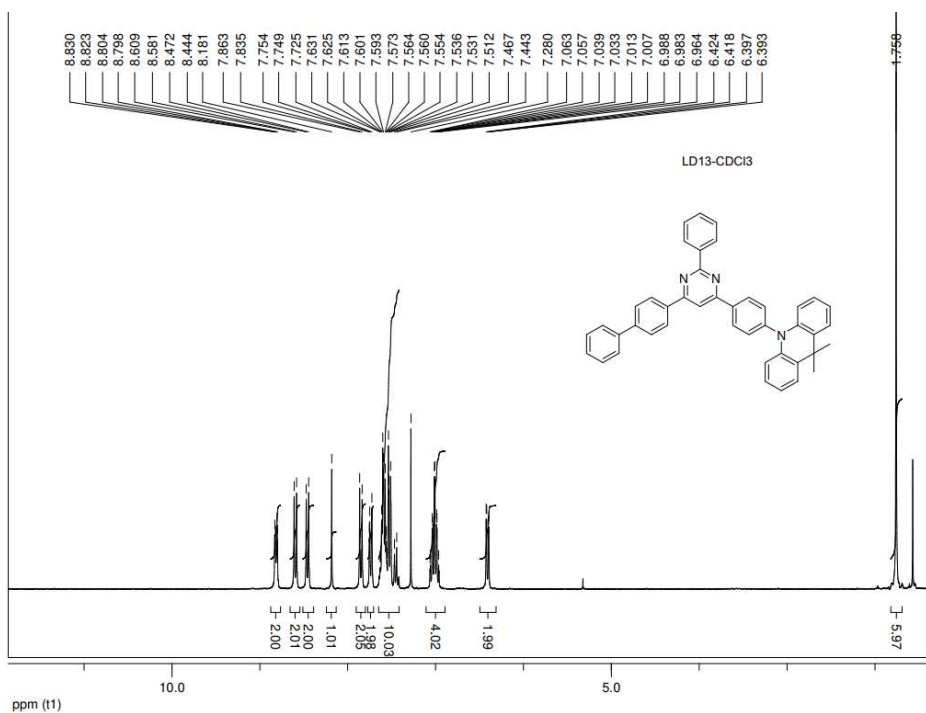


Figure S2: ¹H nmr spectrum (300 MHz) of compound **1**.

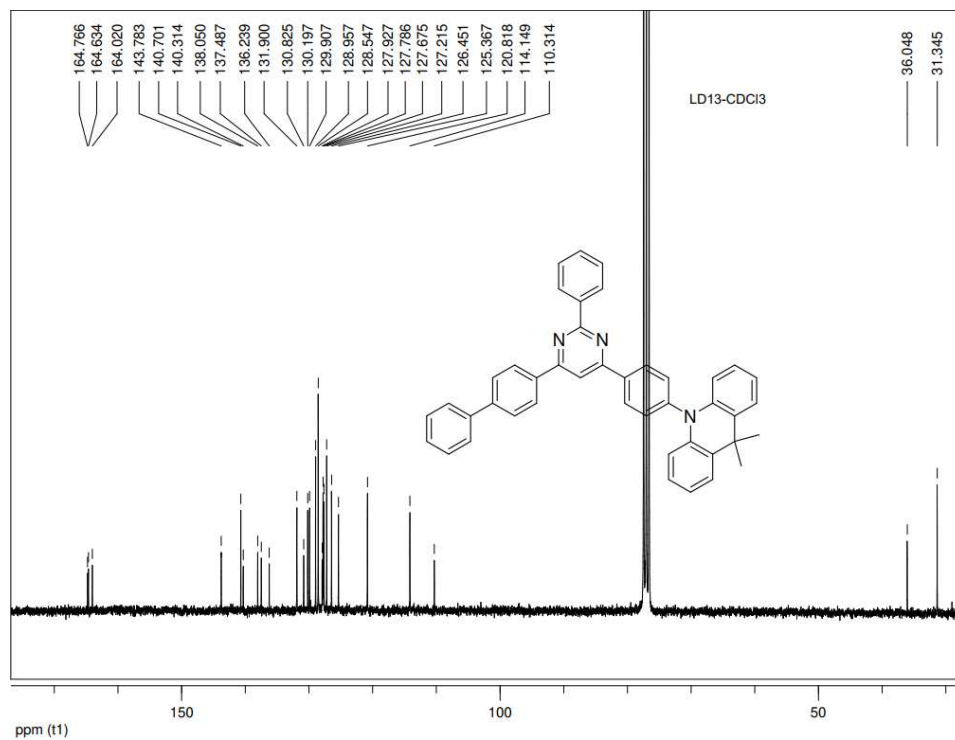


Figure S3: ¹³C NMR spectrum (300 MHz) of compound **1**.